Maximum Likelihood Estimates
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Jeremy Orloff and Jonathan Bloom

1 Learning Goals

1. Be able to define the likelihood function for a parametric model given data.

2. Be able to compute the maximum likelihood estimate of unknown parameter(s).

2 Introduction

Suppose we know we have data consisting of values $x_1, \dots, x_n$ drawn from an exponential distribution. The question remains: which exponential distribution?!

We have casually referred to *the* exponential distribution or *the* binomial distribution or *the* normal distribution. In fact the exponential distribution $\exp(\lambda)$ is not a single distribution but rather a one-parameter family of distributions. Each value of λ defines a different distribution in the family, with pdf $f_\lambda(x) = \lambda e^{-\lambda x}$ on $[0, \infty)$. Similarly, a binomial distribution $\text{bin}(n, p)$ is determined by the two parameters n and p, and a normal distribution $N(\mu, \sigma^2)$ is determined by the two parameters μ and σ^2 (or equivalently, μ and σ). Parameterized families of distributions are often called parametric distributions or parametric models.

We are often faced with the situation of having random data which we know (or believe) is drawn from a parametric model, whose parameters we do not know. For example, in an election between two candidates, polling data constitutes draws from a Bernoulli(p) distribution with unknown parameter p. In this case we would like to use the data to estimate the value of the parameter p, as the latter predicts the result of the election. Similarly, assuming gestational length follows a normal distribution, we would like to use the data of the gestational lengths from a random sample of pregnancies to draw inferences about the values of the parameters μ and σ^2.

Our focus so far has been on computing the probability of data arising from a parametric model with known parameters. Statistical inference flips this on its head: we will estimate the probability of parameters given a parametric model and observed data drawn from it. In the coming weeks we will see how parameter values are naturally viewed as hypotheses, so we are in fact estimating the probability of various hypotheses given the data.

3 Maximum Likelihood Estimates

There are many methods for estimating unknown parameters from data. We will first consider the maximum likelihood estimate (MLE), which answers the question:

> For which parameter value does the observed data have the biggest probability?

The MLE is an example of a point estimate because it gives a single value for the unknown parameter (later our estimates will involve intervals and probabilities). Two advantages of the MLE are that it is often easy to compute and that it agrees with our intuition in simple examples. We will explain the MLE through a series of examples.

Example 1. A coin is flipped 100 times. Given that there were 55 heads, find the maximum likelihood estimate for the probability p of heads on a single toss.

Before actually solving the problem, let's establish some notation and terms.

We can think of counting the number of heads in 100 tosses as an experiment. For a given value of p, the probability of getting 55 heads in this experiment is the binomial probability

$$P(55 \text{ heads}) = \binom{100}{55} p^{55}(1-p)^{45}.$$

The probability of getting 55 heads depends on the value of p, so let's include p in by using the notation of conditional probability:

$$P(55 \text{ heads} \mid p) = \binom{100}{55} p^{55}(1-p)^{45}.$$

You should read $P(55 \text{ heads} \mid p)$ as:

'the probability of 55 heads given p,'

or more precisely as

'the probability of 55 heads given that the probability of heads on a single toss is p.'

Here are some standard terms we will use as we do statistics.

- Experiment: Flip the coin 100 times and count the number of heads.
- Data: The data is the result of the experiment. In this case it is '55 heads'.
- Parameter(s) of interest: We are interested in the value of the unknown parameter p.
- Likelihood, or likelihood function: this is $P(\text{data} \mid p)$. Note it is a function of both the data and the parameter p. In this case the likelihood is

$$P(55 \text{ heads} \mid p) = \binom{100}{55} p^{55}(1-p)^{45}.$$

Notes: **1.** The likelihood $P(\text{data} \mid p)$ changes as the parameter of interest p changes.

2. Look carefully at the definition. One typical source of confusion is to mistake the likelihood $P(\text{data} \mid p)$ for $P(p \mid \text{data})$. We know from our earlier work with Bayes' theorem that $P(\text{data} \mid p)$ and $P(p \mid \text{data})$ are usually very different.

