CHAPTER 5

EVALUATING HYPOTHESES

Empirically evaluating the accuracy of hypotheses is fundamental to machine learning. This chapter presents an introduction to statistical methods for estimating hypothesis accuracy, focusing on three questions. First, given the observed accuracy of a hypothesis over a limited sample of data, how well does this estimate its accuracy over additional examples? Second, given that one hypothesis outperforms another over some sample of data, how probable is it that this hypothesis is more accurate in general? Third, when data is limited what is the best way to use this data to both learn a hypothesis and estimate its accuracy? Because limited samples of data might misrepresent the general distribution of data, estimating true accuracy from such samples can be misleading. Statistical methods, together with assumptions about the underlying distributions of data, allow one to bound the difference between observed accuracy over the sample of available data and the true accuracy over the entire distribution of data.

5.1 MOTIVATION

In many cases it is important to evaluate the performance of learned hypotheses as precisely as possible. One reason is simply to understand whether to use the hypothesis. For instance, when learning from a limited-size database indicating the effectiveness of different medical treatments, it is important to understand as precisely as possible the accuracy of the learned hypotheses. A second reason is that evaluating hypotheses is an integral component of many learning methods. For example, in post-pruning decision trees to avoid overfitting, we must evaluate

the impact of possible pruning steps on the accuracy of the resulting decision tree. Therefore it is important to understand the likely errors inherent in estimating the accuracy of the pruned and unpruned tree.

Estimating the accuracy of a hypothesis is relatively straightforward when data is plentiful. However, when we must learn a hypothesis and estimate its future accuracy given only a limited set of data, two key difficulties arise:

- *Bias in the estimate.* First, the observed accuracy of the learned hypothesis over the training examples is often a poor estimator of its accuracy over future examples. Because the learned hypothesis was derived from these examples, they will typically provide an optimistically biased estimate of hypothesis accuracy over future examples. This is especially likely when the learner considers a very rich hypothesis space, enabling it to overfit the training examples. To obtain an unbiased estimate of future accuracy, we typically test the hypothesis on some set of test examples chosen independently of the training examples and the hypothesis.
- *Variance in the estimate.* Second, even if the hypothesis accuracy is measured over an unbiased set of test examples independent of the training examples, the measured accuracy can still vary from the true accuracy, depending on the makeup of the particular set of test examples. The smaller the set of test examples, the greater the expected variance.

This chapter discusses methods for evaluating learned hypotheses, methods for comparing the accuracy of two hypotheses, and methods for comparing the accuracy of two learning algorithms when only limited data is available. Much of the discussion centers on basic principles from statistics and sampling theory, though the chapter assumes no special background in statistics on the part of the reader. The literature on statistical tests for hypotheses is very large. This chapter provides an introductory overview that focuses only on the issues most directly relevant to learning, evaluating, and comparing hypotheses.

5.2 ESTIMATING HYPOTHESIS ACCURACY

When evaluating a learned hypothesis we are most often interested in estimating the accuracy with which it will classify future instances. At the same time, we would like to know the probable error in this accuracy estimate (i.e., what error bars to associate with this estimate).

Throughout this chapter we consider the following setting for the learning problem. There is some space of possible instances X (e.g., the set of all people) over which various target functions may be defined (e.g., people who plan to purchase new skis this year). We assume that different instances in X may be encountered with different frequencies. A convenient way to model this is to assume there is some unknown probability distribution $\mathcal{D}$ that defines the probability of encountering each instance in X (e.g., $\mathcal{D}$ might assign a higher probability to encountering 19-year-old people than 109-year-old people). Notice $\mathcal{D}$ says nothing

about whether x is a positive or negative example; it only determines the probability that x will be encountered. The learning task is to learn the target concept or target function f by considering a space H of possible hypotheses. Training examples of the target function f are provided to the learner by a trainer who draws each instance independently, according to the distribution $\mathcal{D}$, and who then forwards the instance x along with its correct target value $f(x)$ to the learner.

To illustrate, consider learning the target function "people who plan to purchase new skis this year," given a sample of training data collected by surveying people as they arrive at a ski resort. In this case the instance space X is the space of all people, who might be described by attributes such as their age, occupation, how many times they skied last year, etc. The distribution $\mathcal{D}$ specifies for each person x the probability that x will be encountered as the next person arriving at the ski resort. The target function $f : X \rightarrow \{0, 1\}$ classifies each person according to whether or not they plan to purchase skis this year.

Within this general setting we are interested in the following two questions:

1. Given a hypothesis h and a data sample containing n examples drawn at random according to the distribution $\mathcal{D}$, what is the best estimate of the accuracy of h over future instances drawn from the same distribution?
2. What is the probable error in this accuracy estimate?

5.2.1 Sample Error and True Error

To answer these questions, we need to distinguish carefully between two notions of accuracy or, equivalently, error. One is the error rate of the hypothesis over the sample of data that is available. The other is the error rate of the hypothesis over the entire unknown distribution $\mathcal{D}$ of examples. We will call these the *sample error* and the *true error* respectively.

The *sample error* of a hypothesis with respect to some sample S of instances drawn from X is the fraction of S that it misclassifies:

Definition: The **sample error** (denoted $error_S(h)$) of hypothesis h with respect to target function f and data sample S is

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

Where n is the number of examples in S, and the quantity $\delta(f(x), h(x))$ is 1 if $f(x) \neq h(x)$, and 0 otherwise.

The *true error* of a hypothesis is the probability that it will misclassify a single randomly drawn instance from the distribution $\mathcal{D}$.

Definition: The **true error** (denoted $error_{\mathcal{D}}(h)$) 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 $\mathcal{D}$.

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

Here the notation $\Pr_{x \in \mathcal{D}}$ denotes that the probability is taken over the instance distribution $\mathcal{D}$.

What we usually wish to know is the true error $error_{\mathcal{D}}(h)$ of the hypothesis, because this is the error we can expect when applying the hypothesis to future examples. All we can measure, however, is the sample error $error_S(h)$ of the hypothesis for the data sample S that we happen to have in hand. The main question considered in this section is "How good an estimate of $error_{\mathcal{D}}(h)$ is provided by $error_S(h)$?"

5.2.2 Confidence Intervals for Discrete-Valued Hypotheses

Here we give an answer to the question "How good an estimate of $error_{\mathcal{D}}(h)$ is provided by $error_S(h)$?" for the case in which h is a discrete-valued hypothesis. More specifically, suppose we wish to estimate the true error for some discrete-valued hypothesis h, based on its observed sample error over a sample S, where

- the sample S contains n examples drawn independent of one another, and independent of h, according to the probability distribution $\mathcal{D}$
- $n \geq 30$
- hypothesis h commits r errors over these n examples (i.e., $error_S(h) = r/n$).

