## Maximum likelihood estimation

Peter Hoff Duke STA 610 Estimation frameworks

Review of ML estimation

ML for HNM

### Method of moments

```
aovfit<-anova(lm(y~as.factor(g)) )</pre>
MSG<-aovfit[1,3]
MSE<-aovfit[2,3]
t2<-(MSG-MSE)/n
s2<-MSE
t2; sqrt(t2)
##
## 0.3840768
## 1
## 0.6197393
s2; sqrt(s2)
## [1] 1.787206
## [1] 1.336864
mean(y)
## [1] 16.3064
```

### Maximum likelihood estimation

lmer

package:lme4

 ${\tt R} \ {\tt Documentation}$ 

Fit Linear Mixed-Effects Models

Description:

Fit a linear mixed-effects model (LMM) to data, via REML or maximum likelihood.

#### Usage:

```
lmer(formula, data = NULL, REML = TRUE, control = lmerControl(),
    start = NULL, verbose = OL, subset, weights, na.action,
    offset, contrasts = NULL, devFunOnly = FALSE)
```

```
library(lme4)
lmer(y~1+(1|g))
## Linear mixed model fit by REML ['lmerMod']
## Formula: y ~ 1 + (1 | g)
## REML criterion at convergence: 177.9876
## Random effects:
## Groups Name
                       Std.Dev.
## g
         (Intercept) 0.6197
## Residual
                        1.3369
## Number of obs: 50, groups: g, 10
## Fixed Effects:
## (Intercept)
##
        16.31
```

### A more complicated example

```
nels[1:10,]
##
      school enroll flp public urbanicity hwh
                                                  ses mscore
## 1
        1011
                   5
                                              2 -0.23
                       3
                                      urban
                                                       52.11
## 2
        1011
                   5
                       3
                                     urban
                                              0 0.69
                                                       57.65
## 3
        1011
                                     urban
                                              4 -0.68
                                                       66.44
## 4
        1011
                                     urban
                                              5 -0.89
                                                       44.68
## 5
        1011
                                     urban
                                              3 -1.28
                                                       40.57
                       3
## 6
        1011
                                     urban
                                              5 -0.93
                                                       35.04
## 7
        1011
                       3
                                     urban
                                              1 0.36
                                                       50.71
                       3
## 8
        1011
                                     urban
                                              4 -0.24
                                                       66.17
                                                       46.17
## 10
        1011
                                     urban
                                              8 -1.07
## 11
        1011
                              1
                                      urban
                                              2 -0.10
                                                       58.76
```

# A more complicated example

$$\mathbf{y}_{i,j} = \left(\beta_0 + \frac{\beta_{0,j}}{\beta_{0,j}}\right) + \beta_1 \times \mathsf{flp}_j + \beta_2 \times \mathsf{enroll}_j + \left(\beta_3 + \frac{\beta_{3,j}}{\beta_{3,j}}\right) \times \mathsf{ses}_{i,j} + \epsilon_{i,j}$$

 $\verb|fit<-lmer(mscore"flp+enroll+ses+(ses|school), data=nels, REML=FALSE)|$ 

```
summary(fit)
## Linear mixed model fit by maximum likelihood ['lmerMod']
## Formula: mscore ~ flp + enroll + ses + (ses | school)
     Data: nels
##
##
       ATC
##
               BIC logLik deviance df.resid
## 92397.7 92457.5 -46190.9 92381.7 12966
##
## Scaled residuals:
      Min 1Q Median 3Q
                                   Max
## -3.9797 -0.6399 0.0180 0.6681 4.5053
##
## Random effects:
## Groups Name
                    Variance Std.Dev. Corr
## school (Intercept) 9.004 3.001
##
           ses
                     1.600 1.265
                                      0.05
                      67.260 8.201
## Residual
## Number of obs: 12974, groups: school, 684
##
## Fixed effects:
             Estimate Std. Error t value
## (Intercept) 55.429341 0.402910 137.573
## flp
        -2.411521 0.185312 -13.013
            0.007095 0.082024 0.087
## enroll
## ses
            4.116881 0.125381 32.835
##
## Correlation of Fixed Effects:
##
        (Intr) flp enroll
## flp -0.815
## enroll -0.300 -0.193
## ses
        -0.202 0.212 0.007
```

