Hypothesis Evaluation

- 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 :

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

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

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

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

- Problems of estimating error

. $error_S(h)$ is an estimator of $error_D(h)$.

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

. bias of $error_S(h)$ as an estimator of $error_D(h)$:

$$b_{error_D}(error_s) = E[error_s] - error_D$$

if $b_{error_D}(error_s) = 0$ for all $error_D$, we say $error_s$ is an unbiased estimator of $error_D$.

. The mean square error of $error_s$ is given as follows:

$$
\begin{aligned}
E[(error_s - error_D)^2] &= E[(error_s - E[error_s] + E[error_s] - error_D)^2] \\
&= E[(error_s - E[error_s])^2] + E[(E[error_s] - error_D)^2] + \\
&\quad 2E[(E[error_s] - error_D](error_s - E[error_s])] \\
&= E[(error_s - E[error_s])^2] + (E[error_s] - error_D)^2 \\
&= Var(error_s) + b^2_{error_D}(error_s)
\end{aligned}
$$

That is, the mean square error of $error_s$ is equivalent to the variance of $error_s$ plus the square of bias of $error_s$.

. Let $X_i \in \{0, 1\}$ be a random variable which has the mean $error_D$, that is, $E[X_i] = error_D$. Here, we assume that X_is are

independent and identically distributed.
Then, $error_s$ can be described by

$$error_S = \frac{1}{N}\sum_{i=1}^{N} X_i$$

where N represents the total number of trials.

In this case,

$$E[error_S] = E[\frac{1}{N}\sum_{i=1}^{N} X_i] = \frac{1}{N}\sum_{i=1}^{N} E[X_i] = error_D.$$

That is, $error_S$ is an unbiased estimator of $error_D$.

. example:

Hypothesis h misclassifies 50 of the 100 samples in S.

In this case,

$$error_S(h) = \frac{50}{100} = 0.50.$$

Then, what is $error_D(h)$?

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

- Binomial probability distribution

. Let X be a binomial random variable with parameters (n, p). Then, X represents the number of successes in n trials and p represents the probability of success.

. example: tossing a coin.

Probability $\Pr(r)$ of r heads in n coin flips can be described by

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

where $p = \Pr(head)$.

In this case, the mean value of X is

$$E[X] = \sum_{i=0}^{n} i \Pr(i) = np \quad \text{and}$$

the variance of X is

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

. $error_S(h)$ follows a binomial distribution, that is,

$$error_S(h) = \frac{X}{n},$$

$$E[error_S] = E[\frac{X}{n}] = \frac{1}{n} E[X] = p = error_D, \text{ and}$$

$$Var(error_S) = Var(\frac{X}{n}) = \frac{1}{n^2} Var(X) = \frac{p(1-p)}{n} = \frac{error_D(1-error_D)}{n}.$$

- Normal distribution approximates Binomial

. Let X_i be a random variable which has the value of 0 or 1 and $\Pr[X_i = 1] = p$.

Then, the random variable X having binomial distribution with parameters (n, p) can be described by

$$X = \sum_{i=1}^{n} X_i.$$

Here, the mean of X_i is

$$E[X_i] = 1 \cdot p + 0 \cdot (1-p) = p \quad \text{and}$$

the variance of X_i is

$$Var(X_i) = E[X_i^2] - E^2[X_i] = p - p^2 = p(1-p).$$

. Central Limit Theorem:

Consider a set of independent, identically distributed (i. i. d.) random variables $X_1, X_2, \cdots, X_n$ all governed by an arbitrary probability distribution with mean μ and finite variance σ^2. Let us define a new random vector

$$X = \sum_{i=1}^{n} X_i.$$

Then, as n goes to infinity, the distribution governing X approaches a normal (or Gaussian) distribution, with mean $n\mu$ and variance $n\sigma^2$. That is,

$$X \sim N(n\mu, n\sigma^2).$$

cf. In the case of Bernoulli trial, $X \stackrel{\cdot}{\sim} N(n\mu, n\sigma^2)$ when $n \geqq 30$. That is, X has an approximately Normal distribution with mean $n\mu$ and variance $n\sigma^2$. Here, the sample error of h can be described by

$$error_S(h) = \frac{X}{n} \stackrel{\cdot}{\sim} N(\mu, \frac{\sigma^2}{n})$$

where

$$\mu = error_D(h) \quad \text{and}$$

$$\frac{\sigma^2}{n} = \frac{error_D(1 - error_D)}{n} \approx \frac{error_S(1 - error_S)}{n}.$$

- Normal distribution

. The probability density function is given by

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

. The mean value of X: $E[X] = \mu$.

