Evaluation of Classifiers

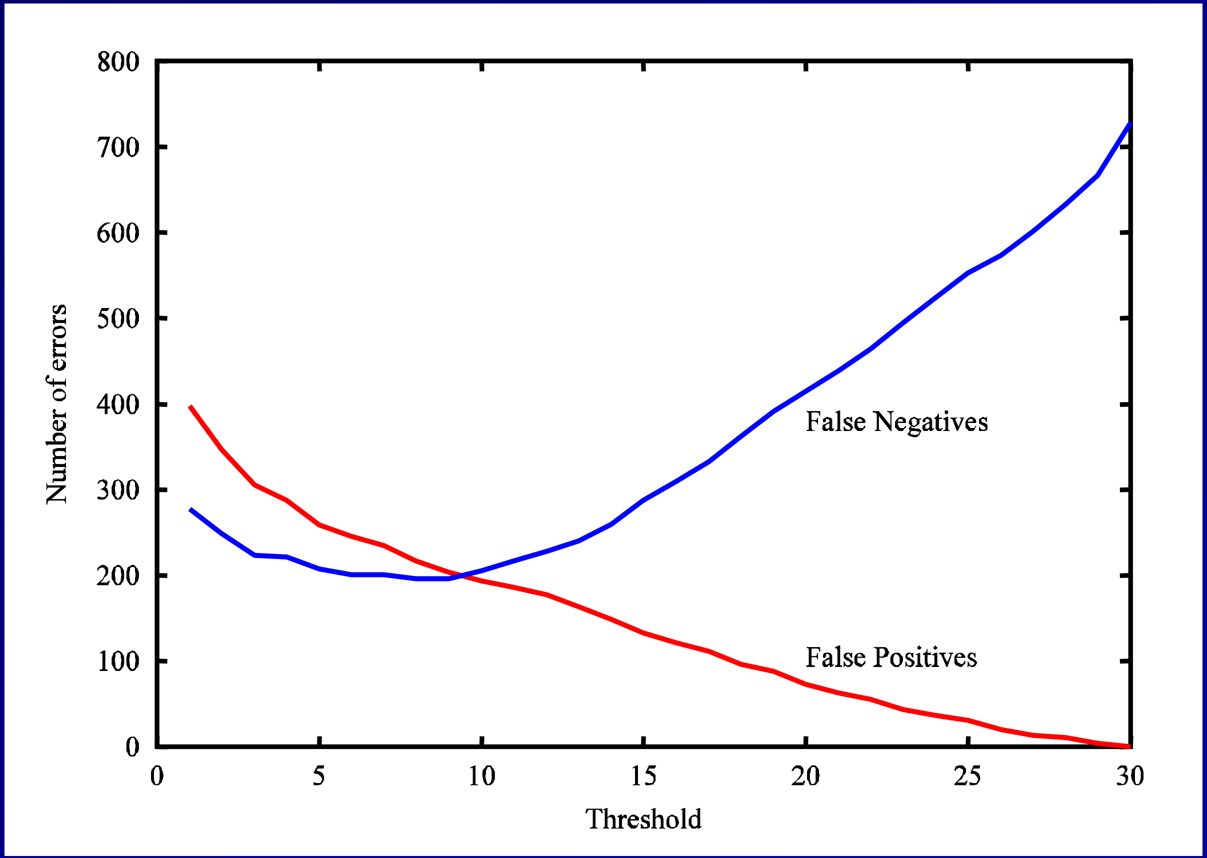
- ROC Curves
- Reject Curves
- Precision-Recall Curves
- Statistical Tests
  - Estimating the error rate of a classifier
  - Comparing two classifiers
  - Estimating the error rate of a learning algorithm
  - Comparing two algorithms

Cost-Sensitive Learning

- In most applications, false positive and false negative errors are not equally important. We therefore want to adjust the tradeoff between them. Many learning algorithms provide a way to do this:
  – probabilistic classifiers: combine cost matrix with decision theory to make classification decisions
  – discriminant functions: adjust the threshold for classifying into the positive class
  – ensembles: adjust the number of votes required to classify as positive