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- Θ is the set of parameter values
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$$\{p(y|\mu,\sigma^2) = (2\pi\sigma^2)^{-1/2} \exp\{-(y-\mu)^2/(2\sigma^2)\}, \mu \in \mathbb{R}, \sigma^2 \in \mathbb{R}^+\}.$$

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- $\theta = \{\mu, \sigma^2\}$  is the parameter (or are the parameters)
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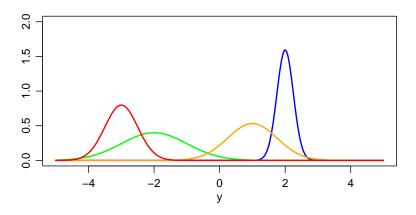
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Estimation: Obtaining a value  $\hat{\theta} \in \Theta$  that "best" represents the population.

Inference: Describing how well  $\hat{\theta}$  represents the population.

Inference includes things like: confidence intervals, hypotheses tests.

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$$Pr(A \text{ and } B) = Pr(A) \times Pr(B).$$

Independent observations: If  $y_1$  and  $y_2$  are independent observations, then

$$\begin{aligned} \rho_{y_1y_2}(y_1, y_2|\theta) &= \rho(y_1|\theta) \times \rho(y_2|\theta) \\ &= \prod_{i=1}^2 \rho(y_i|\theta) \end{aligned}$$

**Independent sample:** If  $y = (y_1, \dots, y_n)$  are independent observations, then

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# Suppose we are sampling people from a population and recording whether or not they have a particular disease.

Let  $y_i \in \{0,1\}$  depending on if they are uninfected or infected.

A natural model is the binomial/binary model

$$y_1, \ldots, y_n \sim \text{i.i.d. binary}(\theta), \ \theta \in [0, 1]$$

#### In this model

- The parameter is  $heta \in [0,1]$
- The probability density is

$$p(y|\theta) = \begin{cases} (1-\theta) & \text{if } y = 0\\ \theta & \text{if } y = 1 \end{cases}$$

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#### **Foreshadowing**

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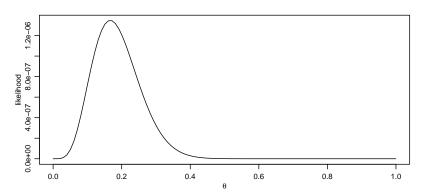
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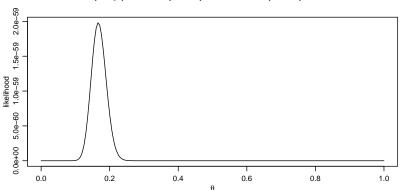
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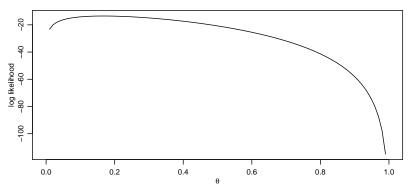
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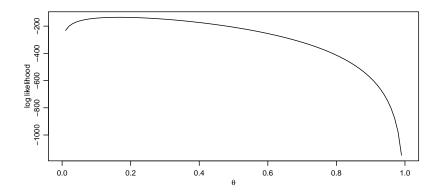
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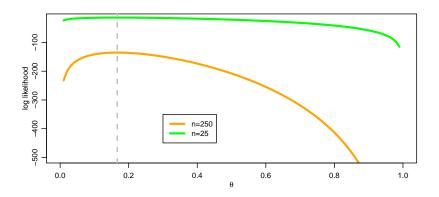
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# Comparing log-likelihoods



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# Finding the MLE

Recall from calculus that the *tangent* or *derivative* of a function, at a local maximum, will be zero. This tells us how to find the MLE:

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$$egin{aligned} rac{d}{d heta}I( heta:m{y}) &= rac{d}{d heta}\left(\sum y_i imes \log heta + (n-\sum y_i) imes \log(1- heta)
ight) \ &= rac{\sum y_i}{ heta} - rac{n-\sum y_i}{1- heta} \end{aligned}$$

#### Therefore

$$\frac{dl(\theta:y)}{d\theta}|_{\theta=\hat{\theta}} = \frac{\sum y_i}{\hat{\theta}} - \frac{n - \sum y_i}{1 - \hat{\theta}} = 0 \text{ if}$$

$$\frac{\sum y_i}{\hat{\theta}} = \frac{n - \sum y_i}{1 - \hat{\theta}}$$

$$\sum y_i - \hat{\theta} \sum y_i = \hat{\theta} n - \hat{\theta} \sum y_i$$

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So not surprisingly, the MLE is the sample proportion  $\sum y_i/n$ .

