Sampling and maximum likelihood estimation

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Outline Today

- An orchid example
- Sampling variation
- Maximum likelihood estimation
- Normal distribution
- Linear models

Sampling data

Figure 1: www.ugent.be

A nice field with orchids.

How do we find the proportion of orchids?

What is the proportion of orchids?

We decide to walk through the field and at 10 places record when we find an orchid (1) or not (0)

1. First time: 5 orchids from 10 picks ($5/10 = 0.5$)

What is the proportion of orchids?

We decide to walk through the field and at 10 places record when we find an orchid (1) or not (0)

1. First time: 5 orchids from 10 picks ($5/10 = 0.5$)
2. Second time: 2 orchids from 10 picks ($2/10 = 0.2$)
3. Third time: 8 orchids from 10 picks ($8/10 = 0.8$)

What is the proportion of orchids?

We conclude, half of the flowers are orchids ($15/30 = 0.5$). But encounter this guy:

- What caused our estimate of the proportion of orchids to be inaccurate?
- And why did we not get the same proportion of orchids every time?

He tells us that the true proportion of orchids is 0.4.

The data

For such (binary) data: $y_i \sim Binom(p, n_{picks})$, with $p(orchid) = p$

The binomial distribution

$$f(y_i; n_{picks}, p) = y_i \log\{p\} + (n_{picks} - y_i) \log\{1 - p\} + constant \qquad (1)$$

R-functions

- Density: `dbinom`
- Number generator: `rbinom`

Simulation: counting orchids once

```r
set.seed(12345) # For reproducibility
p.orchid = 0.4 # The true proportion of orchids
n.picks = 10 # The number of picks in the field
n.times = 1
# Collect data
y <- rbinom(n.times, size = n.picks, prob = p.orchid)
y/n.picks # Proportion of orchids
```

```
## [1] 0.5
```

Simulation: counting orchids once

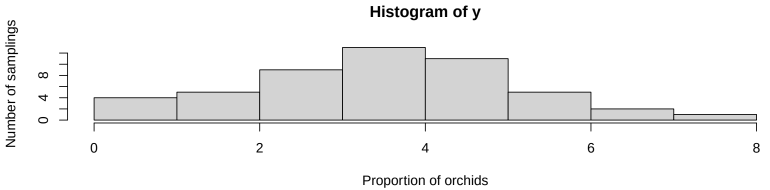
What if we sample the whole field once?

```
set.seed(12345) # For reproducibility
n.times = 1e5 # The number of picks in the field
n.picks <- 1
 # Collect data
y <- rbinom(n.times, size = n.picks, prob = p.orchid)
mean(y/n.picks) # Proportion of orchids
```

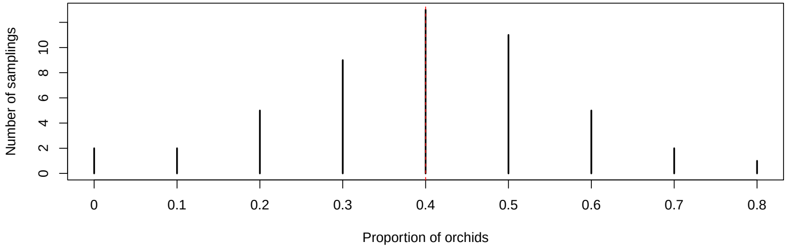
```
## [1] 0.40021
```

Simulation: counting orchids 50x10 times

```
set.seed(12345) # For reproducibility
n.times <- 50
n.picks = 10 # The number of picks in the field
# Collect data
y <- rbinom(n.times, size = n.picks, prob = p.orchid)
hist(y, xlab = "Proportion of orchids",
     ylab = "Number of samplings")
```



Simulation: counting orchids 50x10 times



As you see, we have variability in our estimate of the proportion of orchids.

- Can we summarize this variation?
- Preferably without collecting data many times

The strategy

- Collect data
- Learn about the variation in that data
  - We need a model for that
- Work out distribution of the estimates
  - And find the "best" estimate
- Conclude if our answer is robust
  - Q: Are more than half of the flowers in this field orchids?

Q: Are more than half of the flowers in this field orchids?