Definition: Given data the maximum likelihood estimate (MLE) for the parameter p is the value of p that maximizes the likelihood $P(\text{data} \mid p)$. That is, the MLE is the value of p for which the data is most likely.

Solution: For the problem at hand, we saw above that the likelihood

$$P(55 \text{ heads} \mid p) = \binom{100}{55} p^{55}(1-p)^{45}.$$

We'll use the notation $\hat{p}$ for the MLE. We use calculus to find it by taking the derivative of the likelihood function and setting it to 0.

$$\frac{d}{dp}P(\text{data }|p) = \binom{100}{55}(55p^{54}(1-p)^{45} - 45p^{55}(1-p)^{44}) = 0.$$

Solving this for p we get

$$\begin{aligned}
&55p^{54}(1-p)^{45} = 45p^{55}(1-p)^{44} \\
&55(1-p) = 45p \\
&55 = 100p \\
&\text{the MLE is } \hat{p} = 0.55
\end{aligned}$$

Note: **1.** The MLE for p turned out to be exactly the fraction of heads we saw in our data.

2. The MLE is computed from the data. That is, it is a statistic.

3. Officially we need to check that this critical point is actually the maximum. We could use the second derivative test. Another way is to notice that we are interested only in $0 \le p \le 1$; that the probability is bigger than zero for $0 < p < 1$; and that the probability is equal to zero for $p = 0$ and for $p = 1$. From these facts it follows that the critical point must be the unique maximum.

3.1 Log likelihood

If is often easier to work with the natural log of the likelihood function. For short this is simply called the log likelihood. Since $\ln(x)$ is an increasing function, the maxima of the likelihood and log likelihood coincide.

Example 2. Redo the previous example using log likelihood.

Solution: We had the likelihood $P(55 \text{ heads} \,|\, p) = \binom{100}{55}p^{55}(1-p)^{45}$. Therefore the log likelihood is

$$\ln(P(55 \text{ heads} \,|\, p) = \ln\left(\binom{100}{55}\right) + 55\ln(p) + 45\ln(1-p).$$

Maximizing likelihood is the same as maximizing log likelihood. We check that calculus gives us the same answer as before:

$$\begin{aligned}
\frac{d}{dp}(\text{log likelihood}) &= \frac{d}{dp}\left[\ln\left(\binom{100}{55}\right) + 55\ln(p) + 45\ln(1-p)\right] \\
&= \frac{55}{p} - \frac{45}{1-p} = 0 \\
&\Rightarrow 55(1-p) = 45p \\
&\Rightarrow \hat{p} = 0.55
\end{aligned}$$

3.2 Maximum likelihood for continuous distributions

For continuous distributions, we use the probability density function to define the likelihood. We show this in a few examples. In the next section we explain how this is analogous to what we did in the discrete case.

Example 3. Light bulbs
Suppose that the lifetime of *Badger* brand light bulbs is modeled by an exponential distribution with (unknown) parameter λ. We test 5 bulbs and find they have lifetimes of 2, 3, 1, 3, and 4 years, respectively. What is the MLE for λ?

Solution: We need to be careful with our notation. With five different values it is best to use subscripts. Let X_i be the lifetime of the i^{th} bulb and let x_i be the value X_i takes. Then each X_i has pdf $f_{X_i}(x_i) = \lambda e^{-\lambda x_i}$. We assume the lifetimes of the bulbs are independent, so the joint pdf is the product of the individual densities:

$$f(x_1, x_2, x_3, x_4, x_5 \,|\, \lambda) = (\lambda e^{-\lambda x_1})(\lambda e^{-\lambda x_2})(\lambda e^{-\lambda x_3})(\lambda e^{-\lambda x_4})(\lambda e^{-\lambda x_5}) = \lambda^5 e^{-\lambda(x_1+x_2+x_3+x_4+x_5)}.$$

Note that we write this as a conditional density, since it depends on λ. Viewing the data as fixed and λ as variable, this density is the likelihood function. Our data had values

$$x_1 = 2,\ x_2 = 3,\ x_3 = 1,\ x_4 = 3,\ x_5 = 4.$$

So the likelihood and log likelihood functions with this data are

$$f(2,3,1,3,4 \,|\, \lambda) = \lambda^5 e^{-13\lambda}, \quad \ln(f(2,3,1,3,4 \,|\, \lambda) = 5\ln(\lambda) - 13\lambda$$

Finally we use calculus to find the MLE:

$$\frac{d}{d\lambda}(\text{log likelihood}) = \frac{5}{\lambda} - 13 = 0 \ \Rightarrow \ \boxed{\hat{\lambda} = \frac{5}{13}}.$$

Note: **1.** In this example we used an uppercase letter for a random variable and the corresponding lowercase letter for the value it takes. This will be our usual practice.