The precision of the MLE (how well it estimates the truth) depends on the second derivative, or curvature, of the log-likelihood.

$$\frac{d^2l(\theta:y)}{d\theta^2} = -\frac{\sum y_i}{\theta^2} - \frac{n - \sum y_i}{(1-\theta)^2}$$

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In many problems, the inverse of the information gives a variance estimate:

$$extsf{Var}[\hat{m{ heta}}] pprox 1/I_n$$
  $extsf{sd}(\hat{m{ heta}}) pprox \sqrt{1/I_n}$   $extsf{se}(\hat{m{ heta}}) = \sqrt{1/I_n}$ 

For the binomial model, 
$$I_n=n/[\hat{ heta}(1-\hat{ heta})]$$
, so  ${\sf Var}[\hat{ heta}]pprox \hat{ heta}(1-\hat{ heta})/n$   ${\sf sd}(\hat{ heta})pprox \sqrt{\hat{ heta}(1-\hat{ heta})/n}$   ${\sf se}(\hat{ heta})=\sqrt{\hat{ heta}(1-\hat{ heta})/n}$ 

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 $\{\epsilon_{i,j}\} \sim \text{iid } N(0, \sigma^2)$   
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#### Parameters to estimate:

- Fixed effects: μ
- Variance components:  $\sigma^2$ ,  $\tau^2$
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#### Data:

$$\mathbf{y} = (y_{1,1}, \dots, y_{n_j,1}, \dots, y_{1,m}, \dots, y_{n_m,m})$$
  
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#### Likelihood:

$$I(\mu, \sigma^2, \tau^2 : \mathbf{y}) = p(\mathbf{y}|\mu, \tau^2, \sigma^2)$$

- observations within groups are correlated;
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# Likelihood contribution from a single group

$$y_{i,j} = \mu + a_j + \epsilon_{i,j}$$
  
 $\epsilon_{1,j}, \dots, \epsilon_{n_j,j} \sim \text{iid } N(0, \sigma^2)$   
 $a_j \sim N(0, \tau^2)$ 

As we've discussed, the  $y_{i,j}$ 's are normal with

- $\mathsf{E}[y_{i,j}|\mu] = \mu$
- $Var[y_{i,j}|\mu] = \sigma^2 + \tau^2$
- $Cov[y_{i_1,j}, y_{i_2,j}|\mu] = \tau^2$

In vector form, we can express this as follows:

$$\mathsf{E}[\mathbf{y}_{j}|\mu] = \begin{pmatrix} \mu \\ \mu \\ \vdots \\ \mu \end{pmatrix} = \mu \mathbf{1} \quad \mathsf{Cov}[\mathbf{y}_{j}|\mu] = \begin{pmatrix} \sigma^{2} + \tau^{2} & \tau^{2} & \cdots & \tau^{2} \\ \tau^{2} & \sigma^{2} + \tau^{2} & \cdots & \tau^{2} \\ \vdots & \vdots & & \vdots \\ \tau^{2} & \tau^{2} & \cdots & \sigma^{2} + \tau^{2} \end{pmatrix}$$

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The density of a general multivariate normal  $(\theta, \Sigma)$  distribution is

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# Computing the (minus) log-likelihood

```
mll.oneway
## function(mus2t2,y,g)
##
## {
##
     mu<-mus2t2[1]; s2<-mus2t2[2]; t2<-mus2t2[3]
##
##
     11<-0
##
     for(gj in sort(unique(g)))
##
##
##
##
##
       nj<-sum(g==gj)
##
       S<-diag(s2,nj) + matrix(t2,nj,nj)
##
##
       11<-11+1dmvnorm(y[g==gi],mu,S)
##
##
##
##
## -11
##
## }
```