. The variance of X: $Var(X) = \sigma^2$

. The standard deviation of X: $\sigma_X = \sigma$.

- Calculating confidence intervals

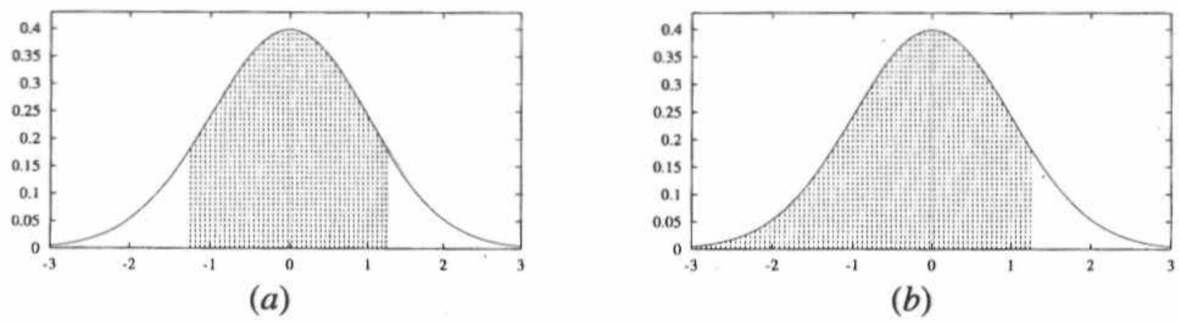


FIGURE 5.1
A Normal distribution with mean 0, standard deviation 1. (*a*) With 80% confidence, the value of the random variable will lie in the two-sided interval [-1.28, 1.28]. Note $z_{.80} = 1.28$. With 10% confidence it will lie to the right of this interval, and with 10% confidence it will lie to the left. (*b*) With 90% confidence, it will lie in the one-sided interval [$-\infty$, 1.28].

. $100(1-\alpha)\%$ of area (probability) lies in $\mu \pm z_{\alpha/2}\sigma$.

Values of $z_{\alpha/2}$ for two-sided $100(1-\alpha)\%$ confidence intervals:

$100(1-\alpha)\%$	50%	68%	80%	90%	95%	98%	99%
$z_{\alpha/2}$	0.67	1.00	1.28	1.64	1.96	2.33	2.58

eg. 95% of area lies in $\mu \pm 1.96\sigma$.

Let $\hat{\mu}$ is an estimator of μ and

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} X_i$$

where X_is are i. i. d. random variables having mean $\mu = p$ and variance $\sigma^2 = p(1-p)$. Then,

$$\hat{\mu} \dot{\sim} N(\mu, \frac{\sigma^2}{n}).$$

Let us make a unit (or standard) normal distribution of $\hat{\mu}$:

$$\frac{\hat{\mu} - \mu}{\sigma / \sqrt{n}} \dot{\sim} N(0, 1).$$

This implies that

$$-1.96 < \frac{\hat{\mu} - \mu}{\sigma/\sqrt{n}} < 1.96$$ with the probability of 0.95.

Due to the symmetry of normal distribution,

$$-1.96 < \frac{\mu - \hat{\mu}}{\sigma/\sqrt{n}} < 1.96.$$

Therefore, we get

$$\hat{\mu} - 1.96\frac{\sigma}{\sqrt{n}} < \mu < \hat{\mu} + 1.96\frac{\sigma}{\sqrt{n}}$$

where $\sigma = \sqrt{p(1-p)}$.

-> True mean μ lies in $\hat{\mu} \pm 1.96\frac{\sigma}{\sqrt{n}}$ with the probability of 0.95.

In general, if $\hat{\mu} \sim N(\mu, \sigma^2)$,

the $100(1-\alpha)\%$ confidence interval of $\hat{\mu}$: $\hat{\mu} \pm z_{\alpha/2}\sigma$

-> With a probability of $1-\alpha$, μ lies in interval $\hat{\mu} \pm z_{\alpha/2}\sigma$.

The sample error is given by

$$error_S(h) = \frac{X}{n} \dot{\sim} N(\mu, \frac{\sigma^2}{n})$$

where

$\mu = error_D(h)$ and

$$\frac{\sigma^2}{n} = \frac{error_D(1 - error_D)}{n} \approx \frac{error_S(1 - error_S)}{n}.$$

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

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

example.
Hypothesis h misclassifies 50 of the 100 samples in S.