- Exclude rare events, and decide on an acceptable margin of error (5%)
- What is the range our parameter is estimated to be 95% of the time?

```
quantile(y/n.picks,c(0.025,.975))
```

```
##   2.5%  97.5%
## 0.0225 0.7000
```

So 50 times 10 picks tell us little.

Q: Are more than half of the flowers in this field orchids?

```
set.seed(12345)
n.picks = 100
n.times <- 50
# Collecting data
y <- rbinom(n.times, size = n.picks, prob = p.orchid)
quantile(y/n.picks,c(0.025,.975))
```

```
##    2.5%   97.5%
## 0.31225 0.48000
```

50 times 100 picks reduces the variability in the proportion of observed orchids. Most of the time we will find fewer orchids than other flowers.

On average, we will get it right.

```
set.seed(12345)
n.picks = 1;n.times <- 100
y <- rbinom(n.times, size = n.picks, prob = p.orchid)
quantile(y/n.picks,c(0.025,.975))
```

```
##  2.5% 97.5%
##     0     1
```

```
mean(y/n.picks)
```

```
## [1] 0.45
```

Estimator and Estimand

- Estimand: the parameter we want to estimate, the true population level parameter
- Estimator: how we are estimating it $\hat{p}_{orchid} = \frac{y}{n.picks}$
  - Why is this a good estimator?
- Estimate: the parameter value based on the data

Estimating parameters and quatifying uncertainty

- We do not usually have infinite amounts of data
- So how can we quantify variability of the estimator?
- We need a model for the process that generates the data

The likelihood: single data point

$$\mathcal{L}(y_i; \Theta) = f(y_i; \Theta) \tag{2}$$

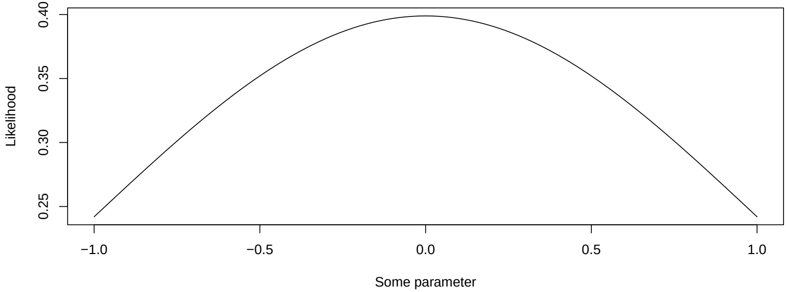
The probability of obtaining our data assuming Θ is the true parameter(s).

The likelihood: multiple data points (2)

$$\mathcal{L}(\mathbf{y};\Theta) = \prod_{i}^{n} f(y_i;\Theta) \tag{3}$$

We just multiply! (assumes independence)

The likelihood (3)

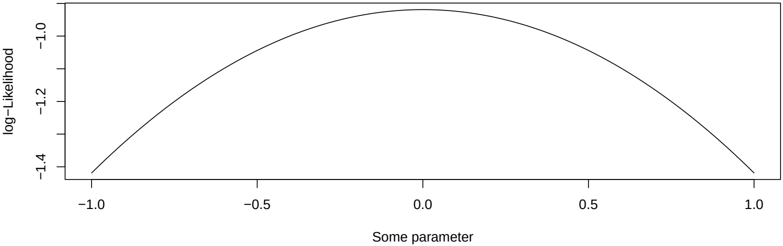


Likelihood tells us about:

- The (set of) parameter estimates that most likely generated the data
- The information contained in our data

The log-likelihood

$$\log\{\mathcal{L}(\mathbf{y};\Theta)\} = \sum_{i}^{n} \log\{f(y_i;\Theta)\} \tag{4}$$



Usually, we work with the log-likelihood. The maximum is the same and it is easier. So we just add things together.

