Maximum Likelihood Estimation

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GV903: Advanced Research Methods, Week 11

University of Essex

1. Conceptual Introduction

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- We can come up with linear models for other outcome distributions, like binary or Poisson-distributed data and plug them in.
- In fact, we can use *any* distribution as an underlying population process.

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- Easy: take the product of all individual probabilities because the probabilities are independent from each other.
- We can leverage this idea for forming a likelihood function, too.

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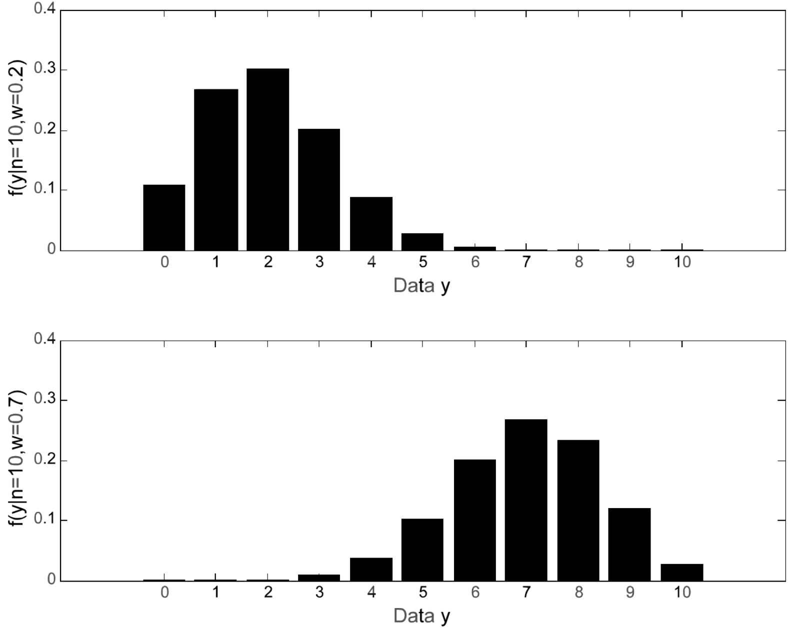
- $\mathcal{L}(\theta|Y)$.
- The two are in principle identical, except you ask the other way around. What is the model, given the observed data? Rather than what are the expected data, given a known model?

2. Example: Binomial Distribution

Binomial Sampling, $n = 10$ and $w = 0.2$ or $w = 0.7$



Binomial Probability Function

Multiplication of probabilities:

$$f(y = (y_1, y_2, \ldots, y_n) \mid w) = f_1(y_1 \mid w)\, f_2(y_2 \mid w) \cdots f_n(y_m \mid w).$$

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Binomial probability function, more generally:

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I. e., we insert the probability parameter first and then get the expected observations.

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$$L(w \mid n = 10, y = 7) = f(y = 7 \mid n = 10, w)$$
$$= \frac{10!}{7!3!} w^7 (1 - w)^3 \quad (0 \leqslant w \leqslant 1).$$

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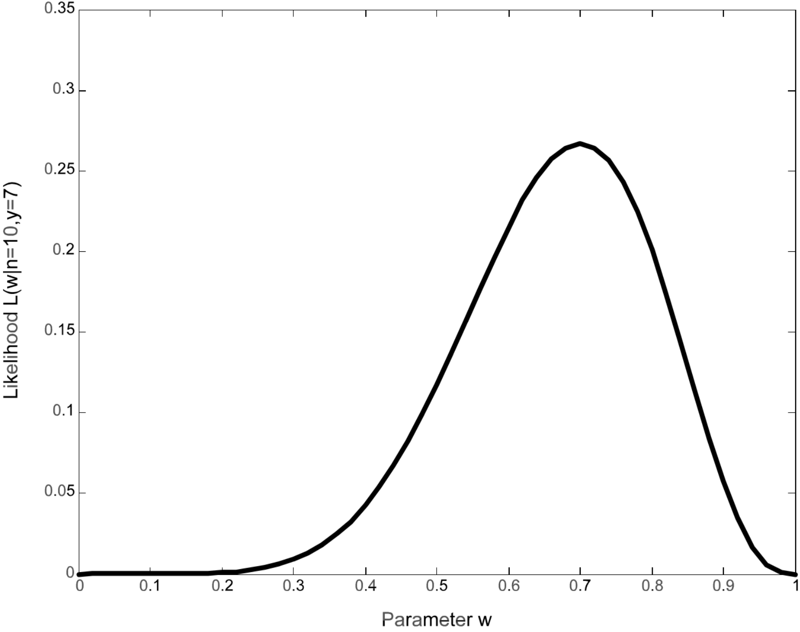
I. e., now we insert the observations first and then solve for the parameter w.

