Data Mining

Practical Machine Learning Tools and Techniques

Slides for Chapter 7 of *Data Mining* by I. H. Witten, E. Frank and M. A. Hall

Data transformations

- Attribute selection
  - Scheme-independent, scheme-specific
- Attribute discretization
  - Unsupervised, supervised, error- vs entropy-based, converse of discretization
- Projections
  - Principal component analysis, random projections, partial least-squares, text, time series
- Sampling
  - Reservoir sampling
- Dirty data
  - Data cleansing, robust regression, anomaly detection
- Transforming multiple classes to binary ones
  - Simple approaches, error-correcting codes, ensembles of nested dichotomies
- Calibrating class probabilities

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
  - Re-calibrating probability estimates

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 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 attribute selection

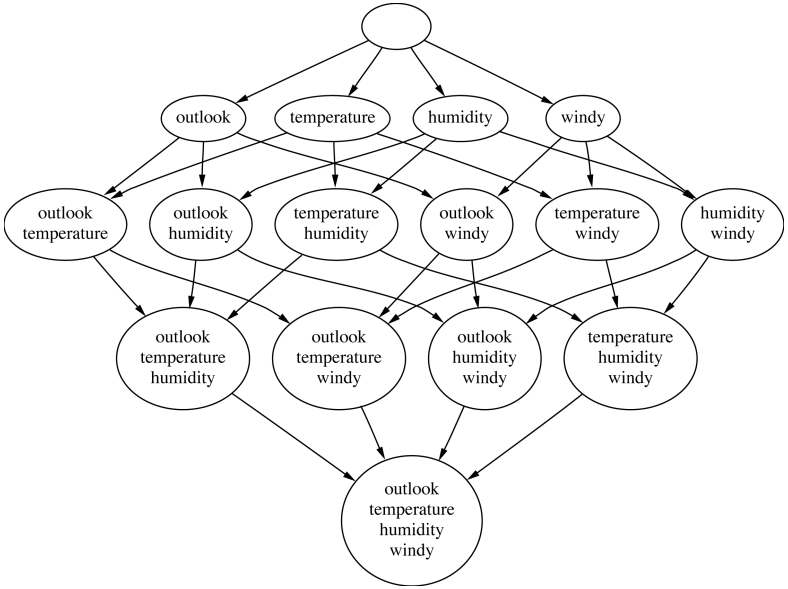
- *Filter* approach: assess based on general characteristics of the data
- One method: find smallest subset of attributes that separates data
- Another method: use different learning scheme
  - e.g. use attributes selected by C4.5 and 1R, or coefficients of linear model, possibly applied recursively (*recursive feature elimination*)
- IBL-based attribute weighting techniques:
  - can't find redundant attributes (but fix has been suggested)
- Correlation-based Feature Selection (CFS):
  - correlation between attributes measured by *symmetric uncertainty*:

$$U(A,B)=2\frac{H(A)+H(B)-H(A,B)}{H(A)+H(B)}\in[0,1]$$

  - goodness of subset of attributes measured by (breaking ties in favor of smaller subsets):

$$\sum_j U(A_j,C)/\sqrt{(\sum_i \sum_j U(A_i,A_j))}$$

Attribute subsets for weather data



Searching attribute space

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

Scheme-specific selection

- *Wrapper* approach to attribute selection
- Implement "wrapper" around learning scheme
  - Evaluation criterion: cross-validation performance
- Time consuming
  - greedy approach, k attributes $\Rightarrow$ $k^2 \times$ time
  - prior ranking of attributes $\Rightarrow$ linear in k
- Can use significance test to stop cross-validation for subset early if it is unlikely to "win" (*race search*)
  - can be used with forward, backward selection, prior ranking, or special-purpose *schemata search*
- Learning decision tables: scheme-specific attribute selection essential
- Efficient for decision tables and Naïve Bayes

Attribute discretization

- Avoids normality assumption in Naïve Bayes and clustering
- 1R: uses simple discretization scheme
- C4.5 performs *local* discretization
- *Global* discretization can be advantageous because it's based on more data
- Apply learner to
  - k-valued discretized attribute *or* to
  - $k-1$ binary attributes that code the cut points