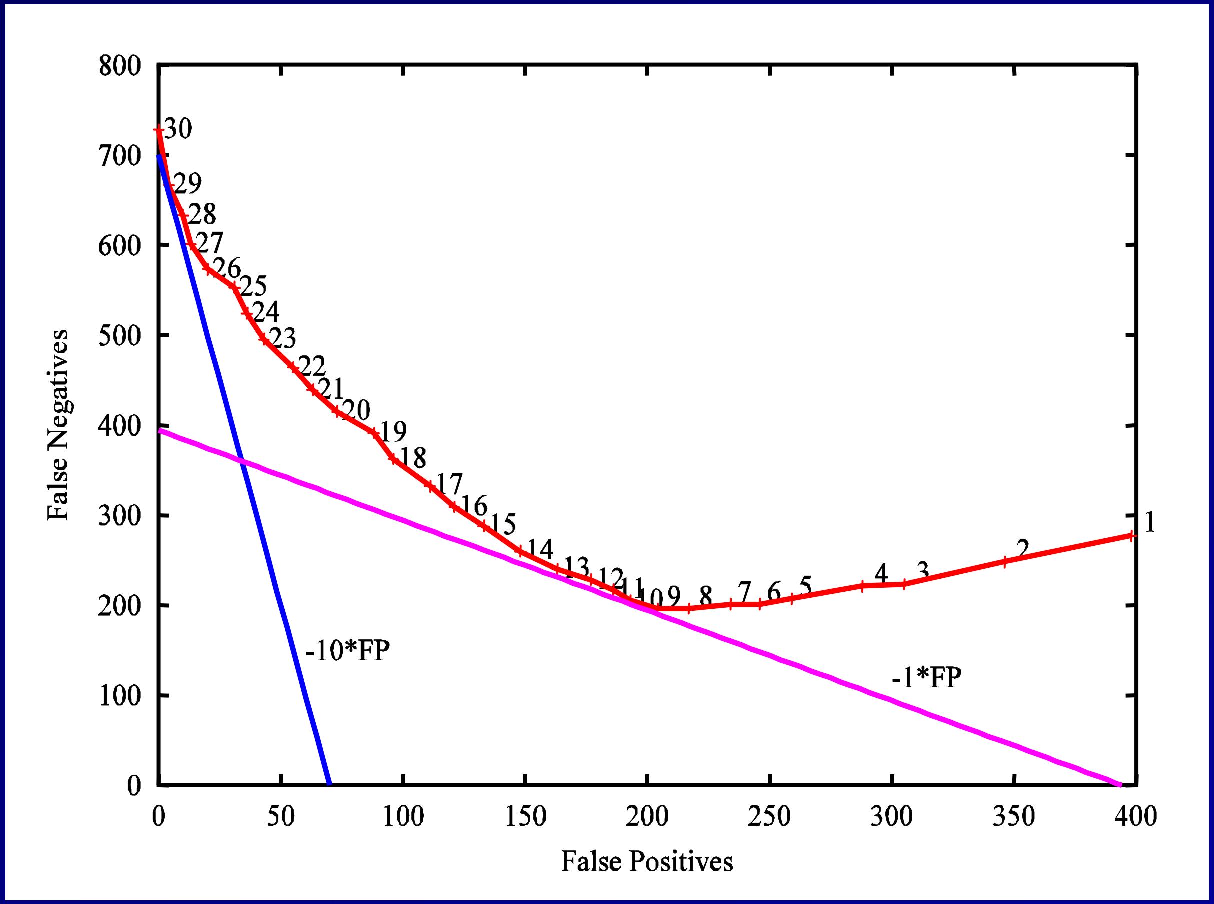
Example: 30 decision trees constructed by bagging

- Classify as positive if K out of 30 trees predict positive. Vary K.



Directly Visualizing the Tradeoff

- We can plot the false positives versus false negatives directly. If L(0,1) = R · L(1,0) (i.e., a FN is R times more expensive than a FP), then the best operating point will be tangent to a line with a slope of –R

