BMEG 802 – Advanced Biomedical Experimental Design and Analysis

Maximum Likelihood Estimation

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Recap

- ANCOVA
  - covariates
  - can use for any combination of between and within designs.

Today

- Maximum Likelihood Estimation (MLE)
  - Probability Distribution Function
  - Likelihood function
  - 3 Ways to find the Maximum Likelihood Estimation
    - Analytical (Calculus)
    - Brute Force (Grid Search)
    - Optimization (Gradient Descent)

Maximum Likelihood Estimation

- Tool for parameter estimation
- good approach for cases when OLS (ordinary least squares) assumptions are violated
- e.g. for non-linear models with non-normal data
- in MLE, we estimate the parameters of a model that maximize the likelihood of your data

Probability Density Function

- assume an observed **data** vector

$$y = (y_1, y_2, ..., y_n)$$

- Goal of MLE: identify the population (the model) that is **most likely** to have generated the data

Probability Density Function

- Here we assume population (model) is associated with a corresponding probability distribution
- Each probability distribution is characterized by a unique value of the model's parameter(s)
- As model parameters change, different probability distributions are generated
- Model = the family of probability distributions indexed by the model's parameter(s)

Probability Density Function

- $f(y|w)$ is the probability density function (PDF) specifying the probability of observing data y, given model parameter(s) w
  - note: w may be a parameter vector, $w = (w_1, w_2, ..., w_n)$
    - e.g. for a normal PDF: $w = (\mu, \sigma)$

Probability Density Function

- If observations yi are i.i.d. (indepedent and identically distributed), then the PDF for the data as a whole, $y = (y_1, y_2, ..., y_n)$ given the parameter vector $\mathbf{w} = (w_1, w_2, ..., w_n)$, can be expressed as the multiplication of PDFs for individual observations:

$$f(y_1, y_2, ..., y_n | \mathbf{w}) = f_1(y_1 | \mathbf{w}) f_2(y_2 | \mathbf{w}), ..., f_n(y_n | \mathbf{w})$$

Or, more concisely $f(\mathbf{y} | \mathbf{w}) = \prod_{i=1}^{n} f_n(y_n | \mathbf{w})$\$

PDF Example with a Normal Distribution

- Let's say our data vector Y is made up of 3 observations: $y_1 = 80, y_2 = 110, y_3 = 130$
- We want to compute the PDF for a Normal distribution:

$$f(y_i|\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i-\mu)}{2\sigma^2}}$$

Let's assume $\mu = 100, \sigma = 15$

$$f(80|\mu = 100, \sigma = 15) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(80-\mu)}{2\sigma^2}} = 0.010934$$

$$f(110|\mu = 100, \sigma = 15) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(110-\mu)}{2\sigma^2}} = 0.010934$$

$$f(130|\mu = 100, \sigma = 15) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(130-\mu)}{2\sigma^2}} = 0.010934$$

$$f(y_1, y_2, y_3|\mu,\sigma) = f(y_1|\mu,\sigma)f(y_2|\mu,\sigma)f(y_3|\mu,\sigma) = (.010934)(.021297)(.003599) = .000000838$$

Binomial Distribution Example

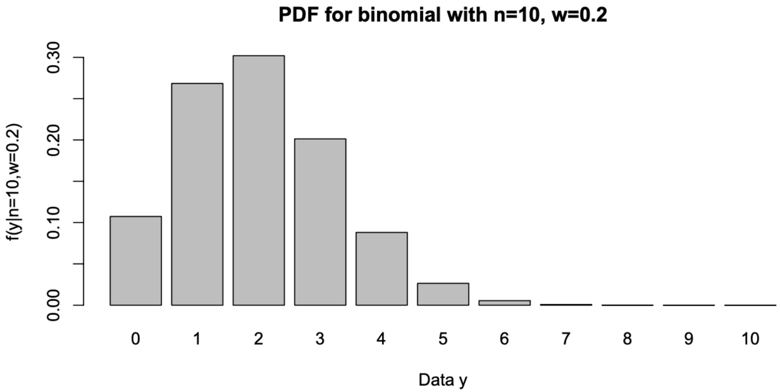
- y is the number of successes in a sequence of 10 Bernoulli trials (e.g. tossing a coin 10 times)
- a Bernoulli trial is an experiment whose outcome is random and can be either of two possible outcomes: success or failure.
- Binomial Distribution PDF:

