Inference I & II

Hyungsuk Tak
Pennsylvania State University

What is Statistics and Why Statistics?

Statistics is a data-driven information science that helps us extract useful information from the observed data and quantify uncertainty in a principled manner. Such information can help us make decisions. It has revolutionized almost all scientific areas in the last 100 years, and has become even more important in the last 10 years due to the computational advances and the advent of the Big Data.

Short review of probability

A random variable X (r.v. hereafter) always accompanies a probability distribution that governs its random realization. That is, an *unrealized* r.v. X is *randomly realized* into a specific value x according to X's probability distribution.

A function of r.v.(s) $g(X)$ is also an r.v., and so the function of r.v.(s) has its own probability distribution.

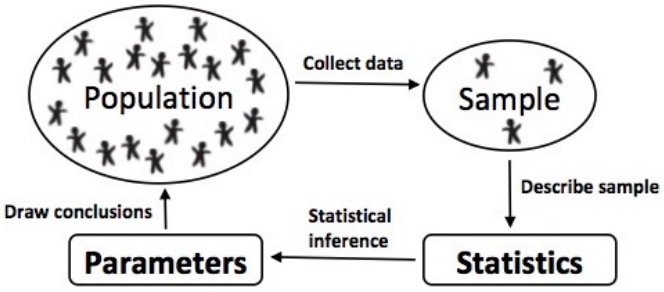
A set of parameters in a probability distribution completely determines the probability distribution, and is denoted by θ.

For example, if $X \sim \text{Normal}(0, 1)$, its realization will be between $(-1, 1)$ with 68%, between $(-2, 2)$ with 95%, and between $(-3, 3)$ with 99%. For example,

If $X \sim \text{Bernoulli}(0.1)$, only one out of ten realizations is expected to be 1. For example,

Terminology in Statistical Inference

Interested in the proportion of Earth-like exoplanets orbiting stars within 10 pc of the Sun.



- _____: The entire group of objects about which we make inferences. The population size is typically denoted by N.

- _____: A fraction of the population on which we actually collect data.

  Let's assume that the sample size is n. Then, we can denote the data (to be collected) by $X_1, X_2, \ldots, X_n$. For example,

  Statisticians treat these data as n *random variables* to model the uncertainty of the data realizations by the probability distributions of the n random variables.

  In statistical modeling, population characteristics of interest are often modeled by unknown parameter(s). For example,

  Thus, estimating the unknown parameter(s) is the main theme of statistical inference.

  For reference, is θ an unknown constant or a value that may vary (r.v.)? For example,

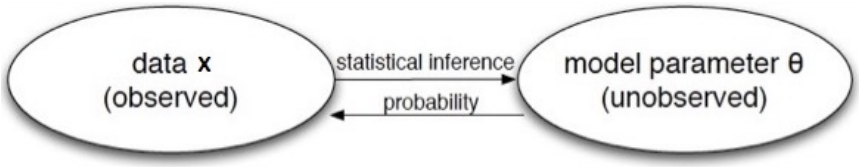
- _____: A numerical summary (i.e., a function) of the data, such as mean, median, maximum, etc.

- _____: A statistic (a function of the data) designed to infer a specific parameter. For example,

  Its realized value is called an estimate.

Probability and Statistical Inference

Probability and statistical inference are two sides of the same coin.



In probability, we have learned several families of probability distributions. For example, Bernoulli, Binomial, Poisson, Normal, Gamma, Beta, etc. These are building blocks to construct a statistical model that is a set of assumptions about *probability distributions of the data* to account for the randomness of the data realizations or data generation process.

Example: We are interested in measuring the brightness of some galaxies. The brightness of galaxy i ($i = 1, 2, \ldots, n$) is measured by a certain telescope, and we assume that it is measured around the unknown true brightness with a Gaussian measurement error (Eddington, 1913). We can express this statistical model as

$$X_i = \mu_i + \epsilon_i, \quad \text{where} \quad \epsilon_i \sim N(0,\ \sigma^2)$$

or equivalently,

$$X_i \sim N(\mu_i,\ \sigma^2).$$

Does the model represent the true data generation process? Absolutely not. But the model can be useful for understanding uncertainty involved in the brightness measurement.

"All models are wrong, but some are useful." — George Box.

In statistical inference, on the other hand, our main interest is about how to obtain the most likely values of the model parameters, $\theta = (\mu_1, \mu_2, \ldots, \mu_n, \sigma^2)$, given the model and observed data of size n, $(X_1 = x_1, \ldots, X_n = x_n)$. In this lecture, we will learn three main topics in statistical inference, i.e., point estimation, interval estimation, and hypothesis testing.

Point Estimation

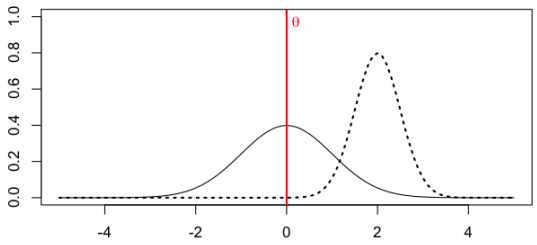
What is a *good* estimator (function of the data) for estimating θ? We first define several criteria by which we evaluate estimators. Also, just providing a point estimator $\hat{\theta}$, without any sense of its uncertainty, is usually unsatisfactory. Thus, statistical inference emphasizes accompanying point estimators with information about their uncertainties, such as standard errors (the standard deviation of an estimator is called the standard error). For example,

Throughout, suppose that we obtain data $x = (x_1, x_2, \ldots, x_n)$ under a statistical model with an unknown parameter vector $\theta = (\theta_1, \theta_2, \ldots, \theta_p)$ that indexes a family of possible distributions for x. The subscript p denotes the number of unknown parameters. For example, when x is a set of 100 realizations from $N(\mu, \sigma^2)$, $n = 100$, $\theta = \{\mu, \sigma^2\}$ and $p = 2$.