Discretization: unsupervised

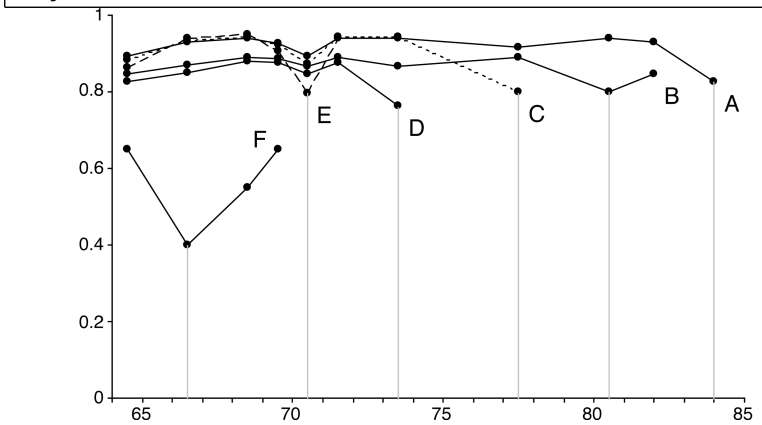
- Determine intervals without knowing class labels
  - When clustering, the only possible way!
- Two strategies:
  - *Equal-interval binning*
  - *Equal-frequency binning* (also called *histogram equalization*)
- Normally inferior to supervised schemes in classification tasks
  - But equal-frequency binning works well with naïve Bayes if number of intervals is set to square root of size of dataset (*proportional k-interval discretization)*

Discretization: supervised

- *Entropy-based* method
- Build a decision tree with pre-pruning on the attribute being discretized
  - Use entropy as splitting criterion
  - Use minimum description length principle as stopping criterion
- Works well: the state of the art
- To apply min description length principle:
  - The "theory" is
    - the splitting point ($\log_2[N-1]$ bits)
    - plus class distribution in each subset
  - Compare description lengths before/after adding split

Example: temperature attribute

Temperature	64	65	68	69	70	71	72	72	75	75	80	81	83	85
Play	Yes	No	Yes	Yes	Yes	No	No	Yes	Yes	Yes	No	Yes	Yes	No



64	65	68	69	70	71	72	75	80	81	83	85
yes	no	yes	yes	yes	no	no yes	yes yes	no	yes	yes	no
		F			E		D	C	B		A
		66.5			70.5		73.5	77.5	80.5		84

Formula for MDLP

- N instances
  - Original set: k classes, entropy E
  - First subset: k_1 classes, entropy E_1
  - Second subset: k_2 classes, entropy E_2

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

- Results in *no* discretization intervals for temperature attribute

Supervised discretization: other methods

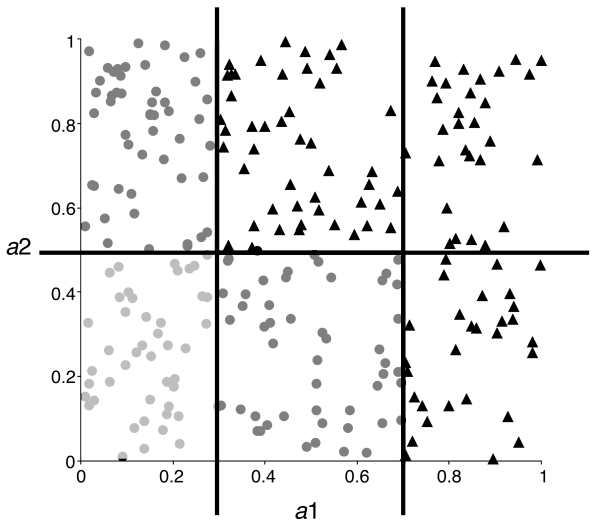
- Can replace top-down procedure by bottom-up method
- Can replace MDLP by chi-squared test
- Can use dynamic programming to find optimum k-way split for given additive criterion
  - Requires time quadratic in the number of instances
  - But can be done in linear time if error rate is used instead of entropy

Error-based vs. entropy-based

- Question:
  could the best discretization ever have two adjacent intervals with the same class?
- Wrong answer: No. For if so,
  - Collapse the two
  - Free up an interval
  - Use it somewhere else
  - *(This is what error-based discretization will do)*
- Right answer: Surprisingly, yes.
  - *(and entropy-based discretization can do it)*

Error-based vs. entropy-based

A 2-class, 2-attribute problem



Entropy-based discretization can detect change of class *distribution*

The converse of discretization

- Make ordinal values into "numeric" ones

1. Indicator attributes (used by IB1)
   - Makes no use of potential ordering information
2. Code an ordinal attribute into binary ones (used by M5')
   - Can be used for any ordered attribute
   - Better than coding ordering into an integer (which implies a metric)

