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

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 ($5/10 = 0.5$)

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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:

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

- 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?

The binomial distribution

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

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

Simulation: counting orchids once

```
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

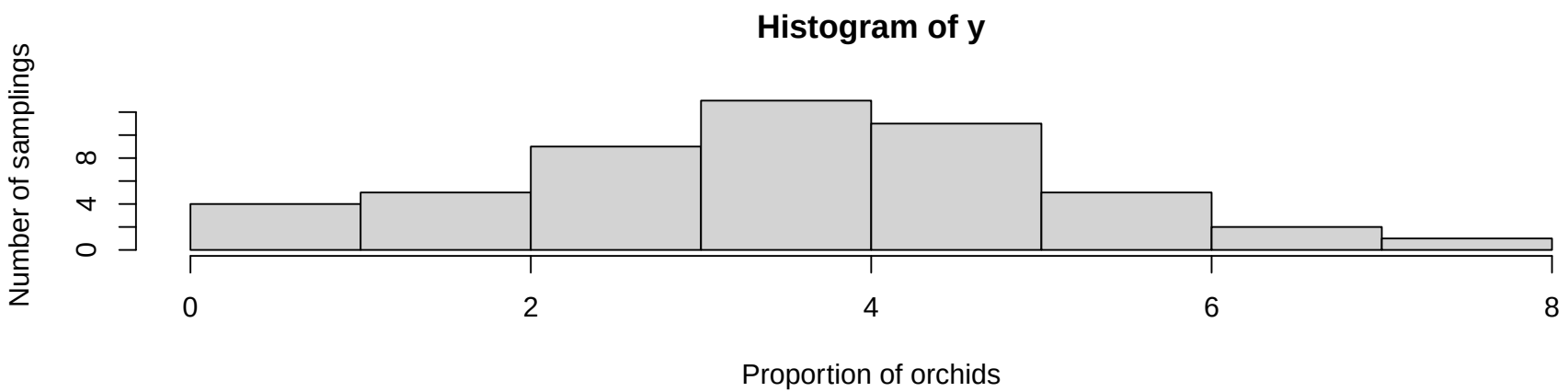
What if we sample the whole field once?

```
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
```

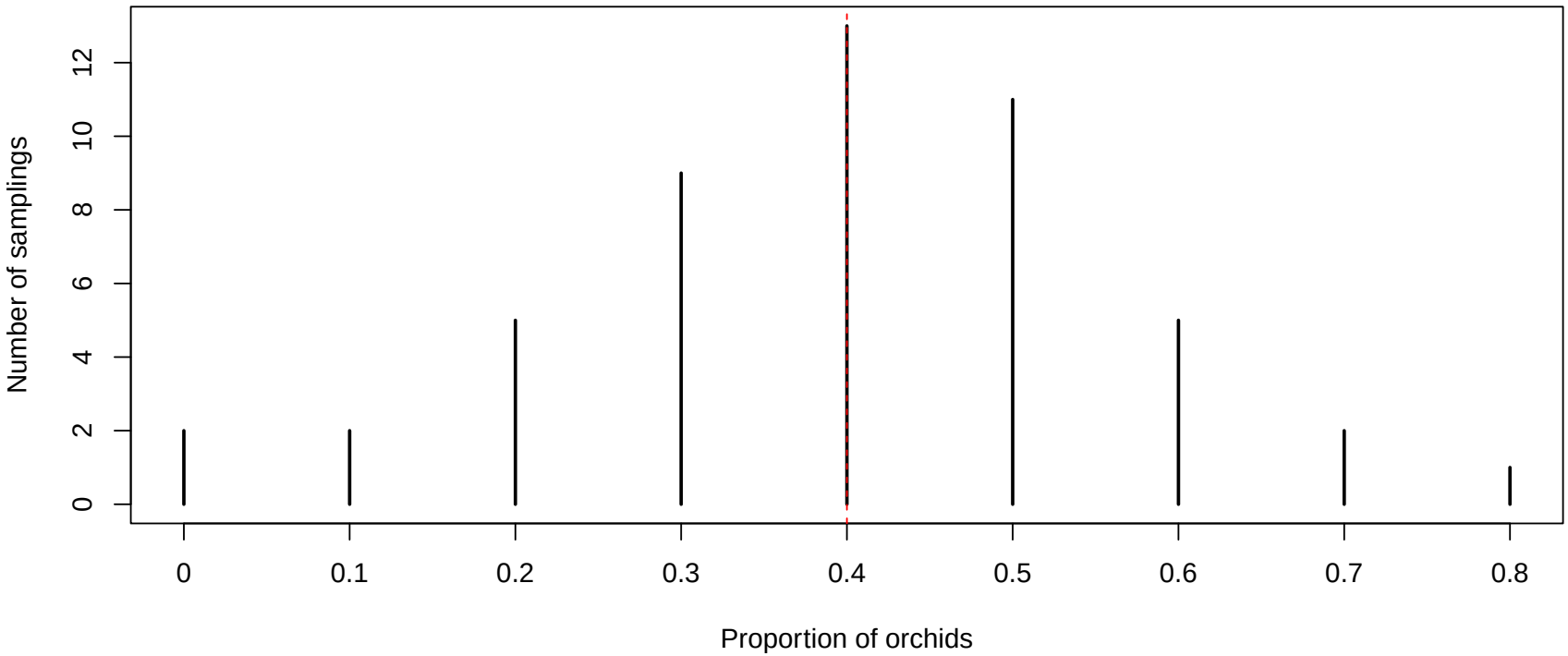
```
## [1] 0.40021
```

Simulation: counting orchids 50x10 times