Criteria to Evaluate Point Estimators

How good is this estimate? What makes an estimate good? Can we say anything about the closeness of an estimate to an unknown parameter?

Unbiasedness: An estimator $\hat{\theta}$ is an r.v. because it is a function of the data (i.e., its value is determined by random realizations of the data). Thus it has its own probability distribution, called a sampling distribution. An estimator of a parameter θ is *unbiased* if the mean of the sampling distribution of $\hat{\theta}$ is θ, i.e., $E(\hat{\theta}) = \theta$.

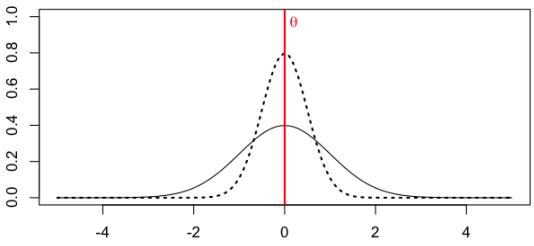


We also define the bias of $\hat{\theta}$ as

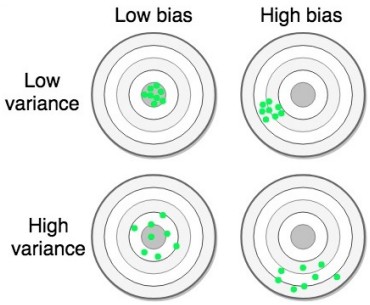
$$\text{Bias}(\hat{\theta}) = E(\hat{\theta}) - \theta.$$

If the bias is positive, then $\hat{\theta}$ tends to overestimate θ on average. On the other hand, if the bias is negative, then then $\hat{\theta}$ tends to underestimate θ on average.

Minimum variance unbiased estimator: Unbiasedness is a nice property, but unbiased estimators are not necessarily "good" estimators. We need some control over the precision of the estimator as well, and it is desirable to have estimators with small variance, $\text{Var}(\hat{\theta})$. If there are several unbiased estimators, one with the smallest variance is preferred. Such an estimator is called a minimum variance unbiased estimator (MVUE).



Mean squared error: The most popular measure of closeness between an estimator and the parameter is the mean squared error (MSE). It is a composite measure of bias and variance, defined as



It strikes a balance between the two, and thus an estimator with smaller MSE is desirable.

Maximum Likelihood Estimation

Likelihood function (R. A. Fisher, 1922) of a model $f(x \mid \theta)$ is the joint probability density or mass function of the observed data $x = \{x_1, x_2, \ldots, x_n\}$ (fixed at constants), viewed as a function of θ. For example, if $X = \{X_1, X_2, \ldots, X_n\}$ are continuous r.v.s,

$$L(\theta) = f(x \mid \theta) = f(x_1, x_2, \ldots, x_n \mid \theta) = \prod_{i=1}^{n} f(x_i \mid \theta), \text{ if independent.}$$

If the data are discrete r.v.s,

$$L(\theta) = P(X = x \mid \theta) = P(X_1 = x_1, \ldots, X_n = x_n \mid \theta) = \prod_{i=1}^{n} P(X_i = x_i \mid \theta), \text{ if independent.}$$

In this discrete case, the likelihood function is the "probability" that we observe the data $\{X = x\}$ under a model with θ. For example, let's say $L(0.8) \gg L(0.2)$. It means that the probability of observing the current data $P(X = x \mid \theta)$ is much higher when $\theta = 0.8$. So, we can say that the data are supporting $\theta = 0.8$ much more than $\theta = 0.2$. In this sense, the likelihood function can be considered as a tool to let the data speak more about which parameter value they prefer!

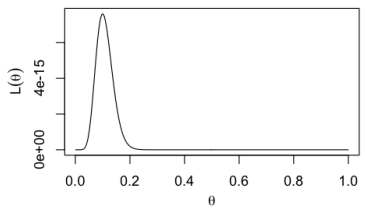
Example: We are interested in the proportion of Earth-like exoplanets orbiting stars within 10 parsecs of the Sun. We have a random sample of 100 exoplanets orbiting stars within 10 parsecs of the Sun. Our statistical model (assumption) for this problem is that there is a Bernoulli r.v. (a binary indicator) for each exoplanet taking on 1 if the exoplanet is Earth-like and 0 otherwise, i.e.,

$$X_1, X_2, \ldots, X_{100} \sim \text{Bernoulli}(\theta),$$

where $\theta \in [0, 1]$ is the true proportion we want to know about. Just for an illustration, let's say we have observed 10 Earth-like exoplanets out of 100.

The probability mass function of the Bernoulli(θ) distribution is $P(X_i = x_i) = \theta^{x_i}(1-\theta)^{1-x_i}$. Then we can derive the likelihood function of the unknown proportion θ given the observed data (100 binary values) as follows.