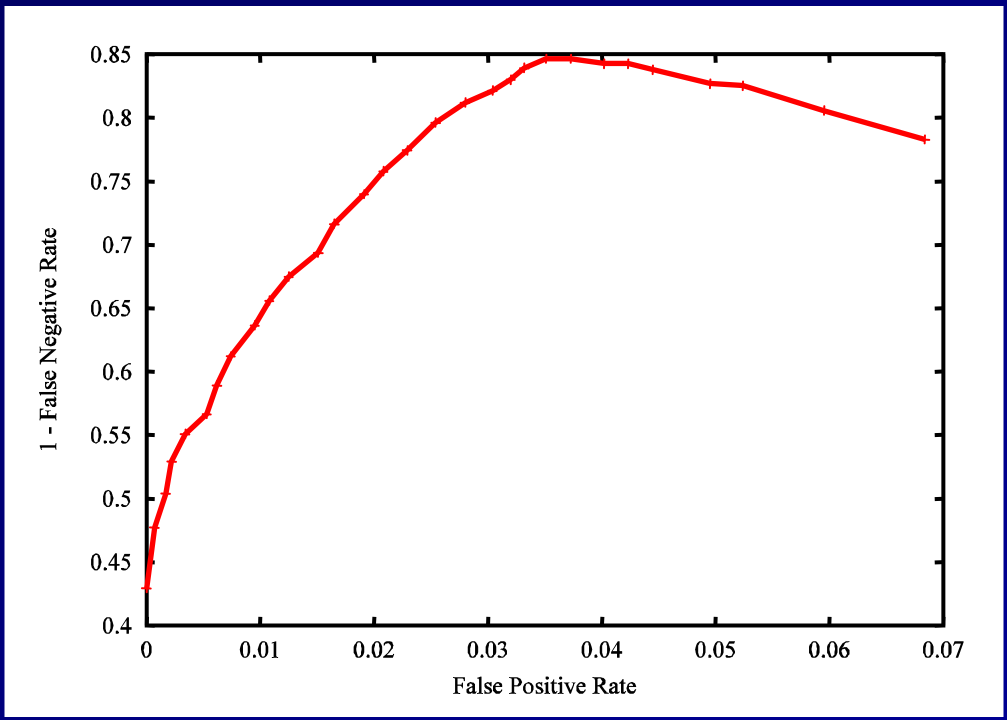


If R=1, we should set the threshold to 10.

If R=10, the threshold should be 29

Receiver Operating Characteristic (ROC) Curve

- It is traditional to plot this same information in a normalized form with 1 – False Negative Rate plotted against the False Positive Rate.



The optimal operating point is tangent to a line with a slope of R

Generating ROC Curves

- Linear Threshold Units, Sigmoid Units, Neural Networks
  – adjust the classification threshold between 0 and 1
- K nearest neighbor
  – adjust number of votes (between 0 and k) required to classify positive
- Naïve Bayes, Logistic Regression, etc.
  – vary the probability threshold for classifying as positive
- Support vector machines
  – require different margins for positive and negative examples

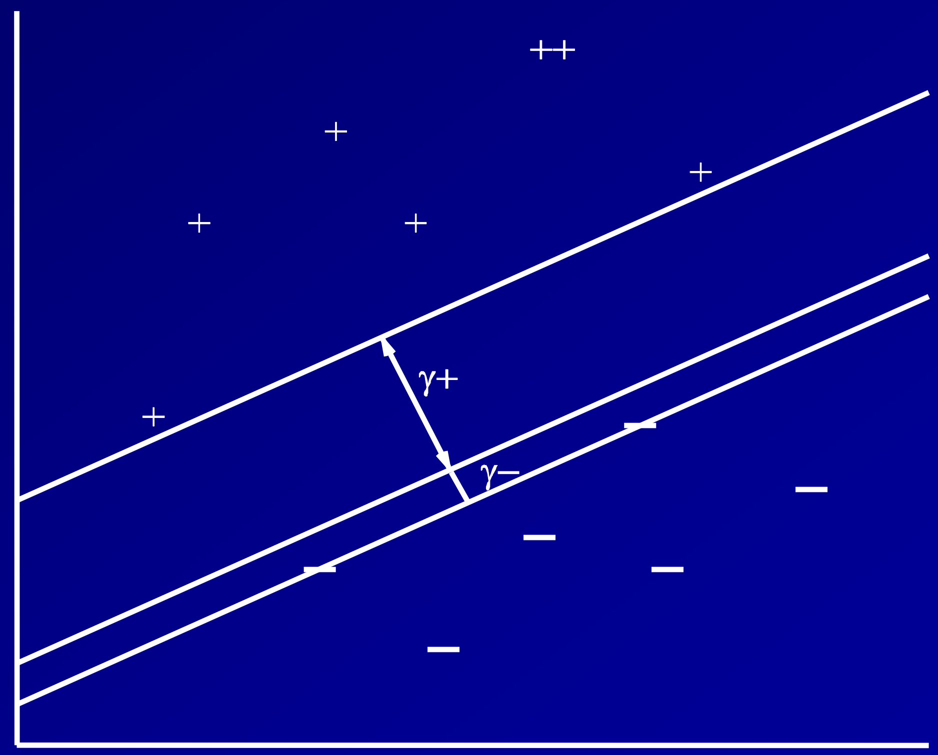
SVM: Asymmetric Margins

Minimize $||w||^2 + C \sum_i \xi_i$

Subject to

$\mathbf{w} \cdot \mathbf{x}_i + \xi_i \geq R$ (positive examples)

