

Evaluating Hypotheses

[Read Ch. 5]

[Recommended exercises: 5.2, 5.3, 5.4]

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

Two Definitions of Error

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

$$error_{\mathcal{D}}(h) \equiv \Pr_{x \in \mathcal{D}}[f(x) \neq h(x)]$$

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

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

Where $\delta(f(x) \neq h(x))$ is 1 if $f(x) \neq h(x)$, and 0 otherwise.

How well does $error_S(h)$ estimate $error_{\mathcal{D}}(h)$?

Problems Estimating Error

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

$$bias \equiv E[error_S(h)] - error_{\mathcal{D}}(h)$$

For unbiased estimate, h and S must be chosen independently

2. *Variance*: Even with unbiased S , $error_S(h)$ may still *vary* from $error_{\mathcal{D}}(h)$

Example

Hypothesis h misclassifies 12 of the 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 \mathcal{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 $error_{\mathcal{D}}(h)$

Given observed $error_S(h)$ what can we conclude about $error_{\mathcal{D}}(h)$?

Confidence Intervals

If

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

Then

- With approximately 95% probability, $error_{\mathcal{D}}(h)$ lies in interval

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

Confidence Intervals

If

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

Then

- With approximately $N\%$ probability, $error_{\mathcal{D}}(h)$ lies in interval

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

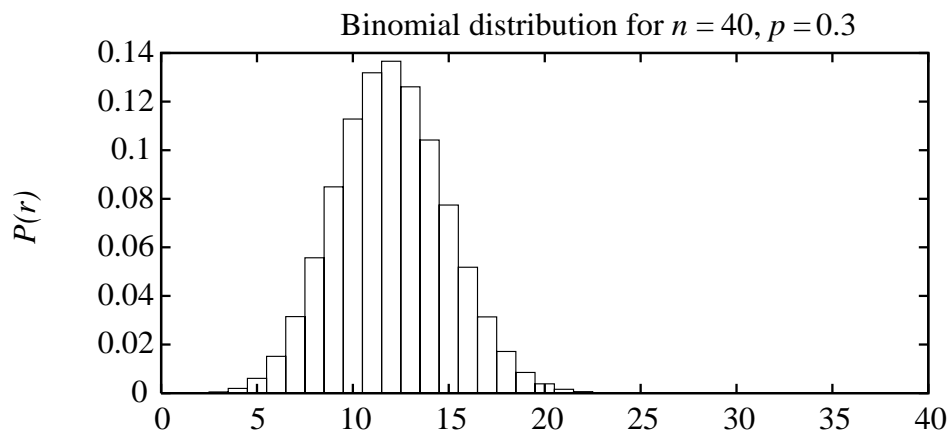
where

$N\%:$	50%	68%	80%	90%	95%	98%	99%
$z_N:$	0.67	1.00	1.28	1.64	1.96	2.33	2.58

$error_S(h)$ is a Random Variable

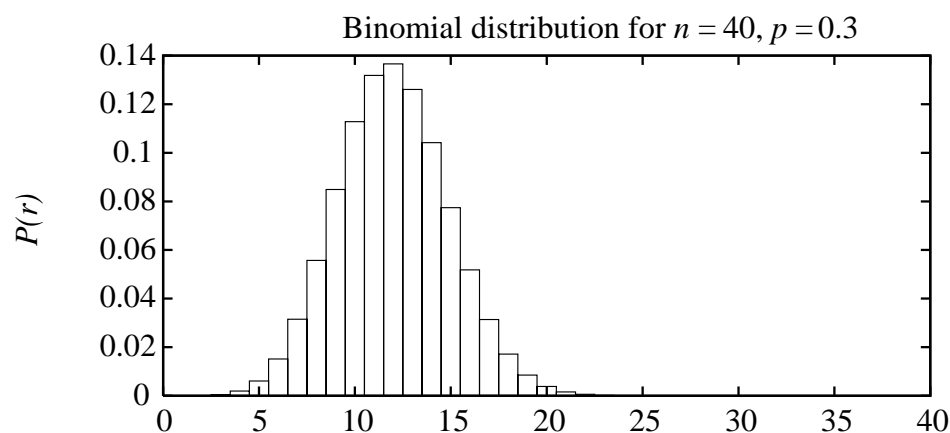
Rerun the experiment with different randomly drawn S (of size n)

Probability of observing r misclassified examples:



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

Binomial Probability Distribution



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

Probability $P(r)$ of r heads in n coin flips, if $p = \Pr(\text{heads})$

- Expected, or mean value of X , $E[X]$, is

$$E[X] \equiv \sum_{i=0}^n iP(i) = np$$

- Variance of X is

$$\text{Var}(X) \equiv E[(X - E[X])^2] = np(1-p)$$

- Standard deviation of X , σ_X , is

$$\sigma_X \equiv \sqrt{E[(X - E[X])^2]} = \sqrt{np(1-p)}$$

Normal Distribution Approximates Binomial

$error_S(h)$ follows a *Binomial* distribution, with

- mean $\mu_{error_S(h)} = error_{\mathcal{D}}(h)$
- standard deviation $\sigma_{error_S(h)}$