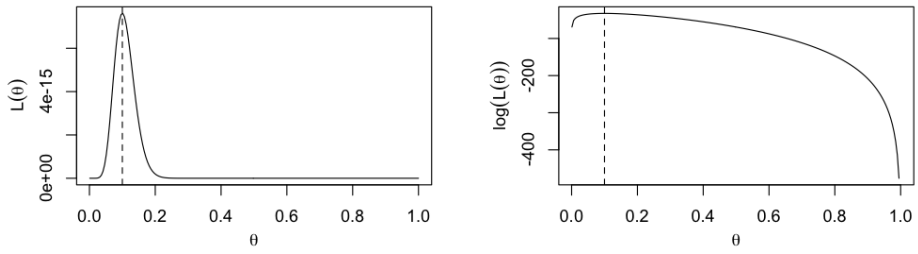
$$\begin{aligned} L(\theta) = P(X = x \mid \theta) = P(X_1 = x_1, \ldots, X_n = x_n \mid \theta) &\overset{\text{indep.}}{=} \prod_{i=1}^{n} P(X_i = x_i \mid \theta) \\ = \prod_{i=1}^{n} \theta^{x_i}(1-\theta)^{1-x_i} &= \theta^{\sum_i x_i}(1-\theta)^{n-\sum_i x_i} = \theta^{10}(1-\theta)^{90}. \end{aligned}$$



Maximum likelihood estimator: A widely used method of obtaining a point estimate for a parameter θ is to find the maximum likelihood estimate (MLE). As the name suggests, the MLE is defined as a value maximizing $L(\theta)$.

In practice, we obtain the MLE by maximizing $\ell(\theta) = \log_e(L(\theta))$ instead of maximizing $L(\theta)$ for a few reasons; (i) since $L(\theta)$ involves a multiplication when the data are independent, it is mathematically more convenient to work with the natural logarithm of the likelihood function. (Summation is easier to handle than product!); (ii) Also, the logarithmic function is strictly increasing, preserving the maximizing value, i.e., the value of θ that maximizes $\ell(\theta)$ also maximizes $L(\theta)$; (iii) lastly, when an analytic solution is not available, we need to find a numerical solution. In this case it is computationally more stable to find the value of θ that maximizes $\ell(\theta)$.

Example: In the previous example, we have obtained the likelihood function.



The value 0.4 is the most likely value of θ that might have generated the observed data because it maximizes the probability of observing the current data,

Example: The length of the cosmic ray path is modeled by an Exponential distribution with scale θ (Protheroe et al., 1981). Let X be the length of a path. Given $\theta > 0$, its probability density function is

$$f(x \mid \theta) = \frac{1}{\theta} \exp\left(-\frac{x}{\theta}\right).$$

To derive the MLE of θ given a random sample of n cosmic ray path lengths, $x_1, \ldots, x_n$, we first derive log-likelihood function:

$$L(\theta) \overset{\text{indep.}}{=} \prod_{i=1}^{n} f(x_i \mid \theta) = \frac{1}{\theta^n} \exp\left(-\frac{\sum_{i=1}^{n} x_i}{\theta}\right).$$

$$\ell(\theta) = \ln(L(\theta)) = -n \ln(\theta) - \frac{\sum_{i=1}^{n} x_i}{\theta}$$

Next we find a value (estimate) that maximizes $\ell(\theta)$:

$$\frac{d}{d\theta}\ell(\theta) = -\frac{n}{\theta} + \frac{\sum_{i=1}^{n} x_i}{\theta^2} = 0 \quad \rightarrow \quad \theta = \frac{1}{n}\sum_{i=1}^{n} x_i = \bar{x} \quad \rightarrow \quad \hat{\theta}_{\text{MLE}} = \bar{x}.$$

Thus, the maximum likelihood estimateof θ is $\hat{\theta}_{\text{MLE}} = \bar{x}$.

Example: van den Bergh (1985) considers the luminosity function for globular clusters in various galaxies, and conclude that the luminosity function for clusters in the Milky Way is adequately described by a Gaussian (Normal) distribution. Its probability density function is

$$f(x \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right),$$

where μ is the mean visual absolute magnitude and σ is the standard deviation of visual absolute magnitude.

To find the MLEs for μ & σ^2 given a sample of n globular clusters, $x_1, \ldots, x_n$, we first derive the log-likelihood function:

$$L(\mu, \sigma^2) \overset{\text{indep.}}{=} \prod_{i=1}^{n} f(x_i \mid \mu, \sigma^2) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^n \exp\left(-\frac{\sum_{i=1}^{n}(x_i-\mu)^2}{2\sigma^2}\right),$$

$$\ell(\mu, \sigma^2) = \ln(L(\mu, \sigma^2)) = -\frac{n}{2}\ln(2\pi\sigma^2) - \frac{\sum_{i=1}^{n}(x_i-\mu)^2}{2\sigma^2}.$$

Then, we find values (estimates) that maximize $\ell(\mu, \sigma^2)$:

$$\frac{\partial}{\partial\mu}\ell(\mu, \sigma^2) = \frac{\sum_{i=1}^{n}(x_i-\mu)}{\sigma^2} = 0 \quad \rightarrow \quad \hat{\mu}_{\text{MLE}} = \frac{1}{n}\sum_{i=1}^{n} x_i = \bar{x}$$

$$\frac{\partial}{\partial\sigma^2}\ell(\mu, \sigma^2) = -\frac{n}{2\sigma^2} + \frac{\sum_{i=1}^{n}(x_i-\mu)^2}{2\sigma^4} = 0 \quad \rightarrow \quad \hat{\sigma}^2_{\text{MLE}} = \frac{1}{n}\sum_{i=1}^{n}(x_i-\bar{x})^2$$

Why MLE? Asymptotic optimality of MLE: As $n \uparrow$, MLE becomes an unbiased, most efficient (smallest variance), and approximately Normally distributed estimator:

$$\hat{\theta}_{\text{MLE}} \dot{\sim} N\left(\theta,\ \hat{\sigma}^2\right).$$

As n becomes very large, no other estimator can have the mean squared error smaller than $\hat{\sigma}^2$. So for many (not all!) problems involving a large number of observations, the MLE becomes the Normally-distributed MVUE.