In this case,

$$error_S(h) = \frac{50}{100} = 0.50 \quad \text{and}$$

$$Var(error_S(h)) = \frac{0.5 \cdot 0.5}{100}.$$

Then, with approximately 95% probability, $error_D(h)$ lies in interval

$$0.50 \pm 1.96\sqrt{\frac{0.50 \cdot 0.50}{100}} = 0.50 \pm 0.098.$$

That is, the 95% confidence interval of $error_S(h)$ is

$$0.50 \pm 0.098.$$

- Comparing two hypotheses

. Problem: What is the probability that

$error_D(h_1) > error_D(h_2)$?

. Let

$d \equiv error_D(h_1) - error_D(h_2)$

and an estimator of d

$\hat{d} \equiv error_{S_1}(h_1) - error_{S_2}(h_2)$.

If $error_{S_i}(h_i)$, $i = 1, 2$ are unbiased estimators,

$E[\hat{d}] = d$.

. Variance of $\hat{d}$:

$Var(\hat{d}) = Var(error_{S_1}(h_1)) + Var(error_{S_2}(h_2))$

assuming $error_{S_1}(h_1)$ and $error_{S_2}(h_2)$ are independent each other.

From the previous results,

$$Var(error_{S_1}(h_1)) \approx \frac{error_{S_1}(h_1)(1 - error_{S_1}(h_1))}{n_1} \text{ and}$$

$$Var(error_{S_2}(h_2)) \approx \frac{error_{S_2}(h_2)(1 - error_{S_2}(h_2))}{n_2}.$$

Therefore,

$$Var(\hat{d}) \approx \frac{error_{S_1}(h_1)(1 - error_{S_1}(h_1))}{n_1} + \frac{error_{S_2}(h_2)(1 - error_{S_2}(h_2))}{n_2}.$$

Example:

What is the probability that $d = error_D(h_2) - error_D(h_1) > 0$ when $error_{S_1}(h_1) = 0.2$ and $error_{S_2}(h_2) = 0.3$ using two sample sets of 100 instances?

Let $\hat{d} = error_{S_2}(h_2) - error_{S_1}(h_1)$. Then,

$\mu_{\hat{d}} = 0.3 - 0.2 = 0.1$ and

$$\sigma_{\hat{d}} = \sqrt{Var(\hat{d})} = \sqrt{\frac{0.2 \cdot 0.8}{100} + \frac{0.3 \cdot 0.7}{100}} = 0.0608.$$

For the given problem, $\mu_{\hat{d}} - z_\alpha \sigma_{\hat{d}} \geqq 0$, that is,

$$z_\alpha \leqq \frac{0.1}{0.0608} = 1.644.$$

From the table of z_α,

$z_\alpha = 1.644$; that is, $\alpha = 0.05$.

Since this is one-sided confidence interval,

the probability of $d > 0$

is $\Pr[d > 0] = 1 - 0.05 = 0.95$.

That is, h_1 is better than h_2 with 95% confidence.

- k-fold cross-validation

. Evaluation of learning algorithms
. Partition the available data into k disjoint subsets.
. k-1 disjoint sets are used to training samples and
the remaining 1 disjoint set is used to test samples.
. Usually, k is set to 10.

<u>k-fold cross-validation method</u>

Step 1. Partition the available data D_0 into k disjoint subsets
$T_1, T_2, \cdots, T_k$ of equal size, where this size is at least 30.

Step 2. For i from 1 to k, do
use T_i for the test set, and the remaining data for
training set S_i:

(1) $S_i \leftarrow \{D_0 - T_i\}$

(2) $h_i \leftarrow L(S_i)$

(3) Evaluate $error_{T_i}(h_i)$.

Step 3. Evaluate the error mean $\hat{\mu}$ and standard deviation s:

$$\hat{\mu} = \frac{1}{k}\sum_{i=1}^{k} error_{T_i}(h_i)$$

$$s = \sqrt{\frac{1}{k-1}\sum_{i=1}^{k}(error_{T_i}(h_i) - \hat{\mu})^2}$$

What is the relationship between $\hat{\mu}$ and μ?

