

Difficulties in Classifier Evaluation and Comparison

- ◆ Training error is not a good indicator of testing error
- ◆ Data with known class labels are often in short supply
- ◆ *Costs* of errors need to be taken into account
- ◆ Evaluation results must be evaluated themselves

Accuracy and Error Rate

- ◆ Accuracy $Acc(M)$ of a classifier on a given test set is the percentage of the test records that are correctly classified
- ◆ Error rate: $1 - Acc(M)$

Confusion Matrix

		Predicted Class	
		cancer	not cancer
Actual Class	cancer	20	5
	not cancer	10	1000

Confusion Matrix for Binary Classification

		Predicted Class	
		C1	C2
Actual Class	C1	true positive (t_{pos})	false negative (f_{neg})
	C2	false positive (f_{pos})	true_negative (t_{neg})

C1 is the main class of interests

Costs of Misclassification

- ◆ The costs (or risks) of a false negative tend to be far greater than that of a false positive
 - E.g. cancer vs. not cancer

Precision and Recall

$$precision = \frac{t_pos}{t_pos + f_pos}$$

$$recall = \frac{t_pos}{t_pos + f_neg}$$

Sensitivity and Specificity

- ◆ Sensitivity = Recall
- ◆ Specificity = $t_neg / (t_neg + f_pos)$

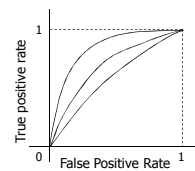
Accuracy Measure Examples

		Predicted Class	
		cancer	not cancer
Actual Class	cancer	20	5
	not cancer	10	1000

- ◆ Accuracy and error rate??
- ◆ Precision and Recall??
- ◆ Sensitivity and specificity??

ROC Curve

- ◆ Receive Operating Characteristic Curve
- ◆ Assumptions
 - Two-class problem
 - Classifier returns a probability



ROC Examples

	1	2	3	4	5	6	7	8	9	10
Prob.	0.9	0.8	0.7	0.6	0.55	0.54	0.53	0.51	0.5	0.4
M ₁	P	P	N	P	P	N	N	N	P	N
M ₂	P	P	P	P	P	N	N	N	N	N
M ₃	P	N	P	N	P	N	P	N	P	N

Utilizing Records with Known Class Labels

- ◆ For both training and testing
 - More training records → better classifier
 - More testing records → better accuracy estimate

The Holdout Method

- ◆ Randomly partition the given records into two non-overlapping subsets: a training set and a testing set
 - ◆ Typically 2/3 for training and 1/3 for testing

Problems of the Holdout Method

- ◆ More records for training means less for testing, and vice versa
- ◆ Distribution of the data in the training/testing set may be different from the original dataset
- ◆ Some classifiers are sensitive to random fluctuations in the training data

Random Subsampling

- ◆ Repeat the holdout method k times
- ◆ Take the average accuracy over the k iterations
- ◆ Random subsampling methods
 - Bootstrap Method
 - Cross-validation

Bootstrap Method

- ◆ Each iteration uses a sample to train the classifier, and the remaining records for testing
- ◆ Uniform sampling with replacement – *bootstrapping*
 - A sample record may be selected more than once

.632 Bootstrap ...

- ◆ Select d samples out of a dataset of size d and use them as the training set, and the rest are used for testing
- ◆ On average, 63.2% of the records will be selected into the training set
- ◆ The probability of not being selected:

$$(1 - 1/d)^d \xrightarrow{d \rightarrow \infty} e^{-1} = 2.718^{-1} = 0.368$$

... .632 Bootstrap

- ◆ Overall accuracy over k iterations

$$\frac{1}{k} \sum_{i=1}^k (0.632 \times \text{Acc}(M_i)_{\text{test_set}} + 0.368 \times \text{Acc}(M_i)_{\text{all_records}})$$

K-fold Cross Validation

- ◆ Randomly divide the data into k non-overlapping subsets of roughly equal size called *folds*
- ◆ Each iteration uses $(k-1)$ subsets for training, and the remaining subset for testing

Variants of K-fold Cross Validation

- ◆ Stratified folds: the class distribution in each fold is roughly the same as in the original dataset
- ◆ Leave-one-out
- ◆ 10-fold Cross Validation