```r
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

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

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

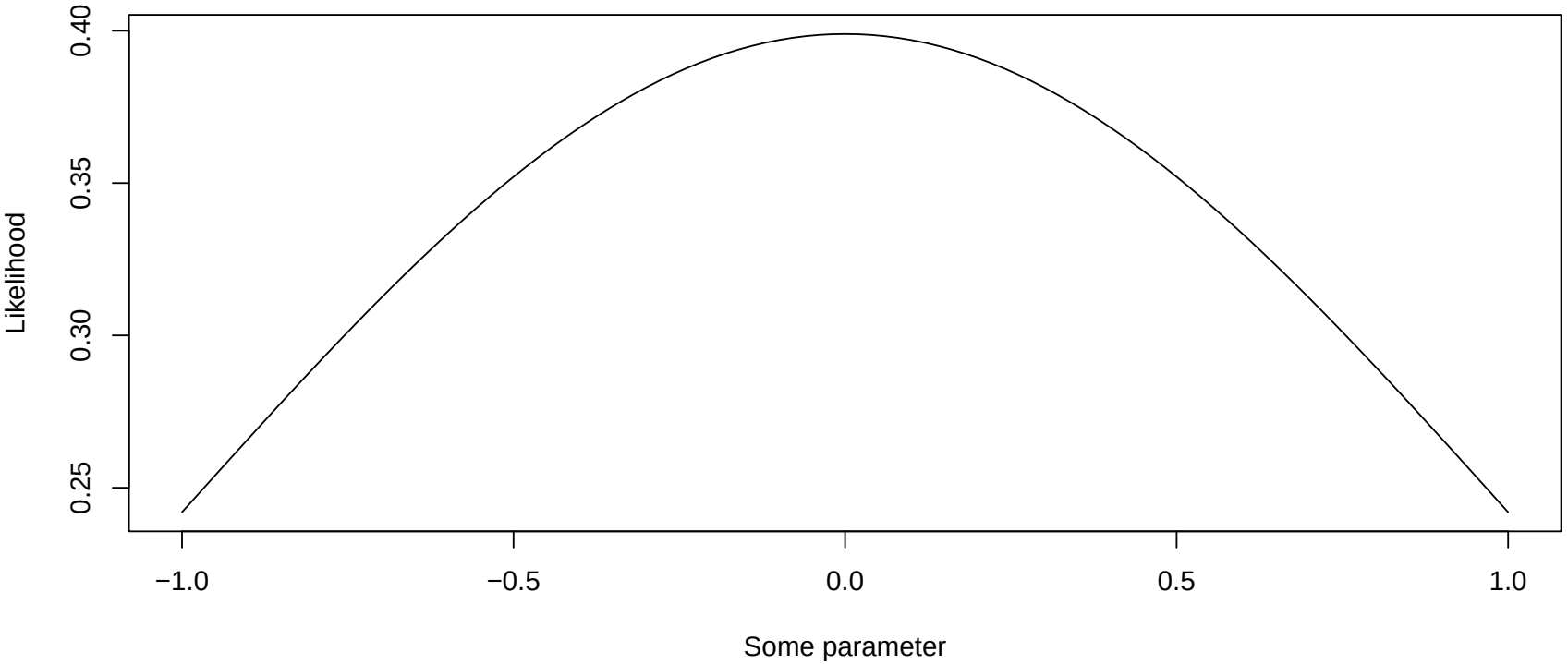
The probability of obtaining our data assuming Θ is the true parameter(s).

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)