Limitations: The MLE is sometimes biased with the sample size is small. Also, it does not always provide a closed-form solution. In this case, algorithms for optimization, such as Newton-Raphson and Expectation-Maximization algorithms, are used.

Interval Estimation

In addition to a point estimate, we also want a margin of error around this estimate to give a sense of uncertainty around the point estimate.

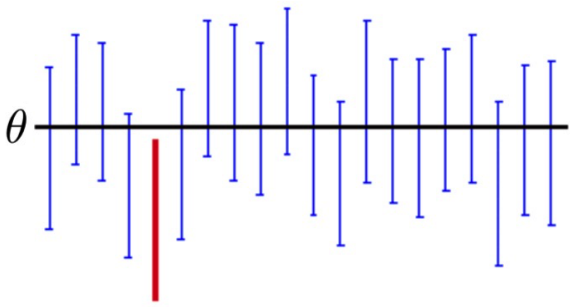
Confidence Interval

For a given value of $\alpha \in (0, 1)$ (typically $\alpha = 0.05$ in statistics and $\alpha = 0.32$ in astronomy), an $100(1 - \alpha)\%$ confidence interval of an estimator for some parameter θ is defined as an interval $(l(X),\ u(X))$ such that

This probability is taken over all possible (random) realizations of the data X for a single (fixed and unknown) value of θ. Note that it is the interval that is random, not the parameter θ. The randomness comes from which data we observe, e.g., the realization of $\bar{X}$ (i.e., $\bar{x}$). This is why we call it "a" 95% confidence interval (out of infinitely many possible intervals according to which random sample we get), not "the" 95% confidence interval.

After the data are observed $(X = x)$, we end up with a single realization of this interval $(l(x),\ u(x))$, which is also called a 95% confidence interval of θ. Once the interval is crystalized, it either covers θ or does not. Thus we cannot say that θ is in $(l(x),\ u(x))$ with 95% chance.

Instead, it actually means that if the experiment of interest (or random sampling of the data) were repeated 100 times under the same condition, computing 100 confidence intervals from the resulting 100 data sets (in the same way), then 95 confidence intervals out of 100 are expected to contain the unknown true parameter θ. That is, we would expect 95% of the intervals obtained from the repeated experiments to cover the true parameter we are estimating.



Example: In the example of the luminosity function for clusters in the Milky Way (vdB, 1985), σ is completely known as $\sigma = 1.2$ mag. Given a random sample of globular clusters, $X_1, \ldots, X_n \sim N(\mu, \sigma^2)$, what is a 95% confidence interval for μ?

From the property of the standard Normal distribution, we can say that

$$P(-1.96 < Z < 1.96) = P\left(-1.96 < \frac{\bar{X} - \mu}{\sigma/\sqrt{n}} < 1.96\right) = 0.95.$$

Next, we derive lower and upper bounds for the parameter of interest, re-arranging the inequalities inside the above probability as follows.

$$P\left(\bar{X} - 1.96\frac{\sigma}{\sqrt{n}} < \mu < \bar{X} + 1.96\frac{\sigma}{\sqrt{n}}\right) = 0.95.$$

The resulting interval is a 95% confidence interval for μ when σ is a known constant.

Example: In the vdB example, the observed data are magnitudes of 148 ($= n$) galactic globular clusters, and the average brightness is $\bar{x} = -7.1$ mag. Assuming that $\sigma = 1.2$ mag, find a 95% confidence interval for the population average brightness μ.

$$\left(-7.1 - 1.96\frac{1.2}{\sqrt{148}}, \quad -7.1 + 1.96\frac{1.2}{\sqrt{148}}\right) = (-7.29, \ -6.91).$$

If we repeated the data collection process, computing a 95% confidence interval each time, then 95% of these intervals would contain μ. The observed interval $(-7.29, \ -6.91)$ is just one of these possible intervals.