## Example: Wheat data

```
mll.oneway( c(16.3, 1.787, 0.31 ), y,g)
##
            [,1]
## [1,] 88.58541
mll.oneway( c(15, 1.787, 0.31 ), y,g)
##
            [,1]
## [1,] 101.3711
mll.oneway( c(16.3, 2, 0.31 ), y,g)
            [,1]
##
## [1,] 88.71672
mll.oneway( c(16.3, 1.787, 0.4), y,g)
##
            [,1]
## [1,] 88.62378
```

## Optimization in R

```
fit.ml<-optim(c(15,1,1),mll.oneway,gr=NULL,y=y,g=g,lower=c(-Inf,0,0),method="L-BFGS-B",hessian=TRUE)
fit.ml
## $par
## [1] 16.3063995 1.7872063 0.3099255
##
## $value
## [1] 88.5851
##
## $counts
## function gradient
##
        16
                 16
##
## $convergence
## [1] 0
##
## $message
## [1] "CONVERGENCE: REL_REDUCTION_OF_F <= FACTR*EPSMCH"
##
## $hessian
##
                     [,2]
## [1,] 1,498426e+01 2,186695e-06 1,090683e-05
## [2,] 2,186695e-06 6,710598e+00 2,245294e+00
## [3,] 1.090683e-05 2.245294e+00 1.122654e+01
```

#### The MLEs are

$$\hat{\mu} = 16.3063995$$
,  $\hat{\sigma}^2 = 1.7872063$ ,  $\hat{\tau}^2 = 0.3099255$ 

### For maximum likelihood estimation in general,

- $\hat{\theta}_{MLE} \rightarrow \theta$  as the sample size goes to infinity (if the model is correct);
- $\hat{\theta} \sim \text{normal}(\theta, \text{Var}[\hat{\theta}])$ , where
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The observed information matrix is the (matrix of) second derivative(s) of the negative log-likelihood function at the MLE (aka the Hessian):

$$I_n(\hat{\theta}: \mathbf{y}) = \{-\frac{\partial^2 I(\theta: \mathbf{y})}{\partial \theta_i \partial \theta_k}\}|_{\theta = \hat{\theta}}$$

The inverse of the information matrix gives an estimate of the variance/covariance of the MLE's:

$$Var[\hat{\theta}:y] \approx I_n^{-1}(\hat{\theta}:y)$$

- $\sqrt{I_{ii}^{-1}}$  gives an approximate standard error for  $\theta_k$
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- The MLE plus and minus 2 standard errors gives a rough confidence interval for the parameters.

$$\Pr(\theta \in \hat{\theta} \pm 2 \times se[\hat{\theta}]) \approx 0.95$$

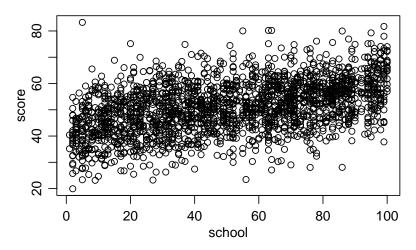
```
theta.wheat <- fit.ml $par
theta wheat
## [1] 16.3063995 1.7872063 0.3099255
I<-fit.ml$hessian
V.wheat<-solve(I)
V.wheat
##
                [,1] [,2]
                                           [.3]
## [1.] 6.673668e-02 -5.694851e-11 -6.482475e-08
## [2,] -5.694851e-11 1.597051e-01 -3.194081e-02
## [3.] -6.482475e-08 -3.194081e-02 9.546274e-02
sqrt(diag(V.wheat))
## [1] 0.2583344 0.3996312 0.3089705
theta.wheat+2*sqrt(diag(V.wheat))
## [1] 16.8230684 2.5864686 0.9278664
theta.wheat-2*sqrt(diag(V.wheat))
## [1] 15.7897307 0.9879440 -0.3080154
```

