Computational learning and discovery

CSI 873 / MATH 689

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Wednesday 7:20 - 10 pm

Evaluating Hypotheses

We need to address three basic questions:

- Given the observed accuracy of a hypothesis over a limited sample data, how well does this estimates its accuracy over additional examples?

- Given that one hypothesis outperforms another over some sample of data, how probable is it that this hypothesis is more accurate in general?

- When data is limited, what is the best way to use this data to both learn a hypothesis and estimate its accuracy?

Why these questions are challenging?

Limited samples of data might misrepresent the general distribution of data, therefore estimating true accuracy from such samples can be misleading.

Why do we need to address these questions?

We need to know how to compare accuracy of learning algorithms in order to select the best one.

Key difficulties:

- **Bias in the estimate.** The observed accuracy of the learned hypotheses over the training examples typically provide an optimistically biased estimate of the hypothesis accuracy over the future examples, especially if overfitting occurs.

- **Variance in the estimate.** The measured accuracy varies from the true accuracy because the set training example is usually smaller than the set of all possible examples.

Key idea:

We specify the probable error of using the observed accuracy of the learned hypotheses over the training examples as the hypothesis accuracy over the future examples.

Setting for the learning problem

X is some space of possible instances over which various target functions can be defined

D is the probability distribution that defines the probability of encountering each instance in X

f(x) is the target function defined on X

H is the space of all possible hypotheses

1. **Given a hypothesis h and a data sample containing n examples drawn at random according to the distribution 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 of this accuracy estimate?**

Sample Error and True Error

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 $\mathcal{D}$.

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

Sample Error and True Error

We would like to know the true error, however only the sample error is available to us!

$$\lim_{n\to\infty} error_s(h) = error_D(h)$$

We do not know have infinite number of the training or testing examples!

Therefore, we want to know how well the sample error estimates the true error!

Sample Error and True Error

Example:

Hypothesis *h* misclassifies 12 out of 40 instances in the sample *S*. What is the true error?

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

What is $error_D(h)$?

Estimators

Experiment:

1. choose sample S of size n according to distribution $\mathcal{D}$
2. measure $error_S(h)$

$error_S(h)$ is a random variable (i.e., result of an experiment)

$error_S(h)$ is an unbiased *estimator* for $error_{\mathcal{D}}(h)$

Given observed $error_S(h)$ what can we conclude about $error_{\mathcal{D}}(h)$?

Confidence intervals for Discrete-Valued Hypotheses

- the sample S contains n examples drawn independent of one another, and independent of h, according to the probability distribution $\mathcal{D}$
- $n\, error_S(h)(1 - error_S(h)) \geq 5$
- 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

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

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

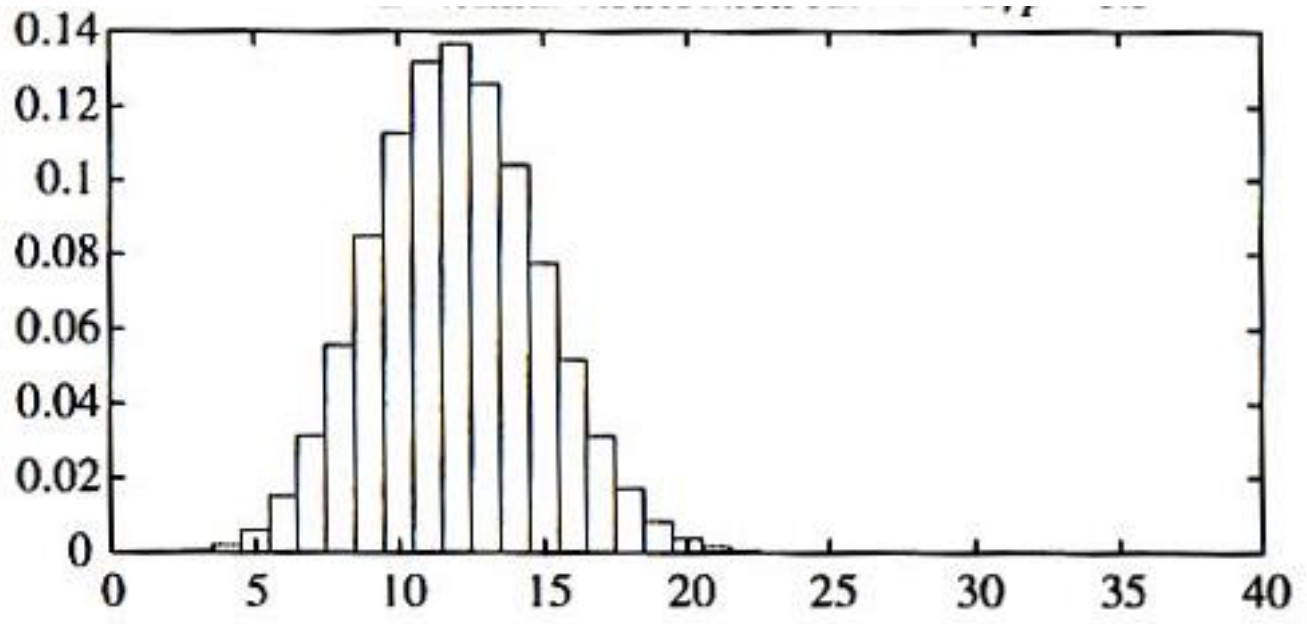
Basics of sampling theory

- 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 $N\%$.