Confidence interval for μ when $X_1, \ldots, X_n \sim N(\mu, \sigma^2)$ with σ unknown

Previously, we use the following quantity to derive the confidence interval:

What if we do not know the value of σ above? *A principle in statistics is to replace any unknown quantity with its good estimator.*

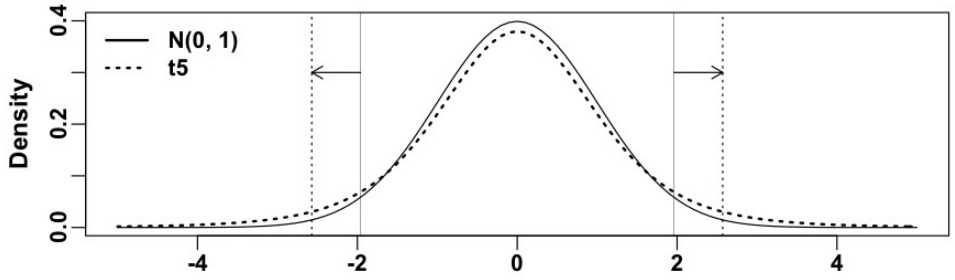
When a random sample of size n (observed data) comes from a Normally distributed population with mean μ and variance σ^2 like the vdB example, a good estimator for σ^2 is the sample variance:

$$S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2$$

If we replace σ with S, it is known that

$$T = \frac{\bar{X} - \mu}{S/\sqrt{n}} \sim t_{n-1}$$

The t_ν-distribution is heavy-tailed: For example, if $T \sim t_5$ with a sample size $n = 6$,



$$P(-1.96 < Z < 1.96) = P(-2.57 < T < 2.57) = 0.95.$$

For the same confidence level, the t_ν-distribution results in an interval wider than a Normal-based interval to account for the additional uncertainty of not knowing σ^2 (i.e., uncertainty of using an estimator S^2 for the unknown σ^2).

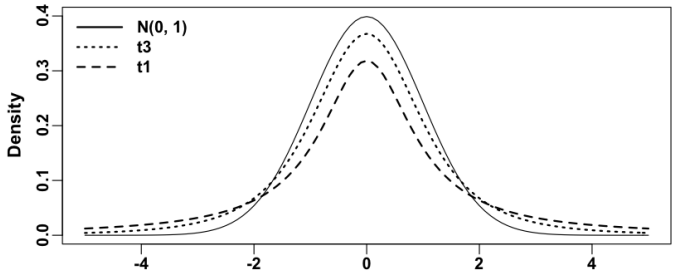
In this case, a 95% confidence interval for μ with unknown σ^2 is

$$\left(\bar{X} - 2.57\frac{S}{\sqrt{6}}, \quad \bar{X} + 2.57\frac{S}{\sqrt{6}}\right)$$

because

$$P\left(-2.57 < \frac{\bar{X}-\mu}{S/\sqrt{6}} < 2.57\right) = P\left(\bar{X} - 2.57\frac{S}{\sqrt{6}} < \mu < \bar{X} + 2.57\frac{S}{\sqrt{6}}\right) = 0.95.$$

As the sample size n increases, the t_{n-1} distribution approaches the standard Normal distribution.



Thus, if n is large (typically $n > 30$), $t_{n-1} \dot{\sim} N(0,1)$, and a 95% confidence interval for μ becomes close to

$$\left(\bar{X} - 1.96\frac{S}{\sqrt{n}}, \quad \bar{X} + 1.96\frac{S}{\sqrt{n}}\right).$$

Summary of confidence interval for μ

Let $X_1, X_n, \ldots, X_n$ be a random sample from $N(\mu, \sigma^2)$.

1. If σ^2 is known, a $100(1-\alpha)\%$ confidence interval for μ is

$$\left(\bar{X} - q_{1-\alpha/2}\frac{\sigma}{\sqrt{n}}, \quad \bar{X} + q_{1-\alpha/2}\frac{\sigma}{\sqrt{n}}\right),$$

   where $q_{1-\alpha/2}$ is a constant satisfying $P(Z < q_{1-\alpha/2}) = 1 - \alpha/2$ when $Z \sim N(0,1)$.

2. If σ^2 is unknown, a $100(1-\alpha)\%$ confidence interval for μ is

$$\left(\bar{X} - q_{1-\alpha/2}\frac{S}{\sqrt{n}}, \quad \bar{X} + q_{1-\alpha/2}\frac{S}{\sqrt{n}}\right),$$

   where $q_{1-\alpha/2}$ is a constant such that $P(T < q_{1-\alpha/2}) = 1 - \alpha/2$ when $T \sim t_{n-1}$.

3. If σ^2 is unknown and n is large ($n > 30$), a $100(1-\alpha)\%$ confidence interval for μ is

$$\left(\bar{X} - q_{1-\alpha/2}\frac{S}{\sqrt{n}}, \quad \bar{X} + q_{1-\alpha/2}\frac{S}{\sqrt{n}}\right),$$

where $q_{1-\alpha/2}$ is a constant satisfying $P(Z < q_{1-\alpha/2}) = 1 - \alpha/2$ when $Z \sim N(0,1)$.

Hypothesis Testing

Estimation is about pinning down the underlying values of unknown parameters from a potentially large number of possibilities with plausible ranges of parameter values. On the other hand, hypothesis testing asks the following: Given two hypotheses about the parameter value, which one do the data support more?

Motivation and Terminology

The average brightness of the M31 globular clusters, denoted by μ, is known to be -7.7 magnitude. Tak feels that the brightness may not be -7.7 magnitude, and so he collects a random sample from M31 to check whether the data are consistent to his feeling. The question is

"Are the data strongly in support of Tak's claim that $\mu \neq -7.7$ magnitude?"

Statistical hypothesis (or hypothesis) is a statement about parameter(s) θ of a population.

Null vs alternative: The null hypothesis H_0 indicates status quo (default or baseline case), and the alternative hypothesis H_a represents what a researcher wants to argue.