Under these conditions, statistical theory allows us to make the following assertions:

1. Given no other information, the most probable value of $error_{\mathcal{D}}(h)$ is $error_S(h)$
2. With approximately 95% probability, the true error $error_{\mathcal{D}}(h)$ lies in the interval

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

To illustrate, suppose the data sample S contains $n = 40$ examples and that hypothesis h commits $r = 12$ errors over this data. In this case, the sample error $error_S(h) = 12/40 = .30$. Given no other information, the best estimate of the true error $error_{\mathcal{D}}(h)$ is the observed sample error .30. However, we do not expect this to be a perfect estimate of the true error. If we were to collect a second sample S' containing 40 new randomly drawn examples, we might expect the sample error $error_{S'}(h)$ to vary slightly from the sample error $error_S(h)$. We expect a difference due to the random differences in the makeup of S and S'. In fact, if we repeated this experiment over and over, each time drawing a new sample S_i containing 40 new examples, we would find that for approximately 95% of these experiments, the calculated interval would contain the true error. For this reason, we call this interval the 95% confidence interval estimate for $error_{\mathcal{D}}(h)$. In the current example, where $r = 12$ and $n = 40$, the 95% confidence interval is, according to the above expression, $0.30 \pm (1.96 \cdot .07) = 0.30 \pm .14$.

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

TABLE 5.1
Values of z_N for two-sided $N\%$ confidence intervals.

The above expression for the 95% confidence interval can be generalized to any desired confidence level. The constant 1.96 is used in case we desire a 95% confidence interval. A different constant, z_N, is used to calculate the $N\%$ confidence interval. The general expression for approximate $N\%$ confidence intervals for $error_{\mathcal{D}}(h)$ is

$$error_S(h) \pm z_N \sqrt{\frac{error_S(h)(1 - error_S(h))}{n}} \tag{5.1}$$

where the constant z_N is chosen depending on the desired confidence level, using the values of z_N given in Table 5.1.

Thus, just as we could calculate the 95% confidence interval for $error_{\mathcal{D}}(h)$ to be $0.30 \pm (1.96 \cdot .07)$ (when $r = 12$, $n = 40$), we can calculate the 68% confidence interval in this case to be $0.30 \pm (1.0 \cdot .07)$. Note it makes intuitive sense that the 68% confidence interval is smaller than the 95% confidence interval, because we have reduced the probability with which we demand that $error_{\mathcal{D}}(h)$ fall into the interval.

Equation (5.1) describes how to calculate the confidence intervals, or error bars, for estimates of $error_{\mathcal{D}}(h)$ that are based on $error_S(h)$. In using this expression, it is important to keep in mind that this applies only to discrete-valued hypotheses, that it assumes the sample S is drawn at random using the same distribution from which future data will be drawn, and that it assumes the data is independent of the hypothesis being tested. We should also keep in mind that the expression provides only an approximate confidence interval, though the approximation is quite good when the sample contains at least 30 examples, and $error_S(h)$ is not too close to 0 or 1. A more accurate rule of thumb is that the above approximation works well when

$$n\, error_S(h)(1 - error_S(h)) \geq 5$$

Above we summarized the procedure for calculating confidence intervals for discrete-valued hypotheses. The following section presents the underlying statistical justification for this procedure.

5.3 BASICS OF SAMPLING THEORY

This section introduces basic notions from statistics and sampling theory, including probability distributions, expected value, variance, Binomial and Normal distributions, and two-sided and one-sided intervals. A basic familiarity with these

- A *random variable* can be viewed as the name of an experiment with a probabilistic outcome. Its value is the outcome of the experiment.
- A *probability distribution* for a random variable Y specifies the probability $\Pr(Y = y_i)$ that Y will take on the value y_i, for each possible value y_i.
- The *expected value*, or *mean*, of a random variable Y is $E[Y] = \sum_i y_i \Pr(Y = y_i)$. The symbol μ_Y is commonly used to represent E[Y].
- The *variance* of a random variable is $Var(Y) = E[(Y - \mu_Y)^2]$. The variance characterizes the width or dispersion of the distribution about its mean.
- The *standard deviation* of Y is $\sqrt{Var(Y)}$. The symbol σ_Y is often used used to represent the standard deviation of Y.
- The *Binomial distribution* gives the probability of observing r heads in a series of n independent coin tosses, if the probability of heads in a single toss is p.
- The *Normal distribution* is a bell-shaped probability distribution that covers many natural phenomena.
- The *Central Limit Theorem* is a theorem stating that the sum of a large number of independent, identically distributed random variables approximately follows a Normal distribution.
- An *estimator* is a random variable Y used to estimate some parameter p of an underlying population.
- The *estimation bias* of Y as an estimator for p is the quantity $(E[Y] - p)$. An unbiased estimator is one for which the bias is zero.
- A *N% confidence interval* estimate for parameter p is an interval that includes p with probability $N\%$.

TABLE 5.2
Basic definitions and facts from statistics.

concepts is important to understanding how to evaluate hypotheses and learning algorithms. Even more important, these same notions provide an important conceptual framework for understanding machine learning issues such as overfitting and the relationship between successful generalization and the number of training examples considered. The reader who is already familiar with these notions may skip or skim this section without loss of continuity. The key concepts introduced in this section are summarized in Table 5.2.

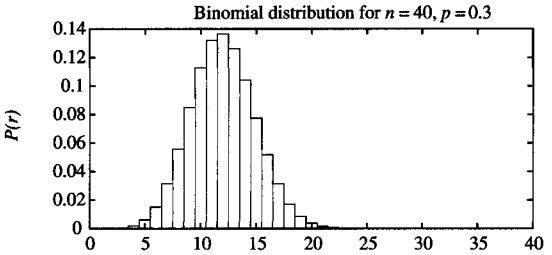
5.3.1 Error Estimation and Estimating Binomial Proportions

Precisely how does the deviation between sample error and true error depend on the size of the data sample? This question is an instance of a well-studied problem in statistics: the problem of estimating the proportion of a population that exhibits some property, given the observed proportion over some random sample of the population. In our case, the property of interest is that h misclassifies the example.

The key to answering this question is to note that when we measure the sample error we are performing an experiment with a random outcome. We first collect a random sample S of n independently drawn instances from the distribution $\mathcal{D}$, and then measure the sample error $error_S(h)$. As noted in the previous

section, if we were to repeat this experiment many times, each time drawing a different random sample S_i of size n, we would expect to observe different values for the various $error_{S_i}(h)$, depending on random differences in the makeup of the various S_i. We say in such cases that $error_{S_i}(h)$, the outcome of the ith such experiment, is a *random variable*. In general, one can think of a random variable as the name of an experiment with a random outcome. The value of the random variable is the observed outcome of the random experiment.

Imagine that we were to run k such random experiments, measuring the random variables $error_{S_1}(h), error_{S_2}(h) \ldots error_{S_k}(h)$. Imagine further that we then plotted a histogram displaying the frequency with which we observed each possible error value. As we allowed k to grow, the histogram would approach the form of the distribution shown in Table 5.3. This table describes a particular probability distribution called the *Binomial distribution*.



A *Binomial distribution* gives the probability of observing r heads in a sample of n independent coin tosses, when the probability of heads on a single coin toss is p. It is defined by the probability function

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

If the random variable X follows a Binomial distribution, then:

- The probability $\Pr(X = r)$ that X will take on the value r is given by $P(r)$
- The expected, or mean value of X, $E[X]$, is

$$E[X] = np$$

- The variance of X, $Var(X)$, is

$$Var(X) = np(1-p)$$

- The standard deviation of X, σ_X, is

$$\sigma_X = \sqrt{np(1-p)}$$

For sufficiently large values of n the Binomial distribution is closely approximated by a Normal distribution (see Table 5.4) with the same mean and variance. Most statisticians recommend using the Normal approximation only when $np(1-p) \geq 5$.

