Machine Learning
Chapter 5. Credibility

5 Credibility:
Evaluating what's been learned

- Issues: training, testing, tuning
- Predicting performance: confidence limits
- Holdout, cross-validation, bootstrap
- Comparing schemes: the t-test
- Predicting probabilities: loss functions
- Cost-sensitive measures
- Evaluating numeric prediction
- The Minimum Description Length principle

Evaluation: the key to success

- How predictive is the model we learned?
- Error on the training data is *not* a good indicator of performance on future data
  - Otherwise 1-NN would be the optimum classifier!
- Simple solution that can be used if lots of (labeled) data is available:
  - Split data into training and test set
- However: (labeled) data is usually limited
  - More sophisticated techniques need to be used

Issues in evaluation

- Statistical reliability of estimated differences in performance ($\rightarrow$ significance tests)
- Choice of performance measure:
  - Number of correct classifications
  - Accuracy of probability estimates
  - Error in numeric predictions
- Costs assigned to different types of errors
  - Many practical applications involve costs

Training and testing I

- Natural performance measure for classification problems: *error rate*
  - *Success*: instance's class is predicted correctly
  - *Error*: instance's class is predicted incorrectly
  - Error rate: proportion of errors made over the whole set of instances
- *Resubstitution error:* error rate obtained from training data
- Resubstitution error is (hopelessly) optimistic!

Training and testing II

- *Test set*: independent instances that have played no part in formation of classifier
  - Assumption: both training data and test data are representative samples of the underlying problem
- Test and training data may differ in nature
  - Example: classifiers built using customer data from two different towns *A* and *B*
    - To estimate performance of classifier from town *A* in completely new town, test it on data from *B*

Note on parameter tuning

- It is important that the test data is not used *in any way* to create the classifier
- Some learning schemes operate in two stages:
  - Stage 1: build the basic structure
  - Stage 2: optimize parameter settings
- The test data can't be used for parameter tuning!
- Proper procedure uses *three* sets: *training data*, *validation data*, and *test data*
  - Validation data is used to optimize parameters

Making the most of the data

- Once evaluation is complete, *all the data* can be used to build the final classifier
- Generally, the larger the training data the better the classifier (but returns diminish)
- The larger the test data the more accurate the error estimate
- *Holdout* procedure: method of splitting original data into training and test set
  - Dilemma: ideally both training set *and* test set should be large!

Predicting performance

- Assume the estimated error rate is 25%. How close is this to the true error rate?
  - Depends on the amount of test data
- Prediction is just like tossing a (biased!) coin
  - "Head" is a "success", "tail" is an "error"
- In statistics, a succession of independent events like this is called a *Bernoulli process*
  - Statistical theory provides us with confidence intervals for the true underlying proportion

Confidence intervals

- We can say: p lies within a certain specified interval with a certain specified confidence
- Example: S=750 successes in N=1000 trials
  - Estimated success rate: 75%
  - How close is this to true success rate p?
    - Answer: with 80% confidence $p \in [73.2,76.7]$
- Another example: S=75 and N=100
  - Estimated success rate: 75%
  - With 80% confidence $p \in [69.1,80.1]$

Mean and variance

- Mean and variance for a Bernoulli trial: p, $p(1-p)$
- Expected success rate $f = S/N$
- Mean and variance for f: p, $p(1-p)/N$
- For large enough N, f follows a Normal distribution
- c% confidence interval $[-z \leq X \leq z]$ for random variable with 0 mean is given by:

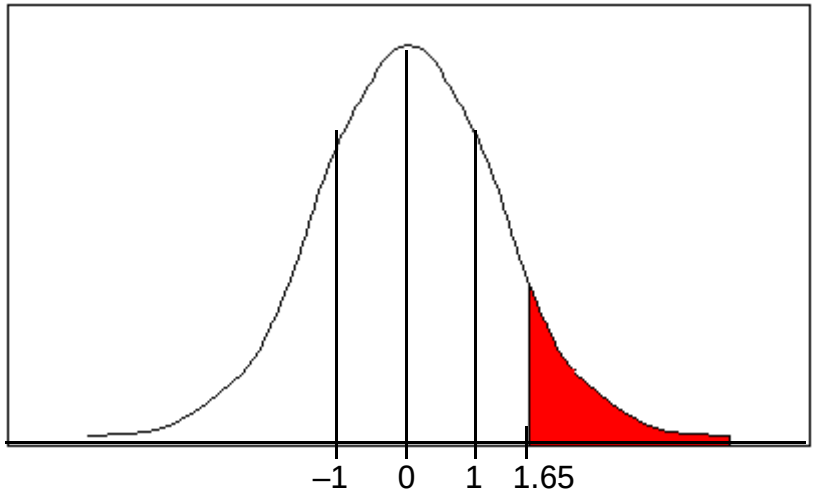
$$\Pr[-z \leq X \leq z] = c$$

- With a symmetric distribution:

$$\Pr[-z \leq X \leq z] = 1 - 2 \times \Pr[X \geq z]$$

Confidence limits

- Confidence limits for the normal distribution with 0 mean and a variance of 1:



Pr[$X \geq z$]	z
0.1%	3.09
0.5%	2.58
1%	2.33
5%	1.65
10%	1.28
20%	0.84
40%	0.25

- Thus:

$$\Pr[-1.65 \leq X \leq 1.65] = 90\%$$

- To use this we have to reduce our random variable f to have 0 mean and unit variance

Transforming *f*

- Transformed value for *f* : $\frac{f-p}{\sqrt{p(1-p)/N}}$

  (i.e. subtract the mean and divide by the *standard deviation*)

- Resulting equation:

$$\Pr\left[-z \le \frac{f-p}{\sqrt{p(1-p)/N}} \le z\right] = c$$

- Solving for *p* :

$$p = \left(f + \frac{z^2}{2N} \pm z\sqrt{\frac{f}{N} - \frac{f^2}{N} + \frac{z^2}{4N^2}} \right) \Big/ \left(1 + \frac{z^2}{N}\right)$$

Examples

- f = 75%, N = 1000, c = 80% (so that z = 1.28):

$$p \in [0.732, 0.767]$$

- f = 75%, N = 100, c = 80% (so that z = 1.28):

$$p \in [0.691, 0.801]$$

- Note that normal distribution assumption is only valid for large N (i.e. $N > 100$)
- f = 75%, N = 10, c = 80% (so that z = 1.28):

$$p \in [0.549, 0.881]$$

(should be taken with a grain of salt)

Holdout estimation

- What to do if the amount of data is limited?
- The *holdout* method reserves a certain amount for testing and uses the remainder for training
  - Usually: one third for testing, the rest for training
- Problem: the samples might not be representative
  - Example: class might be missing in the test data
- Advanced version uses *stratification*
  - Ensures that each class is represented with approximately equal proportions in both subsets

Repeated holdout method

- Holdout estimate can be made more reliable by repeating the process with different subsamples
  - In each iteration, a certain proportion is randomly selected for training (possibly with stratificiation)
  - The error rates on the different iterations are averaged to yield an overall error rate
- This is called the *repeated holdout* method
- Still not optimum: the different test sets overlap
  - Can we prevent overlapping?

Cross-validation

- *Cross-validation* avoids overlapping test sets
  - First step: split data into *k* subsets of equal size
  - Second step: use each subset in turn for testing, the remainder for training
- Called *k-fold cross-validation*
- Often the subsets are stratified before the cross-validation is performed
- The error estimates are averaged to yield an overall error estimate

More on cross-validation

- Standard method for evaluation: stratified ten-fold cross-validation
- Why ten?
  - Extensive experiments have shown that this is the best choice to get an accurate estimate
  - There is also some theoretical evidence for this
- Stratification reduces the estimate's variance
- Even better: repeated stratified cross-validation
  - E.g. ten-fold cross-validation is repeated ten times and results are averaged (reduces the variance)

Leave-One-Out cross-validation

- Leave-One-Out:
  a particular form of cross-validation:
  - Set number of folds to number of training instances
  - I.e., for *n* training instances, build classifier *n* times
- Makes best use of the data
- Involves no random subsampling
- Very computationally expensive
  - (exception: NN)

Leave-One-Out-CV and stratification

- Disadvantage of Leave-One-Out-CV: stratification is not possible
  - It *guarantees* a non-stratified sample because there is only one instance in the test set!
- Extreme example: random dataset split equally into two classes
  - Best inducer predicts majority class
  - 50% accuracy on fresh data
  - Leave-One-Out-CV estimate is 100% error!