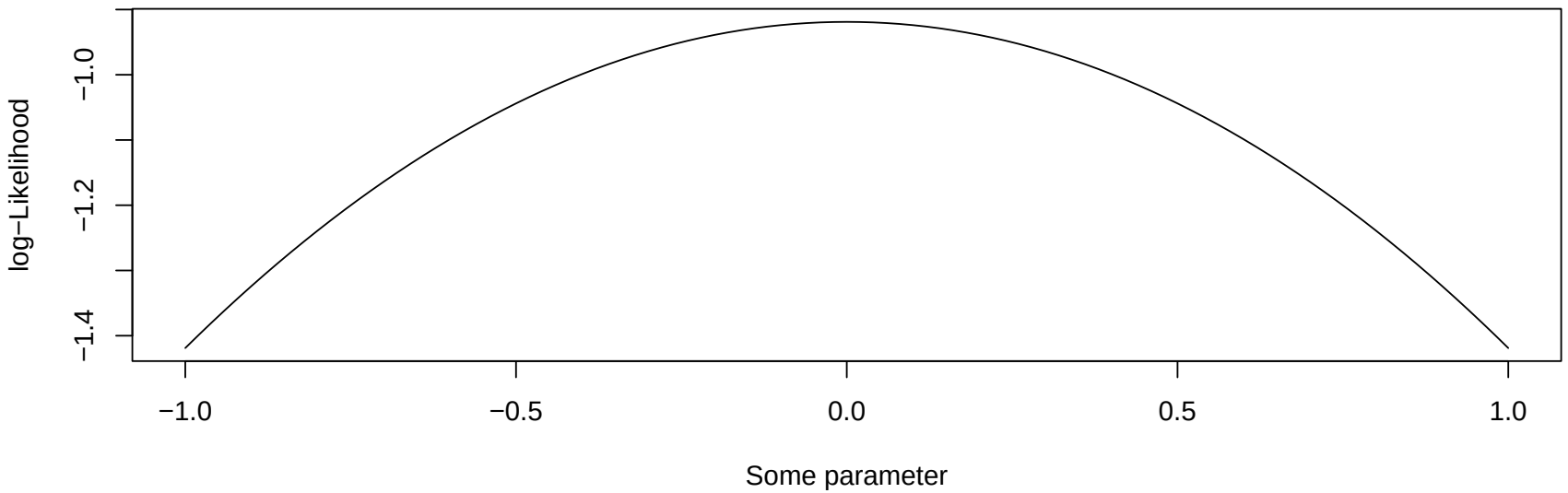


Likelihood tells us about:

- 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)

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

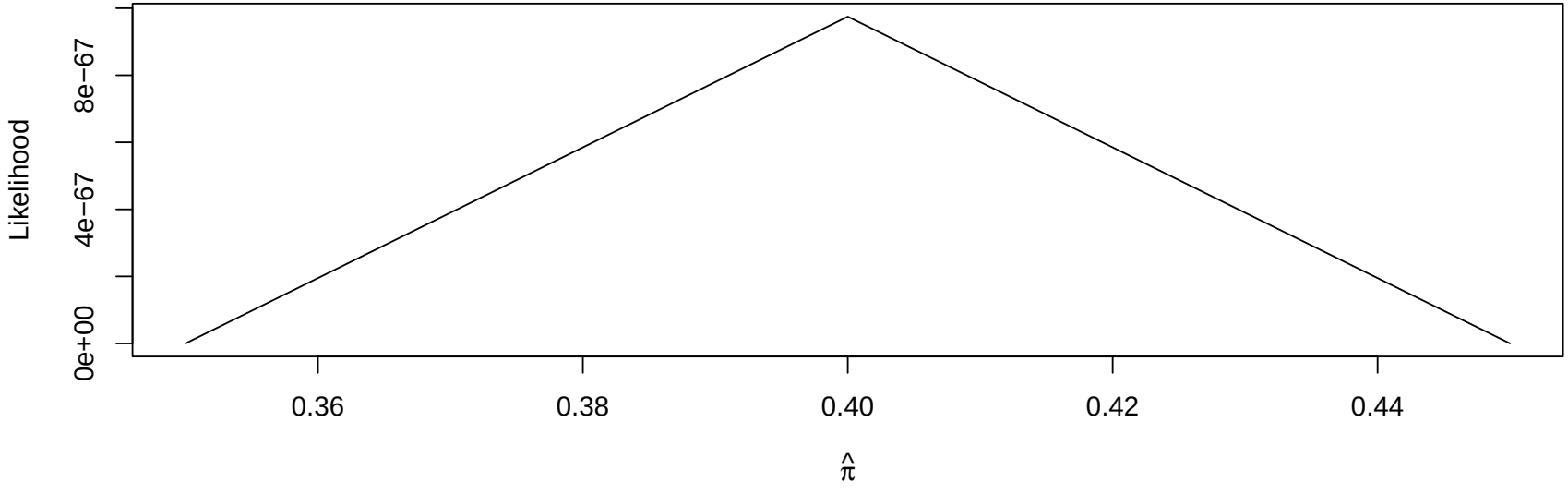
- $N = n_{picks}$ trials
- $r = y_i$ successes (orchids)
- π the probability of success (proportion of orchids)