$$f(y|n, w) = \frac{n!}{y!(n-y)!} w^y (1-w)^{n-y}$$

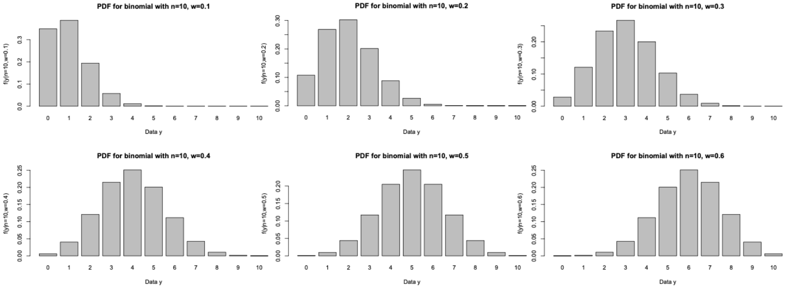
- assume probability of a success on any one trial is 0.2 (a biased coin)
- parameter vector w is n=10, w=0.2

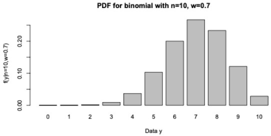
$$f(y|n=10, w=0.2) = \frac{10!}{y!(10-y)!} 0.2^y (1-0.2)^{10-y}; (y = 0, 1, ..., 10)$$

Binomial Distribution



Binomial Distribution - Varying a Parameter

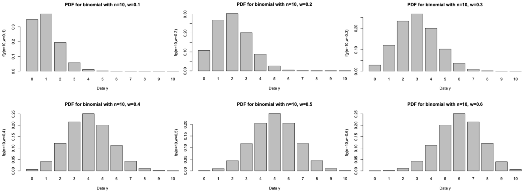


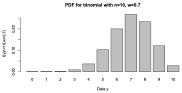


and so on ...

Binomial Distribution - A Model

The collection of all such PDFs generated by varying the parameter across its range defines a **model**





and so on ...

Likelihood Function

Likelihood Function

- Given a set of parameter values, the corresponding PDF will show that some data are more probable than other data
- In fact we have already observed the data

Likelihood Function

- We are faced with the inverse problem
- Given the observed data, and a model of the process by which the data was generated
  - find the one PDF, among all the probability densities that the model prescribes, that is **most likely to have produced the data**

Likelihood Function

- we define the likelihood function by reversing the roles of the data vector y and the parameter vector w in $f(y|w)$:

$$\mathcal{L}(w|y) = f(y|w)$$

$\mathcal{L}(w|y)$ represents the likelihood of the parameter w given the observed data y

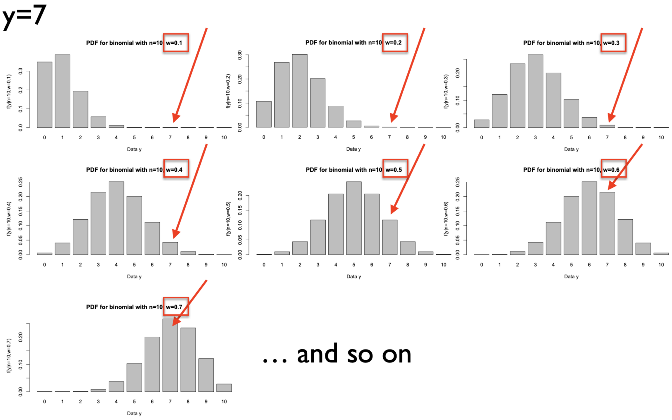
- note: a likelihood function does not need to sum to 1.0
- For our one-dimensional binomial example the likelihood function for y=7 and n=10 is

$$\mathcal{L}(w|n=10, y=7) = \frac{10!}{7!(10-7)!} w^7 (1-w)^{10-7}; (0 \le w \le 1)$$

But, what is the value of w???

