Machine Learning

Evaluating Hypothesis

Prof. Dr. Martin Riedmiller
AG Maschinelles Lernen und Natürlichsprachliche Systeme
Institut für Informatik
Technische Fakultät
Albert-Ludwigs-Universität Freiburg

Martin.Riedmiller@uos.de

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

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

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

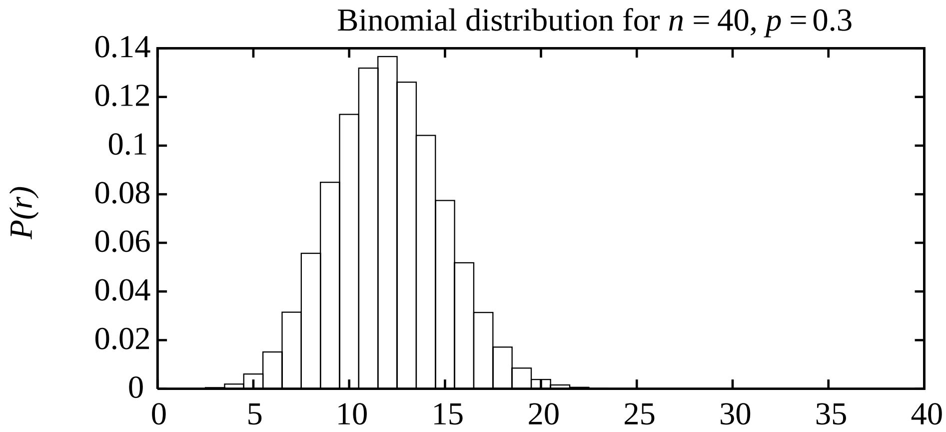
where

$N\%$:	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

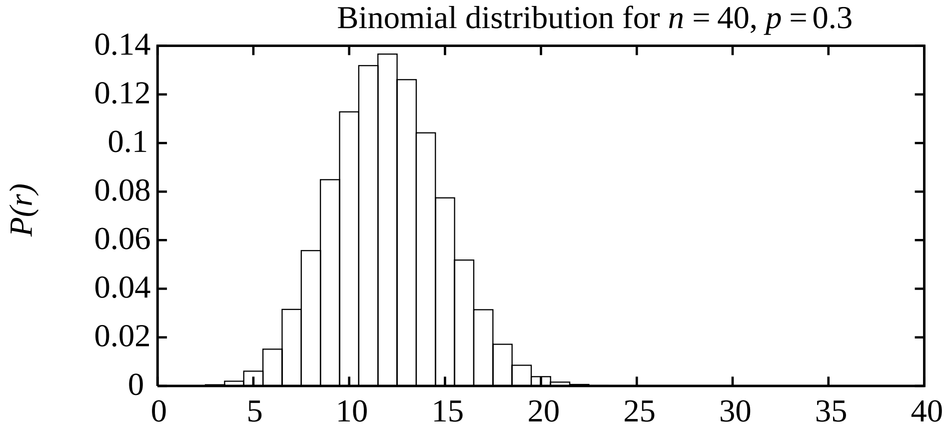
Rerun the experiment with different randomly drawn S (of size n)

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 $p = \Pr(heads)$

- 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 $\sigma_{error_S(h)}$

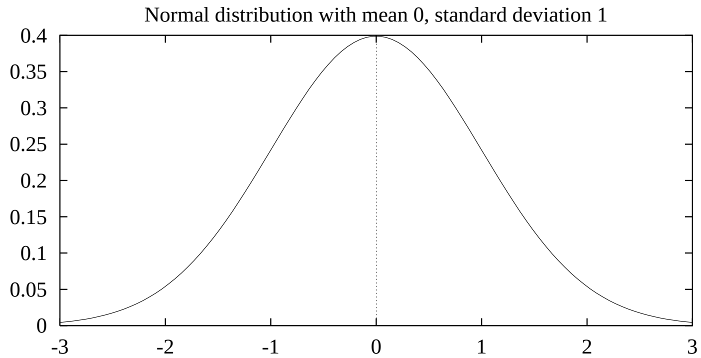
$$\sigma_{error_S(h)} = \sqrt{\frac{error_{\mathcal{D}}(h)(1 - error_{\mathcal{D}}(h))}{n}}$$

Approximate this by a *Normal* distribution with

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

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

Normal Probability Distribution



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

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

$$E[X] = \mu$$

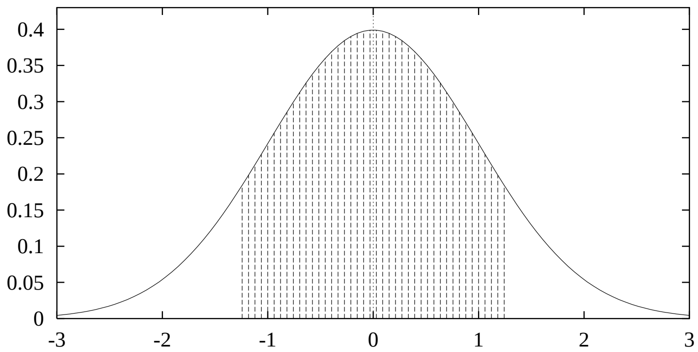
- Variance of X is

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

- Standard deviation of X, 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 $Y_1 \ldots Y_n$, 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 $\frac{\sigma^2}{n}$.

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 $T_1, T_2, \ldots, T_k$ 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

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

$d :=\leftarrow error_D(h_A) - error_D(h_B)$
N% confidence interval estimate for d:

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

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

where
$t_{N,k-1}$ are constants (comparable to the z_N) depending on the confidence level N and the number of test sets, k. For growing k, $t_{N,k-1}$ approxiates z_N.

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

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

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

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

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

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

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