The Likelihood Function for $w = 0.7$



3. MLE: The General Procedure

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3. Take the first derivative and set zero to find the maximum:

$$\frac{\partial \ln L(w|y)}{\partial w_i} = 0$$

4. Take the second derivative to verify this is a maximum, not a minimum:

$$\frac{\partial^2 \ln L(w|y)}{\partial w_i^2} < 0.$$

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Step 1: formulate the correct PMF:

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Step 4: Second derivative:

$$\frac{d^2 \ln L(w \mid n = 10, y = 7)}{dw^2} = -\frac{7}{w^2} - \frac{3}{(1-w)^2}$$

$$= -47.62 < 0$$

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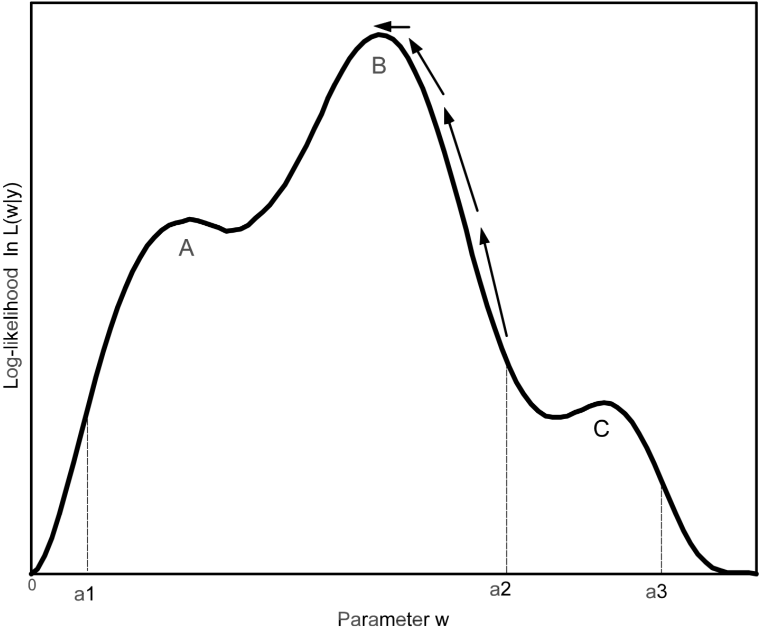
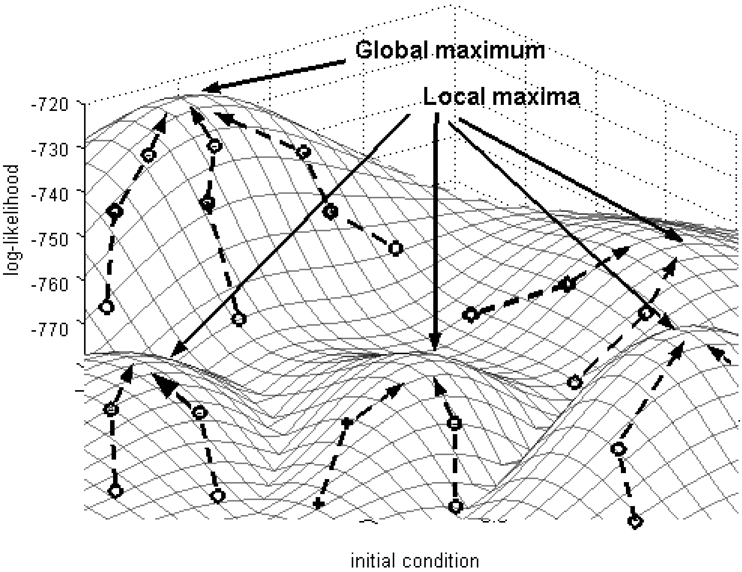
An optimization algorithm needs to find the maximum, for example Newton-Raphson or BFGS.