Assumptions

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

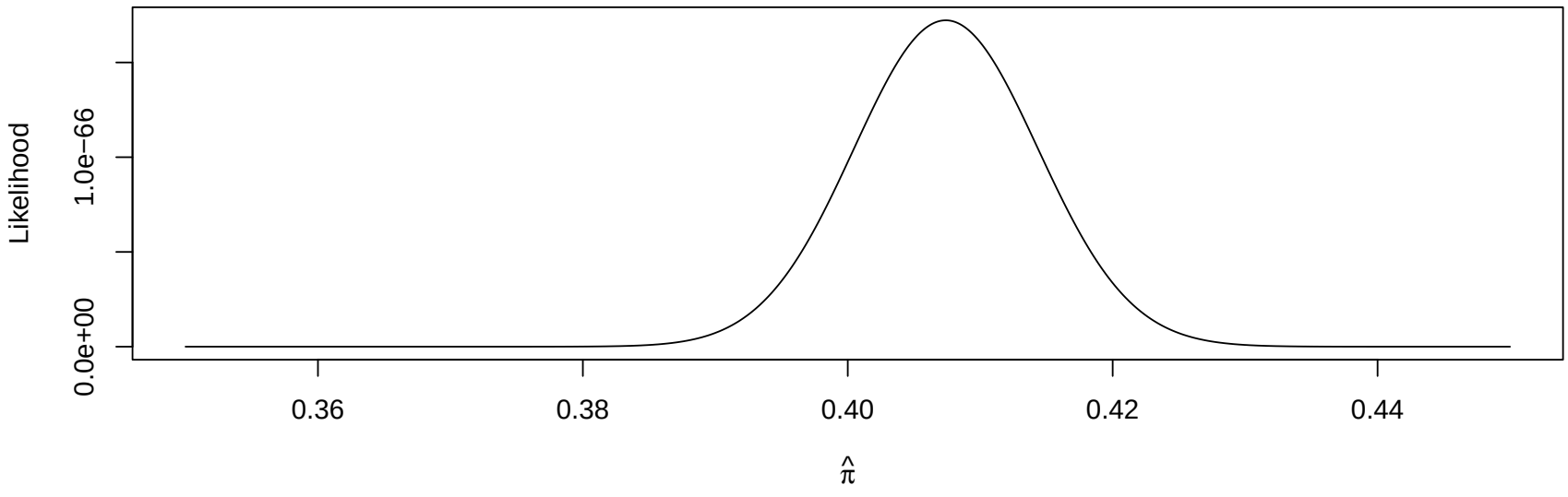
Finding the proportion of orchids

```
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(pi)), ylab="Li
```