- t-distribution

. If Z and χ_n^2 are independent random variables, with Z having standard normal distribution and χ_n^2 having a chi-square distribution with n degrees of freedom, then the random variable T_n defined by

$$T_n = \frac{Z}{\sqrt{\chi_n^2 / n}}$$

is said to have a t-distribution with n degrees of freedom.

. The t-density is symmetric about zero.
If n becomes larger, it becomes more and more like a standard normal density since

$$E[\chi_n^2/n] = E[\sum_{i=1}^{n} Z_i^2/n] \approx E[Z_i^2] = 1.$$

. The mean and variance of T_n:

$$E[T_n] = 0, \quad n > 1$$

$$Var(T_n) = \frac{n}{n-2}, \quad n > 2$$

Thus the variance of T_n decreases to 1 as n increases to ∞.

- t-Test

. From the result of k-fold cross-validation method,

$$\frac{\hat{\mu} - \mu}{s/\sqrt{k}} \sim T_{k-1}.$$

. This implies that with the probability of $1-\alpha$,

$$\hat{\mu} - t_{\alpha/2,k-1}\frac{s}{\sqrt{k}} < \mu < \hat{\mu} + t_{\alpha/2,k-1}\frac{s}{\sqrt{k}}$$

where $t_{\alpha/2,k-1}$ represents a constant such that

$$\Pr[T_{k-1} \geqq t_{\alpha/2,k-1}] = \alpha/2.$$

Values of $t_{\alpha/2,n}$:

	$\alpha=0.1$	$\alpha=0.05$	$\alpha=0.02$	$\alpha=0.01$
$n=2$	2.92	4.30	6.96	9.92
$n=5$	2.02	2.57	3.36	4.03
$n=10$	1.81	2.23	2.76	3.17
$n=20$	1.72	2.09	2.53	2.84
$n=30$	1.70	2.04	2.46	2.75
$n=120$	1.66	1.98	2.36	2.62
$n=\infty$	1.64	1.96	2.33	2.58

Note that n=k-1.

Example: k-fold cross-validation method

11 subsets and each subset has 30 instances.

After measuring the performance of learning algorithm using the k-fold cross-validation method, we get

$\hat{\mu}=0.1$ and $s=0.01$.

In this case, k=11. Let $\alpha=0.05$. Then, $t_{0.025,10}=2.23$.

Then, with the probability of 0.95,

$0.1-2.23 \cdot 0.01 < \mu < 0.1+2.23 \cdot 0.01$, that is,

$0.0819 < \mu < 0.1181$.

- Comparing two learning algorithms

. What we would like to estimate is

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

where $L(S)$ is the hypothesis output by the learning algorithm L using training set S.

That is, the expected difference in true error between hypotheses output by learning algorithms 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?

(1) We could partition D_0 into training set S and test set T_0, and measure

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

(2) Even better, repeat this many times and average the results. That is, apply the k-fold cross-validation method.

k-fold cross-validation method

Step 1. Partition the available data D_0 into k disjoint subsets $T_1, T_2, \cdots, T_k$ of equal size, where this size is at least 30.

Step 2. For i from 1 to k, do

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

(1) $S_i \leftarrow \{D_0 - T_i\}$

(2) $h_A \leftarrow L_A(S_i)$

(3) $h_B \leftarrow L_B(S_i)$

(4) $\delta_i \leftarrow error_{T_i}(h_A) - error_{T_i}(h_B)$

Step 3. Return the average value of δ_i:

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

. From the t-distribution, the approximate $(1-\alpha)\times 100\%$ confidence interval for δ is

$$\bar{\delta} \pm t_{\delta/2,k-1}\frac{s_\delta}{\sqrt{k}}$$

where

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

. k-fold cross-validation method comments

(1) Every example gets used as a test example.
(2) Every test set is independent.
(3) Training sets overlap significantly.
(4) 10 is a standard number of folds, that is, k=10.
(5) No method for comparing learning systems with limited data is perfect. However, some statistical analysis is preferable to ignoring the issue of random variation in testing and training.

Reference: T. Mitchell, "Machine Learning," chapter 5.

- Bootstrap method

. Bootstrap method is a general tool for accessing statistical accuracy.

