Evaluating Hypotheses

- Sample error, true error
- Confidence intervals for observed hypothesis error
- Estimators
- Binomial distribution, Normal distribution, Central Limit Theorem
- Paired t-tests
- Comparing Learning Methods

Problems Estimating Error

1. *Bias*: If S is training set, $error_S(h)$ is optimistically biased

$$bias \equiv E[error_S(h)] - error_D(h)$$

For unbiased estimate, h and S must be chosen independently

2. *Variance*: Even with unbiased S, $error_S(h)$ may still vary from $error_D(h)$

Two Definitions of Error

The true error of hypothesis h with respect to target function f and distribution D is the probability that h will misclassify an instance drawn at random according to D.

$$error_D(h) \equiv \Pr_{x \in D}\left[f(x) \neq h(x)\right]$$

The sample error of h with respect to target function f and data sample S is the proportion of examples h misclassifies

$$error_S(h) \equiv \frac{1}{n}\sum_{x \in S} \delta\left(f(x) \neq h(x)\right)$$

where $\delta\left(f(x) \neq h(x)\right)$ is 1 if $f(x) \neq h(x)$, and 0 otherwise

How well does $error_S(h)$ estimate $error_D(h)$?

Example

Hypothesis h misclassifies 12 of 40 examples in S.

$$error_S(h) = \frac{12}{40} = .30$$

What is $error_D(h)$?

Estimators

Experiment:

1. Choose sample S of size n according to distribution D
2. Measure $error_S(h)$

$error_S(h)$ is a random variable (i.e., result of an experiment)

$error_S(h)$ is an unbiased estimator for $error_D(h)$

Given observed $error_S(h)$ what can we conclude about $error_D(h)$?

Confidence Intervals

If

- S contains n examples, drawn independently of h and each other
- $n \geq 30$

Then

- With approximately N% probability, $error_D(h)$ lies in interval

$$error_S(h) \pm z_N \sqrt{\frac{error_S(h)(1-error_S(h))}{n}}$$

where

N%:	50%	68%	80%	90%	95%	98%	99%
z_N:	0.67	1.00	1.28	1.64	1.96	2.33	2.53

Confidence Intervals

If

- S contains n examples, drawn independently of h and each other
- $n \geq 30$

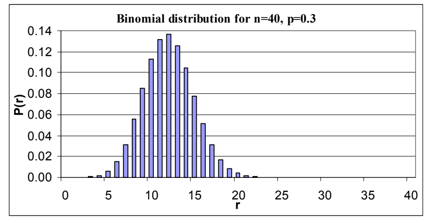
Then

- With approximately 95% probability, $error_D(h)$ lies in interval

$$error_S(h) \pm \mathbf{1.96}\sqrt{\frac{error_S(h)(1-error_S(h))}{n}}$$

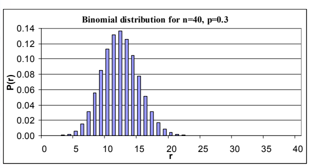
$error_S(h)$ is a Random Variable

- Rerun experiment with different randomly drawn S (size n)
- Probability of observing r misclassified examples:



$$P(r) = \frac{n!}{r!(n-r)!} error_D(h)^r (1-error_D(h))^{n-r}$$

Binomial Probability Distribution

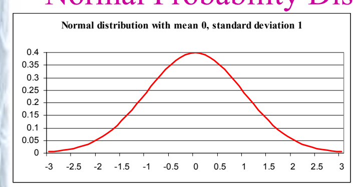


$$P(r) = \frac{n!}{r!(n-r)!} p^r (1-p)^{n-r}$$

Probabilty $P(r)$ of r heads in n coin flips, if $p = \Pr(heads)$

- Expected, or mean value of X: $E[X] \equiv \sum_{i=0}^{n} iP(i) = np$
- Variance of X: $Var(X) \equiv E[(X-E[X])^2] = np(1-p)$
- Standard deviation of X: $\sigma_X \equiv \sqrt{E[(X-E[X])^2]} = \sqrt{np(1-p)}$