TABLE 5.3
The Binomial distribution.

5.3.2 The Binomial Distribution

A good way to understand the Binomial distribution is to consider the following problem. You are given a worn and bent coin and asked to estimate the probability that the coin will turn up heads when tossed. Let us call this unknown probability of heads p. You toss the coin n times and record the number of times r that it turns up heads. A reasonable estimate of p is r/n. Note that if the experiment were rerun, generating a new set of n coin tosses, we might expect the number of heads r to vary somewhat from the value measured in the first experiment, yielding a somewhat different estimate for p. The Binomial distribution describes for each possible value of r (i.e., from 0 to n), the probability of observing exactly r heads given a sample of n independent tosses of a coin whose true probability of heads is p.

Interestingly, estimating p from a random sample of coin tosses is equivalent to estimating $error_{\mathcal{D}}(h)$ from testing h on a random sample of instances. A single toss of the coin corresponds to drawing a single random instance from $\mathcal{D}$ and determining whether it is misclassified by h. The probability p that a single random coin toss will turn up heads corresponds to the probability that a single instance drawn at random will be misclassified (i.e., p corresponds to $error_{\mathcal{D}}(h)$). The number r of heads observed over a sample of n coin tosses corresponds to the number of misclassifications observed over n randomly drawn instances. Thus r/n corresponds to $error_S(h)$. The problem of estimating p for coins is identical to the problem of estimating $error_{\mathcal{D}}(h)$ for hypotheses. The Binomial distribution gives the general form of the probability distribution for the random variable r, whether it represents the number of heads in n coin tosses or the number of hypothesis errors in a sample of n examples. The detailed form of the Binomial distribution depends on the specific sample size n and the specific probability p or $error_{\mathcal{D}}(h)$.

The general setting to which the Binomial distribution applies is:

1. There is a base, or underlying, experiment (e.g., toss of the coin) whose outcome can be described by a random variable, say Y. The random variable Y can take on two possible values (e.g., $Y = 1$ if heads, $Y = 0$ if tails).
2. The probability that $Y = 1$ on any single trial of the underlying experiment is given by some constant p, independent of the outcome of any other experiment. The probability that $Y = 0$ is therefore $(1 - p)$. Typically, p is not known in advance, and the problem is to estimate it.
3. A series of n independent trials of the underlying experiment is performed (e.g., n independent coin tosses), producing the sequence of independent, identically distributed random variables $Y_1, Y_2, \ldots, Y_n$. Let R denote the number of trials for which $Y_i = 1$ in this series of n experiments

$$R \equiv \sum_{i=1}^{n} Y_i$$

4. The probability that the random variable R will take on a specific value r (e.g., the probability of observing exactly r heads) is given by the Binomial distribution

$$\Pr(R = r) = \frac{n!}{r!(n-r)!} p^r (1-p)^{n-r} \tag{5.2}$$

A plot of this probability distribution is shown in Table 5.3.

The Binomial distribution characterizes the probability of observing r heads from n coin flip experiments, as well as the probability of observing r errors in a data sample containing n randomly drawn instances.

5.3.3 Mean and Variance

Two properties of a random variable that are often of interest are its expected value (also called its mean value) and its variance. The expected value is the average of the values taken on by repeatedly sampling the random variable. More precisely

Definition: Consider a random variable Y that takes on the possible values $y_1, \ldots y_n$. The **expected value** of Y, $E[Y]$, is

$$E[Y] \equiv \sum_{i=1}^{n} y_i \Pr(Y = y_i) \tag{5.3}$$

For example, if Y takes on the value 1 with probability .7 and the value 2 with probability .3, then its expected value is $(1 \cdot 0.7 + 2 \cdot 0.3 = 1.3)$. In case the random variable Y is governed by a Binomial distribution, then it can be shown that

$$E[Y] = np \tag{5.4}$$

where n and p are the parameters of the Binomial distribution defined in Equation (5.2).

A second property, the variance, captures the "width" or "spread" of the probability distribution; that is, it captures how far the random variable is expected to vary from its mean value.

Definition: The **variance** of a random variable Y, $Var[Y]$, is

$$Var[Y] \equiv E[(Y - E[Y])^2] \tag{5.5}$$

The variance describes the expected squared error in using a single observation of Y to estimate its mean $E[Y]$. The square root of the variance is called the *standard deviation* of Y, denoted σ_Y.

Definition: The **standard deviation** of a random variable Y, σ_Y, is

$$\sigma_Y \equiv \sqrt{E[(Y - E[Y])^2]} \tag{5.6}$$

In case the random variable Y is governed by a Binomial distribution, then the variance and standard deviation are given by

$$Var[Y] = np(1-p)$$
$$\sigma_Y = \sqrt{np(1-p)} \tag{5.7}$$

5.3.4 Estimators, Bias, and Variance

Now that we have shown that the random variable $error_S(h)$ obeys a Binomial distribution, we return to our primary question: What is the likely difference between $error_S(h)$ and the true error $error_{\mathcal{D}}(h)$?

Let us describe $error_S(h)$ and $error_{\mathcal{D}}(h)$ using the terms in Equation (5.2) defining the Binomial distribution. We then have

$$error_S(h) = \frac{r}{n}$$
$$error_{\mathcal{D}}(h) = p$$

where n is the number of instances in the sample S, r is the number of instances from S misclassified by h, and p is the probability of misclassifying a single instance drawn from $\mathcal{D}$.

Statisticians call $error_S(h)$ an *estimator* for the true error $error_{\mathcal{D}}(h)$. In general, an estimator is any random variable used to estimate some parameter of the underlying population from which the sample is drawn. An obvious question to ask about any estimator is whether on average it gives the right estimate. We define the *estimation bias* to be the difference between the expected value of the estimator and the true value of the parameter.

Definition: The **estimation bias** of an estimator Y for an arbitrary parameter p is

$$E[Y] - p$$

If the estimation bias is zero, we say that Y is an *unbiased estimator* for p. Notice this will be the case if the average of many random values of Y generated by repeated random experiments (i.e., $E[Y]$) converges toward p.

Is $error_S(h)$ an unbiased estimator for $error_{\mathcal{D}}(h)$? Yes, because for a Binomial distribution the expected value of r is equal to np (Equation [5.4]). It follows, given that n is a constant, that the expected value of r/n is p.

Two quick remarks are in order regarding the estimation bias. First, when we mentioned at the beginning of this chapter that testing the hypothesis on the training examples provides an optimistically biased estimate of hypothesis error, it is exactly this notion of estimation bias to which we were referring. In order for $error_S(h)$ to give an unbiased estimate of $error_{\mathcal{D}}(h)$, the hypothesis h and sample S must be chosen independently. Second, this notion of *estimation bias* should not be confused with the *inductive bias* of a learner introduced in Chapter 2. The

estimation bias is a numerical quantity, whereas the inductive bias is a set of assertions.

A second important property of any estimator is its variance. Given a choice among alternative unbiased estimators, it makes sense to choose the one with least variance. By our definition of variance, this choice will yield the smallest expected squared error between the estimate and the true value of the parameter.