The bootstrap

- CV uses sampling *without replacement*
  - The same instance, once selected, can not be selected again for a particular training/test set
- The *bootstrap* uses sampling *with replacement* to form the training set
  - Sample a dataset of *n* instances *n* times *with replacement* to form a new dataset of *n* instances
  - Use this data as the training set
  - Use the instances from the original dataset that don't occur in the new training set for testing

The 0.632 bootstrap

- Also called the *0.632 bootstrap*
  - A particular instance has a probability of 1–1/*n* of *not* being picked
  - Thus its probability of ending up in the test data is:

$$\left(1-\frac{1}{n}\right)^{n} \approx e^{-1} = 0.368$$

  - This means the training data will contain approximately 63.2% of the instances

Estimating error with the bootstrap

- The error estimate on the test data will be very pessimistic
  - Trained on just ~63% of the instances
- Therefore, combine it with the resubstitution error:

$$err = 0.632 \cdot e_{\text{test instances}} + 0.368 \cdot e_{\text{training instances}}$$

- The resubstitution error gets less weight than the error on the test data
- Repeat process several times with different replacement samples; average the results

More on the bootstrap

- Probably the best way of estimating performance for very small datasets
- However, it has some problems
  - Consider the random dataset from above
  - A perfect memorizer will achieve
    0% resubstitution error and
    ~50% error on test data
  - Bootstrap estimate for this classifier:
    $$err = 0.632 \cdot 50\% + 0.368 \cdot 0\% = 31.6\%$$
  - True expected error: 50%

Comparing data mining schemes

- Frequent question: which of two learning schemes performs better?
- Note: this is domain dependent!
- Obvious way: compare 10-fold CV estimates
- Problem: variance in estimate
- Variance can be reduced using repeated CV
- However, we still don’t know whether the results are reliable

Significance tests

- Significance tests tell us how confident we can be that there really is a difference
- *Null hypothesis*: there is no “real” difference
- *Alternative hypothesis*: there is a difference
- A significance test measures how much evidence there is in favor of rejecting the null hypothesis
- Let’s say we are using 10-fold CV
- Question: do the two means of the 10 CV estimates differ significantly?

Paired t-test

- *Student's t-test* tells whether the means of two samples are significantly different
- Take individual samples using cross-validation
- Use a *paired* t-test because the individual samples are paired
  - The same CV is applied twice

William Gosset

Born: 1876 in Canterbury; Died: 1937 in Beaconsfield, England

Obtained a post as a chemist in the Guinness brewery in Dublin in 1899. Invented the t-test to handle small samples for quality control in brewing. Wrote under the name "Student".

Distribution of the means

- $x_1\ x_2\ \ldots\ x_k$ and $y_1\ y_2\ \ldots\ y_k$ are the $2k$ samples for a k-fold CV
- m_x and m_y are the means
- With enough samples, the mean of a set of independent samples is normally distributed

- Estimated variances of the means are σ_x^2/k and σ_y^2/k

- If μ_x and μ_y are the true means then $\frac{m_x - \mu_x}{\sqrt{\sigma_x^2/k}}$ $\frac{m_y - \mu_y}{\sqrt{\sigma_y^2/k}}$ are *approximately* normally distributed with mean 0, variance 1

Student's distribution

- With small samples ($k < 100$) the mean follows *Student's distribution with k–1 degrees of freedom*

- Confidence limits:

9 degrees of freedom

Pr[$X \geq z$]	z
0.1%	4.30
0.5%	3.25
1%	2.82
5%	1.83
10%	1.38
20%	0.88

normal distribution

Pr[$X \geq z$]	z
0.1%	3.09
0.5%	2.58
1%	2.33
5%	1.65
10%	1.28
20%	0.84

Distribution of the differences

- Let $m_d = m_x - m_y$
- The difference of the means (m_d) also has a Student's distribution with k–1 degrees of freedom
- Let σ_d^2 be the variance of the difference
- The standardized version of m_d is called the t-statistic:

$$t = \frac{m_d}{\sqrt{\sigma_d^2 / k}}$$

- We use t to perform the t-test

Performing the test

- Fix a significance level α
  - If a difference is significant at the α% level, there is a (100-α)% chance that there really is a difference
- Divide the significance level by two because the test is two-tailed
  - I.e. the true difference can be +ve or –ve
- Look up the value for z that corresponds to $\alpha/2$
- If $t \leq -z$ or $t \geq z$ then the difference is significant
  - I.e. the null hypothesis can be rejected

Unpaired observations

- If the CV estimates are from different randomizations, they are no longer paired
- (or maybe we used *k* -fold CV for one scheme, and *j* -fold CV for the other one)
- Then we have to use an *un* paired t-test with min(*k* , *j*) – 1 degrees of freedom
- The *t*-statistic becomes:

$$t = \frac{m_d}{\sqrt{\sigma_d^2 / k}} \quad \Rightarrow \quad t = \frac{m_x - m_y}{\sqrt{\frac{\sigma_x^2}{k} + \frac{\sigma_y^2}{j}}}$$

Interpreting the result

- All our cross-validation estimates are based on the same dataset
- Samples are not independent
- Should really use a different dataset sample for each of the *k* estimates used in the test to judge performance across different training sets
- Or, use heuristic test, e.g. *corrected resampled t-test*