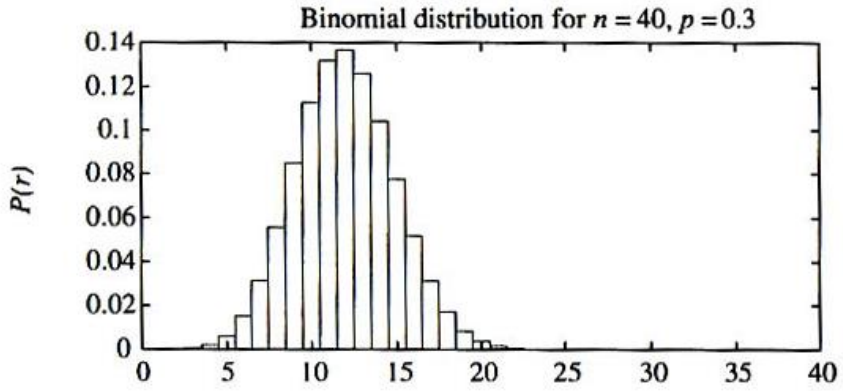
Error Estimation and Estimating Binomial Proportions

$S_i, ..., S_k$ are random samples of size n

$error_{S_1}(h), ..., error_{S_k}(h)$ are random variables



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 $P(r)$
- 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

$$\sigma_X \equiv \sqrt{E[(X - E[X])^2]} = \sqrt{np(1-p)}$$

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 $np(1-p) \geq 5$.

Normal Distribution Approximates Binomial Distribution

$error_S(h)$ follows a *Binomial* distribution, with

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

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

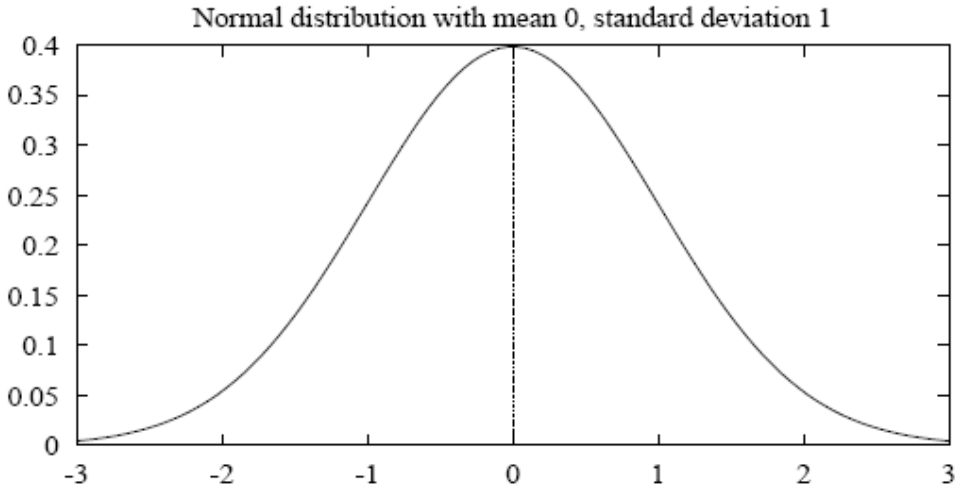
Approximate this by a *Normal* distribution with

- 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 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

$$E[X] = \mu$$

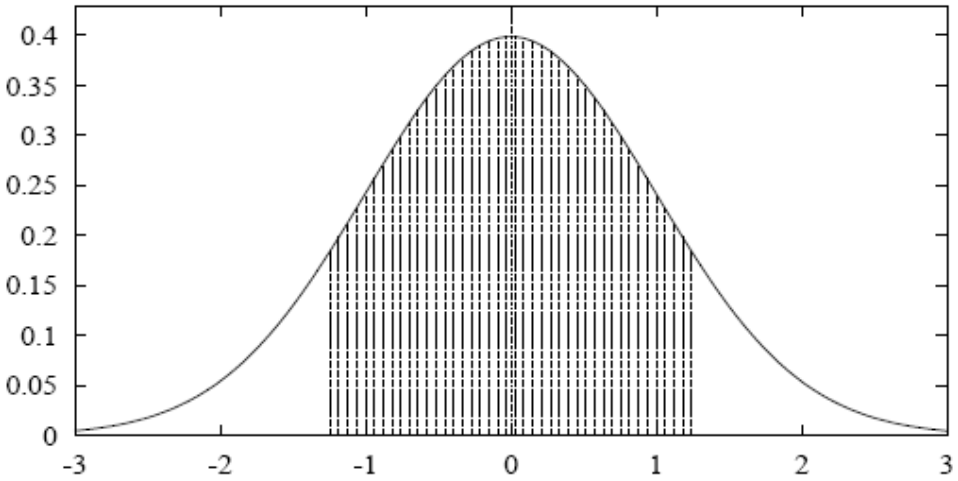
- Variance of X is

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

- Standard deviation of X, σ_X, is

$$\sigma_X = \sigma$$

Normal 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

If

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

Then

- With approximately 95% probability, $error_S(h$
  lies in interval

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

equivalently, $error_D(h)$ lies in interval

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

which is approximately

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

Central Limit Theorem

Consider a set of independent, identically distributed random variables $Y_1 \ldots Y_n$, all governed by an arbitrary probability distribution with mean 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 Interval

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 hypothesis

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

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

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

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

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

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

Paired t test to compare h_A and h_B

1. Partition data into k disjoint test sets $T_1, T_2, \ldots, T_k$ of equal size, where this size is at least 30.

2. For i from 1 to k, do

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

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

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

$N\%$ confidence interval estimate for d:

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

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

Note δ_i approximately Normally distributed

	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

Summary

- **Statistical theory provides a method for estimating the true error of a hypothesis h based on its observed error over a sample S of data.**
- **It is done using confidence intervals**
- **Estimation bias and variance are causes for errors**
- **Comparing of relative effectiveness of two learning algorithms is often done by training algorithms on different subsets of the available data, testing the learned hypothesis on the remaining data, and averaging the results of these experiments**
- **Estimation of true error involves making a number of assumptions. Be aware of them!**