- In general: code subset of attribute values as binary

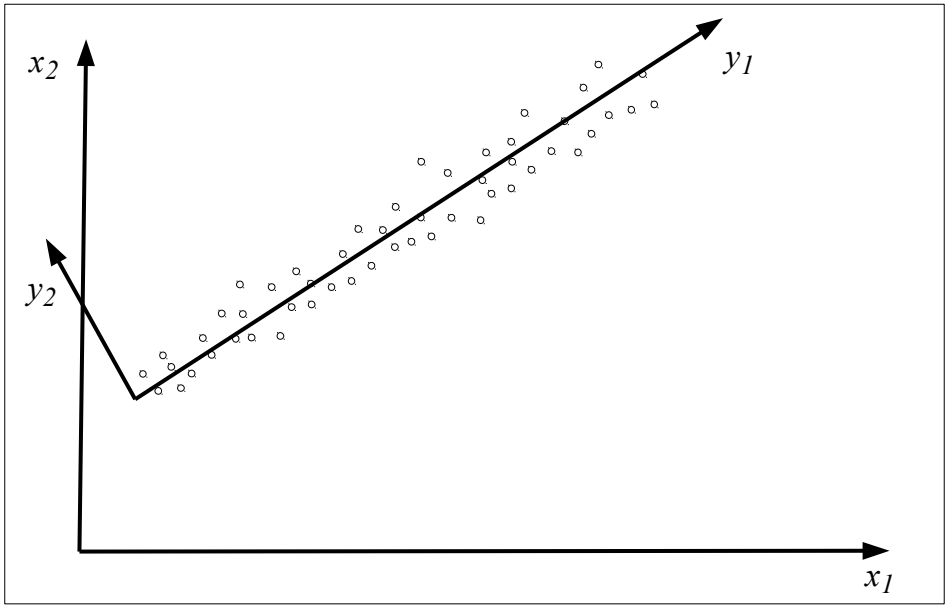
Projections

- 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

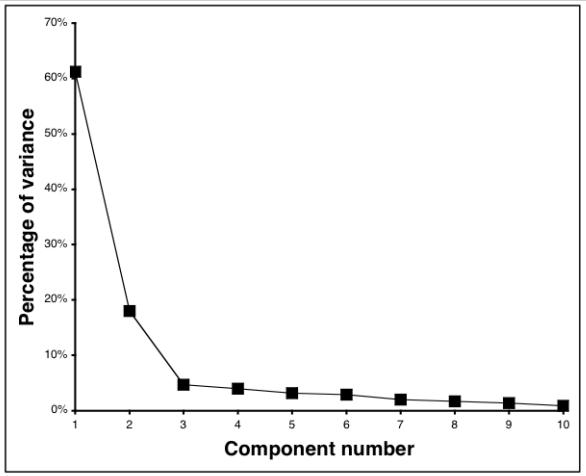
- Method for identifying the important "directions" in the data
- Can rotate data into (reduced) coordinate system that is given by those directions
- Algorithm:
  1. Find direction (axis) of greatest variance
  2. Find direction of greatest variance that is perpendicular to previous direction and repeat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

PCA Example



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

Random projections

- PCA is nice but expensive: cubic in number of attributes
- Alternative: use random directions (projections) instead of principle components
- Surprising: random projections preserve distance relationships quite well (on average)
  - Can use them to apply kD-trees to high-dimensional data
  - Can improve stability by using ensemble of models based on different projections

Partial least-squares regression

- PCA is often a pre-processing step before applying a learning algorithm
  - When linear regression is applied the resulting model is known as *principal components regression*
  - Output can be re-expressed in terms of the original attributes
- Partial least-squares differs from PCA in that it takes the **class** attribute into account
  - Finds directions that have high variance and are strongly correlated with the class

Algorithm

1. Start with *standardized* input attributes
2. Attribute coefficients of the first PLS direction:
   - Compute the dot product between each attribute vector and the class vector in turn
3. Coefficients for next PLS direction:
   - Original attribute values are first replaced by difference (residual) between the attribute's value and the prediction from a simple univariate regression that uses the previous PLS direction as a predictor of that attribute
   - Compute the dot product between each attribute's residual vector and the class vector in turn
4. Repeat from 3

PLS Example (2 attributes only)