Predicting probabilities

- Performance measure so far: success rate
- Also called *0-1 loss function*:

$$\sum_i \begin{cases} 0 \text{ if prediction is correct} \\ 1 \text{ if prediction is incorrect} \end{cases}$$

- Most classifiers produces class probabilities
- Depending on the application, we might want to check the accuracy of the probability estimates
- 0-1 loss is not the right thing to use in those cases

Quadratic loss function

- p_1 ... p_k are probability estimates for an instance
- c is the index of the instance's actual class
- a_1 ... $a_k = 0$, except for a_c which is 1
- *Quadratic loss* is: $\sum_j (p_j - a_j)^2 = \sum_{j \neq c} p_j^2 + (1 - p_c)^2$
- Want to minimize $E\left[\sum_j (p_j - a_j)^2\right]$
- Can show that this is minimized when $p_j = p_j^*$, the true probabilities

Informational loss function

- The informational loss function is $-\log(p_c)$, where c is the index of the instance's actual class
- Number of bits required to communicate the actual class
- Let p_1^* ... p_k^* be the true class probabilities
- Then the expected value for the loss function is:

$$-p_1^* \log_2 p_1 - \ldots - p_k^* \log_2 p_k$$

- Justification: minimized when $p_j = p_j^*$
- Difficulty: *zero-frequency problem*

Discussion

- Which loss function to choose?
  - Both encourage honesty
  - Quadratic loss function takes into account all class probability estimates for an instance
  - Informational loss focuses only on the probability estimate for the actual class
  - Quadratic loss is bounded:
    it can never exceed 2
    $1+\sum_j p_j^2$
  - Informational loss can be infinite

- Informational loss is related to *MDL principle* [later]

Counting the cost

- In practice, different types of classification errors often incur different costs
- Examples:
  - Terrorist profiling
    - "Not a terrorist" correct 99.99% of the time
  - Loan decisions
  - Oil-slick detection
  - Fault diagnosis
  - Promotional mailing

Counting the cost

- The *confusion matrix*:

		Predicted class	
		Yes	No
Actual class	Yes	True positive	False negative
	No	False positive	True negative

- There many other types of cost!
  - E.g.: cost of collecting training data

Lift charts

- In practice, costs are rarely known
- Decisions are usually made by comparing possible scenarios
- Example: promotional mailout to 1,000,000 households
  - Mail to all; 0.1% respond (1000)
  - Data mining tool identifies subset of 100,000 most promising, 0.4% of these respond (400)
    40% of responses for 10% of cost may pay off
  - Identify subset of 400,000 most promising, 0.2% respond (800)
- A *lift chart* allows a visual comparison