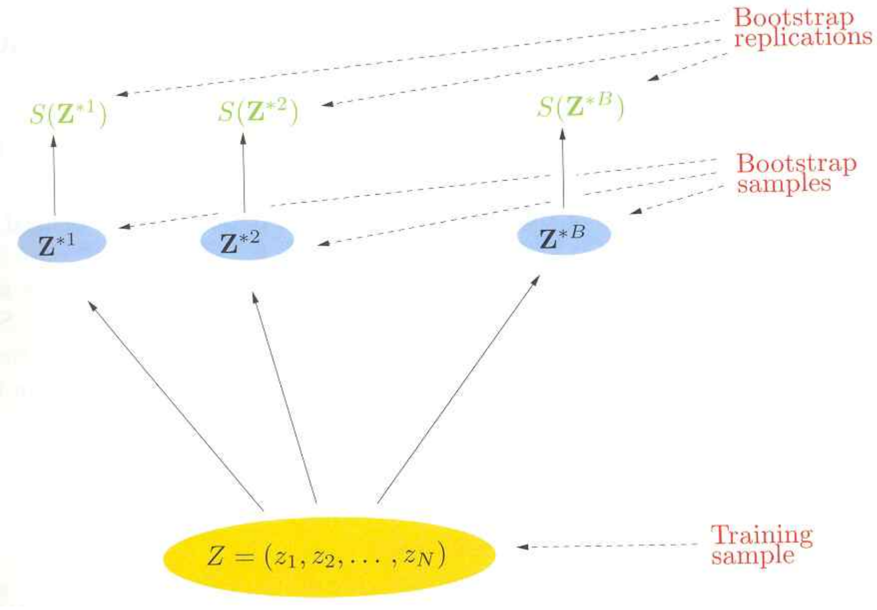
. Let us consider the sample set

$Z = (z_1, z_2, \cdots, z_N)$ and

. the statistical quantity $S(Z)$ computed from the sample set Z.
eg. sample mean:

$$S(Z) = \frac{1}{N}\sum_{i=1}^{N} Z_i$$

. bootstrap process



Z^{*b}, $b = 1, 2, \cdots, B$ are bootstrap samples in which each sample is drawn randomly with replacement from Z.

. variance estimation

From the bootstrap process, variance can be estimated as

$$\widehat{Var}(S(Z)) = \frac{1}{B-1}\sum_{b=1}^{B}(S(Z^{*b}) - \overline{S}^*)^2$$

where

$$\overline{S}^* = \frac{1}{B}\sum_{b=1}^{B} S(Z^{*b}).$$

We can consider $\widehat{Var}(S(Z))$ as a Monte-Carlo estimation of $Var(S(Z))$ under the sampling from the empirical distribution $\hat{F}$ for the data $Z=(Z_1, Z_2, \cdots, Z_N)$.
For this estimation, the proper value of B is typically between 25 and 200.

Bootstrap theorem shows that

$$\lim_{B\to\infty} \widehat{Var}(S(Z)) = Var(S(Z))$$

under the distribution of $\hat{F}$.

. confidence interval

From the bootstrap process, percentile interval is obtained.
Let $\hat{\theta}$ be an estimation of parameter θ

eg. $\hat{\theta}= S(Z) = \dfrac{1}{N}\sum_{i=1}^{N} Z_i$

and $\hat{\theta}^*$ be $\hat{\theta}$ for bootstrap samples, that is,

$$\hat{\theta}^* = S(Z^*).$$

Then, $1-2\alpha$ percentile interval is given by

$$\left[\hat{\theta}_{\%lo}, \hat{\theta}_{\%up}\right]= \left[\hat{G}^{-1}(\alpha), \hat{G}^{-1}(1-\alpha)\right]$$

where $\hat{G}$ represents the cumulative distribution function of $\hat{\theta}^*$.

eg. If $\alpha = 0.05$ and $B = 1000$,

$\hat{\theta}_{\%lo}$ and $\hat{\theta}_{\%up}$ represent the 50th and 950th samples from the sorted $\hat{\theta}^*$ in ascending order respectively.

This estimate of confidence interval is good for unbiased estimate of θ.

. bias

The bias of bootstrap estimate is defined by

$$bias_B = \frac{1}{B}\sum_{b=1}^{B} \hat{\theta}^{*b}$$

where

$$\hat{\theta}^{*b} = S(Z^{*b}).$$

If $bias_B \ll (\widehat{Var}(S(Z))^{1/2}$, $\hat{\theta}$ is a good estimator. Otherwise, use the bias corrected estimator $\overline{\theta} = \hat{\theta} - bias_B$.

Reference: B. Fron and R. Tibshirani, "An Introduction to the Bootstrap," Chapman and Hall, 1993.