Data Mining

Practical Machine Learning Tools and Techniques

Slides for Chapter 5, Evaluation

of *Data Mining* by I. H. Witten, E. Frank,
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Credibility: Evaluating what's been learned

- Issues: training, testing, tuning
- Predicting performance: confidence limits
- Holdout, cross-validation, bootstrap
- Hyperparameter selection
- Comparing machine learning schemes
- Predicting probabilities
- Cost-sensitive evaluation
- Evaluating numeric prediction
- The minimum description length principle
- Model selection using a validation set

Evaluation: the key to success

- How predictive is the model we have 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 a large amount 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 by evaluating model on 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 cannot 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* is located 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 $[–z \leqslant X \leqslant z]$ for a random variable X is determined using:

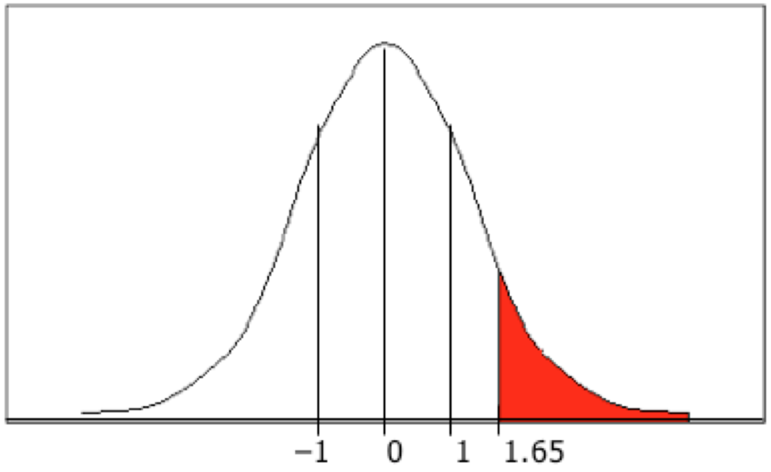
$$P(-z \leq X \leq z) = c.$$

- For a symmetric distribution such as the normal distribution we have:

$$P(-z \leqslant X \leqslant z) = 1-2*P(x \geqslant z)$$

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:

$$P(-1.65 \leq X \leq 1.65) = 90\%.$$

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

Transforming *f*

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

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

- Resulting equation: $P\left(-z < \dfrac{f-p}{\sqrt{p(1-p)/N}} < z\right) = c$

- Solving for *p* yields an expression for the confidence limits:

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

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)

$p \in [0.691, 0.801]$

Holdout estimation

- What should we do if we only have a single dataset?
- The *holdout* method reserves a certain amount for testing and uses the remainder for training, after shuffling
  - 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

- *K-fold cross-validation* avoids overlapping test sets
  - First step: split data into *k* subsets of equal size
  - Second step: use each subset in turn for **T**esting, the remainder for training (**L**earning)
  - This means the learning algorithm is applied to *k* different training sets

Round	S1	S2	S3
1	T	L	L
2	L	T	L
3	L	L	T

- Often the subsets are stratified before the cross-validation is performed to yield stratified *k*-fold cross-validation
- The error estimates are averaged to yield an overall error estimate; also, standard deviation is often computed
- Alternatively, predictions and actual target values from the *k* folds are pooled to compute one estimate
  - Does not yield an estimate of standard deviation

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 *k*-fold 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: using lazy classifiers such as the nearest-neighbor classifier)

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 gives 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 do not 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 0.632 bootstrap

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

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

- The resubstitution error gets less weight than the error on the test data
- Repeat process several times with different 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:

$$(0.632 \times 50\% + 0.368 \times 0\%) = 31.6\%$$

  - True expected error: 50%

Hyperparameter selection

- *Hyperparameter*: parameter that can be tuned to optimize the performance of a learning algorithm
  - Different from basic parameter that is part of a model, such as a coefficient in a linear regression model
  - Example hyperparameter: *k* in the *k*-nearest neighbour classifier
- We are not allowed to peek at the final test data to choose the value of this parameter
  - Adjusting the hyperparameter to the test data will lead to optimistic performance estimates on this test data!
  - Parameter tuning needs to be viewed as part of the learning algorithm and must be done using the training data only
- But how to get a useful estimate of performance for different parameter values so that we can choose a value?
  - Answer: split the data into a smaller “training” set and a validation set” (normally, the data is shuffled first)
  - Build models using different values of *k* on the new, smaller training set and evaluate them on the validation set
  - Pick the best value of *k* and rebuild the model on the full original training set

Hyperparameters and cross-validation

- Note that *k*-fold cross-validation runs *k* different train-test evaluations
  - The above parameter tuning process using validation sets must be applied separately to each of the *k* training sets!
- This means that, when hyperparameter tuning is applied, *k* different hyperparameter values may be selected
  - This is OK: hyperparameter tuning is part of the learning process
  - Cross-validation evaluates the quality of the learning process, not the quality of a particular model
- What to do when the training sets are very small, so that performance estimates on a validation set are unreliable?
- We can use *nested cross-validation* (expensive!)
  - For each training set of the "outer" *k*-fold cross-validation, run "inner" *p*-fold cross-validations to choose the best hyperparameter value
  - Outer cross-validation is used to estimate quality of learning process
  - Inner cross-validations are used to choose hyperparameter values
  - Inner cross-validations are part of the learning process!