To illustrate these concepts, suppose we test a hypothesis and find that it commits $r = 12$ errors on a sample of $n = 40$ randomly drawn test examples. Then an unbiased estimate for $error_{\mathcal{D}}(h)$ is given by $error_S(h) = r/n = 0.3$. The variance in this estimate arises completely from the variance in r, because n is a constant. Because r is Binomially distributed, its variance is given by Equation (5.7) as $np(1-p)$. Unfortunately p is unknown, but we can substitute our estimate r/n for p. This yields an estimated variance in r of $40 \cdot 0.3(1 - 0.3) = 8.4$, or a corresponding standard deviation of $\sqrt{8.4} \approx 2.9$. This implies that the standard deviation in $error_S(h) = r/n$ is approximately $2.9/40 = .07$. To summarize, $error_S(h)$ in this case is observed to be 0.30, with a standard deviation of approximately 0.07. (See Exercise 5.1.)

In general, given r errors in a sample of n independently drawn test examples, the standard deviation for $error_S(h)$ is given by

$$\sigma_{error_S(h)} = \frac{\sigma_r}{n} = \sqrt{\frac{p(1-p)}{n}} \tag{5.8}$$

which can be approximated by substituting $r/n = error_S(h)$ for p

$$\sigma_{error_S(h)} \approx \sqrt{\frac{error_S(h)(1 - error_S(h))}{n}} \tag{5.9}$$

5.3.5 Confidence Intervals

One common way to describe the uncertainty associated with an estimate is to give an interval within which the true value is expected to fall, along with the probability with which it is expected to fall into this interval. Such estimates are called *confidence interval* estimates.

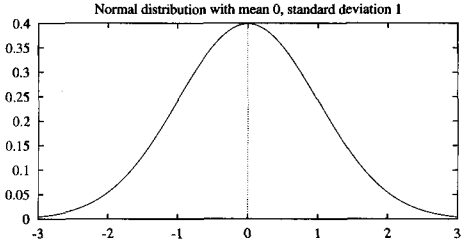
> ***Definition:*** An $N\%$ **confidence interval** for some parameter p is an interval that is expected with probability $N\%$ to contain p.

For example, if we observe $r = 12$ errors in a sample of $n = 40$ independently drawn examples, we can say with approximately 95% probability that the interval 0.30 ± 0.14 contains the true error $error_{\mathcal{D}}(h)$.

How can we derive confidence intervals for $error_{\mathcal{D}}(h)$? The answer lies in the fact that we know the Binomial probability distribution governing the estimator $error_S(h)$. The mean value of this distribution is $error_{\mathcal{D}}(h)$, and the standard deviation is given by Equation (5.9). Therefore, to derive a 95% confidence interval, we need only find the interval centered around the mean value $error_{\mathcal{D}}(h)$,

which is wide enough to contain 95% of the total probability under this distribution. This provides an interval surrounding $error_{\mathcal{D}}(h)$ into which $error_S(h)$ must fall 95% of the time. Equivalently, it provides the size of the interval surrounding $error_S(h)$ into which $error_{\mathcal{D}}(h)$ must fall 95% of the time.

For a given value of N how can we find the size of the interval that contains $N\%$ of the probability mass? Unfortunately, for the Binomial distribution this calculation can be quite tedious. Fortunately, however, an easily calculated and very good approximation can be found in most cases, based on the fact that for sufficiently large sample sizes the Binomial distribution can be closely approximated by the Normal distribution. The Normal distribution, summarized in Table 5.4, is perhaps the most well-studied probability distribution in statistics. As illustrated in Table 5.4, it is a bell-shaped distribution fully specified by its



A Normal distribution (also called a Gaussian distribution) is a bell-shaped distribution defined by the probability density function

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

A Normal distribution is fully determined by two parameters in the above formula: μ and σ.

If the random variable X follows a normal distribution, then:

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

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

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

$$E[X] = \mu$$

- The variance of X, $Var(X)$, is

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

- The standard deviation of X, σ_X, is

$$\sigma_X = \sigma$$

The Central Limit Theorem (Section 5.4.1) states that the sum of a large number of independent, identically distributed random variables follows a distribution that is approximately Normal.

TABLE 5.4
The Normal or Gaussian distribution.

mean μ and standard deviation σ. For large n, any Binomial distribution is very closely approximated by a Normal distribution with the same mean and variance.

One reason that we prefer to work with the Normal distribution is that most statistics references give tables specifying the size of the interval about the mean that contains $N\%$ of the probability mass under the Normal distribution. This is precisely the information needed to calculate our $N\%$ confidence interval. In fact, Table 5.1 is such a table. The constant z_N given in Table 5.1 defines the width of the smallest interval about the mean that includes $N\%$ of the total probability mass under the bell-shaped Normal distribution. More precisely, z_N gives half the width of the interval (i.e., the distance from the mean in either direction) measured in standard deviations. Figure 5.1(a) illustrates such an interval for $z_{.80}$.

To summarize, if a random variable Y obeys a Normal distribution with mean μ and standard deviation σ, then the measured random value y of Y will fall into the following interval $N\%$ of the time

$$\mu \pm z_N \sigma \tag{5.10}$$

Equivalently, the mean μ will fall into the following interval $N\%$ of the time

$$y \pm z_N \sigma \tag{5.11}$$

We can easily combine this fact with earlier facts to derive the general expression for $N\%$ confidence intervals for discrete-valued hypotheses given in Equation (5.1). First, we know that $error_S(h)$ follows a Binomial distribution with mean value $error_{\mathcal{D}}(h)$ and standard deviation as given in Equation (5.9). Second, we know that for sufficiently large sample size n, this Binomial distribution is well approximated by a Normal distribution. Third, Equation (5.11) tells us how to find the $N\%$ confidence interval for estimating the mean value of a Normal distribution. Therefore, substituting the mean and standard deviation of $error_S(h)$ into Equation (5.11) yields the expression from Equation (5.1) for $N\%$ confidence

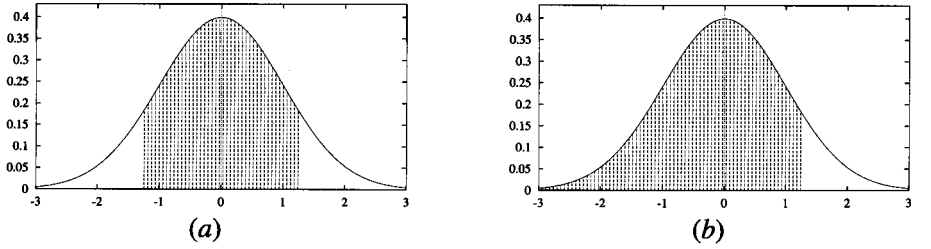


FIGURE 5.1
A Normal distribution with mean 0, standard deviation 1. (a) With 80% confidence, the value of the random variable will lie in the two-sided interval $[-1.28, 1.28]$. Note $z_{.80} = 1.28$. With 10% confidence it will lie to the right of this interval, and with 10% confidence it will lie to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

intervals for discrete-valued hypotheses

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

Recall that two approximations were involved in deriving this expression, namely:

1. in estimating the standard deviation σ of $error_S(h)$, we have approximated $error_{\mathcal{D}}(h)$ by $error_S(h)$ [i.e., in going from Equation (5.8) to (5.9)], and
2. the Binomial distribution has been approximated by the Normal distribution.