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(pi)), ylab="Li
```



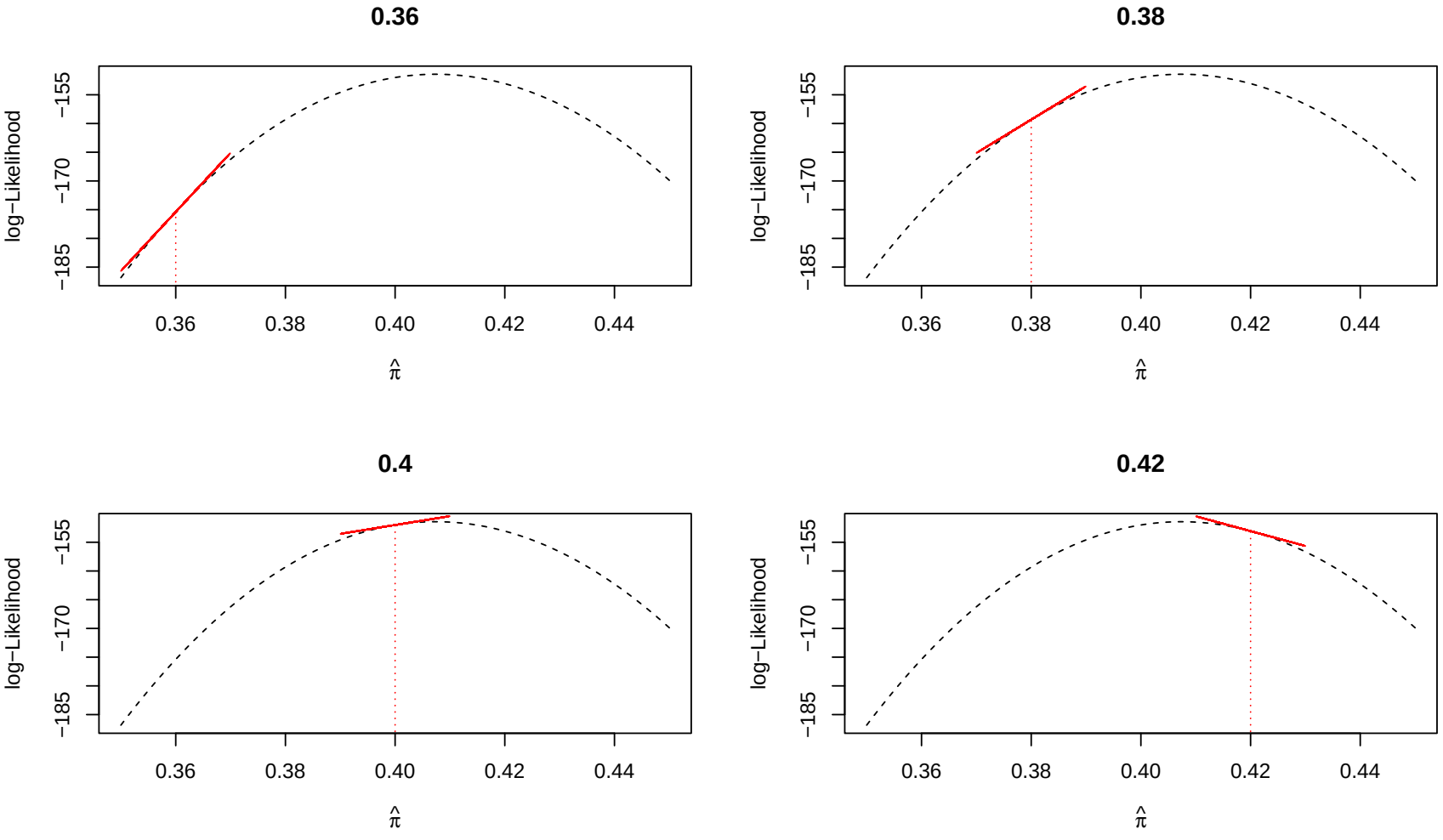
Maximising the likelihood

Trying many values (grid) is very inefficient

We can:

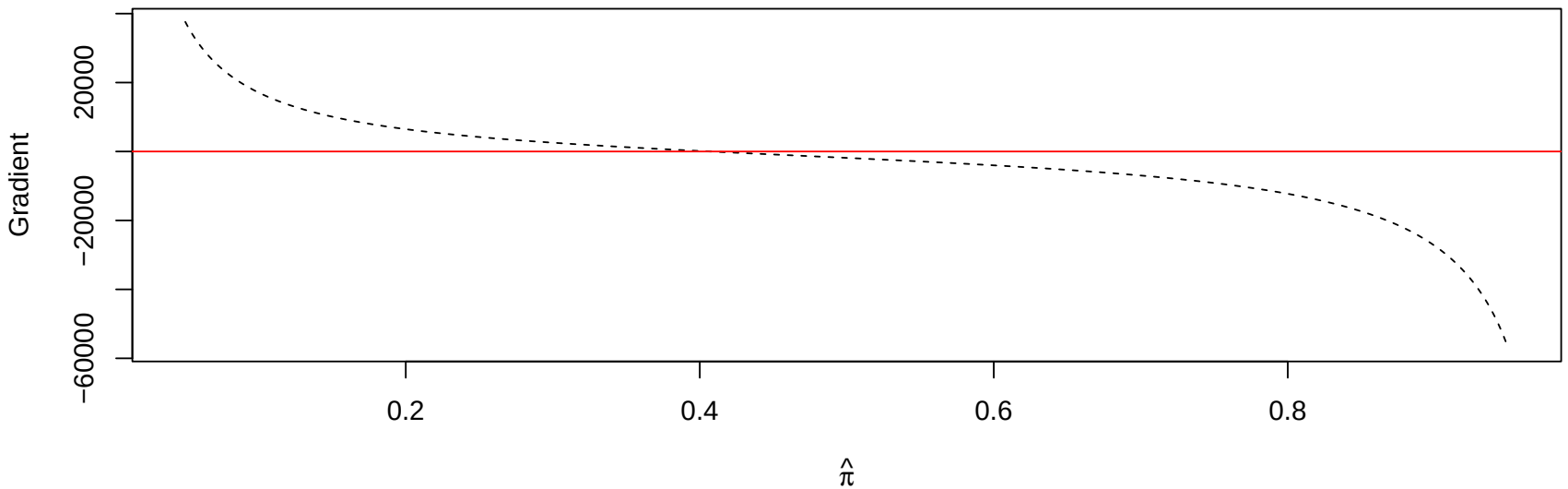
- analytically: do mathematics
- numerically: use an algorithm (as in GLMs)
- simulation: try many values

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(pi)),
     ylab="Gradient", lty = "dashed")
abline(h=0, col = "red")
```



Finding the maximum: mathy bits

Our function:

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

Slope of the likelihood:

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

Estimator:

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

(i.e., the proportion of successes!)