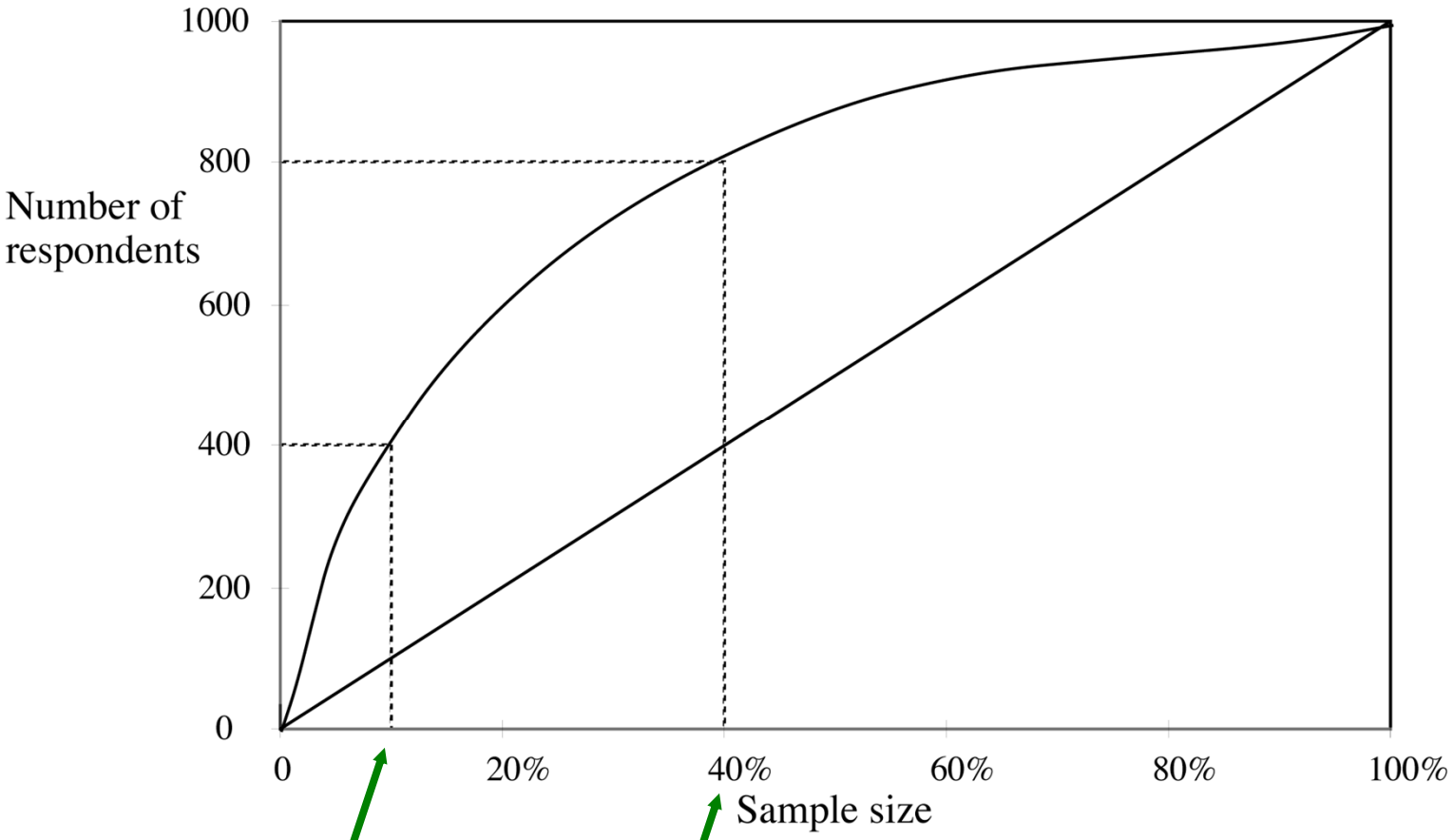
Generating a lift chart

- Sort instances according to predicted probability of being positive:

	Predicted probability	Actual class
1	0.95	Yes
2	0.93	Yes
3	0.93	No
4	0.88	Yes
...	...	...