The common rule of thumb in statistics is that these two approximations are very good as long as $n \geq 30$, or when $np(1-p) \geq 5$. For smaller values of n it is wise to use a table giving exact values for the Binomial distribution.

5.3.6 Two-Sided and One-Sided Bounds

Notice that the above confidence interval is a *two-sided* bound; that is, it bounds the estimated quantity from above and from below. In some cases, we will be interested only in a *one-sided* bound. For example, we might be interested in the question "What is the probability that $error_{\mathcal{D}}(h)$ is at most U?" This kind of one-sided question is natural when we are only interested in bounding the maximum error of h and do not mind if the true error is much smaller than estimated.

There is an easy modification to the above procedure for finding such one-sided error bounds. It follows from the fact that the Normal distribution is symmetric about its mean. Because of this fact, any two-sided confidence interval based on a Normal distribution can be converted to a corresponding one-sided interval with twice the confidence (see Figure 5.1(*b*)). That is, a $100(1-\alpha)\%$ confidence interval with lower bound L and upper bound U implies a $100(1-\alpha/2)\%$ confidence interval with lower bound L and no upper bound. It also implies a $100(1-\alpha/2)\%$ confidence interval with upper bound U and no lower bound. Here α corresponds to the probability that the correct value lies outside the stated interval. In other words, α is the probability that the value will fall into the *unshaded* region in Figure 5.1(*a*), and $\alpha/2$ is the probability that it will fall into the unshaded region in Figure 5.1(*b*).

To illustrate, consider again the example in which h commits $r = 12$ errors over a sample of $n = 40$ independently drawn examples. As discussed above, this leads to a (two-sided) 95% confidence interval of 0.30 ± 0.14. In this case, $100(1-\alpha) = 95\%$, so $\alpha = 0.05$. Thus, we can apply the above rule to say with $100(1-\alpha/2) = 97.5\%$ confidence that $error_{\mathcal{D}}(h)$ is at most $0.30 + 0.14 = 0.44$, making no assertion about the lower bound on $error_{\mathcal{D}}(h)$. Thus, we have a one-sided error bound on $error_{\mathcal{D}}(h)$ with double the confidence that we had in the corresponding two-sided bound (see Exercise 5.3).

5.4 A GENERAL APPROACH FOR DERIVING CONFIDENCE INTERVALS

The previous section described in detail how to derive confidence interval estimates for one particular case: estimating $error_{\mathcal{D}}(h)$ for a discrete-valued hypothesis h, based on a sample of n independently drawn instances. The approach described there illustrates a general approach followed in many estimation problems. In particular, we can see this as a problem of estimating the mean (expected value) of a population based on the mean of a randomly drawn sample of size n. The general process includes the following steps:

1. Identify the underlying population parameter p to be estimated, for example, $error_{\mathcal{D}}(h)$.
2. Define the estimator Y (e.g., $error_S(h)$). It is desirable to choose a minimum-variance, unbiased estimator.
3. Determine the probability distribution $\mathcal{D}_Y$ that governs the estimator Y, including its mean and variance.
4. Determine the $N\%$ confidence interval by finding thresholds L and U such that $N\%$ of the mass in the probability distribution $\mathcal{D}_Y$ falls between L and U.

In later sections of this chapter we apply this general approach to several other estimation problems common in machine learning. First, however, let us discuss a fundamental result from estimation theory called the *Central Limit Theorem.*

5.4.1 Central Limit Theorem

One essential fact that simplifies attempts to derive confidence intervals is the Central Limit Theorem. Consider again our general setting, in which we observe the values of n independently drawn random variables $Y_1 \ldots Y_n$ that obey the same unknown underlying probability distribution (e.g., n tosses of the same coin). Let μ denote the mean of the unknown distribution governing each of the Y_i and let σ denote the standard deviation. We say that these variables Y_i are *independent, identically distributed* random variables, because they describe independent experiments, each obeying the same underlying probability distribution. In an attempt to estimate the mean μ of the distribution governing the Y_i, we calculate the sample mean $\bar{Y}_n \equiv \frac{1}{n}\sum_{i=1}^{n} Y_i$ (e.g., the fraction of heads among the n coin tosses). The Central Limit Theorem states that the probability distribution governing $\bar{Y}_n$ approaches a Normal distribution as $n \to \infty$, *regardless of the distribution that governs the underlying random variables* Y_i. Furthermore, the mean of the distribution governing $\bar{Y}_n$ approaches μ and the standard deviation approaches $\frac{\sigma}{\sqrt{n}}$. More precisely,

Theorem 5.1. Central Limit Theorem. Consider a set of independent, identically distributed random variables $Y_1 \ldots Y_n$ governed by an arbitrary probability distribution with mean μ and finite variance σ^2. Define the sample mean, $\bar{Y}_n \equiv \frac{1}{n}\sum_{i=1}^{n} Y_i$.

Then as $n \to \infty$, the distribution governing

$$\frac{\bar{Y}_n - \mu}{\frac{\sigma}{\sqrt{n}}}$$

approaches a Normal distribution, with zero mean and standard deviation equal to 1.

This is a quite surprising fact, because it states that we know the form of the distribution that governs the sample mean $\bar{Y}$ even when we do not know the form of the underlying distribution that governs the individual Y_i that are being observed! Furthermore, the Central Limit Theorem describes how the mean and variance of $\bar{Y}$ can be used to determine the mean and variance of the individual Y_i.

The Central Limit Theorem is a very useful fact, because it implies that whenever we define an estimator that is the mean of some sample (e.g., $error_S(h)$ is the mean error), the distribution governing this estimator can be approximated by a Normal distribution for sufficiently large n. If we also know the variance for this (approximately) Normal distribution, then we can use Equation (5.11) to compute confidence intervals. A common rule of thumb is that we can use the Normal approximation when $n \geq 30$. Recall that in the preceding section we used such a Normal distribution to approximate the Binomial distribution that more precisely describes $error_S(h)$.

5.5 DIFFERENCE IN ERROR OF TWO HYPOTHESES

Consider the case where we have two hypotheses h_1 and h_2 for some discrete-valued target function. Hypothesis h_1 has been tested on a sample S_1 containing n_1 randomly drawn examples, and h_2 has been tested on an independent sample S_2 containing n_2 examples drawn from the same distribution. Suppose we wish to estimate the difference d between the true errors of these two hypotheses.

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

We will use the generic four-step procedure described at the beginning of Section 5.4 to derive a confidence interval estimate for d. Having identified d as the parameter to be estimated, we next define an estimator. The obvious choice for an estimator in this case is the difference between the sample errors, which we denote by $\hat{d}$

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

Although we will not prove it here, it can be shown that $\hat{d}$ gives an unbiased estimate of d; that is $E[\hat{d}\,] = d$.