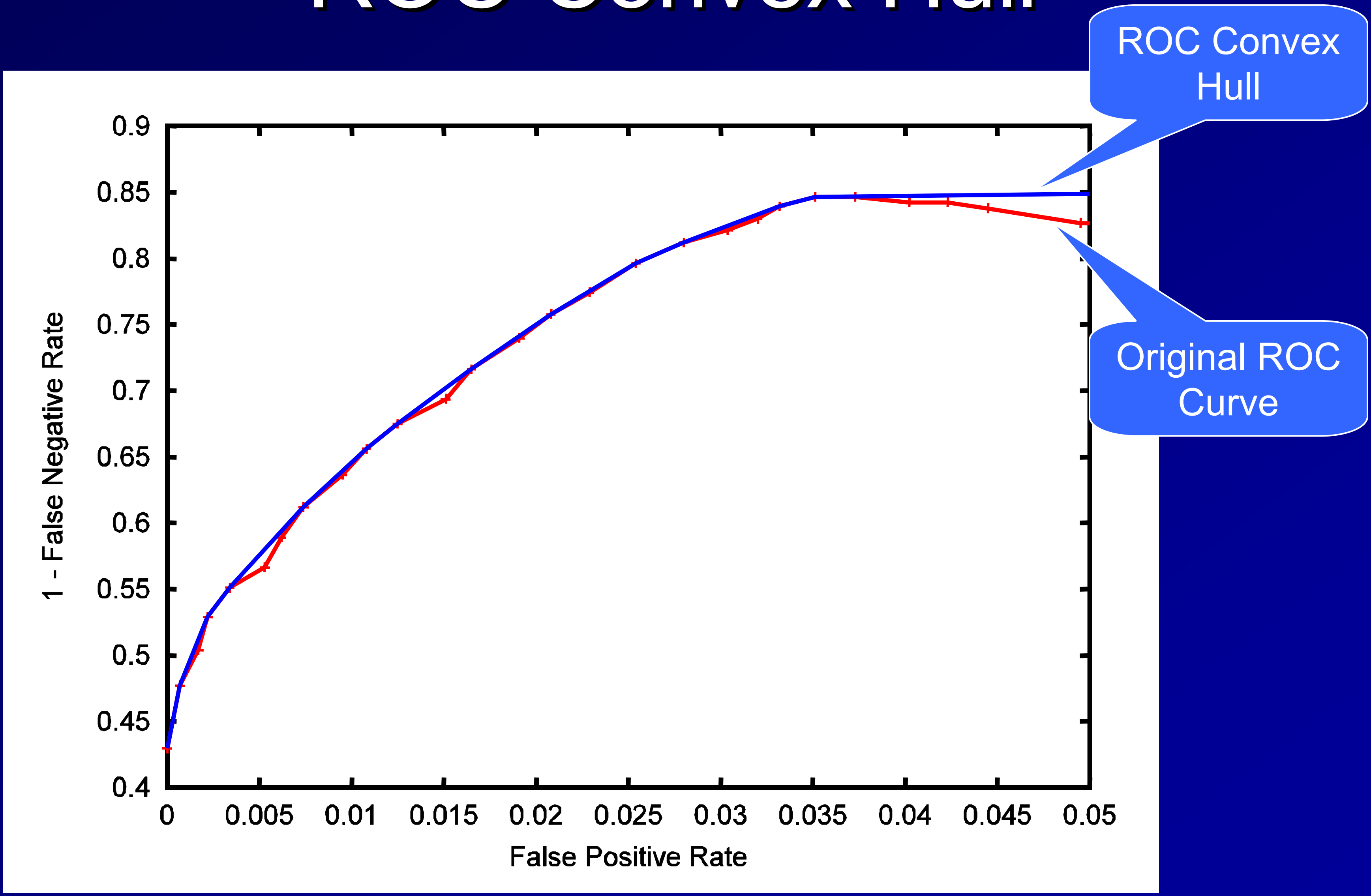
$-\mathbf{w} \cdot \mathbf{x}_i + \xi_i \geq 1$ (negative examples)



ROC Convex Hull

- If we have two classifiers h_1 and h_2 with (fp1,fn1) and (fp2,fn2), then we can construct a stochastic classifier that interpolates between them. Given a new data point **x**, we use classifier h_1 with probability p and h_2 with probability (1-p). The resulting classifier has an expected false positive level of p fp1 + (1 – p) fp2 and an expected false negative level of p fn1 + (1 – p) fn2.
- This means that we can create a classifier that matches any point on the convex hull of the ROC curve

ROC Convex Hull



Maximizing AUC

- At learning time, we may not know the cost ratio R. In such cases, we can maximize the Area Under the ROC Curve (AUC)
- Efficient computation of AUC
  - Assume $h(\mathbf{x})$ returns a real quantity (larger values => class 1)
  - Sort $\mathbf{x}_i$ according to $h(\mathbf{x}_i)$. Number the sorted points from 1 to N such that r(i) = the rank of data point $\mathbf{x}_i$
  - AUC = probability that a randomly chosen example from class 1 ranks above a randomly chosen example from class 0 = the Wilcoxon-Mann-Whitney statistic

Computing AUC

- Let S_1 = sum of r(i) for $y_i = 1$ (sum of the ranks of the positive examples)

$$\widehat{AUC} = \frac{S_1 - N_1(N_1+1)/2}{N_0 N_1}$$

where N_0 is the number of negative examples and N_1 is the number of positive examples