Simple vs composite: Simple hypotheses are hypotheses where θ can only take on a single value, e.g., $H_0 : \theta = 0$ or $H_a : \theta = 3$. Composite hypotheses are hypotheses where θ can take on multiple or a range of values, e.g., $H_0 : \theta \leq 0$ or $H_a : \theta \in \{1, 2, 3\}$. In a particular problem, null and alternative hypotheses can have any combination of simple and composite hypotheses.

One-sided vs two-sided: If an alternative hypothesis is composite and represent one-side of the parameter space around some value c, we call this a one-sided test. For example,

$$\begin{aligned}
H_0 &: \theta \leq c \quad \text{vs} \quad H_a : \theta > c \\
H_0 &: \theta = c \quad \text{vs} \quad H_a : \theta > c \\
H_0 &: \theta \geq c \quad \text{vs} \quad H_a : \theta < c \\
H_0 &: \theta = c \quad \text{vs} \quad H_a : \theta > c
\end{aligned}$$

If H_0 is a simple hypothesis and H_a represents the rest of the parameter space of θ, we call this a two-sided test. For instance,

$$H_0 : \mu = -7.7 \quad \text{vs} \quad H_a : \mu \neq -7.7$$

Test statistic and rejection region: Let $X_1, \ldots, X_n$ be a random sample from a distribution with parameter θ. Let $T = h(X_1, \ldots, X_n)$ be a statistic (a function of the data, but not of a parameter) and let R be a subset of the real line. For a specific set of hypotheses (H_0 vs H_a) in a testing problem, suppose we choose to "*reject* H_0 *if* $T \in R$". Then T is called a test statistic and R is called the critical region or rejection region of the test.

Likelihood Ratio Test

Now, we learn the most fundamental theoretical background of hypothesis testing. Let's consider the simplest situation where we test two simple hypotheses:

$$H_0 : \theta = \theta_0 \quad \text{vs} \quad H_a : \theta = \theta_1$$

(Each of θ_0 and θ_1 is a value in the parameter space Ω). We make a choice between these two possibilities based on the data we observe. Let us consider this as a binary decision problem—reject or do not reject H_0.

A test (or equivalently a decision rule) for choosing one of the two hypotheses based on the data, can be specified by the rejection region R:

$$\begin{aligned} &\text{If } X \in R, \text{ then we reject } H_0 \\ &\text{If } X \notin R, \text{ then we cannot reject } H_0 \end{aligned}$$

So constructing a test boils down to choosing the corresponding rejection region R, i.e., choosing the data values corresponding to each decision.

The question is "How do we choose the rejection region R?" It turns out that there is a general procedure with which one can construct good tests. The idea is related to the maximum likelihood principle we have used for the estimation problem. Let's start with the testing of simple vs simple hypothesis above.

Comparing likelihoods: How about comparing the likelihoods under the two hypotheses? Then, we can choose a hypothesis with the higher likelihood (i.e., a hypothesis that the data support more). That is

The "best" (and optimal) hypothesis testing is very much along this line!

Likelihood ratio test statistic $L(\theta_1)/L(\theta_0)$ measures the relative evidence from the data under the two hypotheses. A rejection region based on this statistic is

A test with a rejection region of this form is called a *likelihood ratio test*. Although the above rejection region appears mysterious at first glance, it is always simplified to an inequality with respect to a test statistic (a function of an MLE in the end), for example, $R = \{x : T(x) > c'\}$, $R = \{x : T(x) < c'\}$, etc. It turns out that likelihood tests are the "best" tests under certain criteria. Let's first check which test is a good test and why the likelihood ratio test is the best.

What is a "good" test? Let us describe our testing problem as making a choice between

$$H_0 : \theta = \theta_0 \quad \text{versus} \quad H_a : \theta = \theta_1.$$

Intuitively, a test is "good" if

when H_0 is true, we are *less likely* to reject H_0, and
when H_0 is false, we are *more likely* to reject H_0.

Two kinds of error: Correspondingly, there are two types of errors that one can make:

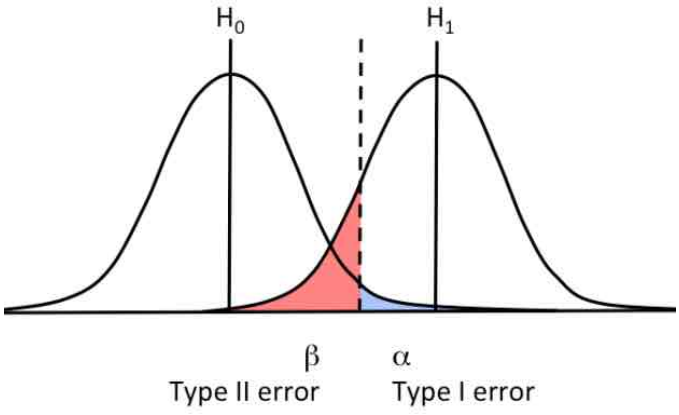
Type I error: Reject H_0 when H_0 is true.
Type II error: Do not reject H_0 when H_a is true.

In addition, we can define two quantities

$$\text{Type I error rate} = \alpha = P(\text{Reject } H_0 \mid H_0 \text{ is true})$$
$$\text{Type II error rate} = \beta = P(\text{Do not reject } H_0 \mid H_a \text{ is true})$$

Using the characterization of tests by rejection regions

$$\alpha = P(\text{Data } X \text{ are in the rejection region } R \mid H_0) = P(X \in R \mid H_0)$$
$$\beta = P(\text{Data } X \text{ are not in the rejection region } R \mid H_a) = P(X \notin R \mid H_a)$$



Example: When searching for a faint signal from a noisy background, we may want to test the following hypotheses

$$H_0 : \text{Signal does not exist} \quad \text{vs} \quad H_a : \text{Signal exists}$$

_____ occurs when we incorrectly conclude that a signal is present although it truly is not.

How do the error rates change with the size of the rejection region R? If R is large, the data X are _____ likely to be in R. That means, α is _____ and β is _____, if R is large. If R is small, the data X are _____ likely to be in R, resulting in _____ α and _____ β.