What is the probability distribution governing the random variable $\hat{d}$? From earlier sections, we know that for large n_1 and n_2 (e.g., both ≥ 30), both $error_{S_1}(h_1)$ and $error_{S_2}(h_2)$ follow distributions that are approximately Normal. Because the difference of two Normal distributions is also a Normal distribution, $\hat{d}$ will also

follow a distribution that is approximately Normal, with mean d. It can also be shown that the variance of this distribution is the sum of the variances of $error_{S_1}(h_1)$ and $error_{S_2}(h_2)$. Using Equation (5.9) to obtain the approximate variance of each of these distributions, we have

$$\sigma_{\hat{d}}^2 \approx \frac{error_{S_1}(h_1)(1 - error_{S_1}(h_1))}{n_1} + \frac{error_{S_2}(h_2)(1 - error_{S_2}(h_2))}{n_2} \quad (5.12)$$

Now that we have determined the probability distribution that governs the estimator $\hat{d}$, it is straightforward to derive confidence intervals that characterize the likely error in employing $\hat{d}$ to estimate d. For a random variable $\hat{d}$ obeying a Normal distribution with mean d and variance σ^2, the N% confidence interval estimate for d is $\hat{d} \pm z_N\sigma$. Using the approximate variance $\sigma_{\hat{d}}^2$ given above, this approximate $N\%$ confidence interval estimate for d is

$$\hat{d} \pm z_N \sqrt{\frac{error_{S_1}(h_1)(1 - error_{S_1}(h_1))}{n_1} + \frac{error_{S_2}(h_2)(1 - error_{S_2}(h_2))}{n_2}} \quad (5.13)$$

where z_N is the same constant described in Table 5.1. The above expression gives the general two-sided confidence interval for estimating the difference between errors of two hypotheses. In some situations we might be interested in one-sided bounds—either bounding the largest possible difference in errors or the smallest, with some confidence level. One-sided confidence intervals can be obtained by modifying the above expression as described in Section 5.3.6.

Although the above analysis considers the case in which h_1 and h_2 are tested on independent data samples, it is often acceptable to use the confidence interval seen in Equation (5.13) in the setting where h_1 and h_2 are tested on a single sample S (where S is still independent of h_1 and h_2). In this later case, we redefine $\hat{d}$ as

$$\hat{d} \equiv error_S(h_1) - error_S(h_2)$$

The variance in this new $\hat{d}$ will usually be smaller than the variance given by Equation (5.12), when we set S_1 and S_2 to S. This is because using a single sample S eliminates the variance due to random differences in the compositions of S_1 and S_2. In this case, the confidence interval given by Equation (5.13) will generally be an overly conservative, but still correct, interval.

5.5.1 Hypothesis Testing

In some cases we are interested in the probability that some specific conjecture is true, rather than in confidence intervals for some parameter. Suppose, for example, that we are interested in the question "what is the probability that $error_{\mathcal{D}}(h_1) > error_{\mathcal{D}}(h_2)$?" Following the setting in the previous section, suppose we measure the sample errors for h_1 and h_2 using two independent samples S_1 and S_2 of size 100 and find that $error_{S_1}(h_1) = .30$ and $error_{S_2}(h_2) = .20$, hence the observed difference is $\hat{d} = .10$. Of course, due to random variation in the data sample,

we might observe this difference in the sample errors even when $error_{\mathcal{D}}(h_1) \leq error_{\mathcal{D}}(h_2)$. What is the probability that $error_{\mathcal{D}}(h_1) > error_{\mathcal{D}}(h_2)$, given the observed difference in sample errors $\hat{d} = .10$ in this case? Equivalently, what is the probability that $d > 0$, given that we observed $\hat{d} = .10$?

Note the probability $\Pr(d > 0)$ is equal to the probability that $\hat{d}$ has not overestimated d by more than .10. Put another way, this is the probability that $\hat{d}$ falls into the one-sided interval $\hat{d} < d + .10$. Since d is the mean of the distribution governing $\hat{d}$, we can equivalently express this one-sided interval as $\hat{d} < \mu_{\hat{d}} + .10$.

To summarize, the probability $\Pr(d > 0)$ equals the probability that $\hat{d}$ falls into the one-sided interval $\hat{d} < \mu_{\hat{d}} + .10$. Since we already calculated the approximate distribution governing $\hat{d}$ in the previous section, we can determine the probability that $\hat{d}$ falls into this one-sided interval by calculating the probability mass of the $\hat{d}$ distribution within this interval.

Let us begin this calculation by re-expressing the interval $\hat{d} < \mu_{\hat{d}} + .10$ in terms of the number of standard deviations it allows deviating from the mean. Using Equation (5.12) we find that $\sigma_{\hat{d}} \approx .061$, so we can re-express the interval as approximately

$$\hat{d} < \mu_{\hat{d}} + 1.64\sigma_{\hat{d}}$$

What is the confidence level associated with this one-sided interval for a Normal distribution? Consulting Table 5.1, we find that 1.64 standard deviations about the mean corresponds to a two-sided interval with confidence level 90%. Therefore, the one-sided interval will have an associated confidence level of 95%.

Therefore, given the observed $\hat{d} = .10$, the probability that $error_{\mathcal{D}}(h_1) > error_{\mathcal{D}}(h_2)$ is approximately .95. In the terminology of the statistics literature, we say that we accept the hypothesis that "$error_{\mathcal{D}}(h_1) > error_{\mathcal{D}}(h_2)$" with confidence 0.95. Alternatively, we may state that we reject the opposite hypothesis (often called the null hypothesis) at a $(1 - 0.95) = .05$ level of significance.

5.6 COMPARING LEARNING ALGORITHMS

Often we are interested in comparing the performance of two learning algorithms L_A and L_B, rather than two specific hypotheses. What is an appropriate test for comparing learning algorithms, and how can we determine whether an observed difference between the algorithms is statistically significant? Although there is active debate within the machine-learning research community regarding the best method for comparison, we present here one reasonable approach. A discussion of alternative methods is given by Dietterich (1996).

As usual, we begin by specifying the parameter we wish to estimate. Suppose we wish to determine which of L_A and L_B is the better learning method on average for learning some particular target function f. A reasonable way to define "on average" is to consider the relative performance of these two algorithms averaged over all the training sets of size n that might be drawn from the underlying instance distribution $\mathcal{D}$. In other words, we wish to estimate the expected value

of the difference in their errors

$$\underset{S \subset \mathcal{D}}{E}[error_{\mathcal{D}}(L_A(S)) - error_{\mathcal{D}}(L_B(S))] \tag{5.14}$$

where $L(S)$ denotes the hypothesis output by learning method L when given the sample S of training data and where the subscript $S \subset \mathcal{D}$ indicates that the expected value is taken over samples S drawn according to the underlying instance distribution $\mathcal{D}$. The above expression describes the expected value of the difference in errors between learning methods L_A and L_B.

Of course in practice we have only a limited sample D_0 of data when comparing learning methods. In such cases, one obvious approach to estimating the above quantity is to divide D_0 into a training set S_0 and a disjoint test set T_0. The training data can be used to train both L_A and L_B, and the test data can be used to compare the accuracy of the two learned hypotheses. In other words, we measure the quantity

$$error_{T_0}(L_A(S_0)) - error_{T_0}(L_B(S_0)) \tag{5.15}$$

Notice two key differences between this estimator and the quantity in Equation (5.14). First, we are using $error_{T_0}(h)$ to approximate $error_{\mathcal{D}}(h)$. Second, we are only measuring the difference in errors for one training set S_0 rather than taking the expected value of this difference over all samples S that might be drawn from the distribution $\mathcal{D}$.