Example : Hyperparameters in Cross-Validation

Round	S1	S2	S3
1		L	V
		V	L
	T	L	L
2	L		V
	V		L
	L	T	L
3	L	V	
	V	L	
	L	L	T

Comparing machine learning schemes

- Frequent question: which of two learning schemes performs better?
- Note: this is domain dependent!
- Obvious way: compare 10-fold cross-validation estimates
- Generally sufficient in applications (we do not loose if the chosen method is not truly better)
- However, what about machine learning research?
- Need to show convincingly that a particular method works better in a particular domain from which data is taken

Comparing learning schemes II

- Want to show that scheme A is better than scheme B in a particular domain
  - For a given amount of training data (i.e., data size)
  - On average, across all possible training sets from that domain
- Let's assume we have an infinite amount of data from the domain
- Then, we can simply
  - sample infinitely many datasets of a specified size
  - obtain a cross-validation estimate on each dataset for each scheme
  - check if the mean accuracy for scheme A is better than the mean accuracy for scheme B

Paired t-test

- In practice, we have limited data and a limited number of estimates for computing the mean
- *Student's t-test* tells us whether the means of two samples are significantly different
- In our case the samples are cross-validation estimates, one for each dataset we have sampled
- We can use a *paired* t-test because the individual samples are paired
  - The same cross-validation is applied twice, ensuring that all the training and test sets are exactly the same

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 2*k* samples for the *k* different datasets
- m_x and m_y are the means
- With enough samples, the mean of a set of independent samples is normally distributed
  (*central limit theorem* from statistics)
- 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
  $$\frac{m_x - \mu_x}{\sqrt{\sigma_x^2 / k}} \quad \frac{m_y - \mu_y}{\sqrt{\sigma_y^2 / k}}$$

  are *approximately* normally distributed with mean 0, variance 1

Student's distribution

- With small sample sizes (k < 100) the mean follows *Student's distribution with k–1 degrees of freedom*
- Confidence limits from Student's distribution:

Assuming we have 10 estimates

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 differences
- 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 paired *t*-test

Performing the test

- Fix a significance level
  - If a difference is significant at the a% level,
    there is a (100-a)% chance that the true means differ
- 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 a/2
- Compute the value of *t* based on the observed performance estimates for the schemes being compared
- If $t \leq -z$ or $t \geq z$ then the difference is significant
  - I.e., the *null hypothesis* (that the difference is zero) can be rejected

Unpaired observations

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

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

Dependent estimates

- Unfortunately, we have assumed that we have enough data to create several datasets of the desired size
- Need to re-use data if that is not the case
  - E.g., running cross-validations with different randomizations on the same data
- Samples become dependent → insignificant differences can become significant
- A heuristic test that tries to combat this is the *corrected resampled t-test*
  - Assume we use the repeated hold-out method with *k* runs, with n_1 instances for training and n_2 for testing
  - The new test statistic is:

$$t = \frac{m_d}{\sqrt{\left(\frac{1}{k} + \frac{n_2}{n_1}\right)\sigma_d^2}}$$

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 produce 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

- $p_1 \ldots p_k$ are probability estimates for an instance
- *c* is the index of the instance's actual class
- $a_1 \ldots a_k = 0$, except for a_c which is 1
- *Quadratic loss* is: $\sum_j (p_j - a_j)^2$
- Want to minimize $1 - 2p_c + \sum_j p_j^2$
- Can show that the expected value of this is minimized when $p_i = p_i^*$, where the latter are the true probabilities:

$$E\left[\sum_j (p_j - a_j)^2\right] = \sum_j (E[p_j^2] - 2E[p_j a_j] + E[a_j^2])$$
$$= \sum_j (p_j^2 - 2p_j p_j^* + p_j^*) = \sum_j ((p_j - p_j^*)^2 + p_j^*(1 - p_j^*))$$

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:

$$-p_1^*\log_2 p_1 - p_2^*\log_2 p_2 - \ldots - p_k^*\log_2 p_k$$

- Justification for informational loss is that this is minimized when $p_j = p_j^*$:

$$-p_1^*\log_2 p_1^* - p_2^*\log_2 p_2^* - \ldots - p_k^*\log_2 p_k^*$$

- Difficulty with informational loss : *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 by $1 + \sum_j p_j^2$

    it can never exceed 2
  - Informational loss can be infinite
- Informational loss is related to the *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

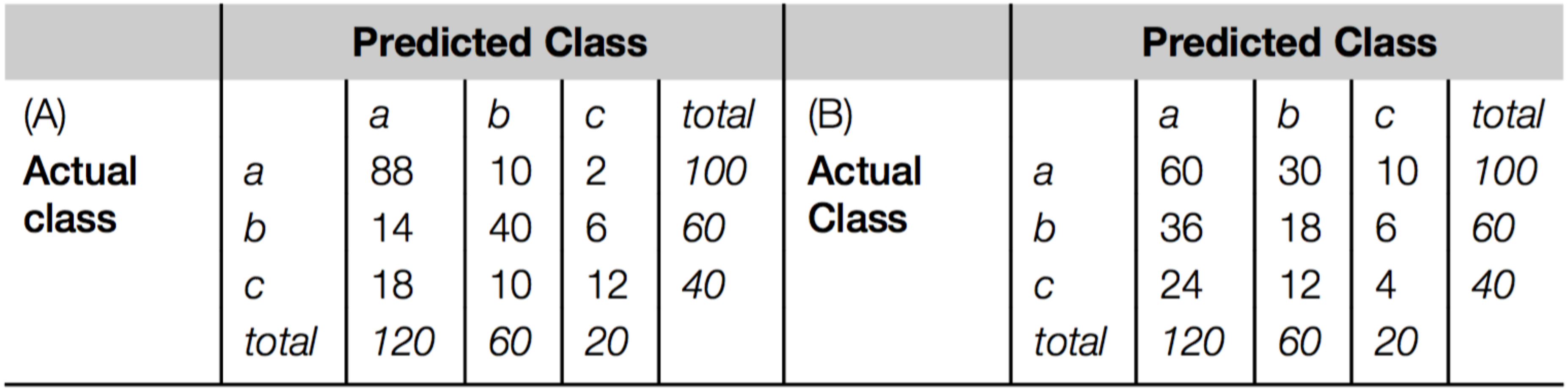
- The *confusion matrix*:

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

- Different misclassification costs can be assigned to false positives and false negatives
- There are many other types of cost!
  - E.g., cost of collecting training data

Aside: the kappa statistic

- Two confusion matrices for a 3-class problem: actual predictor (left) vs. random predictor (right)

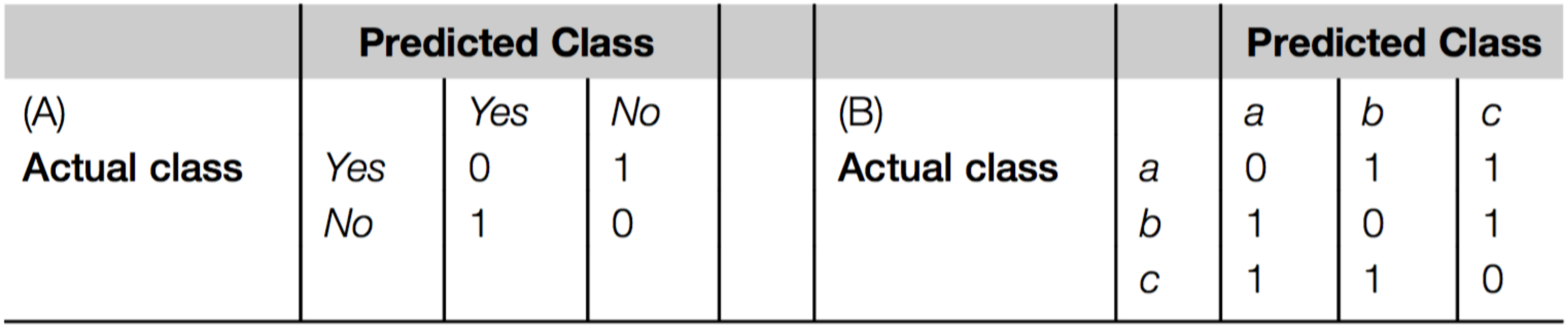


	Predicted Class						Predicted Class				
(A)		*a*	*b*	*c*	*total*	(B)		*a*	*b*	*c*	*total*
Actual class	*a*	88	10	2	*100*	**Actual Class**	*a*	60	30	10	*100*
	b	14	40	6	*60*		*b*	36	18	6	*60*
	c	18	10	12	*40*		*c*	24	12	4	*40*
	total	*120*	*60*	*20*			*total*	*120*	*60*	*20*	

- Number of successes: sum of entries in diagonal (*D*)
- *Kappa* statistic: (success rate of actual predictor - success rate of random predictor) / (1 - success rate of random predictor)
- Measures relative improvement on random predictor: 1 means perfect accuracy, 0 means we are doing no better than random

Classification with costs

- Two cost matrices:



		Predicted Class	
(A)		*Yes*	*No*
Actual class	*Yes*	0	1
	No	1	0

		Predicted Class		
(B)		*a*	*b*	*c*
Actual class	*a*	0	1	1
	b	1	0	1
	c	1	1	0

- In cost-sensitive evaluation of classification methods, success rate is replaced by average cost per prediction
  - Cost is given by appropriate entry in the cost matrix

Cost-sensitive classification

- Can take costs into account when making predictions
  - Basic idea: only predict high-cost class when very confident about prediction
- Given: predicted class probabilities
  - Normally, we just predict the most likely class
  - Here, we should make the prediction that minimizes the expected cost
    - Expected cost: dot product of vector of class probabilities and appropriate column in cost matrix
    - Choose column (class) that minimizes expected cost
- This is the minimum-expected cost approach to cost-sensitive classification

Cost-sensitive classification: Example

Cost Matrix		predicted class	
		Spam	Ham
actual class	Spam	0	1
	Ham	10	0

- Let p_S =Pr(X=Spam)
- Regard expected costs for each class
  (dot product of vector of class probabilities and appropriate column in cost matrix)
  - EC(Spam)=p_S *0 + (1-p_S)*10
  - EC(Ham)=p_S *1 + (1-p_S)*0
- E.g. p_S=*0.7*: EC(Spam)=3, EC(Ham)=0.7
- Decide for Spam iff EC(Spam) < EC(Ham):
  - p_S > 10/11