- *x* axis is sample size
  y axis is number of true positives

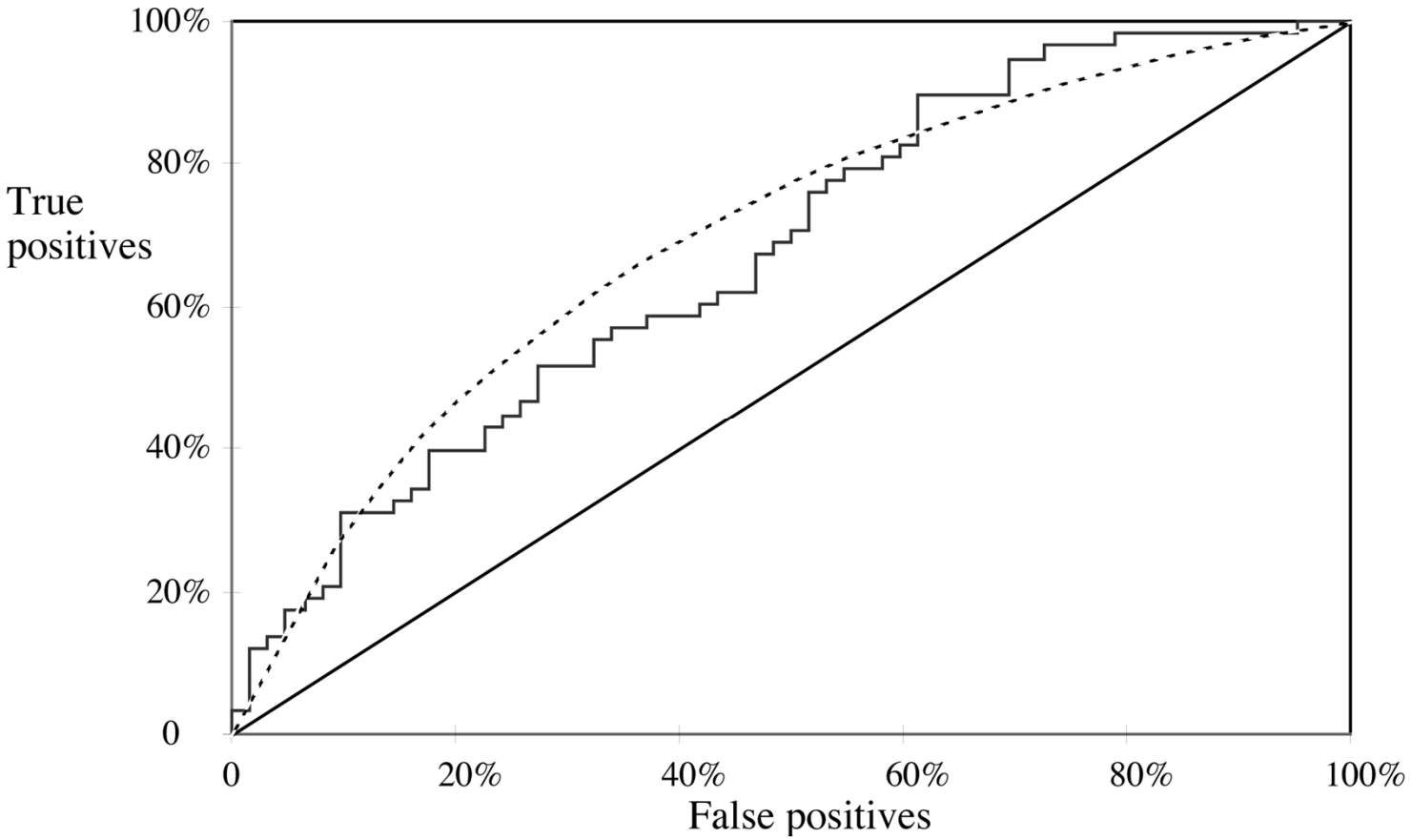
A hypothetical lift chart



ROC curves

- *ROC curves* are similar to lift charts
  - Stands for “receiver operating characteristic”
  - Used in signal detection to show tradeoff between hit rate and false alarm rate over noisy channel
- Differences to lift chart:
  - *y* axis shows percentage of true positives in sample *rather than absolute number*
  - *x* axis shows percentage of false positives in sample *rather than sample size*