Accuracy Using K-fold Cross Validation

Total # of correctly classified records over k iterations

Total # of records in the original dataset

Interpret Testing Results

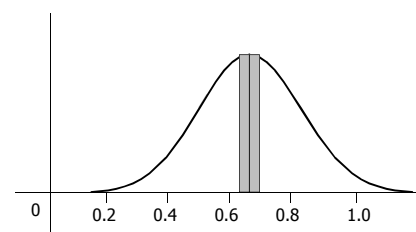
Round	1	2	3	4	5	Avg
Acc(M_1)	0.62	0.47	0.70	0.72	0.69	0.64
Acc(M_2)	0.57	0.57	0.63	0.53	0.72	0.604

- ◆ How confident are we about the average accuracy?
- ◆ Is M_1 really better than M_2 ?

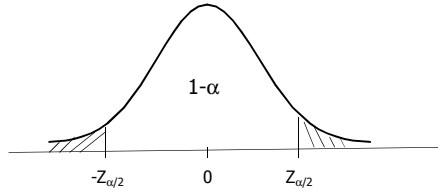
Confidence Interval

- ◆ Accuracies are *estimated*
- ◆ We want to say something like: the accuracy is in the range of 0.66 ± 0.04 with 99% confidence
 - Confidence interval: 0.66 ± 0.04
 - Degree of confidence (a.k.a. confidence level): 99%

Probabilistic Distribution of Accuracy



Confidence Interval of Standard Normal Distribution



$1-\alpha$	0.99	0.98	0.95	0.9	0.8	0.7	0.5
$Z_{\alpha/2}$	2.58	2.33	1.96	1.65	1.28	1.04	0.67

Confidence Interval for Accuracy

$$\frac{2N \cdot \text{Acc} + Z_{\alpha/2}^2 \pm Z_{\alpha/2} \sqrt{Z_{\alpha/2}^2 + 4N \cdot \text{Acc} - 4N \cdot \text{Acc}^2}}{2(N + Z_{\alpha/2}^2)}$$

N: number of testing records
Acc: average accuracy

Confidence Interval Examples

- ◆ Average accuracy: 80%
- ◆ Confidence level (i.e. $1-\alpha$): 95%

N	Confidence Interval
50	[0.67, 0.89]
100	[0.71, 0.87]
500	[0.76, 0.83]
1000	[0.77, 0.82]

Comparing Classifiers

- ◆ Is a classifier with 72% accuracy better than one with 68% accuracy? Or in other words, is the 4% difference statistically significant?

t-test

- ◆ Test whether the means of two normally distributed populations are the same

1. Null hypothesis: $\mu_1 - \mu_2 = 0$
2. Choose significance level: α
3. Calculate t statistic
4. Reject hypothesis if $t > t_{v, \alpha}$ where v is the degree of freedom

t-test Example

- ◆ Two classifiers M_1 and M_2
- ◆ 5-fold cross validation, and at each round M_1 and M_2 use the same training/testing partition(s)

Round	1	2	3	4	5
Acc(M_1)	0.62	0.47	0.70	0.72	0.69
Acc(M_2)	0.57	0.57	0.63	0.53	0.72

t Statistic

Accuracy difference in round i : $d_i = Acc(M_1)_i - Acc(M_2)_i$

Mean accuracy difference: $\bar{d} = \frac{1}{k} \sum_{i=1}^k d_i$

Standard deviation of accuracy differences: $S_d = \sqrt{\frac{1}{k-1} \sum_{i=1}^k (d_i - \bar{d})^2}$

t Statistic: $t = \frac{\bar{d}}{S_d / \sqrt{k}}$

t Statistic Calculation Example

Round	1	2	3	4	5
Acc(M ₁)	0.62	0.47	0.70	0.72	0.69
Acc(M ₂)	0.57	0.57	0.63	0.53	0.72
d _i	0.05	-0.10	0.07	0.19	-0.03

$$\bar{d} = 0.036$$

$$S_d = 0.109 \quad t = \frac{0.036}{0.109 / \sqrt{5}} = 0.74$$

t Value Table Lookup

α	0.1	0.05	0.025	0.01	0.005	v
	1.53	2.13	2.78	3.75	4.60	4
	1.38	1.83	2.26	2.82	3.25	9

In our example

- Choose significance level $\alpha = 0.05$
- Degree of freedom $v = k - 1 = 4$

Readings

- ◆ Textbook 8.5