Likelihood Function - Iterate Through Variable

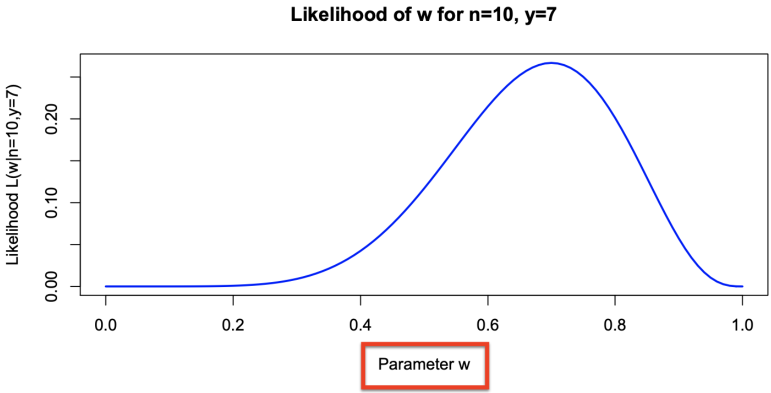
Let's try all value of w between 0 and 1



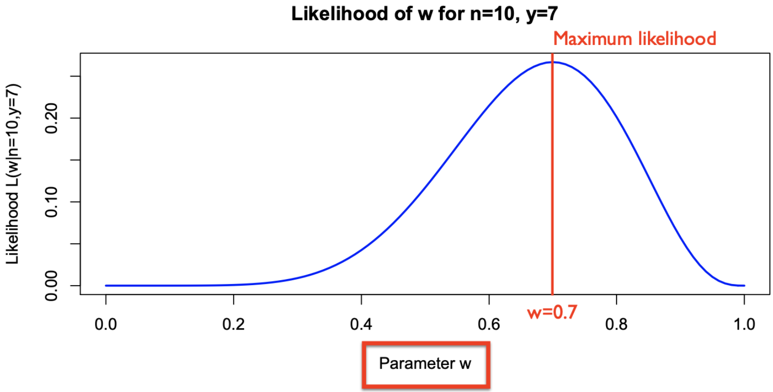
... and so on

Notice $\mathcal{L}(w|n = 10, y = 7)$ is highest when $w = 0.7$

Graphing the Likelihood Function



Graphing the Likelihood Function



$w = 0.7$ is the Maximum Likelihood Estimate!!!

Maximum Likelihood Estimate (MLE)

- find the probability distribution (the model) that makes the observed data most likely
- seek the value of the parameter vector w that maximizes the likelihood function

$\mathcal{L}(w|y)$ - the resulting parameter vector w is known as the MLE estimate

Maximum Likelihood Estimate (MLE)

Three ways of finding the MLE

1. Analytical: use calculus to solve for the parameter value(s) w that result in a peak
2. Brute Force: exhaustive search through parameter space in a grid
3. Optimization: use non-linear optimization (e.g. gradient descent) to iteratively find the peak

Numerical Considerations

- we saw before that the PDF for observed data, $y = (y_1, y_2, ..., y_n)$ given a parameter vector w, can be expressed as the **product (multiply) of PDFs for individual observations**

$$\mathcal{L}(w|y_1, y_2, ..., y_n) = \mathcal{L}_1(w|y_1)\mathcal{L}_2(w|y_2)...\mathcal{L}_n(w|y_n)$$

- multiplying together a lot of values that lie between 0 and 1, (as many as there are data points) will result in a very small number
- in fact the more data, the smaller the resulting product will be
- computers are not good at representing very small numbers

Numerical Considerations

- solution: take the logarithm
- this reformulates the series of products, as a series of sums
- the more data, the higher the resulting sum

$$ln[\mathcal{L}_1(w|y_1)\mathcal{L}_2(w|y_2)...\mathcal{L}_n(w|y_n)] = ln[\mathcal{L}_1(w|y_1) + \mathcal{L}_2(w|y_2)+, ..., \mathcal{L}_n(w|y_n)]$$

Numerical Considerations

- another problem: most optimization algorithms are formulated in terms of minimizing an objective function, not maximizing
- solution: rather than maximizing the log-likelihood, we will minimize the negative log-likelihood
- find w that minimizes:

$$argmin_w \Bigg[-1.0 \Bigg(ln \Bigg[\mathcal{L}_1(w|y_1) + \mathcal{L}_2(w|y_2)+, ..., \mathcal{L}_n(w|y_n) \Bigg] \Bigg) \Bigg]$$

An Example

- Let's say I claim I can correctly identify coffee quality between Little Goat and Starbucks coffee
- My lab designs an experiment to test me
- They give me 20 cups of coffee in random order and I have to say "Goat" or "Starbucks"
- Observed data: I get 16 correct, 4 incorrect
- what model explains the observed data?