Iterative Optimization to Find the MLE

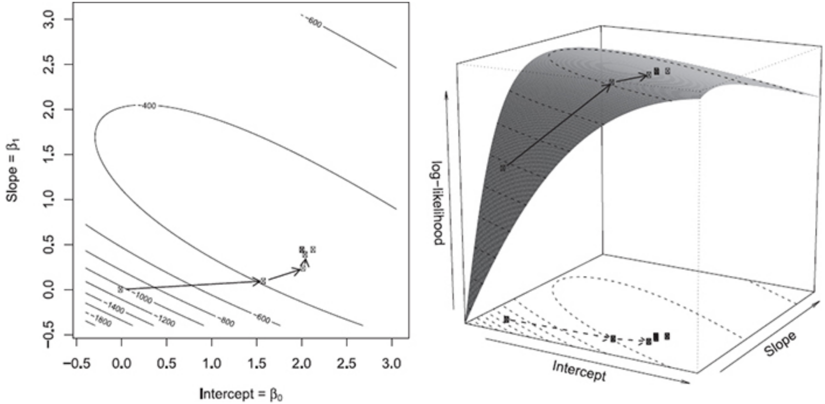


Multidimensional Likelihood and Local Maxima

Source: Akbar et al 2019: Statistical Analysis of Wireless Systems Using Markov Models



Newton-Raphson Optimization for Linear Models



4. Example: Sample Mean

You should know the PDF of the normal distribution (here with $\sigma = 1$ fixed):

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

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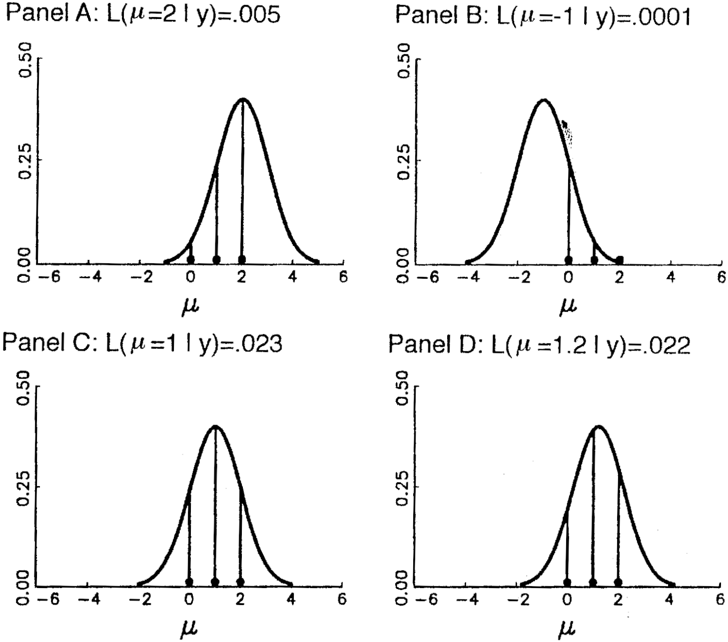
Let's say the three observed values are 0, 1, and 2. We can take a few "guesses" of μ and evaluate the likelihood...

Four Guesses of μ: $\mu = 1$ Maximizes the Likelihood



5. Re-Interpreting the Linear Model

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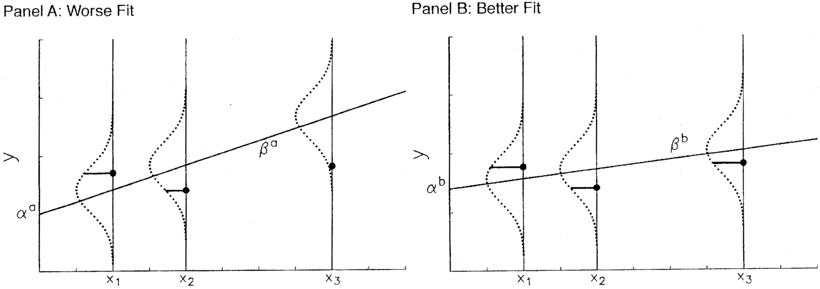