One way to improve on the estimator given by Equation (5.15) is to repeatedly partition the data D_0 into disjoint training and test sets and to take the mean of the test set errors for these different experiments. This leads to the procedure shown in Table 5.5 for estimating the difference between errors of two learning methods, based on a fixed sample D_0 of available data. This procedure first partitions the data into k disjoint subsets of equal size, where this size is at least 30. It then trains and tests the learning algorithms k times, using each of the k subsets in turn as the test set, and using all remaining data as the training set. In this way, the learning algorithms are tested on k independent test sets, and the mean difference in errors $\bar{\delta}$ is returned as an estimate of the difference between the two learning algorithms.

The quantity $\bar{\delta}$ returned by the procedure of Table 5.5 can be taken as an estimate of the desired quantity from Equation 5.14. More appropriately, we can view $\bar{\delta}$ as an estimate of the quantity

$$\underset{S \subset D_0}{E}[error_{\mathcal{D}}(L_A(S)) - error_{\mathcal{D}}(L_B(S))] \tag{5.16}$$

where S represents a random sample of size $\frac{k-1}{k}|D_0|$ drawn uniformly from D_0. The only difference between this expression and our original expression in Equation (5.14) is that this new expression takes the expected value over subsets of the available data D_0, rather than over subsets drawn from the full instance distribution $\mathcal{D}$.

1. Partition the available data D_0 into k disjoint subsets $T_1, T_2, \ldots, T_k$ 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

$$\bar{\delta} \equiv \frac{1}{k} \sum_{i=1}^{k} \delta_i \tag{T5.1}$$

TABLE 5.5
A procedure to estimate the difference in error between two learning methods L_A and L_B. Approximate confidence intervals for this estimate are given in the text.

The approximate $N\%$ confidence interval for estimating the quantity in Equation (5.16) using $\bar{\delta}$ is given by

$$\bar{\delta} \pm t_{N,k-1}\, s_{\bar{\delta}} \tag{5.17}$$

where $t_{N,k-1}$ is a constant that plays a role analogous to that of z_N in our earlier confidence interval expressions, and where $s_{\bar{\delta}}$ is an estimate of the standard deviation of the distribution governing $\bar{\delta}$. In particular, $s_{\bar{\delta}}$ is defined as

$$s_{\bar{\delta}} \equiv \sqrt{\frac{1}{k(k-1)} \sum_{i=1}^{k} (\delta_i - \bar{\delta})^2} \tag{5.18}$$

Notice the constant $t_{N,k-1}$ in Equation (5.17) has two subscripts. The first specifies the desired confidence level, as it did for our earlier constant z_N. The second parameter, called the number of *degrees of freedom* and usually denoted by ν, is related to the number of independent random events that go into producing the value for the random variable $\bar{\delta}$. In the current setting, the number of degrees of freedom is $k - 1$. Selected values for the parameter t are given in Table 5.6. Notice that as $k \rightarrow \infty$, the value of $t_{N,k-1}$ approaches the constant z_N.

Note the procedure described here for comparing two learning methods involves testing the two learned hypotheses on identical test sets. This contrasts with the method described in Section 5.5 for comparing hypotheses that have been evaluated using two independent test sets. Tests where the hypotheses are evaluated over identical samples are called *paired tests*. Paired tests typically produce tighter confidence intervals because any differences in observed errors in a paired test are due to differences between the hypotheses. In contrast, when the hypotheses are tested on separate data samples, differences in the two sample errors might be partially attributable to differences in the makeup of the two samples.

	Confidence level N			
	90%	95%	98%	99%
$\nu = 2$	2.92	4.30	6.96	9.92
$\nu = 5$	2.02	2.57	3.36	4.03
$\nu = 10$	1.81	2.23	2.76	3.17
$\nu = 20$	1.72	2.09	2.53	2.84
$\nu = 30$	1.70	2.04	2.46	2.75
$\nu = 120$	1.66	1.98	2.36	2.62
$\nu = \infty$	1.64	1.96	2.33	2.58

TABLE 5.6
Values of $t_{N,\nu}$ for two-sided confidence intervals. As $\nu \to \infty$, $t_{N,\nu}$ approaches z_N.

5.6.1 Paired t Tests

Above we described one procedure for comparing two learning methods given a fixed set of data. This section discusses the statistical justification for this procedure, and for the confidence interval defined by Equations (5.17) and (5.18). It can be skipped or skimmed on a first reading without loss of continuity.

The best way to understand the justification for the confidence interval estimate given by Equation (5.17) is to consider the following estimation problem:

- We are given the observed values of a set of independent, identically distributed random variables $Y_1, Y_2, \ldots, Y_k$.
- We wish to estimate the mean μ of the probability distribution governing these Y_i.
- The estimator we will use is the sample mean $\bar{Y}$

$$\bar{Y} \equiv \frac{1}{k} \sum_{i=1}^{k} Y_i$$

This problem of estimating the distribution mean μ based on the sample mean $\bar{Y}$ is quite general. For example, it covers the problem discussed earlier of using $error_S(h)$ to estimate $error_{\mathcal{D}}(h)$. (In that problem, the Y_i are 1 or 0 to indicate whether h commits an error on an individual example from S, and $error_{\mathcal{D}}(h)$ is the mean μ of the underlying distribution.) The t test, described by Equations (5.17) and (5.18), applies to a special case of this problem—the case in which the individual Y_i follow a Normal distribution.

Now consider the following idealization of the method in Table 5.5 for comparing learning methods. Assume that instead of having a fixed sample of data D_0, we can request new training examples drawn according to the underlying instance distribution. In particular, in this idealized method we modify the procedure of Table 5.5 so that on each iteration through the loop it generates a new random training set S_i and new random test set T_i by drawing from this underlying instance distribution instead of drawing from the fixed sample D_0. This idealized method

perfectly fits the form of the above estimation problem. In particular, the δ_i measured by the procedure now correspond to the independent, identically distributed random variables Y_i. The mean μ of their distribution corresponds to the expected difference in error between the two learning methods [i.e., Equation (5.14)]. The sample mean $\bar{Y}$ is the quantity $\bar{\delta}$ computed by this idealized version of the method. We wish to answer the question "how good an estimate of μ is provided by $\bar{\delta}$?"

First, note that the size of the test sets T_i has been chosen to contain at least 30 examples. Because of this, the individual δ_i will each follow an approximately Normal distribution (due to the Central Limit Theorem). Hence, we have a special case in which the Y_i are governed by an approximately Normal distribution. It can be shown in general that when the individual Y_i each follow a Normal distribution, then the sample mean $\bar{Y}$ follows a Normal distribution as well. Given that $\bar{Y}$ is Normally distributed, we might consider using the earlier expression for confidence intervals (Equation [5.11]) that applies to estimators governed by Normal distributions. Unfortunately, that equation requires that we know the standard deviation of this distribution, which we do not.