An Example

- This experiment can be modelled as 20 Bernoulli trials (outcome of each trial is random and can be either of two possible outcomes, "success" and "failure")
- we know PDF is binomial, which has 2 parameters: n ($\#$ trials) and w (prob of a success on a given trial)
- equivalent to asking, what is the value of the parameter w?
- high w (e.g. near 1.0) means I have a good ability to discriminate
- w near 0.5 means I am flipping a coin

Likelihood Function

Likelihood Function:

$$\mathcal{L}(w|n, y) = \frac{n!}{y!(n-y)!} w^y (1-w)^{n-y}$$

Log Likelihood Function:

$$ln[\mathcal{L}(w|n, y)] = ln\left(\frac{n!}{y!(n-y)!}\right) + y \cdot ln(w) + (n-y) \cdot ln(1-w)$$

Tips: $ln(x \cdot y) = ln(x) + ln(y)$; $ln(e) = 1$; $\frac{d[ln(x)]}{dx} = \frac{1}{x}$

MLE - ANALYTICAL

MLE - ANALYTICAL

We want:

$$\frac{d}{dw}\left(ln[\mathcal{L}(w|n,y)]\right) = 0$$

Log Likelihood Function:

$$ln[\mathcal{L}(w|n,y)] = ln\left(\frac{n!}{y!(n-y)!}\right) + y \cdot ln(w) + (n-y) \cdot ln(1-w)$$

Taking the partial derivative of the log likelihood function:

$$\frac{d}{dw}\left(ln[\mathcal{L}(w|n,y)]\right) = \frac{d}{dw}\left(ln\left(\frac{n!}{y!(n-y)!}\right) + y \cdot ln(w) + (n-y) \cdot ln(1-w)\right) = 0$$

$$\frac{d}{dw}\left(ln[\mathcal{L}(w|n,y)]\right) = 0 + \frac{n}{w} - \frac{n-y}{1-w} = 0$$

MLE - ANALYTICAL

$$\frac{n}{w} - \frac{n-y}{1-w} = 0$$

Finding the common denominator:

$$\frac{y(1-w)}{w(1-w)} - \frac{w(n-y)}{w(1-w)} = 0$$

$$\frac{y(1-w) - w(n-y)}{w(1-w)} = 0$$

$$\frac{y - y \cdot w - w \cdot n + y \cdot w}{w(1-w)} = 0$$

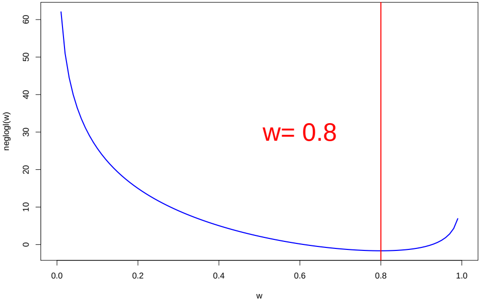
$$w = \frac{y}{n}$$

MLE $= 0.8 = \frac{16}{20}$

MLE - BRUTE FORCE

MLE - BRUTE FORCE

```r
neglogl <- function(w) {
  loglik <- log(116280) + 16 * log(w) + 4 * log(1-w)
  return(-1 * loglik)
}
w <- seq(0,1,.01) # iterate through a range of w's
plot(w, neglogl(w), type="l", col="blue", lwd=2)
imin <- which(neglogl(w)==min(neglogl(w)))
abline(v=w[imin], col="red", lwd=2)
text(.6, 30, paste("w=",w[imin]),col="red", cex = 3)
```