Normal Probability Distribution



$$P(r) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

The probability that X will fall into the interval (a,b) is given by

$$\int_a^b p(x)dx$$

- Expected, or mean value of X: $E[X] = \mu$
- Variance of X: $Var(X) = \sigma^2$
- Standard deviation of X: $\sigma_X = \sigma$

Normal Distribution Approximates Binomial

$error_s(h)$ follows a Binomial distribution, with

- mean $\mu_{error_S(h)} = error_D(h)$
- standard deviation

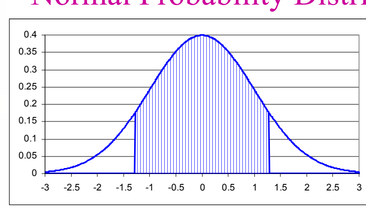
$$\sigma_{error_S(h)} = \sqrt{\frac{error_D(h)(1-error_D(h))}{n}}$$

Approximate this by a Normal distribution with

- mean $\mu_{error_S(h)} = error_D(h)$
- standard deviation

$$\sigma_{error_S(h)} \approx \sqrt{\frac{error_S(h)(1-error_S(h))}{n}}$$

Normal Probability Distribution



80% of area (probability) lies in $\mu \pm 1.28\sigma$

N% of area (probability) lies in $\mu \pm z_N \sigma$

N%:	50%	68%	80%	90%	95%	98%	99%
z_N:	0.67	1.00	1.28	1.64	1.96	2.33	2.53

Confidence Intervals, More Correctly

If
- S contains n examples, drawn independently of h and each other
- $n \geq 30$

Then
- With approximately 95% probability, $error_S(h)$ lies in interval
$$error_D(h) \pm \mathbf{1.96}\sqrt{\frac{error_D(h)(1-error_D(h))}{n}}$$
- equivalently, $error_D(h)$ lies in interval
$$error_S(h) \pm \mathbf{1.96}\sqrt{\frac{error_D(h)(1-error_D(h))}{n}}$$
- which is approximately
$$error_S(h) \pm \mathbf{1.96}\sqrt{\frac{error_S(h)(1-error_S(h))}{n}}$$

Calculating Confidence Intervals

1. Pick parameter p to estimate
- $error_D(h)$
2. Choose an estimator
- $error_S(h)$
3. Determine probability distribution that governs estimator
- $error_S(h)$ governed by Binomial distribution, approximated by Normal when $n \geq 30$
4. Find interval (L,U) such that N% of probability mass falls in the interval
- Use table of z_N values

Central Limit Theorem

Consider a set of independent, identically distributed random variables $Y_1 \ldots Y_n$, all governed by an arbitrary probability distribution with mean μ and finite variance σ^2. Define the sample mean

$$\bar{Y} \equiv \frac{1}{n}\sum_{i=1}^{n} Y_i$$

Central Limit Theorem. As $n \to \infty$, the distribution governing $\bar{Y}$ approaches a Normal distribution, with mean μ and variance $\frac{\sigma^2}{n}$.

Difference Between Hypotheses

Test h_1 on sample S_1, test h_2 on S_2

1. Pick parameter to estimate
$$d \equiv error_D(h_1) - error_D(h_2)$$
2. Choose an estimator
$$\hat{d} \equiv error_{S_1}(h_1) - error_{S_2}(h_2)$$
3. Determine probability distribution that governs estimator
$$\sigma_{\hat{d}} \approx \sqrt{\frac{error_{S_1}(h_1)(1-error_{S_1}(h_1))}{n_1} + \frac{error_{S_2}(h_2)(1-error_{S_2}(h_2))}{n_2}}$$
4. Find interval (L, U) such that N% of probability mass falls in the interval
$$\hat{d} \pm z_N\sqrt{\frac{error_{S_1}(h_1)(1-error_{S_1}(h_1))}{n_1} + \frac{error_{S_2}(h_2)(1-error_{S_2}(h_2))}{n_2}}$$