Ideally we want both α and β to be small, even both to be zero. However this is not possible because α and β move in the opposite direction according to the size of R.

Since we cannot make both zero, we must strike a balance. A common strategy is to specify a permissible level for one of the two types of errors, most often for the Type I error α. Then given that level for α, we find a test that attains the best level for the other, by custom β.

Neyman-Pearson Lemma: In the problem of testing simple hypotheses

$$H_0 : \theta = \theta_0 \ (X \text{ has distribution } f(x \mid \theta_0)) \ \text{ vs } \ H_a : \theta = \theta_1 \ (X \text{ has distribution } f(x \mid \theta_1)),$$

given a Type I error rate α, no test with the same or lower α has a lower Type II error rate β than the likelihood ratio test. Simply speaking, the Lemma says that the *likelihood ratio test* is the most powerful test for this purpose.

What if we test one-sided hypotheses? It turns out that the likelihood ratio test is *still the most powerful test*. For two-sided tests, however, there does not exist a single test that performs uniformly the best in the Neyman-Pearson sense. In this case, generalized likelihood ratio tests are used to find a test that satisfies some restrictions on the Type I error rate α, while performing *reasonably* well in terms of Type II error rate β. Essentially all testing procedures, specified and summarized in most statistical inference books, are likelihood ratio tests or generalized likelihood ratio tests.

Likelihood Ratio Test via MLE

In the likelihood ratio test, the MLE for the parameter being tested or a function of the MLE (typically a standardized form under H_0) is used as a test statistic T. For example, $\bar{X}$ for testing some value of μ in a Normal case, $\hat{p}$ $(= \bar{X})$ for testing values of p in a Bernoulli or Binomial case, and $\hat{\lambda}$ $(= \bar{X})$ for testing values of λ in a Poisson case. A rejection region is usually in the form of $T \geq c$, $T \leq c$, or $|T| \geq c$. The direction of the inequality is set by the direction of H_a.

Example: Find the rejection region (in particular, direction) when the null hypothesis is $H_0 : \theta = \theta_0$, and the alternative is $H_a : \theta > \theta_0, H_a : \theta < \theta_0$ or $H_a : \theta \neq \theta_0$

Example: One of the most popular likelihood ratio tests is a t-test. In the example of luminosity function for clusters in the Milky Way (vdB), a random sample of 148 measurements has sample mean $\bar{x} = -7.5$ and sample variance $s^2 = 1.1^2$. From the data, Tak feels that $\mu\ (= M_0) \neq -7.7$ mag. We want to test it at the significant level $\alpha = 0.05$.

1. Specify the null and alternative hypotheses:

$$H_0 : \mu = -7.7 \text{ mag} \quad \text{vs} \quad H_a : \mu \neq -7.7 \text{ mag}.$$

2. Set up a test statistic for μ under H_0:

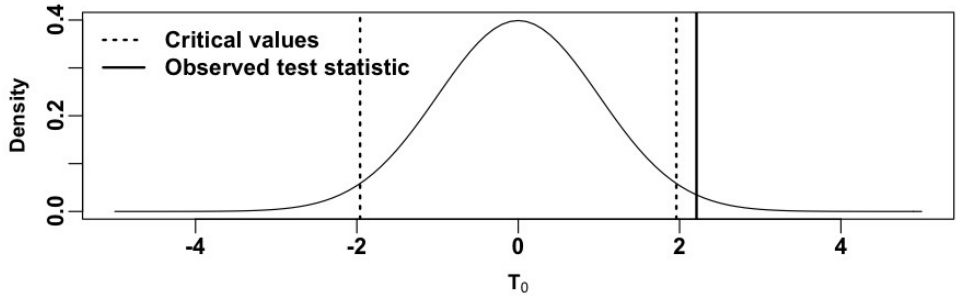
3. Find the distribution of the test statistic under the null: As the data size is large,

$$T = \frac{\bar{X} - \mu_0}{S/\sqrt{n}}$$

4. Set up the rejection rule: Reject H_0 if $|T| > 1.96$. Otherwise, we fail to reject H_0.

5. Calculate the value of the test statistic using the observed data.

$$\frac{\bar{x} - \mu_0}{s/\sqrt{n}} = \frac{-7.5 + 7.7}{1.1/\sqrt{148}} = 2.21.$$



6. We reject the null hypothesis H_0 because the calculated value of the test statistic lies in the rejection region. We report that there is a statistically significant difference between the population mean and the hypothesized value $\mu_0 = -7.7$ mag.

There are two other popular ways to conduct the same hypothesis testing.

Hypothesis testing via confidence interval: A test of level α for a parameter θ can be done by deriving a $100(1-\alpha)\%$ confidence interval for θ. We reject the null if the interval does not contain the hypothesized value of θ under the null (i.e., θ_0) because it is a rare event ($100\alpha\%$) if the null is true.