The t test applies to precisely these situations, in which the task is to estimate the sample mean of a collection of independent, identically and Normally distributed random variables. In this case, we can use the confidence interval given by Equations (5.17) and (5.18), which can be restated using our current notation as

$$\mu = \bar{Y} \pm t_{N,k-1}\, s_{\bar{Y}}$$

where $s_{\bar{Y}}$ is the estimated standard deviation of the sample mean

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

and where $t_{N,k-1}$ is a constant analogous to our earlier z_N. In fact, the constant $t_{N,k-1}$ characterizes the area under a probability distribution known as the t distribution, just as the constant z_N characterizes the area under a Normal distribution. The t distribution is a bell-shaped distribution similar to the Normal distribution, but wider and shorter to reflect the greater variance introduced by using $s_{\bar{Y}}$ to approximate the true standard deviation $\sigma_{\bar{Y}}$. The t distribution approaches the Normal distribution (and therefore $t_{N,k-1}$ approaches z_N) as k approaches infinity. This is intuitively satisfying because we expect $s_{\bar{Y}}$ to converge toward the true standard deviation $\sigma_{\bar{Y}}$ as the sample size k grows, and because we can use z_N when the standard deviation is known exactly.

5.6.2 Practical Considerations

Note the above discussion justifies the use of the confidence interval estimate given by Equation (5.17) in the case where we wish to use the sample mean $\bar{Y}$ to estimate the mean of a sample containing k independent, identically and Normally distributed random variables. This fits the idealized method described

above, in which we assume unlimited access to examples of the target function. In practice, given a limited set of data D_0 and the more practical method described by Table 5.5, this justification does not strictly apply. In practice, the problem is that the only way to generate new δ_i is to resample D_0, dividing it into training and test sets in different ways. The δ_i are not independent of one another in this case, because they are based on overlapping sets of training examples drawn from the limited subset D_0 of data, rather than from the full distribution $\mathcal{D}$.

When only a limited sample of data D_0 is available, several methods can be used to resample D_0. Table 5.5 describes a k-fold method in which D_0 is partitioned into k disjoint, equal-sized subsets. In this k-fold approach, each example from D_0 is used exactly once in a test set, and $k - 1$ times in a training set. A second popular approach is to randomly choose a test set of at least 30 examples from D_0, use the remaining examples for training, then repeat this process as many times as desired. This randomized method has the advantage that it can be repeated an indefinite number of times, to shrink the confidence interval to the desired width. In contrast, the k-fold method is limited by the total number of examples, by the use of each example only once in a test set, and by our desire to use samples of size at least 30. However, the randomized method has the disadvantage that the test sets no longer qualify as being independently drawn with respect to the underlying instance distribution $\mathcal{D}$. In contrast, the test sets generated by k-fold cross validation are independent because each instance is included in only one test set.

To summarize, no single procedure for comparing learning methods based on limited data satisfies all the constraints we would like. It is wise to keep in mind that statistical models rarely fit perfectly the practical constraints in testing learning algorithms when available data is limited. Nevertheless, they do provide approximate confidence intervals that can be of great help in interpreting experimental comparisons of learning methods.

5.7 SUMMARY AND FURTHER READING

The main points of this chapter include:

- Statistical theory provides a basis for estimating the true error ($error_{\mathcal{D}}(h)$) of a hypothesis h, based on its observed error ($error_S(h)$) over a sample S of data. For example, if h is a discrete-valued hypothesis and the data sample S contains $n \geq 30$ examples drawn independently of h and of one another, then the $N\%$ confidence interval for $error_{\mathcal{D}}(h)$ is approximately

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

  where values for z_N are given in Table 5.1.
- In general, the problem of estimating confidence intervals is approached by identifying the parameter to be estimated (e.g., $error_{\mathcal{D}}(h)$) and an estimator

(e.g., $error_S(h)$) for this quantity. Because the estimator is a random variable (e.g., $error_S(h)$ depends on the random sample S), it can be characterized by the probability distribution that governs its value. Confidence intervals can then be calculated by determining the interval that contains the desired probability mass under this distribution.

- One possible cause of errors in estimating hypothesis accuracy is *estimation bias*. If Y is an estimator for some parameter p, the estimation bias of Y is the difference between p and the expected value of Y. For example, if S is the training data used to formulate hypothesis h, then $error_S(h)$ gives an optimistically biased estimate of the true error $error_{\mathcal{D}}(h)$.
- A second cause of estimation error is *variance* in the estimate. Even with an unbiased estimator, the observed value of the estimator is likely to vary from one experiment to another. The variance σ^2 of the distribution governing the estimator characterizes how widely this estimate is likely to vary from the correct value. This variance decreases as the size of the data sample is increased.
- Comparing the relative effectiveness of two learning algorithms is an estimation problem that is relatively easy when data and time are unlimited, but more difficult when these resources are limited. One possible approach described in this chapter is to run the learning algorithms on different subsets of the available data, testing the learned hypotheses on the remaining data, then averaging the results of these experiments.
- In most cases considered here, deriving confidence intervals involves making a number of assumptions and approximations. For example, the above confidence interval for $error_{\mathcal{D}}(h)$ involved approximating a Binomial distribution by a Normal distribution, approximating the variance of this distribution, and assuming instances are generated by a fixed, unchanging probability distribution. While intervals based on such approximations are only approximate confidence intervals, they nevertheless provide useful guidance for designing and interpreting experimental results in machine learning.

The key statistical definitions presented in this chapter are summarized in Table 5.2.

An ocean of literature exists on the topic of statistical methods for estimating means and testing significance of hypotheses. While this chapter introduces the basic concepts, more detailed treatments of these issues can be found in many books and articles. Billingsley et al. (1986) provide a very readable introduction to statistics that elaborates on the issues discussed here. Other texts on statistics include DeGroot (1986); Casella and Berger (1990). Duda and Hart (1973) provide a treatment of these issues in the context of numerical pattern recognition.

Segre et al. (1991, 1996), Etzioni and Etzioni (1994), and Gordon and Segre (1996) discuss statistical significance tests for evaluating learning algorithms whose performance is measured by their ability to improve computational efficiency.

Geman et al. (1992) discuss the tradeoff involved in attempting to minimize bias and variance simultaneously. There is ongoing debate regarding the best way to learn and compare hypotheses from limited data. For example, Dietterich (1996) discusses the risks of applying the paired-difference t test repeatedly to different train-test splits of the data.

EXERCISES

5.1. Suppose you test a hypothesis h and find that it commits $r = 300$ errors on a sample S of $n = 1000$ randomly drawn test examples. What is the standard deviation in $error_S(h)$? How does this compare to the standard deviation in the example at the end of Section 5.3.4?

5.2. Consider a learned hypothesis, h, for some boolean concept. When h is tested on a set of 100 examples, it classifies 83 correctly. What is the standard deviation and the 95% confidence interval for the true error rate for $Error_{\mathcal{D}}(h)$?

5.3. Suppose hypothesis h commits $r = 10$ errors over a sample of $n = 65$ independently drawn examples. What is the 90% confidence interval (two-sided) for the true error rate? What is the 95% one-sided interval (i.e., what is the upper bound U such that $error_{\mathcal{D}}(h) \leq U$ with 95% confidence)? What is the 90% one-sided interval?

5.4. You are about to test a hypothesis h whose $error_{\mathcal{D}}(h)$ is known to be in the range between 0.2 and 0.6. What is the minimum number of examples you must collect to assure that the width of the two-sided 95% confidence interval will be smaller than 0.1?

5.5. Give general expressions for the upper and lower one-sided $N\%$ confidence intervals for the difference in errors between two hypotheses tested on different samples of data. Hint: Modify the expression given in Section 5.5.

5.6. Explain why the confidence interval estimate given in Equation (5.17) applies to estimating the quantity in Equation (5.16), and not the quantity in Equation (5.14).

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