Optimizing AUC

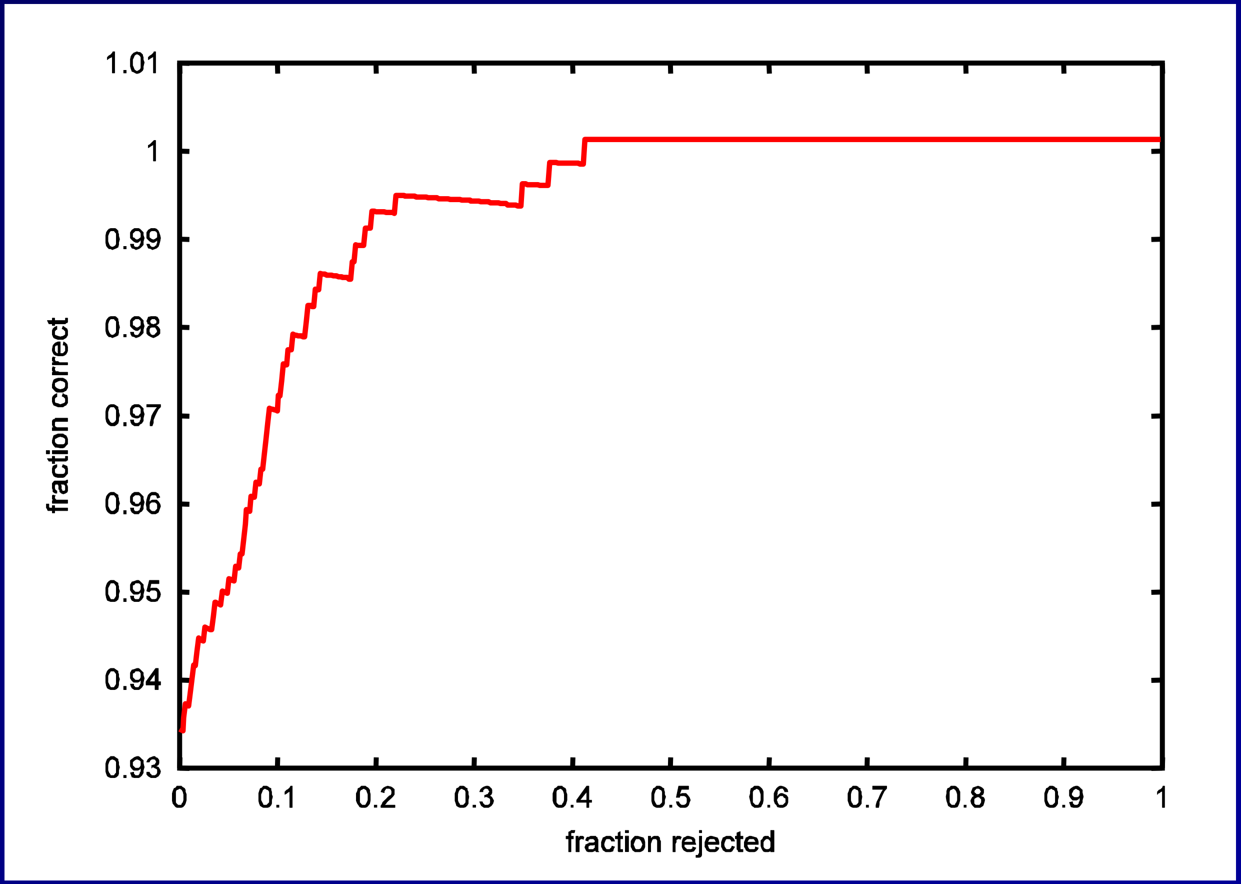
- A hot topic in machine learning right now is developing algorithms for optimizing AUC
- RankBoost: A modification of AdaBoost. The main idea is to define a “ranking loss” function and then penalize a training example **x** by the number of examples of the other class that are misranked (relative to **x**)

Rejection Curves

- In most learning algorithms, we can specify a threshold for making a rejection decision
  - Probabilistic classifiers: adjust cost of rejecting versus cost of FP and FN
  - Decision-boundary method: if a test point **x** is within θ of the decision boundary, then reject
    - Equivalent to requiring that the “activation” of the best class is larger than the second-best class by at least θ

Rejection Curves (2)