In the previous example, we have derived a 95% confidence interval for μ and we can use this to conduct the same hypothesis testing. Since n is large enough,

$$\left(\bar{x} - 1.96\frac{s}{\sqrt{n}}, \quad \bar{x} + 1.96\frac{s}{\sqrt{n}}\right) = (-7.68, \quad -7.32)\,.$$

This 95% confidence interval for μ _____ contain the hypothesized value under the null hypothesis, i.e., $\mu_0 = -7.7$, and thus at the 5% significance level we _____ H_0.

Hypothesis testing via p-value: Compute the p-value, i.e., the probability of observing the current test statistic or a more extreme one (in the direction of the alternative) given that H_0 is correct. If H_a is two-sided,

$$p\text{-value} = P\left(T > \frac{|\bar{x}-\mu_0|}{s/\sqrt{n}} \text{ or } T < -\frac{|\bar{x}-\mu_0|}{s/\sqrt{n}} \;\middle|\; H_0\right) = 2P\left(T > \frac{|\bar{x}-\mu_0|}{s/\sqrt{n}} \;\middle|\; H_0\right).$$

For instance, the p-value in the vdB example is $2P(T > 2.21 \mid H_0) = 0.03$ that is _____ than the significance level 0.05. Thus, at the 5% significant level, there is enough evidence in data to _____ H_0.

Note that the p-value is not the probability of H_0 being correct (the most common misunderstanding!).

Model Comparison via Information Criteria

Penalized likelihood approaches have dominated model selection since the 1980s due to several limitations of the likelihood ratio test.

1. The likelihood ratio test is only applicable to nested models (i.e., one is a special case of the other larger model).
2. Let's say a model M_1 is nested within another model M_2. The largest likelihood achievable by M_2 will always be larger than that achievable by M_1 even when M_1 is the true model. This is because M_2 has more parameters (enabling M_2 to explain the data more elaborately).

If a penalty is applied to compensate for the difference in likelihoods due to the different number of parameters in M_1 and M_2, the desired balance between overfitting and underfitting can be found.

Akaike information criterion (AIC, 1973) is defined as

$$\text{AIC} = -2\ell(\hat{\theta}) + 2p = (\text{goodness-of-fit}) + (\text{penalty}),$$

where $\ell(\hat{\theta})$ is the maximized log likelihood (evaluated at the MLE $\hat{\theta}$) and p is the number of parameters in a model.

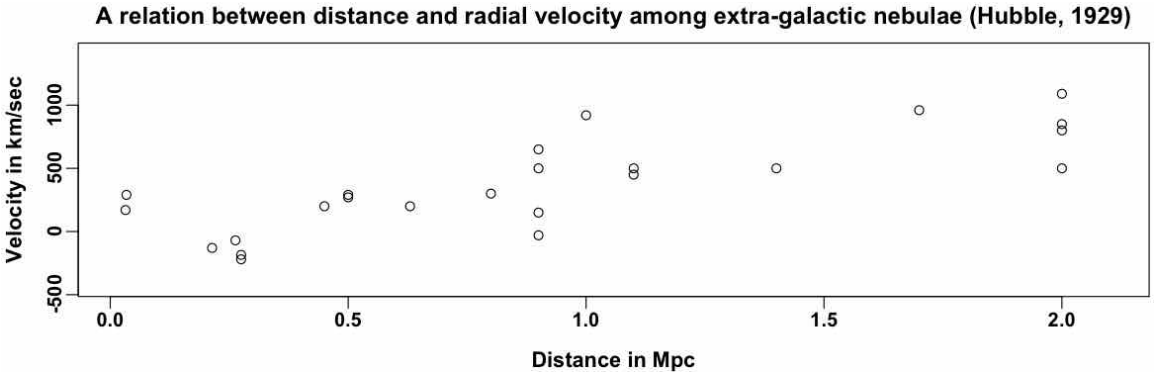
The penalty term, $2p$, increases as the complexity of the model grows, and thus compensates for the necessary increase in the likelihood. A model with the 'smallest' AIC, i.e., a model that explains the data well with a small number of parameters, is preferred.

Bayesian information criterion weights the penalty according to the data size n.

$$\text{BIC} = -2\ell(\hat{\theta}) + p\log(n)$$

As we collect more data, the penalty on an additional parameter becomes stronger than that of AIC. Thus, when n is large, BIC prefers even more parsimonious models than AIC does.

Example: Let's compare the following four models on the original data of Hubble (1929).



Let y denote the velocity and x denote the distance.

Model 1: $y_i = \alpha + \beta x_i + \epsilon_i, \quad \epsilon \sim N(0, \sigma^2)$.
Model 2: $y_i = \alpha + \epsilon_i, \quad \epsilon \sim N(0, \sigma^2)$.
Model 3: $y_i = \beta x_i + \epsilon_i, \quad \epsilon \sim N(0, \sigma^2)$.
Model 4: $y_i = \epsilon_i, \quad \epsilon \sim N(0, \sigma^2)$.

The AIC and BIC are computed for each model as follows.

	Model 1	Model 2	Model 3	Model 4
AIC	333.65	355.10	**331.91**	370.37
BIC	337.19	357.45	**334.27**	371.55

The data prefer Model 3 (no intercept α) in a sense that both AIC and BIC are the smallest under Model 3. This is consistent to the Hubble's reasoning:

$$\text{Velocity} = \beta \times \text{Distance} = H_0 \times \text{Distance}$$