Table 1.5 CPU Performance Data

	Main Memory (Kb)			Channels		
	Cycle Time (ns)	Min	Max	Cache (KB)	Min	Max	Performance
	MYCT	*MMIN*	*MMAX*	*CACH*	*CHMIN*	*CHMAX*	*PRP*
1	125	256	6000	256	16	128	198
2	29	8000	32,000	32	8	32	269
3	29	8000	32,000	32	8	32	220
4	29	8000	32,000	32	8	32	172
5	29	8000	16,000	32	8	16	132
...							
207	125	2000	8000	0	2	14	52
208	480	512	8000	32	0	0	67
209	480	1000	4000	0	0	0	45

Table 7.1 First Five Instances from the CPU Performance Data

	(a)			(b)	(c)		
	chmin	chmax	prp	pls 1	chmin	chmax	prp
1	1.7889	1.7678	198	39.825	0.0436	0.0008	198
2	–0.4472	–0.3536	269	–7.925	–0.0999	–0.0019	269
3	–0.4472	–0.3536	220	–7.925	–0.0999	–0.0019	220
4	–0.4472	–0.3536	172	–7.925	–0.0999	–0.0019	172
5	–0.4472	–0.7071	132	–16.05	0.2562	0.005	132

(a) original values, (b) first partial least-squares direction, and (c) residuals from the first direction.

PLS Example (cont'd)

- PRP*CHMIN= -0.4472, PRP*CHMAX=22.981
  PLS1= -0.4472 CHMIN + 22.981 CHMAX
- Univariate Regression:
  CHMIN= 0.0438 PLS1
  CHMAX=0.0444 PLS1
- PLS2= -23.6002 CHMIN -0.4593 CHMAX
- All attribute residuals are zero now

- Use PLS directions as input for linear regression: *partial least squares regression model*
- If all directions are used, result is the same as with original attributes

Text to attribute vectors

- Many data mining applications involve textual data (eg. string attributes in ARFF)
- Standard transformation: convert string into bag of words by *tokenization*
  - Attribute values are binary, word frequencies (f_{ij}), $\log(1+f_{ij})$, or TF × IDF: $f_{ij} \log \frac{\#\,documents}{\#\,documents\ \ that\ \ include\ \ word\ \ i}$
- Only retain alphabetic sequences?
- What should be used as delimiters?
- Should words be converted to lowercase?
- Should *stopwords* be ignored?
- Should *hapax legomena* be included? Or even just the k most frequent words?

Time series

- In time series data, each instance represents a different time step
- Some simple transformations:
  - Shift values from the past/future
  - Compute difference (*delta*) between instances (i.e. "derivative")
- In some datasets, samples are not regular but time is given by *timestamp* attribute
  - Need to normalize by step size when transforming
- Transformations need to be adapted if attributes represent different time steps

Sampling

- Sampling is typically a simple procedure
- What if training instances arrive one by one but we don't know the total number in advance?
  - Or perhaps there are so many that it is impractical to store them all before sampling?
- Is it possible to produce a uniformly random sample of a fixed size? Yes.
- *Reservoir sampling*
  - Fill the reservoir, of size *r*, with the first *r* instances to arrive
  - Subsequent instances replace a randomly selected reservoir element with probability *r*/*i*, where *i* is the number of instances seen so far

Automatic data cleansing

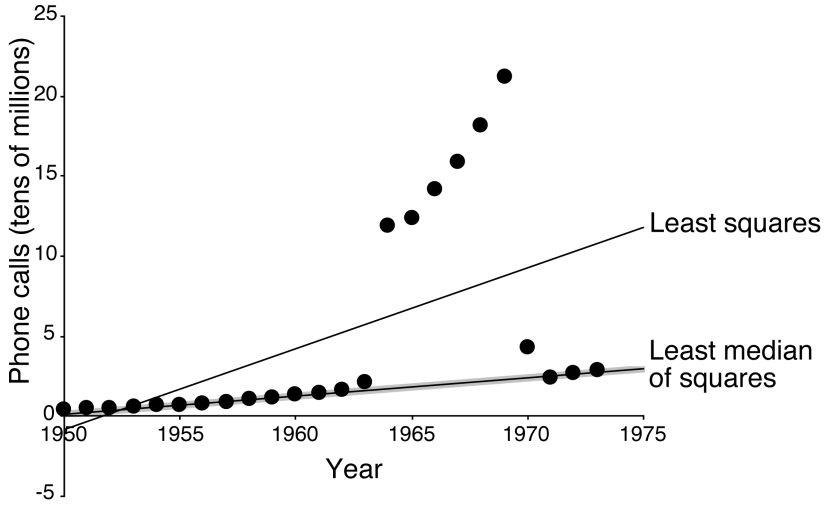
- To improve a decision tree:
  - Remove misclassified instances, then re-learn!
- Better (of course!):
  - Human expert checks misclassified instances
- Attribute noise vs class noise
  - Attribute noise should be left in training set *(don't train on clean set and test on dirty one)*
  - Systematic class noise (e.g. one class substituted for another): leave in training set
  - Unsystematic class noise: eliminate from training set, if possible