Cost-sensitive learning

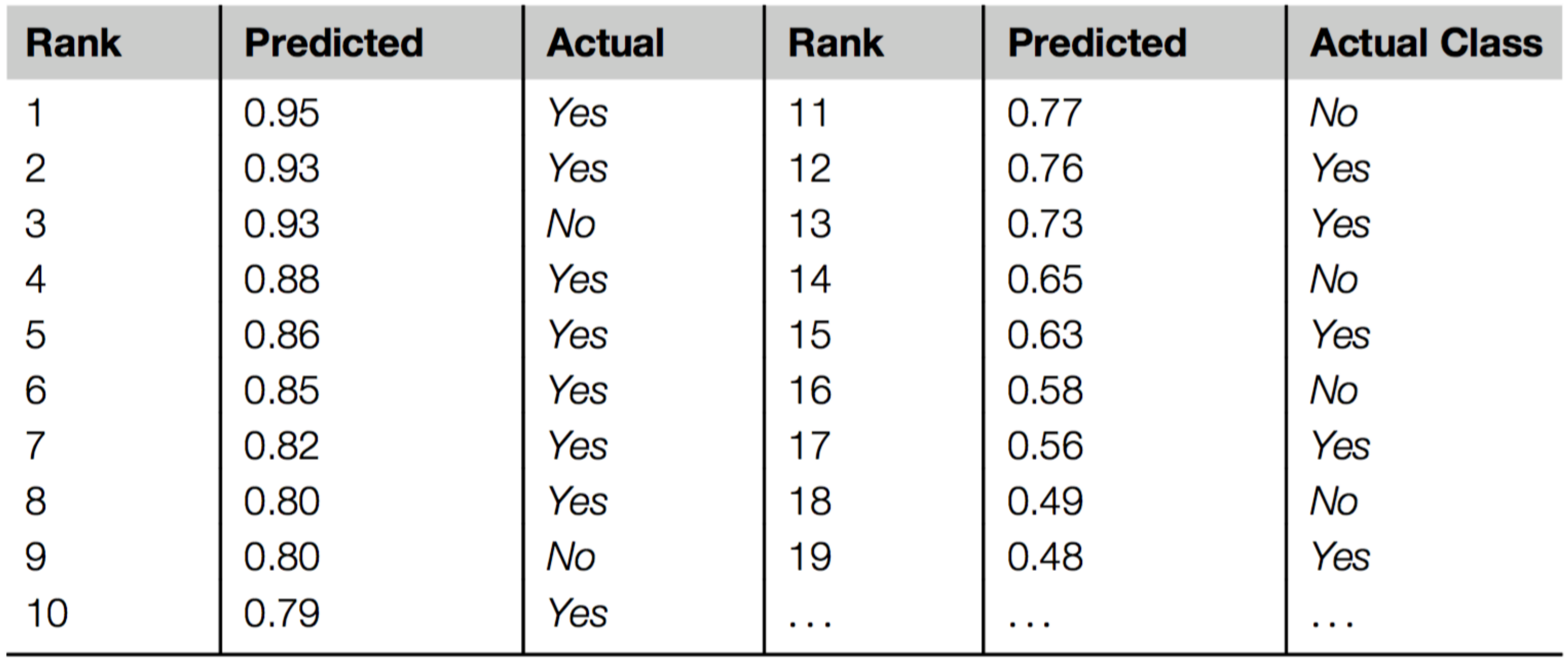
- So far we haven't taken costs into account at training time
- Most learning schemes do not perform cost-sensitive learning
  - They generate the same classifier no matter what costs are assigned to the different classes
  - Example: standard decision tree learner
- Simple methods for cost-sensitive 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

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

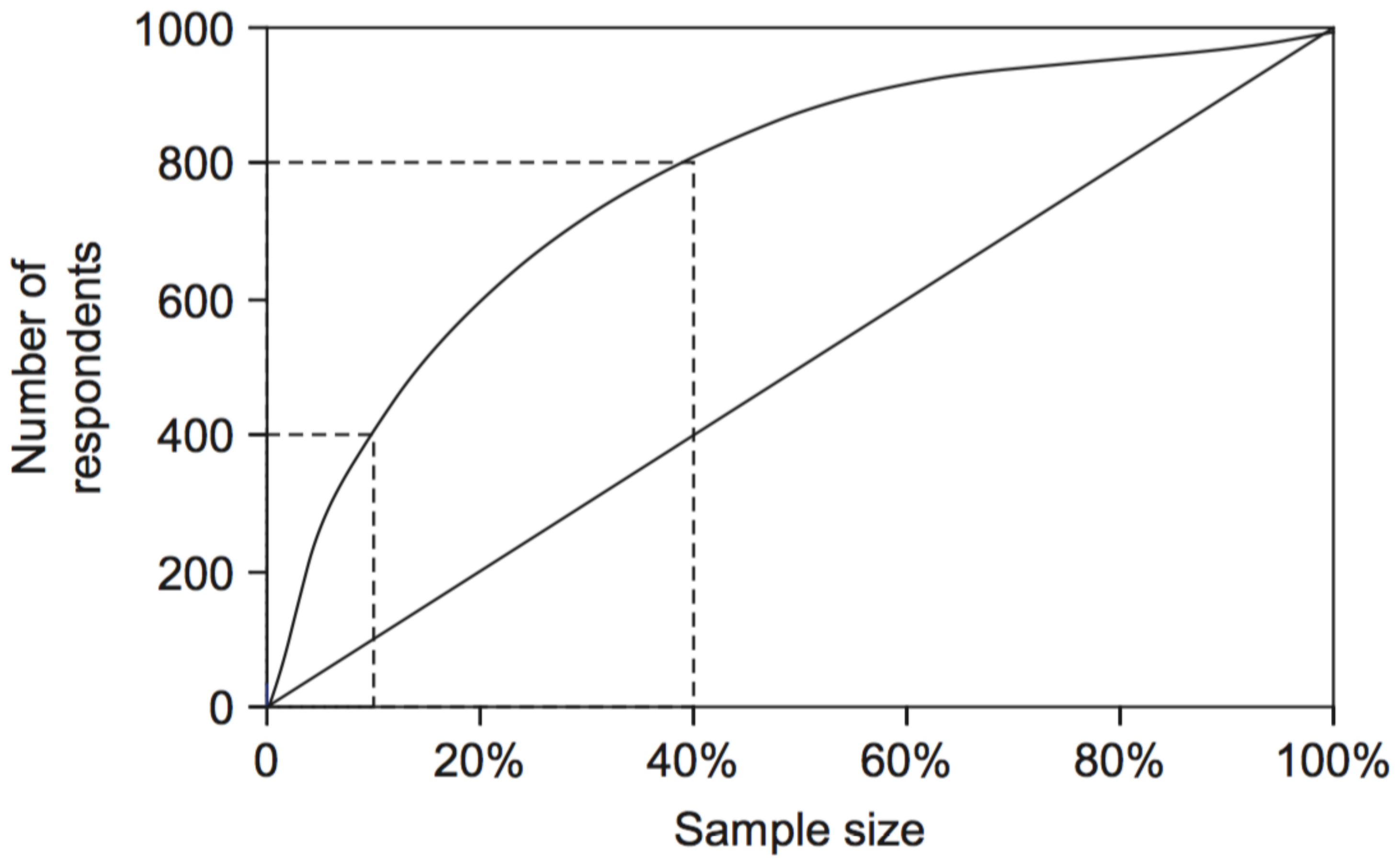
- Sort instances based on predicted probability of being positive:



Rank	Predicted	Actual	Rank	Predicted	Actual Class
1	0.95	*Yes*	11	0.77	*No*
2	0.93	*Yes*	12	0.76	*Yes*
3	0.93	*No*	13	0.73	*Yes*
4	0.88	*Yes*	14	0.65	*No*
5	0.86	*Yes*	15	0.63	*Yes*
6	0.85	*Yes*	16	0.58	*No*
7	0.82	*Yes*	17	0.56	*Yes*
8	0.80	*Yes*	18	0.49	*No*
9	0.80	*No*	19	0.48	*Yes*
10	0.79	*Yes*	...	...	...

- *x* axis in lift chart is sample size for each probability threshold
- *y* axis is number of true positives above threshold

A hypothetical lift chart



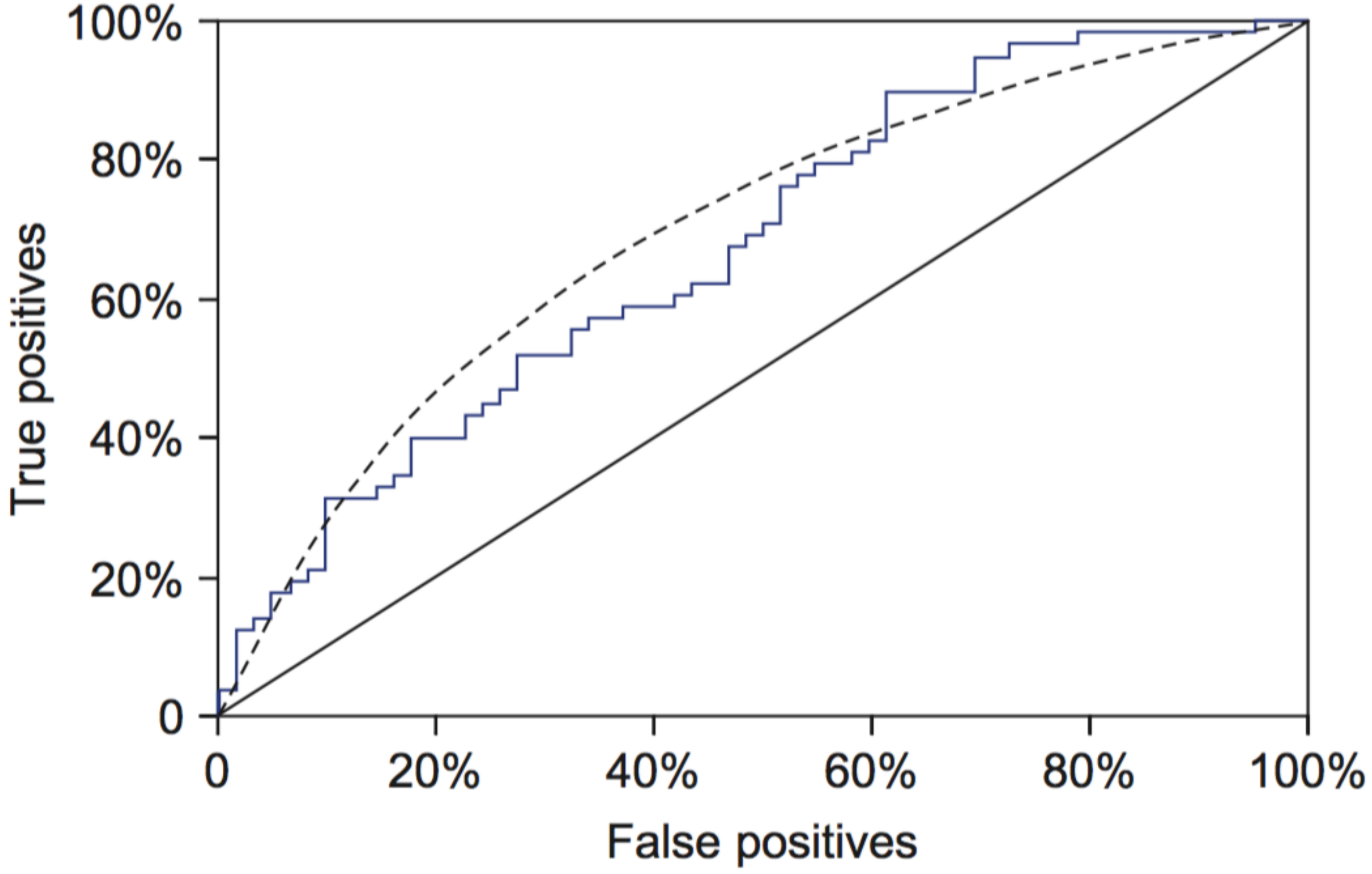
40% of responses for 10% of cost