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The corresponding likelihood function (i. e., for all data):

$$L(\alpha, \beta, \sigma \mid \mathbf{y}, \mathbf{X}) = \prod_{i=1}^{N} \frac{1}{\sigma}\,\phi\left(\frac{y_i - [\alpha + \beta x_i]}{\sigma}\right)$$

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We can now compute the first and second derivative to maximize this likelihood. This will yield $\hat{\boldsymbol{\beta}}$ and $\hat{\sigma}$.

MLE for the Linear Model

Take the log (note how this replaces product by sum operator):

$$\ln L(\alpha, \beta, \sigma \mid \mathbf{y}, \mathbf{X}) = \sum_{i=1}^{N} \ln \frac{1}{\sigma} \phi\left(\frac{y_i - [\alpha + \beta x_i]}{\sigma} \right)$$

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We can now compute the first and second derivative to maximize this likelihood. This will yield $\hat{\boldsymbol{\beta}}$ and $\hat{\sigma}$.

We can do this analytically for the linear model. (In most cases, we would need an optimization algorithm.)

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Think of this as the multivariate version of the second derivative for testing for a maximum of the log likelihood.

Fisher Information Matrix and VCOV

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6. MLE in `R`

MLE in R (see Monogan 2015)

Binomial likelihood function with y heads, n trials, π probability:
$L(\pi|n, y) = \pi^{y}(1 - \pi)^{n-y}$

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Write this as an R function:

```
binomial.loglikelihood <- function(prob, y, n) {
   loglikelihood <- y*log(prob) + (n-y)*log(1-prob)
   return(loglikelihood)
}
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   return(loglikelihood)
}
```

Use the `optim` function to optimize the likelihood given fixed `y`, `n`:

```
test <- optim(c(.5),                # starting value for prob
   binomial.loglikelihood,          # the log-likelihood function
   method="BFGS",                   # optimization method
   hessian=TRUE,                    # return numerical Hessian
   control=list(fnscale=-1),        # maximize instead of minimize
   y=43, n=100)                     # the data
print(test)
```

MLE in R

This yields a list object with several slots:

```
$par
[1] 0.4300015

$value
[1] -68.33149

$counts
function gradient
      13        4

$convergence
[1] 0

$message
NULL

$hessian
          [,1]
[1,] -407.9996
```

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```

par lists the estimated π parameter.

MLE in R

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```

`value` shows the log-likelihood of our final solution.

MLE in R

This yields a list object with several slots:

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$counts
function gradient
      13        4

$convergence
[1] 0

$message
NULL

$hessian
          [,1]
[1,] -407.9996
```

`counts` shows how often `optim` called the function and gradient.

MLE in R

This yields a list object with several slots:

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$value
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function gradient
      13        4

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[1] 0

$message
NULL

$hessian
          [,1]
[1,] -407.9996
```

`convergence`: 0 means successfully converged to maximum.

This yields a list object with several slots:

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```

`message`: Messages from the function during optimization.

MLE in R

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```
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[1] 0

$message
NULL

$hessian
          [,1]
[1,] -407.9996
```

`hessian`: Hessian matrix (here: only one parameter).

MLE in R

We can now proceed to compute the standard error(s):