Robust regression

- "Robust" statistical method ⇒ one that addresses problem of *outliers*
- To make regression more robust:
  - Minimize absolute error, not squared error
  - Remove outliers (e.g. 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

Number of international phone calls from Belgium, 1950–1973



Detecting anomalies

- Visualization can help to detect anomalies
- Automatic approach: committee of different learning schemes
  - E.g.
    - decision tree
    - nearest-neighbor learner
    - linear discriminant function
  - Conservative approach: delete instances incorrectly classified by all of them
  - Problem: might sacrifice instances of small classes

One-Class Learning

- Usually training data is available for all classes
- Some problems exhibit only a single class at training time
  - Test instances may belong to this class or a new class not present at training time
- One-class classification
  - Predict either *target* or *unknown*
- Some problems can be re-formulated into two-class ones
- Other applications truly don't have negative data
  - E.g. password hardening

Outlier detection

- One-class classification is often called *outlier/novelty* detection
- Generic approach: identify outliers as instances that lie beyond distance *d* from percentage *p* of the training data
- Alternatively, estimate density of the target class and mark low probability test instances as outliers
  - Threshold can be adjusted to obtain a suitable rate of outliers

Generating artificial data

- Another possibility is to generate artificial data for the outlier class
  - Can then apply any off-the-shelf classifier
  - Can tune rejection rate threshold if classifier produces probability estimates
- Generate uniformly random data
  - Too much will overwhelm the target class!
    - Can be avoided if learning accurate probabilities rather than minimizing classification error
  - Curse of dimensionality – as # attributes increase it becomes infeasible to generate enough data to get good coverage of the space

Generating artificial data

- Generate data that is *close* to the target class
  - No longer uniformly distributed and must take this distribution into account when computing membership scores for the one-class model
- T – target class, A – artificial class. Want Pr[X | T], for any instance X; we know Pr[X | A]
- Combine some amount of A with instances of T and use a class probability estimator to estimate Pr[T | X]; then by Bayes' rule:

$$Pr[X|T] = \frac{(1-Pr[T])Pr[T|X]}{Pr[T](1-Pr[T|X])} Pr[X|A]$$

- For classification, choose a threshold to tune rejection rate
- How to choose Pr[X | A]? Apply a density estimator to the target class and use resulting function to model the artificial class

Transforming multiple classes to binary ones

- Some learning algorithms only work with two class problems
  - Sophisticated multi-class variants exist in many cases but can be very slow or difficult to implement
- A common alternative is to transform multi-class problems into multiple two-class ones
- Simple methods
  - Discriminate each class agains the union of the others – *one-vs.-rest*
  - Build a classifier for every pair of classes – *pairwise classification*

Error-correcting output codes

- Multiclass problem ⇒ binary problems
  - Simple one-vs.rest scheme: One-per-class coding
- Idea: use *error-correcting codes* instead
  - base classifiers predict 1011111, true class = ??
- Use code words that have large *Hamming distance* between any pair
  - Can correct up to $(d-1)/2$ single-bit errors

class	class vector
a	1000
b	0100
c	0010
d	0001

class	class vector
a	1111111
b	0000111
c	0011001
d	0101010

More on ECOCs

- Two criteria :
  - *Row separation*: minimum distance between rows
  - *Column separation*: minimum distance between columns
    - (and columns' complements)
    - Why? Because if columns are identical, base classifiers will likely make the same errors
    - Error-correction is weakened if errors are correlated
- 3 classes ⇒ only 2^3 possible columns
  - (and 4 out of the 8 are complements)
  - Cannot achieve row and column separation
- Only works for problems with > 3 classes

Exhaustive ECOCs

- *Exhaustive* code for k classes:
  - Columns comprise every possible k-string …
  - … except for complements and all-zero/one strings
  - Each code word contains $2^{k-1} - 1$ bits