80% of responses for 40% of cost

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

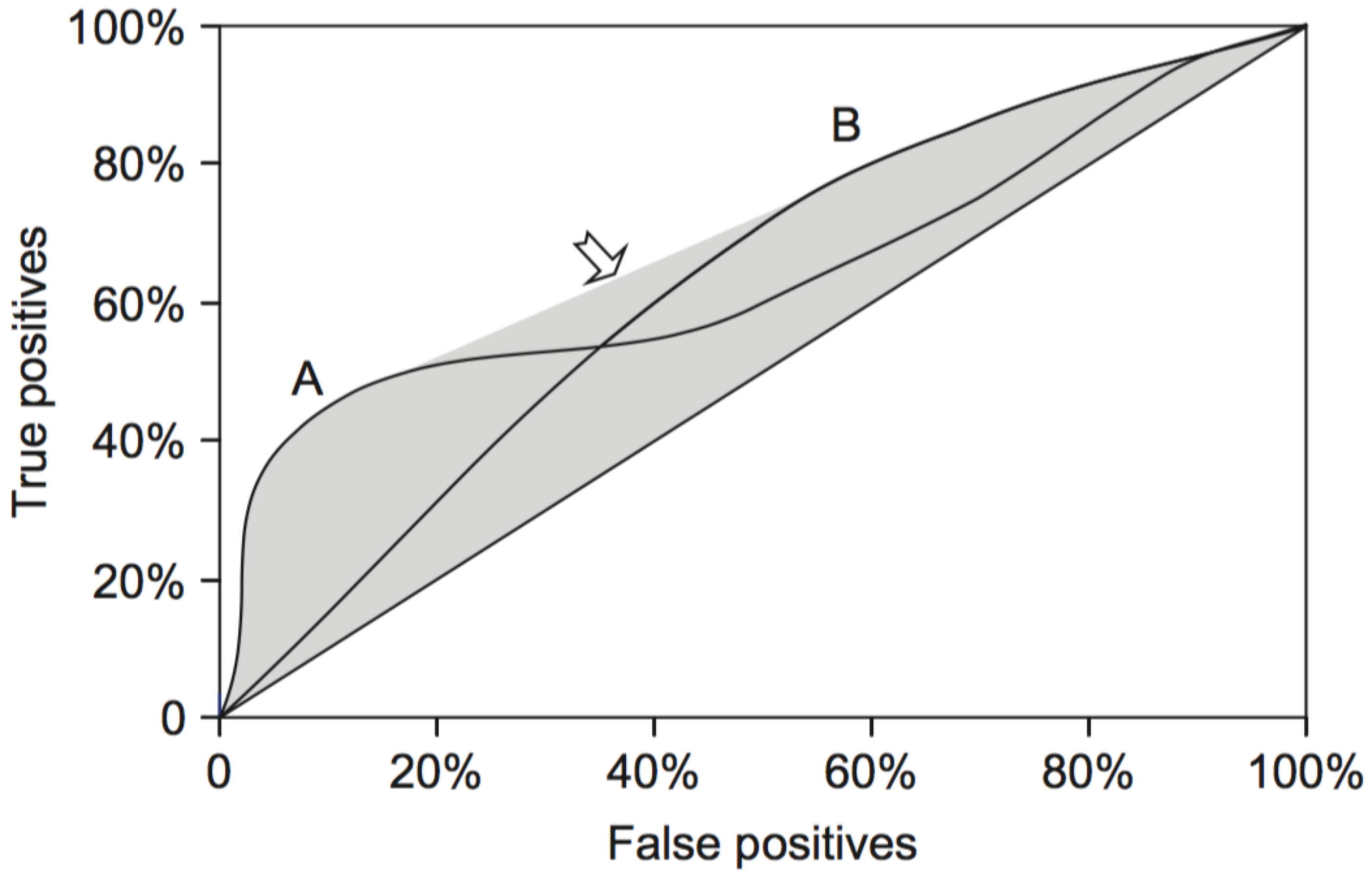


- Jagged curve—one set of test data
- Smoother curve—use cross-validation

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
  - Another possibility is to generate an ROC curve for each fold and average them

ROC curves for two schemes



- For a small, focused sample, use method A
- For a larger one, use method B
- Inbetween, 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:
    $q \times f_1 + (1-q) \times f_2$