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)
```

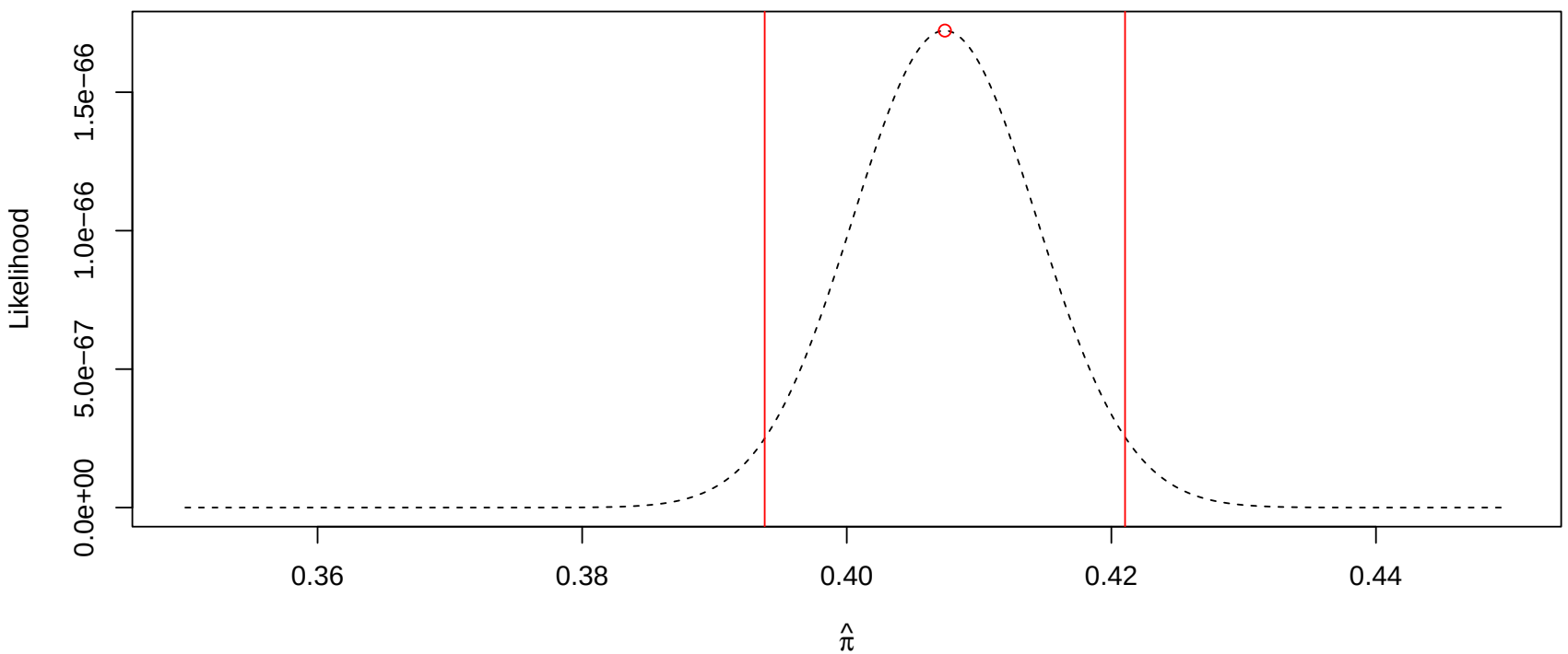
```
## $maximum
## [1] 0.4074027
##
## $objective
## [1] -151.4268
```

- Usually there is more than 1 parameter, much harder

Uncertainty

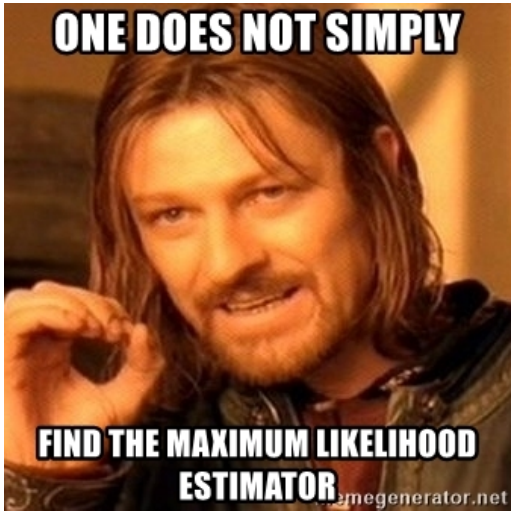
(an estimate of) Width of the likelihood:

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