MLE - OPTIMIZER

MLE - OPTIMIZER

```
neglogl <- function(w) {
  loglik <- log(116280) + 16 * log(w) + 4 * log(1-w)
  return(-1 * loglik)
}
opt <- nlm(f=neglogl, p=0.5)
```

```
## Warning in log(1 - w): NaNs produced

## Warning in nlm(f = neglogl, p = 0.5): NA/Inf replaced by maximum positive value

## Warning in log(1 - w): NaNs produced

## Warning in nlm(f = neglogl, p = 0.5): NA/Inf replaced by maximum positive value
```

```
opt$estimate
```

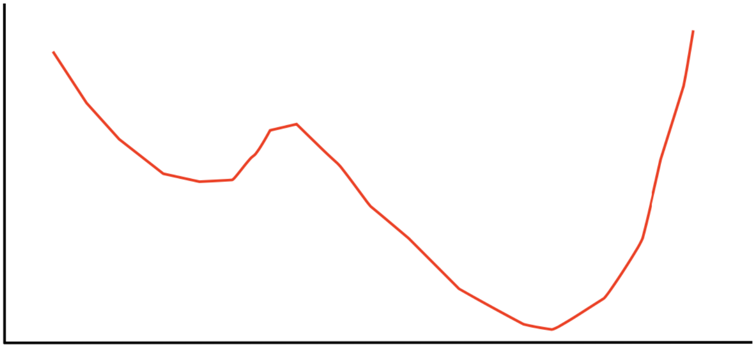
```
## [1] 0.7999995
```

Finds the Maximum Likelihood Estimate: 0.8

MLE in general

- MLE for many distributions are known (look it up)
- MLE for more complex models can sometimes be determined analytically
- Often however not possible/feasible
- Iterative optimization is a common method in these cases
    - local minima

Optimization and Local Minima



General Procedure

- If you can write an equation for the Likelihood function
- i.e. probability of obtaining your observed data, given a model with parameter(s) w
- then you can find the MLE for w
- i.e. you can find the model that is most likely to generate your data

Hypothesis Testing

- We can use the Likelihood Ratio Test to compare two models
- Little Goat and Starbucks Example
- 16 correct out of 20 trials
- our MLE for p was 0.80
- let's test this against a null hypothesis that p=0.50

Likelihood Ratio Test

- test statistic D is a ratio:

$$D = -2 \cdot ln\left(\frac{likelihood\ for\ null\ model}{(likelihood\ for\ alternative\ model}\right)$$

$$D = -2 \cdot ln(likelihood\ for\ null\ model) + (likelihood\ for\ alternative\ model)$$

Likelihood Ratio Test

- the probability distribution of test statistic D is approximately a chi-squared distribution with $df = df_2 - df_1$
- df_1 and df_2 are number of free parameters of models 1 (null) and 2 (alternative), respectively.
  - $df_1 = 0$ for the null model since assuming w is set to 0.5 (not a free parameter)
  - $df_2 = 1$ for the alternative model since assuming w is a free parameter

Likelihood Ratio Test

$$\mathcal{L}(w|n, y) = \frac{n!}{y!(n-y)!} w^y (1-w)^{n-y}$$

- our data: 16 correct and 4 incorrect

$$Null\ model = -2 \cdot ln[L(w = 0.5|y = 16, n = 20)] = 16.29966$$

- MLE of w is, $w = 0.8$.

$$Alternative\ model = -2 \cdot ln[L(w = 0.8|y = 16, n = 20)] = -4.82984$$

$$D = -2 \cdot ln(likelihood\ for\ null\ model) + (likelihood\ for\ alternative\ model)$$

$$D = 16.29966 - 4.82984 = 11.46982$$

Likelihood Ratio Test

$$D = 11.46982$$

- now compute a p-value using chi-square distribution with df = 1-0 = 1

```
pval <- pchisq(q=11.46982, df=1, lower.tail=FALSE)
pval
```

```
## [1] 0.0007073553
```

We can reject the null with a Type 1 error rate of 0.00071. Thus, Josh can detect differences in Little Goat coffee compared to Starbucks coffee compared to chance.

Beyond the Binomial

Maximum Likelihood of

Normal Distribution:

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

Linear Regression:

$$p(y_i|x_i, \beta_0, \beta_1, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i-(\beta_0+\beta_1 \cdot x_i))^2}{2\sigma^2}}$$

Next Week

- Bayesian Statistics
  - Priors, Likelihoods, Posterior Distributions
  - Continually updating probabilities based on new information