Back to the orchid example

- Data is binary or counts
- Which follows a binomial likelihood (only as example, for now)

$$f(y_i; n_{picks}, p) = y_i \log\{p\} + (n_{picks} - y_i) \log\{1 - p\} + constant \tag{5}$$

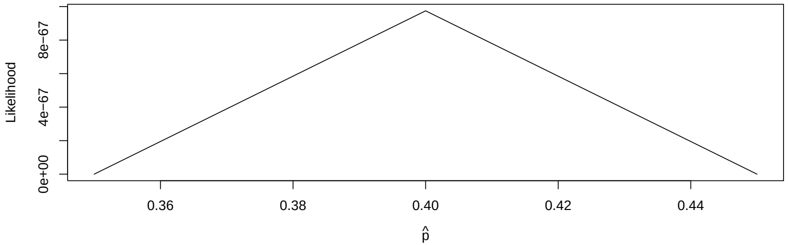
- $N = n_{picks}$ trials
- $r = y_i$ successes (orchids)
- p the probability of success (proportion of orchids)

Assumptions

- Each pick is independent from the next
- p is the same for all observations

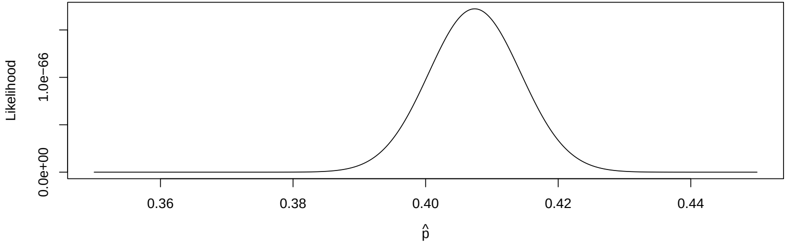
Finding the proportion of orchids

```
ll <- function(p, n.picks, y)prod(dbinom(y, n.picks,p))
phat <- seq(0.35,0.45,length.out=3)
plot(sapply(phat, ll, n.picks = n.picks, y = y),
     x = phat, type = "l", xlab=expression(hat(p)), ylab="Lik
```



Finding the proportion of orchids (2)

```
ll <- function(p, n.picks, y)prod(dbinom(y, n.picks,p))
phat <- seq(0.35,0.45,length.out=1000)
plot(sapply(phat, ll, n.picks = n.picks, y = y),
    x = phat, type = "l", xlab=expression(hat(p)), ylab="Lik
```



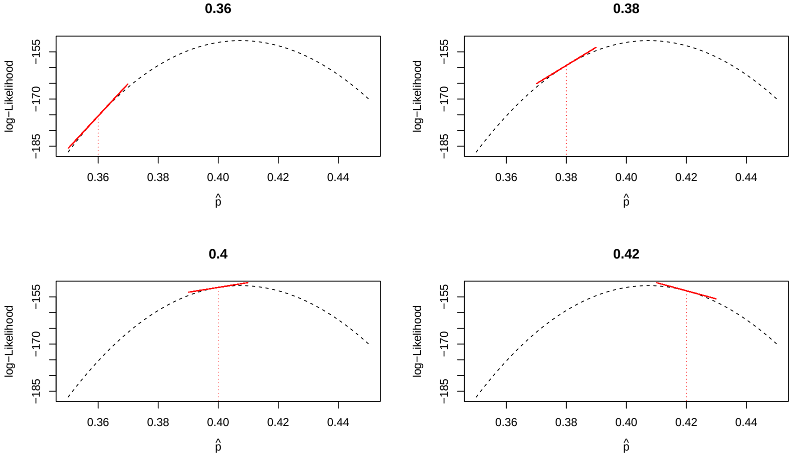
Maximising the likelihood

Trying many values (grid) is very inefficient

We can:

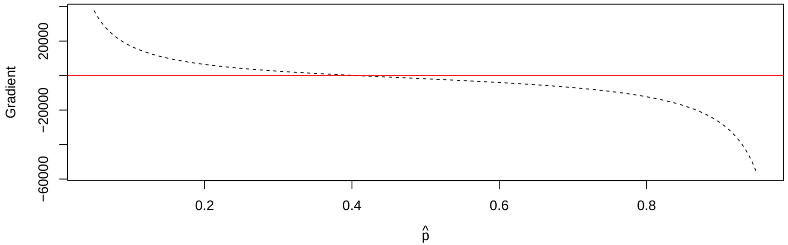
- analytically: do mathematics
- numerically: use an algorithm (as in GLMs)
- simulation: try many values

Finding the maximum



Finding the maximum: gradient

```
phat =  seq(0.05,0.95,length.out=1000)
plot(sapply(phat, grad.dbinom, y=y, n.picks = n.picks),
     x = phat, type = "l", xlab=expression(hat(p)),
     ylab="Gradient", lty = "dashed")
abline(h=0, col = "red")
```