More measures…

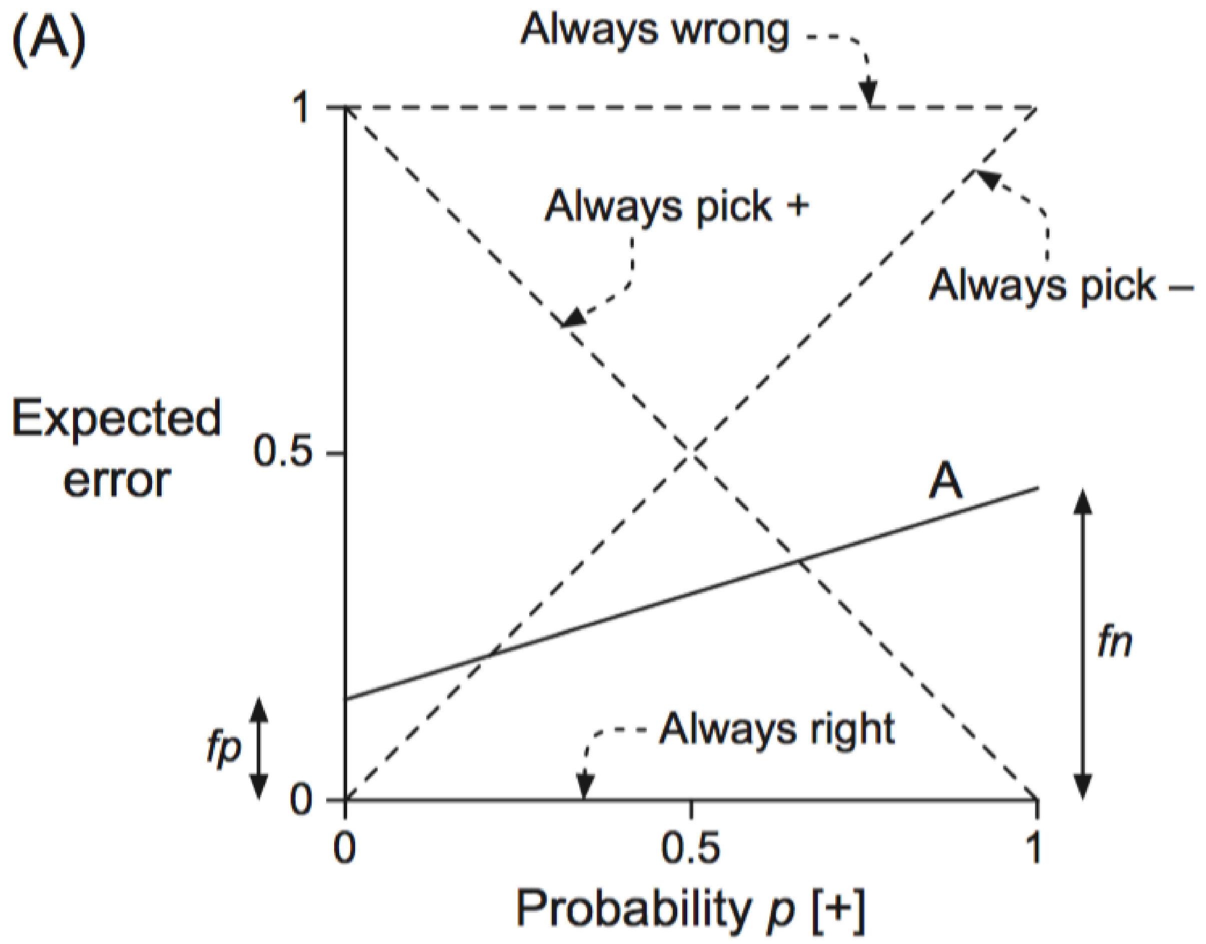
- Percentage of retrieved documents that are relevant: *precision*=TP/(TP+FP)
- Percentage of relevant documents that are returned: *recall* =TP/(TP+FN)
- Precision/recall curves have hyperbolic shape
- Summary measures: *average precision* values at each correct item
- *F-measure*=(2 × recall × precision)/(recall+precision)
- *sensitivity* × specificity = (TP / (TP + FN)) × (TN / (FP + TN))
- Area under the ROC curve (*AUC*):
  probability that randomly chosen positive instance is ranked above randomly chosen negative one

Summary of some measures

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

Cost curves

- *Cost curves* plot expected costs directly
- Example for case with uniform costs (i.e., error)