- Vary θ and plot fraction correct versus fraction rejected

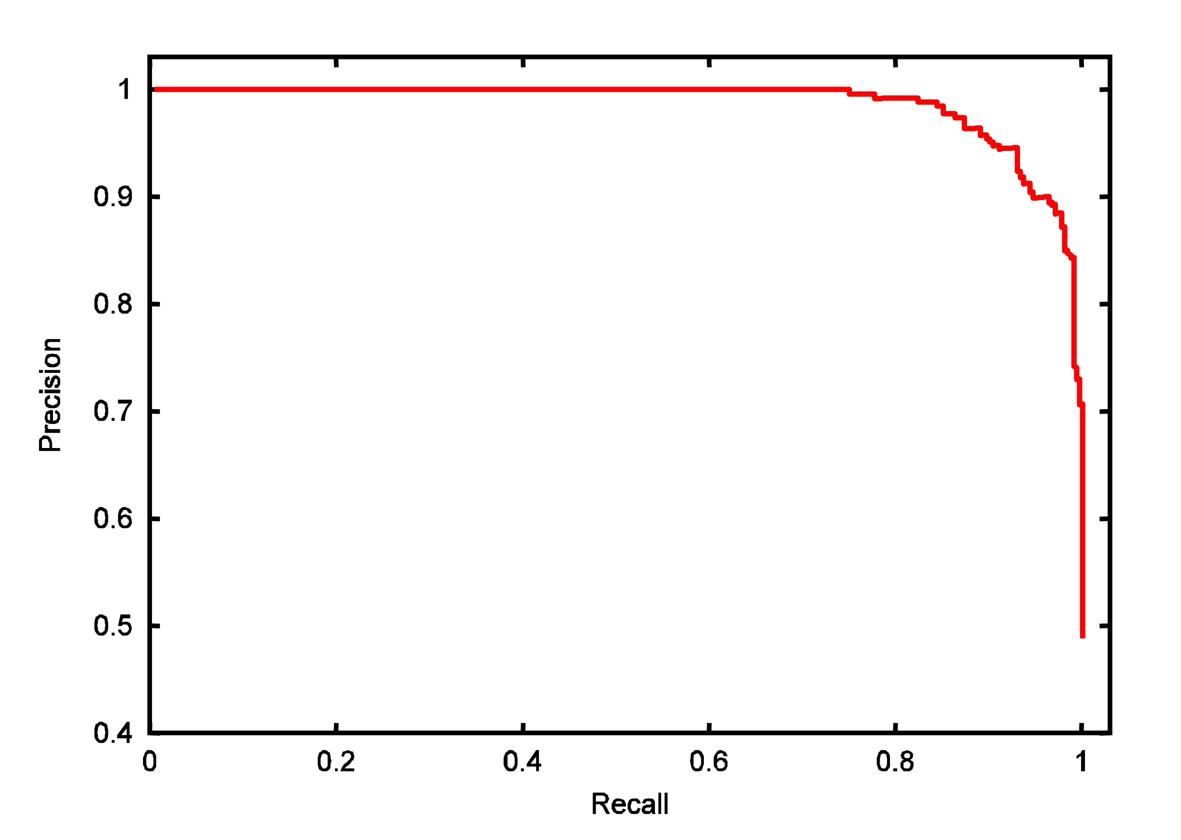


Precision versus Recall

- Information Retrieval:
  - y = 1: document is relevant to query
  - y = 0: document is irrelevant to query
  - K: number of documents retrieved
- Precision:
  - fraction of the K retrieved documents ($\hat{y}$=1) that are actually relevant (y=1)
  - TP / (TP + FP)
- Recall:
  - fraction of all relevant documents that are retrieved
  - TP / (TP + FN) = true positive rate

Precision Recall Graph

- Plot recall on horizontal axis; precision on vertical axis; and vary the threshold for making positive predictions (or vary K)



The F_1 Measure

- Figure of merit that combines precision and recall.

$$F_1 = 2 \cdot \frac{P \cdot R}{P + R}$$

- where P = precision; R = recall. This is twice the harmonic mean of P and R.
- We can plot F_1 as a function of the classification threshold θ

Summarizing a Single Operating Point

- WEKA and many other systems normally report various measures for a single operating point (e.g., $\theta = 0.5$). Here is example output from WEKA:

=== Detailed Accuracy By Class ===

TP Rate	FP Rate	Precision	Recall	F-Measure	Class
0.854	0.1	0.899	0.854	0.876	0
0.9	0.146	0.854	0.9	0.876	1

Visualizing ROC and P/R Curves in WEKA

- Right-click on the result list and choose "Visualize Threshold Curve". Select "1" from the popup window.
- ROC:
  - Plot False Positive Rate on X axis
  - Plot True Positive Rate on Y axis
  - WEKA will display the AUC also
- Precision/Recall:
  - Plot Recall on X axis
  - Plot Precision on Y axis
- WEKA does not support rejection curves

Sensitivity and Selectivity

- In medical testing, the terms "sensitivity" and "selectivity" are used
  – Sensitivity = TP/(TP + FN) = true positive rate = recall
  – Selectivity = TN/(FP + TN) = true negative rate = recall for the negative class = 1 – the false positive rate
- The sensitivity versus selectivity tradeoff is identical to the ROC curve tradeoff

Estimating the Error Rate of a Classifier

- Compute the error rate on hold-out data
  - suppose a classifier makes *k* errors on *n* holdout data points
  - the estimated error rate is ê = *k* / *n*.
- Compute a confidence internal on this estimate
  - the standard error of this estimate is

$$SE = \sqrt{\frac{\hat{\epsilon} \cdot (1 - \hat{\epsilon})}{n}}$$

  - A 1 – α confidence interval on the true error ε is

$$\hat{\epsilon} - z_{\alpha/2} SE <= \epsilon <= \hat{\epsilon} + z_{\alpha/2} SE$$