Finding the maximum: mathy bits

Our function:

$$\log\{\mathcal{L}(\mathbf{y}; n_{picks})\} =$$

Finding the maximum: mathy bits

Our function:

$$\log\{\mathcal{L}(\mathbf{y}; n_{picks})\} = \sum_{i=1}^{n_{times}} y_i \log\{p\} + (n_{picks} - y_i) \log\{1-p\} + constant \tag{6}$$

Finding the maximum: mathy bits

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Slope of the likelihood:

$$\frac{\partial \log\{\mathcal{L}(\mathbf{y}; n_{picks})\}}{\partial p}$$

Finding the maximum: mathy bits

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$$\log\{\mathcal{L}(\mathbf{y}; n_{picks})\} = \sum_{i=1}^{n_{times}} y_i \log\{p\} + (n_{picks} - y_i) \log\{1-p\} + constant \tag{6}$$

Slope of the likelihood:

$$\frac{\partial \log\{\mathcal{L}(\mathbf{y}; n_{picks})\}}{\partial p} = \sum_{i=1}^{n_{times}} \frac{y_i}{p} - \frac{n_{picks} - y_i}{1-p} \tag{7}$$

Estimator for p

$$0 = \sum_{i=1}^{n_{times}} \frac{y_i}{p} - \frac{n_{picks} - y_i}{1-p} \tag{8}$$

Estimator for p

$$\sum_{i=1}^{n_{times}} \frac{n_{picks} - y_i}{1 - p} = \sum_{i=1}^{n_{times}} \frac{y_i}{p} \tag{8}$$

Estimator for p

$$\sum_{i=1}^{n_{times}} (n_{picks} - y_i)p = \sum_{i=1}^{n_{times}} y_i(1-p) \tag{8}$$

Estimator for p

$$n_{times} n_{picks} p - \sum_{i=1}^{n_{times}} y_i p = \sum_{i=1}^{n_{times}} y_i - \sum_{i=1}^{n_{times}} y_i p \qquad (8)$$

Estimator for p

$$\sum_{i=1}^{n_{times}} y_i = n_{times} n_{picks} p \tag{8}$$

Estimator for p

$$\hat{p} = \frac{\sum_{i=1}^{n_{times}} y_i}{n_{times} n_{picks}} \tag{8}$$

Estimator for p

And if we only pick once every time:

$$\hat{p} = \frac{\sum_{i=1}^{n_{times}} y_i}{n_{times}} \tag{8}$$

which is the proportion of 1s in the data!

Maximum likelihood estimation: summary

No ideal properties in finite samples. But as we get more data:

- Get things right with a lot of data (consistency)
- Is the best estimator (in terms of RMSE) in large samples of consistent estimators

Often does well in practice anyway 😄

Letting R do the work

```
optimize(ll, n.picks = n.picks, y=y,
         lower = 0, upper = 1, maximum = TRUE)
```

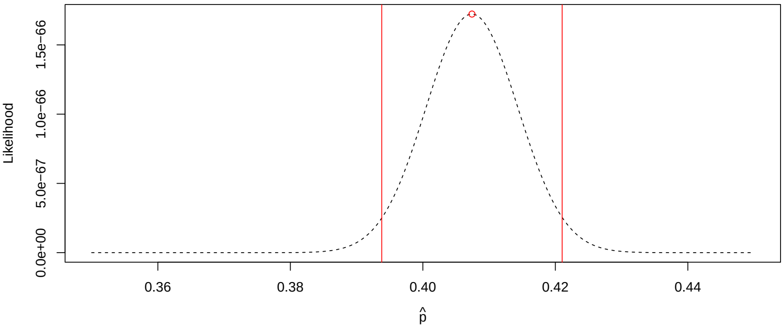
```
## $maximum
## [1] 0.4074027
##
## $objective
## [1] -151.4268
```

- Usually there is more than 1 parameter, much harder

Uncertainty

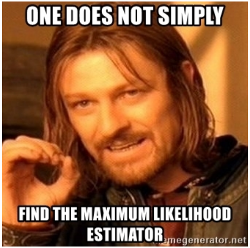
(an estimate of) Width of the likelihood:

$$\frac{\partial^2 \log\{\mathcal{L}(\mathbf{y}; n_{picks})\}}{\partial p^2} = -\sum_{i=1}^{n_{times}} \frac{y_i}{p^2} + \frac{n_{picks} - y_i}{(1-p)^2} \qquad (9)$$



