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, $\text{error}_S(h)$ is optimistically biased

\[
\text{bias} \equiv E[\text{error}_S(h)] - \text{error}_D(h)
\]

For unbiased estimate, $h$ and $S$ must be chosen independently

2. Variance: Even with unbiased $S$, $\text{error}_S(h)$ may still vary from $\text{error}_D(h)$
Example

Hypothesis $h$ misclassifies 12 of the 40 examples in $S$

$$\text{error}_S(h) = \frac{12}{40} = .30$$

What is $\text{error}_D(h)$?
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
- $n \geq 30$

Then

- With approximately 95% probability, $\text{error}_D(h)$ lies in interval

$$\text{error}_S(h) \pm 1.96 \sqrt{\frac{\text{error}_S(h)(1 - \text{error}_S(h))}{n}}$$
Confidence Intervals

If

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

Then

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

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

where

<table>
<thead>
<tr>
<th>$N%$:</th>
<th>50%</th>
<th>68%</th>
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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:

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

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

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

- Standard deviation of \( X \), \( \sigma_X \), is
  \[ \sigma_X \equiv \sqrt{E[(X - E[X])^2]} = \sqrt{np(1 - p)} \]
Normal Distribution Approximates Binomial

$\text{error}_S(h)$ follows a $\textit{Binomial}$ distribution, with

- mean $\mu_{\text{error}_S(h)} = \text{error}_D(h)$
- standard deviation $\sigma_{\text{error}_S(h)}$

$$\sigma_{\text{error}_S(h)} = \sqrt{\frac{\text{error}_D(h)(1 - \text{error}_D(h))}{n}}$$

Approximate this by a $\textit{Normal}$ distribution with

- mean $\mu_{\text{error}_S(h)} = \text{error}_D(h)$
- standard deviation $\sigma_{\text{error}_S(h)}$

$$\sigma_{\text{error}_S(h)} \approx \sqrt{\frac{\text{error}_S(h)(1 - \text{error}_S(h))}{n}}$$
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
  \[ Var(X) = \sigma^2 \]

- Standard deviation of \( X \), \( \sigma_X \), is
  \[ \sigma_X = \sigma \]
Normal Probability Distribution

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

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

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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

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

equivalently, $error_D(h)$ lies in interval

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

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 $Y_1 \ldots Y_n$, all governed by an arbitrary probability distribution with mean $\mu$ and finite variance $\sigma^2$. 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 $\mu$ and variance $\frac{\sigma^2}{n}$. 

Calculating Confidence Intervals

1. Pick parameter $p$ to estimate
   - $\text{error}_D(h)$
2. Choose an estimator
   - $\text{error}_S(h)$
3. Determine probability distribution that governs estimator
   - $\text{error}_S(h)$ 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
   
   $$d \equiv \text{error}_D(h_1) - \text{error}_D(h_2)$$

2. Choose an estimator
   
   $$\hat{d} \equiv \text{error}_{S_1}(h_1) - \text{error}_{S_2}(h_2)$$

3. Determine probability distribution that governs estimator
   
   $$\sigma_{\hat{d}} \approx \sqrt{\frac{\text{error}_{S_1}(h_1)(1 - \text{error}_{S_1}(h_1))}{n_1} + \frac{\text{error}_{S_2}(h_2)(1 - \text{error}_{S_2}(h_2))}{n_2}}$$

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

   $$\hat{d} \pm z_N \sqrt{\frac{\text{error}_{S_1}(h_1)(1 - \text{error}_{S_1}(h_1))}{n_1} + \frac{\text{error}_{S_2}(h_2)(1 - \text{error}_{S_2}(h_2))}{n_2}}$$
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 $\bar{\delta}$, where
   $$
   \bar{\delta} \equiv \frac{1}{k} \sum_{i=1}^{k} \delta_i
   $$

$N\%$ confidence interval estimate for $d$:

$$
\bar{\delta} \pm t_{N,k-1} \cdot s_{\delta}
$$

$$
s_{\bar{\delta}} \equiv \sqrt{\frac{1}{k(k-1)} \sum_{i=1}^{k} (\delta_i - \bar{\delta})^2}
$$

Note $\delta_i$ approximately Normally distributed
Comparing learning algorithms $L_A$ and $L_B$

What we’d like to estimate:

$$E_{S \subseteq D}[error_D(L_A(S)) - error_D(L_B(S))]$$

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 $D$.

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 $L_B$

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 $S_i$
   
   $\cdot S_i \leftarrow \{D_0 - T_i\}$
   
   $\cdot h_A \leftarrow L_A(S_i)$
   
   $\cdot h_B \leftarrow L_B(S_i)$
   
   $\cdot \delta_i \leftarrow error_{T_i}(h_A) - error_{T_i}(h_B)$

3. Return the value $\bar{\delta}$, where
   
   $$\bar{\delta} \equiv \frac{1}{k} \sum_{i=1}^{k} \delta_i$$
Comparing learning algorithms $L_A$ and $L_B$

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

$$E_{S \subseteq D_0}[error_D(L_A(S)) - error_D(L_B(S))]$$

instead of

$$E_{S \subseteq D}[error_D(L_A(S)) - error_D(L_B(S))]$$

but even this approximation is better than no comparison