2. The MLE for λ turned out to be the reciprocal of the sample mean $\bar{x}$, so $X \sim \exp(\hat{\lambda})$ satisfies $E[X] = \bar{x}$.

The following example illustrates how we can use the method of maximum likelihood to estimate multiple parameters at once.

Example 4. Normal distributions
Suppose the data $x_1, x_2, \ldots, x_n$ is drawn from a $\mathrm{N}(\mu, \sigma^2)$ distribution, where μ and σ are unknown. Find the maximum likelihood estimate for the pair (μ, σ^2).

Solution: Let's be precise and phrase this in terms of random variables and densities. Let uppercase $X_1, \ldots, X_n$ be i.i.d. $\mathrm{N}(\mu, \sigma^2)$ random variables, and let lowercase x_i be the value X_i takes. The density for each X_i is

$$f_{X_i}(x_i) = \frac{1}{\sqrt{2\pi}\,\sigma} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}.$$

Since the X_i are independent their joint pdf is the product of the individual pdf's:

$$f(x_1, \ldots, x_n \,|\, \mu, \sigma) = \left(\frac{1}{\sqrt{2\pi}\,\sigma}\right)^n e^{-\sum_{i=1}^n \frac{(x_i-\mu)^2}{2\sigma^2}}.$$

For the fixed data $x_1, \dots, x_n$, the likelihood and log likelihood are

$$f(x_1, \dots, x_n|\mu, \sigma) = \left(\frac{1}{\sqrt{2\pi}\,\sigma}\right)^n \mathrm{e}^{-\sum_{i=1}^n \frac{(x_i-\mu)^2}{2\sigma^2}}, \quad \ln(f(x_1, \dots, x_n|\mu, \sigma)) = -n\ln(\sqrt{2\pi}) - n\ln(\sigma) - \sum_{i=1}^n \frac{(x_i-\mu)^2}{2\sigma^2}.$$

Since $\ln(f(x_1, \dots, x_n|\mu, \sigma))$ is a function of the two variables μ, σ we use partial derivatives to find the MLE. The easy value to find is $\hat{\mu}$:

$$\frac{\partial f(x_1, \dots, x_n|\mu, \sigma)}{\partial \mu} = \sum_{i=1}^n \frac{(x_i-\mu)}{\sigma^2} = 0 \;\Rightarrow\; \sum_{i=1}^n x_i = n\mu \;\Rightarrow\; \hat{\mu} = \frac{\sum_{i=1}^n x_i}{n} = \overline{x}.$$

To find $\hat{\sigma}$ we differentiate and solve for σ:

$$\frac{\partial f(x_1, \dots, x_n|\mu, \sigma)}{\partial \sigma} = -\frac{n}{\sigma} + \sum_{i=1}^n \frac{(x_i-\mu)^2}{\sigma^3} = 0 \;\Rightarrow\; \hat{\sigma}^2 = \frac{\sum_{i=1}^n (x_i-\mu)^2}{n}.$$

We already know $\hat{\mu} = \overline{x}$, so we use that as the value for μ in the formula for $\hat{\sigma}$. We get the maximum likelihood estimates

$$\begin{aligned} \hat{\mu} &= \overline{x} && = \text{the mean of the data} \\ \hat{\sigma}^2 &= \sum_{i=1}^n \frac{1}{n}(x_i - \hat{\mu})^2 = \sum_{i=1}^n \frac{1}{n}(x_i - \overline{x})^2 && = \text{the unadjusted variance of the data.} \end{aligned}$$

(Later we will learn that the sample variance is $\dfrac{\sum_{i=1}^n (x_i - \hat{\mu})^2}{n-1}$.)