Putting it all together

- We collect data
- We estimate a parameter of interest
- If we collected data again, we get many different estimates
  - This forms a *sampling* distribution
- We summarize this variability
- The width of this sampling distribution tells us the variability
- Instead of collecting data many times, we estimate parameters with MLE
  - This also allows us to quantify the variability

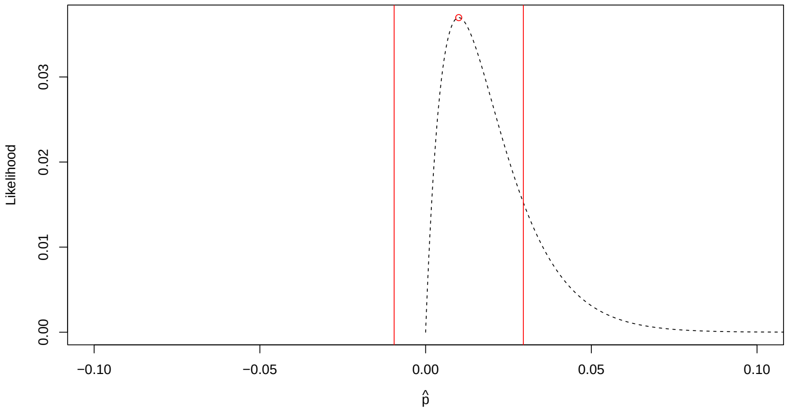


95% Confidence intervals

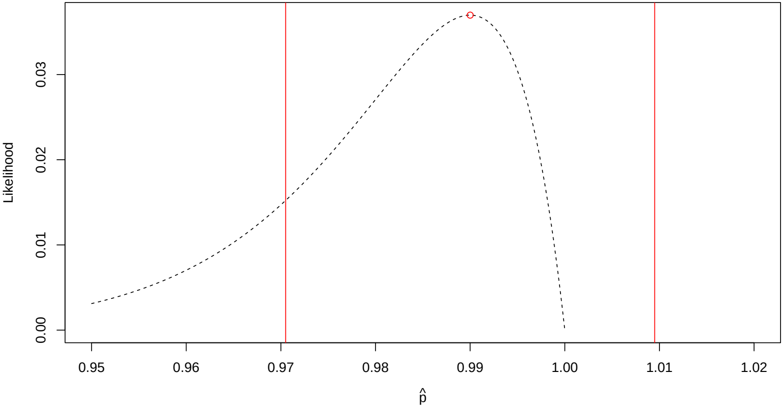
Estimate of the range that the true parameter will fall in 95% of the time.

Different methods exist. Based on MLE not quite correct for the Binomial distribution due to **assumptions**.

Why not?



Why not? (2)



Sampling distribution of $\hat{p}$

But, we have more information about $\hat{p}$

What do we know?

Sampling distribution of $\hat{p}$

We simulated $y_i \sim Binom(1, p)$.

Sampling distribution of $\hat{p}$

We simulated $y_i \sim Binom(1, p)$. In real data, this is an assumption. As long as it holds:

$$\hat{p} = \frac{\sum_{i=1}^{n_{times}} y_i}{n_{times}} \tag{10}$$

is a linear combination of $y_i \sim Binom(1, p)$, from which we know $\left(\sum_{i=1}^{n_{times}} y_i\right) \sim Binom(n_{times}, p)$