Paired t test to Compare h_A, h_B

1. Partition data into k disjoint test sets $T_1, T_2, \ldots, T_k$ of equal size, where this size is at least 30.
2. For i from 1 to k do
$$\delta_i \leftarrow error_{T_i}(h_A) - error_{T_i}(h_B)$$
3. Return the value d, where
$$\bar{\delta} \equiv \frac{1}{k}\sum_{i=1}^{k} \delta_i$$

N% confidence interval estimate for d:
$$\bar{\delta} \pm t_{N,k-1} s_{\bar{\delta}}$$
$$s_{\bar{\delta}} \equiv \sqrt{\frac{1}{k(k-1)}\sum_{i=1}^{k}(\delta_i - \bar{\delta})^2}$$

Note δ_i approximately Normally distributed

N-Fold Cross Validation

- Popular testing methodology
- Divide data into N even-sized random folds
- For n = 1 to N
  - Train set = all folds except n
  - Test set = fold n
  - Create learner with train set
  - Count number of errors on test set
- Accumulate number of errors across N test sets and divide by N (result is error rate)
- For comparing algorithms, use the same set of folds to create learners (results are paired)

N-Fold Cross Validation

- Advantages/disadvantages
  - Estimate of error within a single data set
  - Every point used once as a test point
  - At the extreme (when N = size of data set), called leave-one-out testing
  - Results affected by random choices of folds (sometimes answered by choosing multiple random folds – Dietterich in a paper expressed significant reservations)

Results Analysis: Confusion Matrix

- For many problems (especially multiclass problems), often useful to examine the sources of error
- Confusion matrix:

		Predicted			
		ClassA	ClassB	ClassC	Total
Expected	ClassA	25	5	20	50
	ClassB	0	45	5	50
	ClassC	25	0	25	50
	Total	50	50	50	150

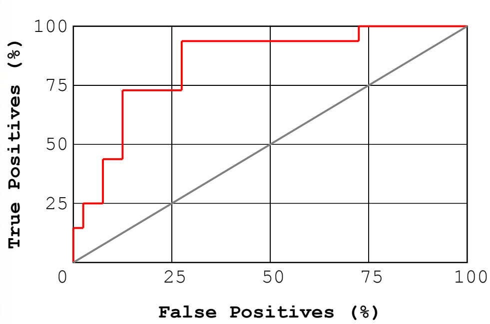
Results Analysis: Confusion Matrix

- Building a confusion matrix
  - Zero all entries
  - For each data point add one in row corresponding to actual class of problem under column corresponding to predicted class
- Perfect prediction has all values down the diagonal
- Off diagonal entries can often tell us about what is being mis-predicted

Receiver Operator Characteristic (ROC) Curves

- Originally from signal detection
- Becoming very popular for ML
- Used in:
  - Two class problems
  - Where predictions are ordered in some way (e.g., neural network activation is often taken as an indication of how strong or weak a prediction is)
- Plotting an ROC curve:
  - Sort predictions (right) by their predicted strength
  - Start at the bottom left
  - For each positive example, go up 1/P units where P is the number of positive examples
  - For each negative example, go right 1/N units where N is the number of negative examples

ROC Curve



ROC Properties

- Can visualize the tradeoff between coverage and accuracy (as we lower the threshold for prediction how many more true positives will we get in exchange for more false positives)
- Gives a better feel when comparing algorithms
  - Algorithms may do well in different portions of the curve
- A perfect curve would start in the bottom left, go to the top left, then over to the top right
  - A random prediction curve would be a line from the bottom left to the top right
- When comparing curves:
  - Can look to see if one curve dominates the other (is always better)
  - Can compare the area under the curve (very popular – some people even do t-tests on these numbers)