A sample ROC curve

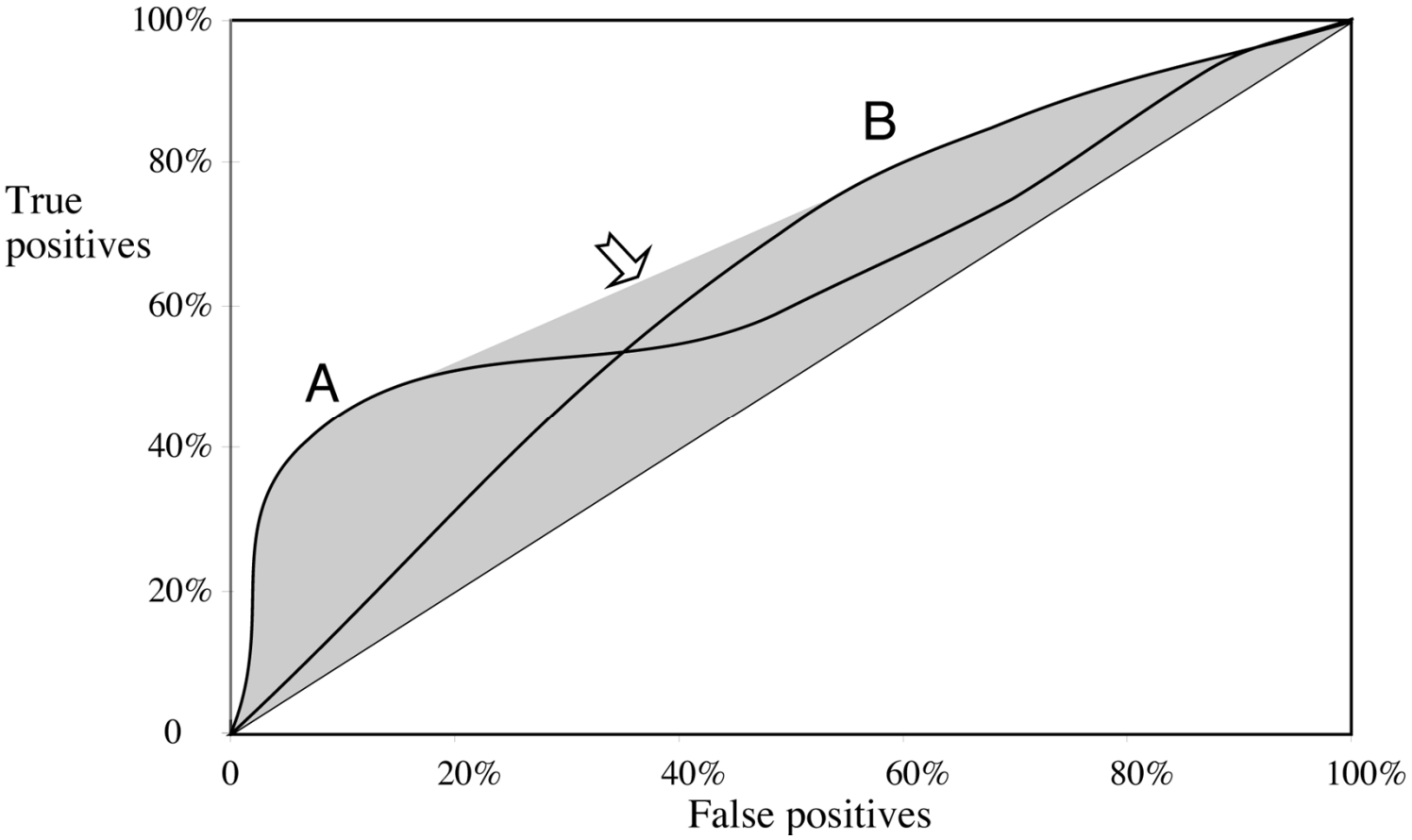


- Jagged curve—one set of test data
- Smooth curve—use cross-validation

Cross-validation and ROC curves

- Simple method of getting a ROC curve using cross-validation:
  - Collect probabilities for instances in test folds
  - Sort instances according to probabilities
- This method is implemented in WEKA
- However, this is just one possibility
  - The method described in the book generates an ROC curve for each fold and averages them

ROC curves for two schemes



- For a small, focused sample, use method A
- For a larger one, use method B
- In between, choose between A and B with appropriate probabilities

The convex hull

- Given two learning schemes we can achieve any point on the convex hull!
- TP and FP rates for scheme 1: t_1 and f_1
- TP and FP rates for scheme 2: t_2 and f_2
- If scheme 1 is used to predict $100 \times q$ % of the cases and scheme 2 for the rest, then
  - TP rate for combined scheme: $q \times t_1 + (1-q) \times t_2$
  - FP rate for combined scheme: $q \times f_1 + (1-q) \times f_2$

Cost-sensitive learning

- Most learning schemes do not perform cost-sensitive learning
  - They generate the same classifier no matter what costs are assigned to the different classes
  - Example: standard decision tree learner
- Simple methods for cost-sensitive learning:
  - Resampling of instances according to costs
  - Weighting of instances according to costs
- Some schemes can take costs into account by varying a parameter, e.g. naïve Bayes

Measures in information retrieval

- Percentage of retrieved documents that are relevant: *precision*=TP/(TP+FP)
- Percentage of relevant documents that are returned: *recall* =TP/(TP+FN)
- Precision/recall curves have hyperbolic shape
- Summary measures: average precision at 20%, 50% and 80% recall (*three-point average recall*)
- *F-measure*=(2×recall×precision)/(recall+precision)

Summary of measures

	Domain	Plot	Explanation
Lift chart	Marketing	TP Subset size	TP (TP+FP) / (TP+FP+TN+FN)
ROC curve	Communications	TP rate FP rate	TP / (TP+FN) FP / (FP+TN)
Recall-precision curve	Information retrieval	Recall Precision	TP / (TP+FN) TP / (TP+FP)

Evaluating numeric prediction

- Same strategies: independent test set, cross-validation, significance tests, etc.
- Difference: error measures
- Actual target values: $a_1\ a_2\ \ldots a_n$
- Predicted target values: $p_1\ p_2\ \ldots\ p_n$
- Most popular measure: *mean-squared error*

$$\frac{(p_1-a_1)^2+\ldots+(p_n-a_n)^2}{n}$$

  - Easy to manipulate mathematically

Other measures

- The *root mean-squared error* :

$$\sqrt{\frac{(p_1 - a_1)^2 + \ldots + (p_n - a_n)^2}{n}}$$

- The *mean absolute error* is less sensitive to outliers than the mean-squared error:

$$\frac{|p_1 - a_1| + \ldots + |p_n - a_n|}{n}$$

- Sometimes *relative* error values are more appropriate (e.g. 10% for an error of 50 when predicting 500)

Improvement on the mean

- How much does the scheme improve on simply predicting the average?
- The *relative squared error* is ($\bar{a}$ is the average):

$$\frac{(p_1 - a_1)^2 + \ldots + (p_n - a_n)^2}{(\bar{a} - a_1)^2 + \ldots + (\bar{a} - a_n)^2}$$

- The *relative absolute error* is:

$$\frac{|p_1 - a_1| + \ldots + |p_n - a_n|}{|\bar{a} - a_1| + \ldots + |\bar{a} - a_n|}$$

Correlation coefficient

- Measures the *statistical correlation* between the predicted values and the actual values

$$\frac{S_{PA}}{\sqrt{S_P S_A}}$$

$$S_{PA} = \frac{\sum_i (p_i - \bar{p})(a_i - \bar{a})}{n-1} \qquad S_P = \frac{\sum_i (p_i - \bar{p})^2}{n-1} \qquad S_A = \frac{\sum_i (a_i - \bar{a})^2}{n-1}$$

- Scale independent, between –1 and +1
- Good performance leads to large values!