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

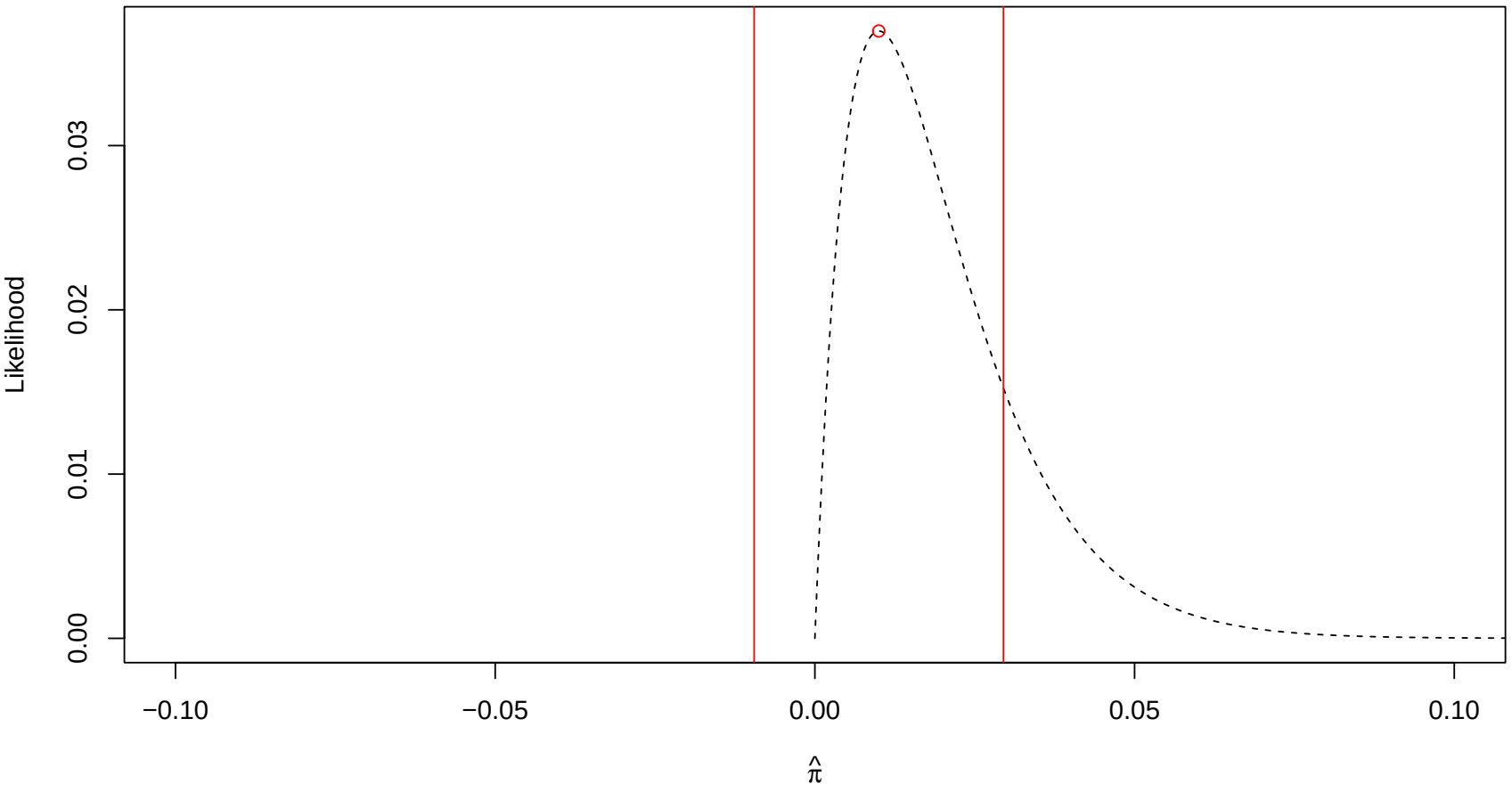


95% Confidence intervals

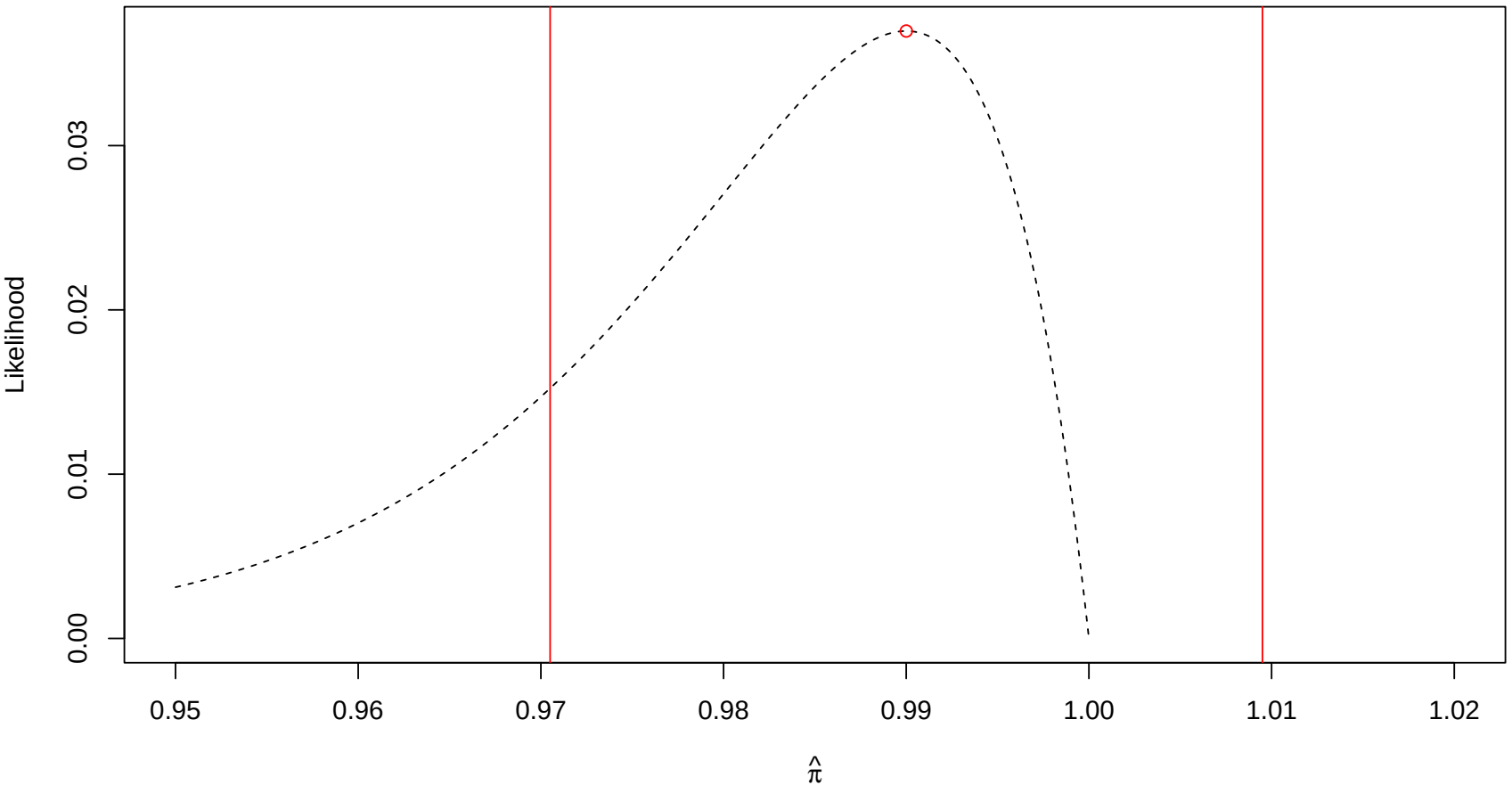
Estimate of the range that the true parameter will fall in 95% of the time.

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

Why not?



Why not? (2)


Likelihood