  - For a 95% confidence interval, $Z_{0.025}$ = 1.96, so we use

$$\hat{\epsilon} - 1.96 SE <= \epsilon <= \hat{\epsilon} + 1.96 SE.$$

Comparing Two Classifiers

- Goal: decide which of two classifiers h_1 and h_2 has lower error rate
- Method: Run them both on the same test data set and record the following information:
  - n_{00}: the number of examples correctly classified by both classifiers
  - n_{01}: the number of examples correctly classified by h_1 but misclassified by h_2
  - n_{10}: The number of examples misclassified by h_1 but correctly classified by h_2
  - n_{00}: The number of examples misclassified by both h_1 and h_2.

n_{00}	n_{01}
n_{10}	n_{11}

McNemar's Test

$$M = \frac{(|n_{01} - n_{10}| - 1)^2}{n_{01} + n_{10}} > \chi^2_{1,\alpha}$$

- M is distributed approximately as χ^2 with 1 degree of freedom. For a 95% confidence test, $\chi^2_{1,095}$ = 3.84. So if M is larger than 3.84, then with 95% confidence, we can reject the null hypothesis that the two classifies have the same error rate

Confidence Interval on the Difference Between Two Classifiers

- Let $p_{ij} = n_{ij}/n$ be the 2x2 contingency table converted to probabilities

$$
\begin{aligned}
SE &= \sqrt{\frac{p_{01} + p_{10} + (p_{01} - p_{10})^2}{n}} \\
p_A &= p_{10} + p_{11} \\
p_B &= p_{01} + p_{11}
\end{aligned}
$$

- A 95% confidence interval on the difference in the true error between the two classifiers is

$$p_A - p_B - 1.96\left(SE + \frac{1}{2n}\right) <= \epsilon_A - \epsilon_B <= p_A - p_B + 1.96\left(SE + \frac{1}{2n}\right)$$

Cost-Sensitive Comparison of Two Classifiers

- Suppose we have a non-0/1 loss matrix $L(\hat{y},y)$ and we have two classifiers h_1 and h_2. Goal: determine which classifier has lower expected loss.
- A method that does not work well:
  - For each algorithm a and each test example $(\mathbf{x}_i,y_i)$ compute $\ell_{a,i} = L(h_a(\mathbf{x}_i),y_i)$.
  - Let $\delta_i = \ell_{1,i} - \ell_{2,i}$
  - Treat the δ's as normally distributed and compute a normal confidence interval
- The problem is that there are only a finite number of different possible values for δ_i. They are not normally distributed, and the resulting confidence intervals are too wide

A Better Method: BDeltaCost

- Let $\Delta = \{\delta_i\}^N_{i=1}$ be the set of δ_i's computed as above
- For *b* from 1 to 1000 do
  - Let T_b be a bootstrap replicate of Δ
  - Let s_b = average of the δ's in T_b
- Sort the s_b's and identify the 26th and 975th items. These form a 95% confidence interval on the average difference between the loss from h_1 and the loss from h_2.
- The bootstrap confidence interval quantifies the uncertainty due to the size of the test set. It does not allow us to compare <u>algorithms</u>, only <u>classifiers</u>.

Estimating the Error Rate of a Learning Algorithm

- Under the PAC model, training examples **x** are drawn from an underlying distribution *D* and labeled according to an unknown function *f* to give (**x**,y) pairs where y = *f*(**x**).
- The error rate of a <u>classifier</u> *h* is

$$\text{error}(h) = P_D(h(\mathbf{x}) \neq f(\mathbf{x}))$$

- Define the error rate of a <u>learning algorithm</u> A for sample size *m* and distribution *D* as

$$\text{error}(A,m,D) = E_S\,[\text{error}(A(S))]$$

- This is the expected error rate of h = A(S) for training sets S of size *m* drawn according to *D*.
- We could estimate this if we had several training sets S_1, …, S_L all drawn from *D*. We could compute $A(S_1)$, $A(S_2)$, …, $A(S_L)$, measure their error rates, and average them.
- Unfortunately, we don't have enough data to do this!