Example 5. Uniform distributions
Suppose our data $x_1, \dots x_n$ are independently drawn from a uniform distribution $U(a, b)$. Find the MLE for a and b.

Solution: This example is different from the previous ones in that we won't use calculus to find the MLE. The density for $U(a, b)$ is $\frac{1}{b-a}$ on $[a, b]$. Therefore our likelihood function is

$$f(x_1, \dots, x_n \,|\, a, b) = \begin{cases} \left(\frac{1}{b-a}\right)^n & \text{if all } x_i \text{ are in the interval } [a, b] \\ 0 & \text{otherwise.} \end{cases}$$

This is maximized by making $b - a$ as small as possible. The only restriction is that the interval $[a, b]$ must include all the data. Thus the MLE for the pair (a, b) is

$$\hat{a} = \min(x_1, \dots, x_n) \qquad \hat{b} = \max(x_1, \dots, x_n).$$

Example 6. Capture/recapture method

The capture/recapture method is a way to estimate the size of a population in the wild. The method assumes that each animal in the population is equally likely to be captured by a trap.

Suppose 10 animals are captured, tagged and released. A few months later, 20 animals are captured, examined, and released. 4 of these 20 are found to be tagged. Estimate the size of the wild population using the MLE for the probability that a wild animal is tagged.

Solution: Our unknown parameter n is the number of animals in the wild. Our data is that 4 out of 20 recaptured animals were tagged (and that there are 10 tagged animals). The likelihood function is

$$P(\text{data} \mid n \text{ animals}) = \frac{\binom{n-10}{16}\binom{10}{4}}{\binom{n}{20}}$$

(The numerator is the number of ways to choose 16 animals from among the $n-10$ untagged ones times the number of was to choose 4 out of the 10 tagged animals. The denominator is the number of ways to choose 20 animals from the entire population of n.) We can use R to compute that the likelihood function is maximized when $n = 50$. This should make some sense. It says our best estimate is that the fraction of all animals that are tagged is 10/50 which equals the fraction of recaptured animals which are tagged.

Example 7. Hardy-Weinberg. Suppose that a particular gene occurs as one of two alleles (A and a), where allele A has frequency θ in the population. That is, a random copy of the gene is A with probability θ and a with probability $1-\theta$. Since a diploid genotype consists of two genes, the probability of each genotype is given by:

genotype	AA	Aa	aa
probability	θ^2	$2\theta(1-\theta)$	$(1-\theta)^2$

Suppose we test a random sample of people and find that k_1 are AA, k_2 are Aa, and k_3 are aa. Find the MLE of θ.

Solution: The likelihood function is given by

$$P(k_1, k_2, k_3 \mid \theta) = \binom{k_1+k_2+k_3}{k_1}\binom{k_2+k_3}{k_2}\binom{k_3}{k_3}\theta^{2k_1}(2\theta(1-\theta))^{k_2}(1-\theta)^{2k_3}.$$

So the log likelihood is given by

$$\text{constant} + 2k_1\ln(\theta) + k_2\ln(\theta) + k_2\ln(1-\theta) + 2k_3\ln(1-\theta)$$

We set the derivative equal to zero:

$$\frac{2k_1+k_2}{\theta} - \frac{k_2+2k_3}{1-\theta} = 0$$

Solving for θ, we find the MLE is

$$\hat{\theta} = \frac{2k_1+k_2}{2k_1+2k_2+2k_3},$$

which is simply the fraction of A alleles among all the genes in the sampled population.