## Fitting via 1me4: Wheat

```
fit.wheat<-lmer(v~1+(1|g),REML=FALSE)
summary(fit.wheat)
## Linear mixed model fit by maximum likelihood ['lmerMod']
## Formula: v ~ 1 + (1 | g)
##
      AIC BIC logLik deviance df.resid
##
## 183.2 188.9 -88.6 177.2 47
##
## Scaled residuals:
## Min 1Q Median 3Q Max
## -2.7913 -0.6035 0.1311 0.6520 1.7262
##
## Random effects:
## Groups Name Variance Std.Dev.
## g (Intercept) 0.3099 0.5567
## Residual
                     1.7872 1.3369
## Number of obs: 50, groups: g, 10
##
## Fixed effects:
  Estimate Std. Error t value
##
## (Intercept) 16.3064 0.2583 63.12
theta.wheat
## [1] 16.3063995 1.7872063 0.3099255
sqrt(diag(V.wheat))
## [1] 0.2583344 0.3996312 0.3089705
```

# **NELS** example

100 randomly sampled schools from the NELS dataset



# Analysis of all schools

```
fit.ml.nels<-optim(c(50, 1, 1), mll.oneway, gr = NULL, y = nels$mscore, g = nels$school, lower = c(-Inf,
fit.ml.nels
## $par
## [1] 50.93914 73.70881 23.63382
##
## $value
## [1] 46956.63
##
## $counts
## function gradient
##
                  27
##
## $convergence
## [1] 0
##
## $message
## [1] "CONVERGENCE: REL_REDUCTION_OF_F <= FACTR*EPSMCH"
##
## $hessian
##
              [,1] [,2] [,3]
## [1,] 24.35837087 -0.01576882 0.04913818
## [2,] -0.01576882 1.13128044 0.03026526
## [3,] 0.04913818 0.03026526 0.42089960
```

#### The MLEs are

$$\hat{\mu} = 50.9391407$$
,  $\hat{\sigma}^2 = 73.708808$ ,  $\hat{\tau}^2 = 23.6338229$ 

```
theta.nels<-fit.ml.nels$par
theta.nels
## [1] 50.93914 73.70881 23.63382
I<-fit.ml.nels$hessian
V.nels<-solve(I)
V.nels
##
                [,1] [,2]
                                          [.3]
## [1.] 0.0410638760 0.0007019913 -0.004844505
## [2,] 0.0007019913 0.8856698641 -0.063767034
## [3,] -0.0048445047 -0.0637670344 2.381014344
sqrt(diag(V.nels))
## [1] 0.2026422 0.9411003 1.5430536
theta.nels+2*sqrt(diag(V.nels))
## [1] 51.34443 75.59101 26.71993
theta.nels-2*sqrt(diag(V.nels))
## [1] 50.53386 71.82661 20.54772
```

## Fitting via 1me4: Math scores

```
fit.nels<-lmer(mscore~1+(1|school),REML=FALSE,data=nels)
summarv(fit.nels)
## Linear mixed model fit by maximum likelihood ['lmerMod']
## Formula: mscore ~ 1 + (1 | school)
##
     Data: nels
##
##
       ATC
                BIC logLik deviance df.resid
## 93919.3 93941.7 -46956.6 93913.3 12971
##
## Scaled residuals:
              1Q Median 3Q
      Min
                                     Max
## -3.8112 -0.6534 0.0093 0.6732 4.6999
##
## Random effects:
## Groups Name
                       Variance Std.Dev.
## school (Intercept) 23.63 4.861
## Residual
                       73.71 8.585
## Number of obs: 12974, groups: school, 684
##
## Fixed effects:
             Estimate Std. Error t value
## (Intercept) 50.9391 0.2026 251.4
theta nels
## [1] 50.93914 73.70881 23.63382
sqrt(diag(V.nels))
## [1] 0.2026422 0.9411003 1.5430536
```

#### ANOVA, method of moments:

- Estimation:  $\hat{\mu} = \bar{y}_{...}$ ,  $\hat{\sigma}^2 = MSE$ ,  $\hat{\tau}^2 = (MSG MSE)/n$
- Inference: *F*-test for across-group differences.

#### Maximum likelihood:

- Estimation: MLEs  $\hat{\mu}, \hat{\sigma}^2, \hat{\tau}^2$
- Inference: Cls for population parameters via likelihood curvature

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