0.00
0.01
0.02
0.03
0.95
0.96
0.97
0.98
0.99
1.00
1.01
1.02
$\hat{\pi}$

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:

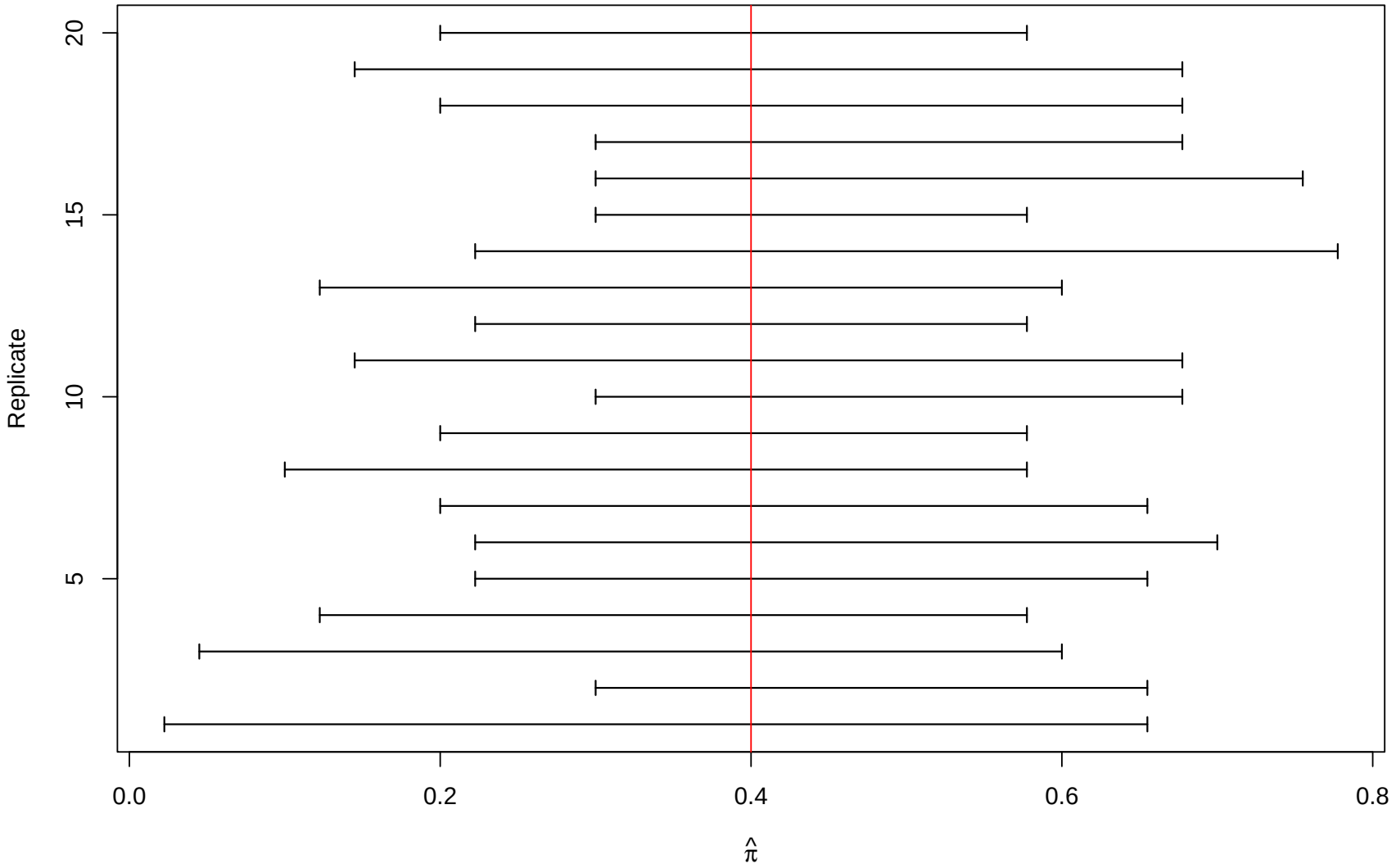
- Asymptotic normality
- inverse Hessian gives covariance of estimators

- 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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