Two Practical Methods

- k-fold Cross Validation
  - This provides an unbiased estimate of error(A, (1 – 1/k)*m*, *D*) for training sets of size (1 – 1/k)*m*
- Bootstrap error estimate (out-of-bag estimate)
  - Construct L bootstrap replicates of S_{train}
  - Train A on each of them
  - Evaluate on the examples that *did not appear* in the bootstrap replicate
  - Average the resulting error rates

Estimating the Difference Between Two Algorithms: the 5x2CV F test

for i from 1 to 5 **do**

perform a 2-fold cross-validation

split S evenly and randomly into S_1 and S_2

for j from 1 to 2 **do**

Train algorithm A on S_j, measure error rate $p_A^{(i,j)}$

Train algorithm B on S_j, measure error rate $p_B^{(i,j)}$

$p_i^{(j)} := p_A^{(i,j)} - p_B^{(i,j)}$ *Difference in error rates on fold* j

end /* for j */

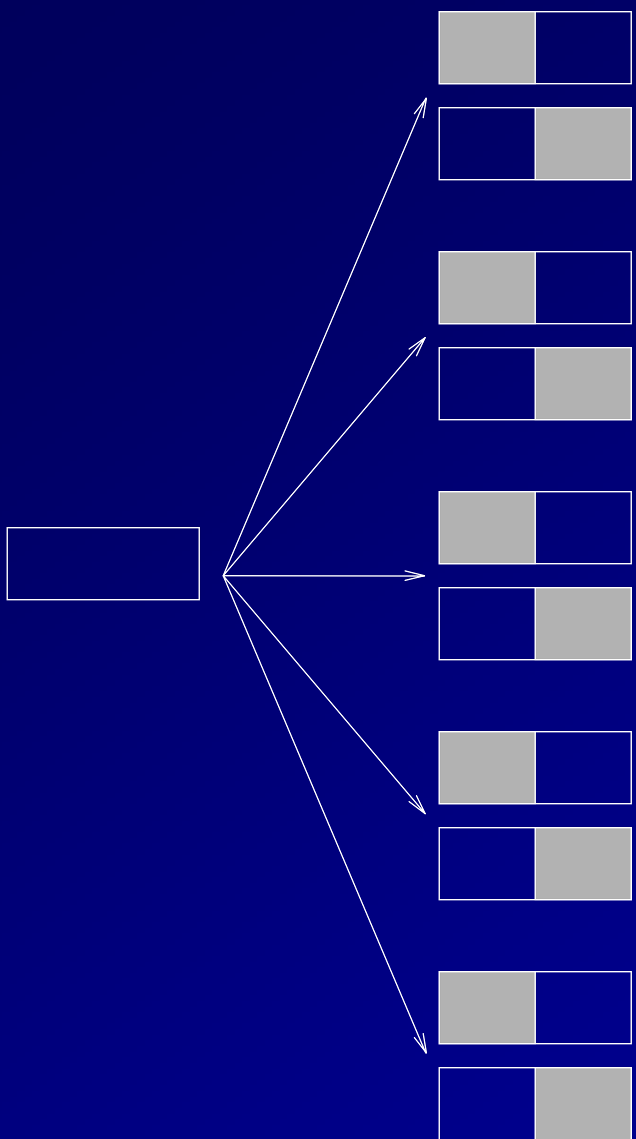
$\overline{p}_i := \dfrac{p_i^{(1)} + p_i^{(2)}}{2}$ *Average difference in error rates in iteration* i

$s_i^2 = \left(p_i^{(1)} - \overline{p}_i\right)^2 + \left(p_i^{(2)} - \overline{p}_i\right)^2$ *Variance in the difference, for iteration* i

end /* for i */

$$F := \frac{\sum_i \overline{p}_i^2}{2 \sum_i s_i^2}$$

5x2cv F test



$p_A^{(1,1)}$	$p_B^{(1,1)}$	$p_1^{(1)}$	$\overline{p}_1$	s_1^2
$p_A^{(1,2)}$	$p_B^{(1,2)}$	$p_1^{(2)}$		
$p_A^{(2,1)}$	$p_B^{(2,1)}$	$p_2^{(1)}$	$\overline{p}_2$	s_2^2
$p_A^{(2,2)}$	$p_B^{(2,2)}$	$p_2^{(2)}$		
$p_A^{(3,1)}$	$p_B^{(3,1)}$	$p_3^{(1)}$	$\overline{p}_3$	s_3^2
$p_A^{(3,2)}$	$p_B^{(3,2)}$	$p_3^{(2)}$		
$p_A^{(4,1)}$	$p_B^{(4,1)}$	$p_4^{(1)}$	$\overline{p}_4$	s_4^2
$p_A^{(4,2)}$	$p_B^{(4,2)}$	$p_4^{(2)}$		
$p_A^{(5,1)}$	$p_B^{(5,1)}$	$p_5^{(1)}$	$\overline{p}_5$	s_5^2
$p_A^{(5,2)}$	$p_B^{(5,2)}$	$p_5^{(2)}$		

5x2CV F test

- If F > 4.47, then with 95% confidence, we can reject the null hypothesis that algorithms A and B have the same error rate when trained on data sets of size *m*/2.

Summary

- ROC Curves
- Reject Curves
- Precision-Recall Curves
- Statistical Tests
  - Estimating error rate of classifier
  - Comparing two classifiers
  - Estimating error rate of a learning algorithm
  - Comparing two algorithms