Exhaustive code, $k = 4$

class	class vector
a	1111111
b	0000111
c	0011001
d	0101010

- Class 1: code word is all ones
- Class 2: 2^{k-2} zeroes followed by $2^{k-2} - 1$ ones
- Class i: alternating runs of 2^{k-i} 0s and 1s
  - last run is one short

More on ECOCs

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

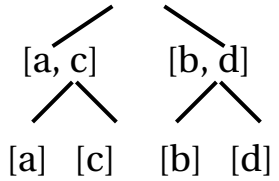
Ensembles of nested dichotomies

- ECOCs produce classifications, but what if we want class probability estimates as well?
  - e.g. for cost-sensitive classification via minimum expected cost
- *Nested dichotomies*
  - Decomposes multi-class to binary
  - Works with two-class classifiers that can produce class probability estimates
  - Recursively split the full set of *classes* into smaller and smaller subsets, while splitting the full dataset of instances into subsets corresponding to these subsets of classes
    - Yields a binary tree of classes called a nested dichotomy

Example

Full set of classes: [a, b, c, d]

Two disjoint subsets:



Nested dichotomy as a code matrix:

Class	Class vector
a	0 0 X
b	1 X 0
c	0 1 X
d	1 X 1

Probability estimation

- Suppose we want to compute Pr[a | x]?
  - Learn two class models for each of the three internal nodes
  - From the two-class model at the root:
    Pr[{a, c} | x]
  - From the left-hand child of the root:
    Pr[{a} | x, {a , c}]
  - Using the chain rule:
    Pr[{a} | x] = Pr[{a} | {a, c}, x] × Pr[{a, c} | x]
- Issues
  - Estimation errors for deep hierarchies
  - How to decide on hierarchical decomposition of classes?

Ensembles of nested dichotomies

- If there is no reason a priori to prefer any particular decomposition then use them all
  - Impractical for any non-trivial number of classes
- Consider a subset by taking a random sample of possible tree structures
  - Caching of models (since a given two class problem may occur in multiple trees)
  - Average probability estimates over the trees
  - Experiments show that this approach yields accurate multiclass classifiers
  - Can even improve the performance of methods that can already handle multiclass problems!

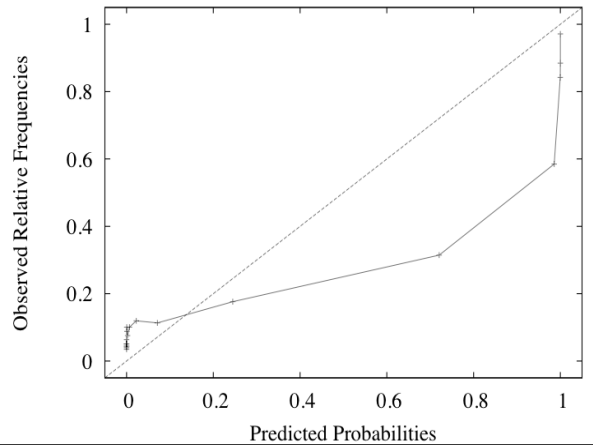
Calibrating class probabilities

- Class probability estimation is harder than classification
  - Classification error is minimized as long as the correct class is predicted with max probability
  - Estimates that yield correct classification may be quite poor with respect to quadratic or informational loss
- Often important to have accurate class probabilities
  - e.g. cost-sensitive prediction using the minimum expected cost method

Calibrating class probabilities

- Consider a two class problem. Probabilities that are correct for classification may be:
  - Too optimistic – too close to either 0 or 1
  - Too pessimistic – not close enough to 0 or 1

Reliability diagram showing overoptimistic probability estimation for a two-class problem



Calibrating class probabilities

- Reliability diagram generated by collecting predicted probabilities and relative frequencies from a 10-fold cross-validation
  - Predicted probabilities discretized into 20 ranges via equal-frequency discretization
  - Correct bias by using post-hoc calibration to map observed curve to the diagonal
  - A rough approach can use the data from the reliability diagram directly
- Discretization-based calibration is fast…
  - But determining the appropriate number of discretization intervals is not easy

Calibrating class probabilities

- View as a function estimation problem
  - One input – estimated class probability – and one output – the calibrated probability
- Assuming the function is piecewise constant and monotonically increasing
  - *Isotonic regression* minimizes the squared error between observed class "probabilities (0/1) and resulting calibrated class probabilities
  - Alternatively, use *logistic regression* to estimate the calibration function
    - Must use the *log-odds* of the estimated class probabilities as input
    - Multiclass logistic regression can be used for calibration in the multiclass case