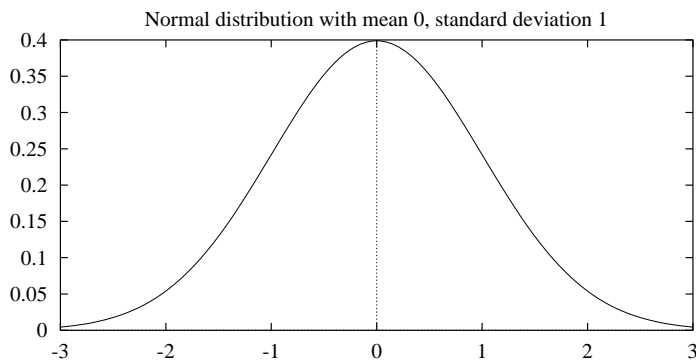
$$\sigma_{error_S(h)} = \sqrt{\frac{error_{\mathcal{D}}(h)(1 - error_{\mathcal{D}}(h))}{n}}$$

Approximate this by a *Normal* distribution with

- mean $\mu_{error_S(h)} = error_{\mathcal{D}}(h)$
- standard deviation $\sigma_{error_S(h)}$

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

Normal Probability Distribution



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

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 , $E[X]$, is

$$E[X] = \mu$$

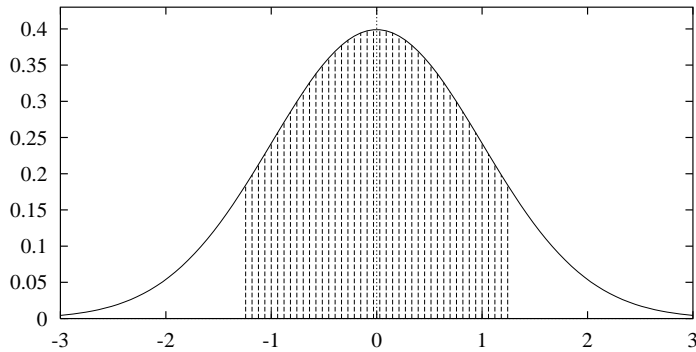
- Variance of X is

$$\text{Var}(X) = \sigma^2$$

- Standard deviation of X , σ_X , is

$$\sigma_X = \sigma$$

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	2.58

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

$$error_{\mathcal{D}}(h) \pm 1.96 \sqrt{\frac{error_{\mathcal{D}}(h)(1 - error_{\mathcal{D}}(h))}{n}}$$

equivalently, $error_{\mathcal{D}}(h)$ lies in interval

$$error_S(h) \pm 1.96 \sqrt{\frac{error_{\mathcal{D}}(h)(1 - error_{\mathcal{D}}(h))}{n}}$$

which is approximately

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

Central Limit Theorem

Consider a set of independent, identically distributed random variables $Y_1 \dots Y_n$, 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 $n \rightarrow \infty$, the distribution governing \bar{Y} approaches a Normal distribution, with mean μ and variance $\frac{\sigma^2}{n}$.

Calculating Confidence Intervals

1. Pick parameter p to estimate
 - $error_{\mathcal{D}}(h)$
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

Difference Between Hypotheses

Test h_1 on sample S_1 , test h_2 on S_2

1. Pick parameter to estimate

$$d \equiv error_{\mathcal{D}}(h_1) - error_{\mathcal{D}}(h_2)$$

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, \dots, T_k of equal size, where this size is at least 30.

2. For i from 1 to k , do

$$\delta_i \leftarrow \text{error}_{T_i}(h_A) - \text{error}_{T_i}(h_B)$$

3. Return the value $\bar{\delta}$, 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

Comparing learning algorithms L_A and L_B

What we'd like to estimate:

$$E_{S \subset \mathcal{D}}[\text{error}_{\mathcal{D}}(L_A(S)) - \text{error}_{\mathcal{D}}(L_B(S))]$$

where $L(S)$ is the hypothesis output by learner L using training set S

i.e., the expected difference in true error between hypotheses output by learners L_A and L_B , when trained using randomly selected training sets S drawn according to distribution \mathcal{D} .

But, given limited data D_0 , what is a good estimator?

- could partition D_0 into training set S and training set T_0 , and measure

$$\text{error}_{T_0}(L_A(S_0)) - \text{error}_{T_0}(L_B(S_0))$$

- even better, repeat this many times and average the results (next slide)

Comparing learning algorithms L_A and L_B

1. Partition data D_0 into k disjoint test sets T_1, T_2, \dots, T_k of equal size, where this size is at least 30.

2. For i from 1 to k , do

use T_i for the test set, and the remaining data for training set S_i

- $S_i \leftarrow \{D_0 - T_i\}$
- $h_A \leftarrow L_A(S_i)$
- $h_B \leftarrow L_B(S_i)$
- $\delta_i \leftarrow \text{error}_{T_i}(h_A) - \text{error}_{T_i}(h_B)$

3. Return the value $\bar{\delta}$, where

$$\bar{\delta} \equiv \frac{1}{k} \sum_{i=1}^k \delta_i$$

Comparing learning algorithms L_A and L_B

Notice we'd like to use the paired t test on $\bar{\delta}$ to obtain a confidence interval

but not really correct, because the training sets in this algorithm are not independent (they overlap!)

more correct to view algorithm as producing an estimate of

$$E_{S \subset D_0}[\text{error}_{\mathcal{D}}(L_A(S)) - \text{error}_{\mathcal{D}}(L_B(S))]$$

instead of

$$E_{S \subset D}[\text{error}_{\mathcal{D}}(L_A(S)) - \text{error}_{\mathcal{D}}(L_B(S))]$$

but even this approximation is better than no comparison