Which measure?

- Best to look at all of them
- Often it doesn't matter
- Example:

	A	B	C	D
Root mean-squared error	67.8	91.7	63.3	57.4
Mean absolute error	41.3	38.5	33.4	29.2
Root rel squared error	42.2%	57.2%	39.4%	35.8%
Relative absolute error	43.1%	40.1%	34.8%	30.4%
Correlation coefficient	0.88	0.88	0.89	0.91

- D best
- C second-best
- A, B arguable

The MDL principle

- MDL stands for *minimum description length*
- The description length is defined as:

  space required to describe a theory

  +

  space required to describe the theory's mistakes
- In our case the theory is the classifier and the mistakes are the errors on the training data
- Aim: we seek a classifier with minimal DL
- MDL principle is a *model selection criterion*

Model selection criteria

- Model selection criteria attempt to find a good compromise between:
  - The complexity of a model
  - Its prediction accuracy on the training data
- Reasoning: a good model is a simple model that achieves high accuracy on the given data
- Also known as *Occam's Razor* : the best theory is the smallest one that describes all the facts

William of Ockham, born in the village of Ockham in Surrey (England) about 1285, was the most influential philosopher of the 14th century and a controversial theologian.

Elegance vs. errors

- Theory 1: very simple, elegant theory that explains the data almost perfectly
- Theory 2: significantly more complex theory that reproduces the data without mistakes
- Theory 1 is probably preferable
- Classical example: Kepler's three laws on planetary motion
  - Less accurate than Copernicus's latest refinement of the Ptolemaic theory of epicycles

MDL and compression

- MDL principle relates to data compression:
  - The best theory is the one that compresses the data the most
  - I.e. to compress a dataset we generate a model and then store the model and its mistakes
- We need to compute
  (a) size of the model, and
  (b) space needed to encode the errors
- (b) easy: use the informational loss function
- (a) need a method to encode the model

MDL and Bayes's theorem

- L[T]="length" of the theory
- L[E|T]=training set encoded wrt the theory
- Description length= L[T] + L[E|T]
- Bayes's theorem gives *a posteriori* probability of a theory given the data:

$$\Pr[T \mid E] = \frac{\Pr[E \mid T]\Pr[T]}{\Pr[E]}$$

- Equivalent to:

$$-\log\Pr[T \mid E] = -\log\Pr[E \mid T] - \log\Pr[T] + \underbrace{\log\Pr[E]}_{\textit{constant}}$$

MDL and MAP

- MAP stands for *maximum a posteriori probability*
- Finding the MAP theory corresponds to finding the MDL theory
- Difficult bit in applying the MAP principle: determining the prior probability Pr[T] of the theory
- Corresponds to difficult part in applying the MDL principle: coding scheme for the theory
- I.e. if we know a priori that a particular theory is more likely we need less bits to encode it

Discussion of MDL principle

- Advantage: makes full use of the training data when selecting a model
- Disadvantage 1: appropriate coding scheme/prior probabilities for theories are crucial
- Disadvantage 2: no guarantee that the MDL theory is the one which minimizes the expected error
- Note: Occam's Razor is an axiom!
- Epicurus's *principle of multiple explanations*: keep all theories that are consistent with the data

Bayesian model averaging

- Reflects Epicurus's principle: all theories are used for prediction weighted according to P[T|E]
- Let *I* be a new instance whose class we must predict
- Let *C* be the random variable denoting the class
- Then BMA gives the probability of *C* given
  - *I*
  - training data *E*
  - possible theories T_j

$$\Pr[C \mid I, E] = \sum_j \Pr[C \mid I, T_j] \Pr[T_j \mid E]$$

MDL and clustering

- Description length of theory:
  bits needed to encode the clusters
  - e.g. cluster centers
- Description length of data given theory:
  encode cluster membership and position relative to cluster
  - e.g. distance to cluster center
- Works if coding scheme uses less code space for small numbers than for large ones
- With nominal attributes, must communicate probability distributions for each cluster