Sampling distribution of $\hat{p}$

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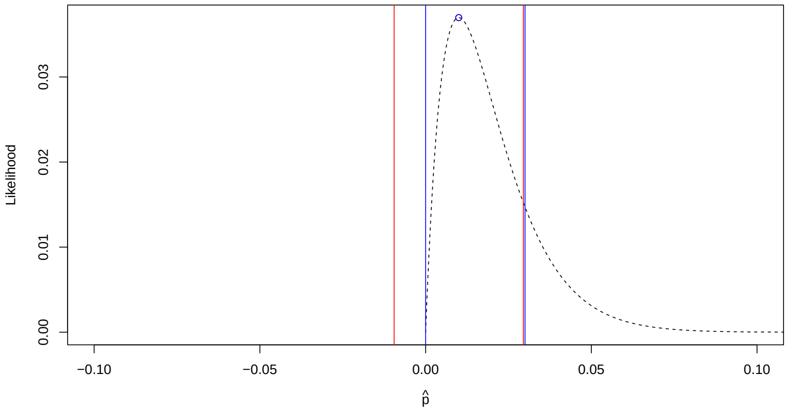
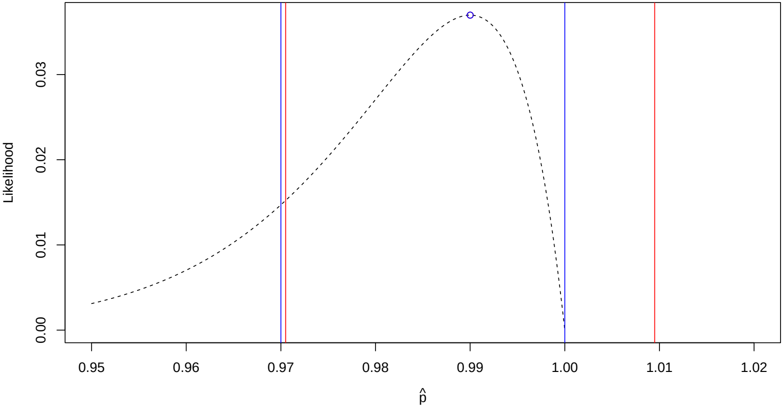
is a linear combination of $y_i \sim Binom(1, p)$, from which we know $\left(\sum_{i=1}^{n_{times}} y_i\right) \sim Binom(n_{times}, p)$

From this we also know $\text{var}(\hat{p}) = \frac{p(1-p)}{n_{times}}$, which gives us a better standard error!

Improved CI for $\hat{p}$ (1)



Improved CI for $\hat{p}$ (2)



Why is uncertainty so important

- Our sampling distribution estimates needs summarizing
- Tells us if we expect our answer to be the same if we repeated the study
- I.e., not so important for the *dataset* but important for *multiple datasets*

Afterall, we are looking for a robust recommendation.

Confidence intervals

An interval that contains the true value in 95% of repeated samples (in large samples)

Be careful with interpretation, and with assumptions.

- Any computed interval either contains the truth, or it does not
- Not the range that the true parameter falls in with 95
- Other misinterpretations

Assumes:

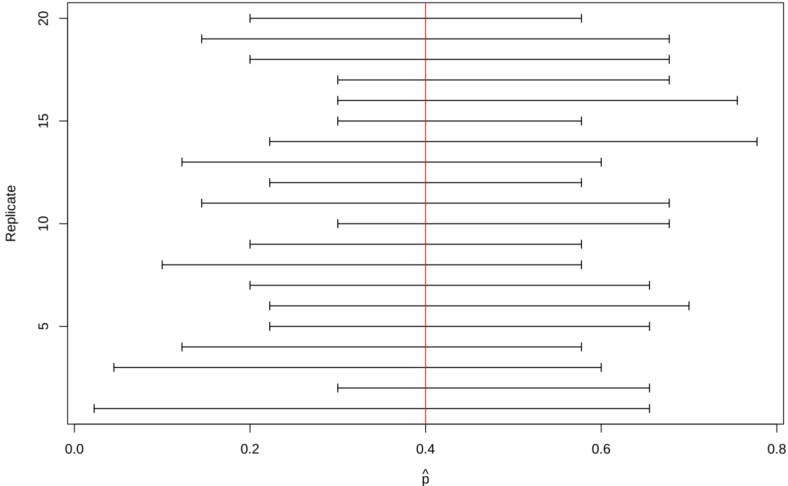
- Asymptotic normality
- inverse Hessian gives covariance of estimators

- Can be interpreted as a kind of statistical test
- Or generally as “evidence”

Gets smaller with:

- More information
- Less variability
- The confidence level

Repetition



Summary

- Our data comes from a population
- That population is generated by a model
- The model has parameters that we want to find
- We do that based on our data
- Our data is a sample, so it is not a perfect representation of the population
- We need to sample many times to get an idea of variability due to our sampling
- We summarize this with a sampling distribution of our estimates
- And use that to draw a conclusion

Questions?


IF YOU HAVE
A QUESTION... ASK
YOU WON'T BE
MAULED, PROMISE
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