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

$$error_S(h) \equiv \frac{1}{n} \mathop{\textstyle \sum}_{x \in S} \delta(f(x) \neq h(x))$$

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

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

Example

Hypothesis h misclassifies 12 of the 40 examples in S

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

What is $error_{\mathcal{D}}(h)$?

75

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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 $error_D(h)$

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 $error_{D}(h)$

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
- $n \ge 30$

Then

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

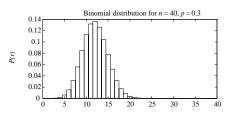
$$error_S(h) \pm 1.96 \sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$

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 $error_S(h)$ is a Random Variable

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

Probability of observing r misclassified examples:



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

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Confidence Intervals

If

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

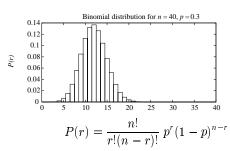
Then

• 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

Binomial Probability Distribution



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

• Expected, or mean value of X, E[X], is

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

• Variance of X is

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

• 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 $\sigma_{error_S(h)}$

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

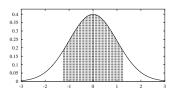
Approximate this by a Normal distribution with

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

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

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Normal Probability Distribution



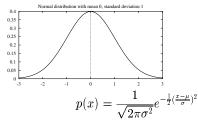
80% of area (probability) lies in $\mu \pm 1.28\sigma$

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

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Normal Probability Distribution



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

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

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

$$E[X] = \mu$$

 \bullet Variance of X is

$$Var(X) = \sigma^2$$

• Standard deviation of X, σ_X , is

$$\sigma_X = \sigma$$

Confidence Intervals, More Correctly

If

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

Then

 \bullet 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

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

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 $\frac{\sigma^2}{n}$.

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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

$$\sigma_{\mathring{\mathbf{d}}} \approx \sqrt{\frac{\mathrm{error}_{\mathbf{S}_1}(\mathbf{h}_1)(1 - \mathrm{error}_{\mathbf{S}_1}(\mathbf{h}_1))}{\mathbf{n}_1} + \frac{\mathrm{error}_{\mathbf{S}_2}(\mathbf{h}_2)(1 - \mathrm{error}_{\mathbf{S}_2}(\mathbf{h}_2))}{\mathbf{n}_2}}$$

4. Find interval (L, U) such that N% of probability mass falls in the interval

$$\hat{d}\pm z_N\sqrt{rac{error_{S_1}(h_1)(1-error_{S_1}(h_1))}{n_1}+rac{error_{S_2}(h_2)(1-error_{S_2}(h_2))}{n_2}}$$

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Calculating Confidence Intervals

- 1. Pick parameter p to estimate
 - $error_{\mathcal{D}}(h)$
- 2. Choose an estimator
 - $\bullet error_S(h)$
- 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

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 $\bar{\delta}$, where

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

N% confidence interval estimate for d:

$$s_{ar{\delta}} \equiv \sqrt{rac{1}{k(k-1)}\sum\limits_{i=1}^k (\delta_i - ar{\delta})^2}$$

Note δ_i approximately Normally distributed

Comparing learning algorithms L_A and L_B

What we'd like to estimate:

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

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

$$error_{T_0}(L_A(S_0)) - error_{T_0}(L_B(S_0))$$

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

Comparing learning algorithms L_A and L_B

Notice we'd like to use the paired t test on $\overline{\delta}$ 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

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

instead of

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

but even this approximation is better than no comparison

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Comparing learning algorithms L_A and L_B

- 1. Partition data D_0 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

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

- $S_i \leftarrow \{D_0 T_i\}$
- \bullet $h_A \leftarrow L_A(S_i)$
- $h_B \leftarrow L_B(S_i)$
- $\delta_i \leftarrow error_{T_i}(h_A) error_{T_i}(h_B)$
- 3. Return the value $\bar{\delta}$, where

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