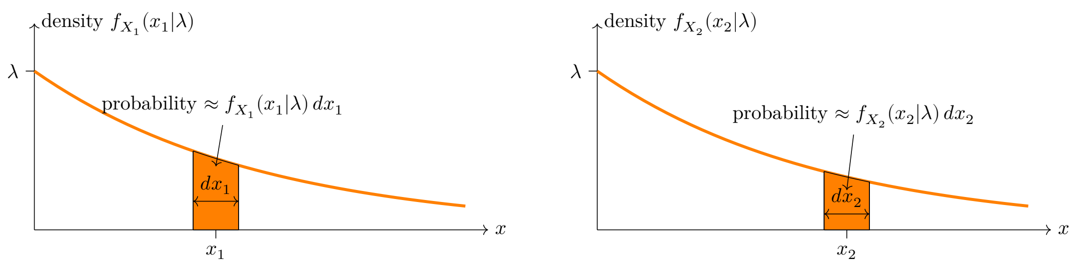
4 Why we use the density to find the MLE for continuous distributions

The idea for the maximum likelihood estimate is to find the value of the parameter(s) for which the data has the highest probability. In this section we 'll see that we're doing this is really what we are doing with the densities. We will do this by considering a smaller version of the light bulb example.

Example 8. Suppose we have two light bulbs whose lifetimes follow an exponential(λ) distribution. Suppose also that we independently measure their lifetimes and get data $x_1 = 2$ years and $x_2 = 3$ years. Find the value of λ that maximizes the probability of this data.

Solution: The main paradox to deal with is that for a continuous distribution the probability of a single value, say $x_1 = 2$, is zero. We resolve this paradox by remembering that a single measurement really means a range of values, e.g. in this example we might check the light bulb once a day. So the data $x_1 = 2$ years really means x_1 is somewhere in a range of 1 day around 2 years.

If the range is small we call it dx_1. The probability that X_1 is in the range is approximated by $f_{X_1}(x_1|\lambda)\,dx_1$. This is illustrated in the figure below. The data value x_2 is treated in exactly the same way.



The usual relationship between density and probability for small ranges.

Since the data is collected independently the joint probability is the product of the individual probabilities. Stated carefully

$$P(X_1 \text{ in range}, X_2 \text{ in range}|\lambda) \approx f_{X_1}(x_1|\lambda)\,dx_1 \cdot f_{X_2}(x_2|\lambda)\,dx_2$$

Finally, using the values $x_1 = 2$ and $x_2 = 3$ and the formula for an exponential pdf we have

$$P(X_1 \text{ in range}, X_2 \text{ in range}|\lambda) \approx \lambda e^{-2\lambda}\,dx_1 \cdot \lambda e^{-3\lambda}\,dx_2 = \lambda^2 e^{-5\lambda}\,dx_1\,dx_2.$$

Now that we have a genuine probability we can look for the value of λ that maximizes it. Looking at the formula above we see that the factor $dx_1\,dx_2$ will play no role in finding the maximum. So for the MLE we drop it and simply call the density the likelihood:

$$\text{likelihood} = f(x_1, x_2|\lambda) = \lambda^2 e^{-5\lambda}.$$

The value of λ that maximizes this is found just like in the example above. It is $\hat{\lambda} = 2/5$.

5 Appendix: Properties of the MLE

For the interested reader, we note several nice features of the MLE. These are quite technical and will not be on any exams.

The MLE behaves well under transformations. That is, if $\hat{p}$ is the MLE for p and g is a one-to-one function, then $g(\hat{p})$ is the MLE for $g(p)$. For example, if $\hat{\sigma}$ is the MLE for the standard deviation σ then $(\hat{\sigma})^2$ is the MLE for the variance σ^2.

Furthermore, under some technical smoothness assumptions, the MLE is asymptotically unbiased and has asymptotically minimal variance. To explain these notions, note that the MLE is itself a random variable since the data is random and the MLE is computed from the data. Let $x_1, x_2, \ldots$ be an infinite sequence of samples from a distribution with parameter p. Let $\hat{p}_n$ be the MLE for p based on the data $x_1, \ldots, x_n$.

Asymptotically unbiased means that as the amount of data grows, the mean of the MLE converges to p. In symbols: $E[\hat{p}_n] \to p$ as $n \to \infty$. Of course, we would like the MLE to be close to p with high probability, not just on average, so the smaller the variance of the MLE the better. Asymptotically minimal variance means that as the amount of data grows, the MLE has the minimal variance among all unbiased estimators of p. In symbols: for any unbiased estimator $\tilde{p}_n$ and $\epsilon > 0$ we have that $\text{Var}(\tilde{p}_n) + \epsilon > \text{Var}(\hat{p}_n)$ as $n \to \infty$.