```
sqrt(diag(solve(-test$hessian)))
```

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```
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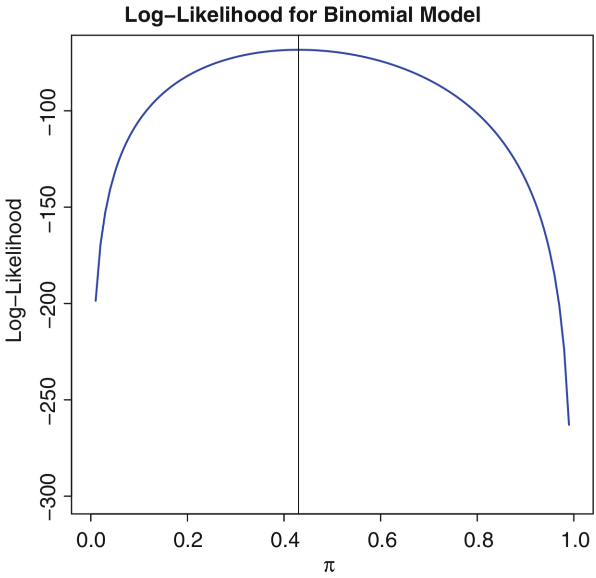
Only one parameter. It's easy to plot the likelihood function:

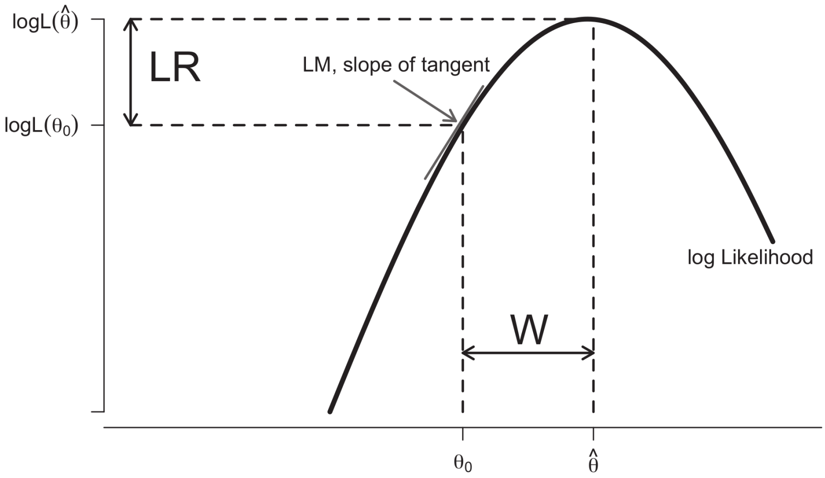
```
ruler <- seq(0,1,0.01)
loglikelihood <- binomial.loglikelihood(ruler, y=43, n=100)
plot(ruler, loglikelihood, type="l", lwd=2, col="blue",
   xlab=expression(pi),ylab="Log-Likelihood",ylim=c(-300,-70),
   main="Log-Likelihood for Binomial Model")
abline(v=.43)
```

MLE in R: The Likelihood Function



7. Diagnostics and Goodness of Fit

Likelihood Ratio Test, Wald Statistic, and LM Test



The Likelihood Ratio Test (LR Test)

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$$\mathrm{LR}(\boldsymbol{\theta}_R, \boldsymbol{\theta}_G \mid \mathbf{x}) = -2 \log \frac{\mathcal{L}(\boldsymbol{\theta}_R \mid \mathbf{x})}{\mathcal{L}(\boldsymbol{\theta}_G \mid \mathbf{x})}$$

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It follows a χ^2_{g-r} distribution with $g - r$ degrees of freedom.

A similar diagnostic is the *model deviance*, the log-likelihood difference between a model and a saturated model (with as many parameters as observations). It is sometimes used to compute the difference between residual deviance and null deviance.

AIC and BIC

The most common goodness-of-fit measures for MLE are AIC and BIC.

Akaike Information Criterion (AIC):

$$\mathsf{AIC} = -2 \log \hat{\mathcal{L}} + 2k$$

Bayesian Information Criterion (BIC):

$$\mathsf{BIC} = -2 \log \hat{\mathcal{L}} + k \log n$$

where k is the number of parameters and n is the number of observations.

Both measures penalise the inclusion of additional parameters.

Smaller values are "better". Only use for model comparison with the same data! Never interpret the absolute value of AIC or BIC!

Concluding Thoughts: Why Do We Need MLE?

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- MLE is much more flexible.
- Flexibility comes at a price: computational cost and complexity.
- Proper theoretical foundation for inference.
- MLE will allow us to look at models for various outcome distributions in the spring, such as binary, count, and ordinal DVs. This is called *generalized linear model* (GLM).

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- MLE will allow us to look at models for various outcome distributions in the spring, such as binary, count, and ordinal DVs. This is called *generalized linear model* (GLM).
- The MLE framework is also the starting point for Bayesian statistics (not covered in this module).