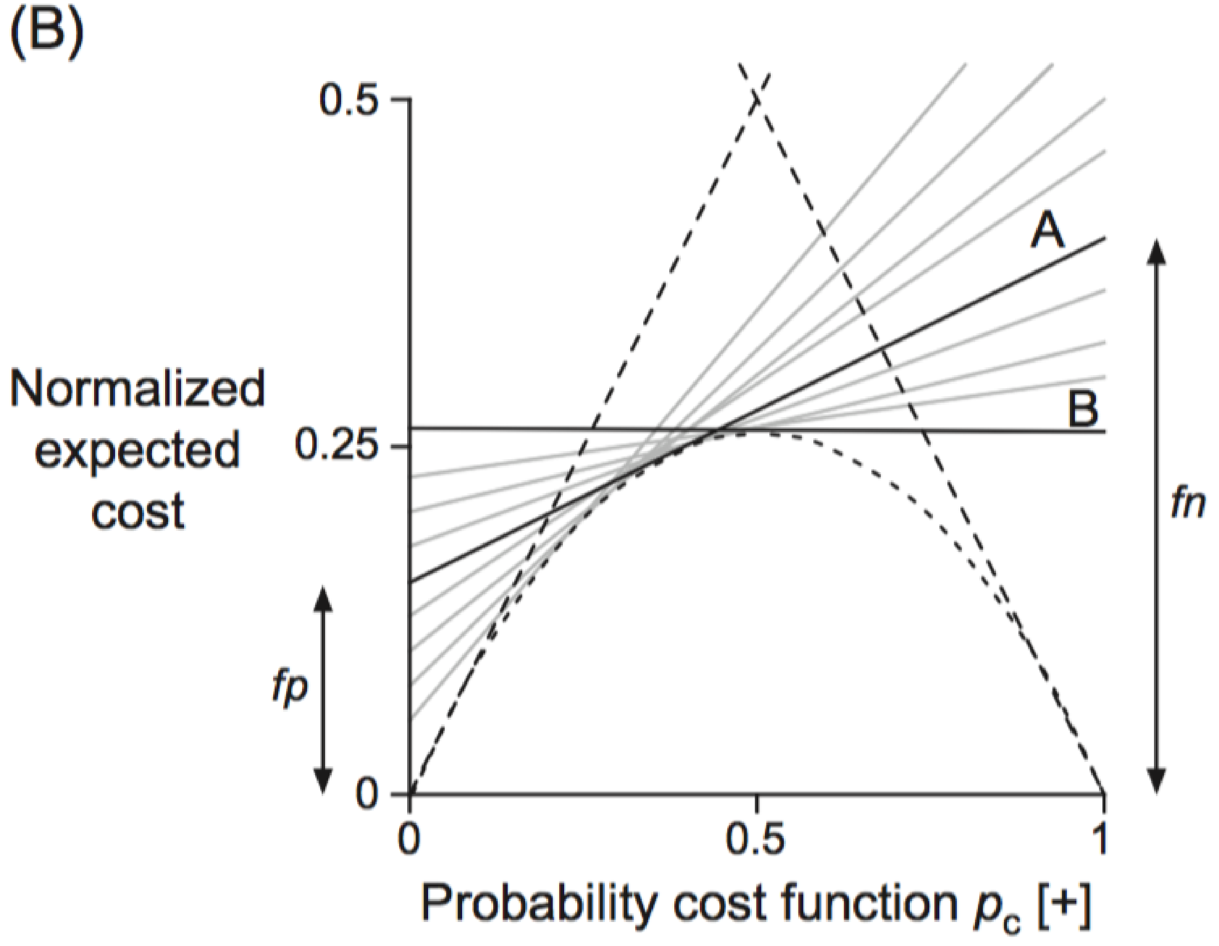
fp – false positive rate

fn - false negative rate

p[+] - average probability on test sample

Cost curves: example with costs

Effect of varying probability threshold



- C[+|-]: Costs for predicting + when -
- C[-|+]: Costs for predicting - when +
- C[+|+] = C[–|–] = 0

$$\text{Normalized expected cost} = fn \times P_C(+) + fp \times (1 - P_C(+))$$

$$\text{Probability cost function } P_C(+) = \frac{P(+)C[-\mid+]}{P(+)C[-\mid+] + P(-)C[+\mid-]}$$

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*

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

  - Easy to manipulate mathematically

Other measures

- The *root mean-squared error* :

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

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

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

- 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:

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

(in this formula and the following two, $\bar{a}$ is the mean value over the training data)

- The *root relative squared error* and the *relative absolute error* are:

$$\sqrt{\frac{(p_1 - a_1)^2 + \cdots + (p_n - a_n)^2}{(a_1 - \bar{a})^2 + \cdots + (a_n - \bar{a})^2}} \qquad \frac{|p_1 - a_1| + \cdots + |p_n - a_n|}{|a_1 - \bar{a}| + \cdots + |a_n - \bar{a}|}$$

Correlation coefficient

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

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

$$S_A = \frac{\sum_i (a_i - \bar{a})^2}{n-1} \text{ (here, } \bar{a} \text{ is the mean value over the test data)}$$

- 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

Choice of Evaluation Measure

- Often strong correlation between different measures
- However, in certain settings choosing the right measure (and underlying criterion) is crucial, e.g.
  - skewed distributions
  - many outliers
  - different cost parameters (e.g. high cost for missing infrequent class)

Evaluation vs. tuning criterion

- Tuning: top speed

- Evaluation: fuel consumption

Evaluation vs. tuning criterion

- All ML algorithms use a (sometimes implicit) tuning criterion, e.g.
  - ID3: information gain
  - linear regression: mean squared error
- Evaluation measure is based on an evaluation criterion
- Ideally, evaluation criterion = tuning criterion
  - ID3: information loss
  - linear regression: mean squared error
- Same criterion especially important for considering costs

➔ Think about evaluation criterion before choosing ML algorithm!

➔ If possible, choose algorithm with tuning criterion $\approx$ evaluation criterion

The MDL principle

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*
  - Enables us to choose a classifier of an appropriate complexity to combat overfitting

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 on the data available at the time

MDL and compression

- MDL principle relates to data compression:
  - The best theory is the one that compresses the data the most
  - In supervised learning, to compress the labels of a dataset, we generate a model and then store the model and its mistakes
- We need to compute
  (a) the size of the model, and
  (b) the 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 can be used to obtain the *a posteriori* probability of a theory given the data:

$$P(T|E) = \frac{P(E|T)P(T)}{P(E)}$$

- Equivalent to:

$$-\log P(T|E) = -\log P(E|T) - \log P(T) + \underbrace{\log P(E)}_{\textit{constant}}.$$

MDL and MAP

- MAP stands for *maximum a posteriori probability*
  - Probabilistic approach to model selection
- Finding the MAP theory is the same as finding the MDL theory, assuming coding scheme corresponds to prior
- Difficult bit in applying the MAP principle: determining the prior probability P(T) of the theory
- Corresponds to difficult part in applying the MDL principle: coding scheme for the theory
- Correspondence is clear: if we know *a priori* that a particular theory is more likely, we need fewer 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

MDL and clustering

- Model selection in clustering: finding the most appropriate number of clusters to model the data
- 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

Using a validation set for model selection

- MDL principle is one example of a model selection criterion
  - Model selection: finding the right model complexity
- Classic model selection problem in statistics:
  - Finding the subset of attributes to use in a linear regression model (yes, linear regression can overfit!)
- Other model selection problems: choosing the size of a decision tree or artificial neural network
- Many model selection criteria exist, based on a variety of theoretical assumptions
- Simple model selection approach: use a validation set
  - Use the model complexity that yields best performance on the validation set
- Alternative approach when data is scarce: internal cross-validation