Review of maximum likelihood estimation 560 Hierarchical modeling

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1me4 software

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```
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
```

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
## 0.3840768
s2
## [1] 1.787206
sqrt(t2)
## 0.6197393
sqrt(s2)
## [1] 1.336864
mean(y)
## [1] 16.3064
```

A more complicated example

```
nels_mathdat[1:10,]
     school enroll flp public urbanicity hwh ses mscore
##
## 1
       1011
                 5
                                 urban 2 -0.23 52.11
                   3
## 2
       1011
                                 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
## 6
      1011
                                 urban 5 -0.93 35.04
## 7
       1011
                                 urban 1 0.36 50.71
## 8
       1011
                 5
                                 urban 4 -0.24 66.17
## 10
       1011
                                 urban 8 -1.07 46.17
## 11
       1011
                           1
                                 urban
                                         2 -0.10 58.76
```

A more complicated example

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

fit<-lmer(mscore~flp+enroll+ses+(ses|school),data=nels_mathdat,REML=FALSE)</pre>

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```
summary(fit)
## Linear mixed model fit by maximum likelihood ['lmerMod']
## Formula: mscore ~ flp + enroll + ses + (ses | school)
     Data: nels_mathdat
##
##
               BIC logLik deviance df.resid
       AIC
## 92397.7 92457.5 -46190.9 92381.7 12966
##
## Scaled residuals:
## Min 10 Median 30
                                   Max
## -3.9797 -0.6399 0.0180 0.6681 4.5053
##
## Random effects:
                    Variance Std.Dev. Corr
## Groups Name
## school (Intercept) 9.004 3.001
##
           ses
                     1.600 1.265 0.05
## Residual
                      67.260 8.201
## Number of obs: 12974, groups: school, 684
##
## Fixed effects:
              Estimate Std. Error t value
##
## (Intercept) 55.429339 0.402907 137.57
## flp -2.411519 0.185311 -13.01
## enroll
            0.007095 0.082023 0.09
## ses
             4.116886 0.125381
                                32.83
##
## 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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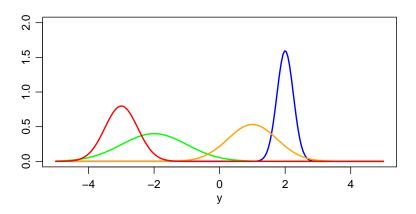
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Estimation: Obtaining a value $\hat{\theta} \in \Theta$ that "best" represents the population.

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

Inference includes things like: confidence intervals, hypotheses tests.

- a type of model based inference
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Independent events: Recall if A and B are independent events,

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

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

$$p_{y_1y_2}(y_1, y_2|\theta) = p(y_1|\theta) \times p(y_2|\theta)$$
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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 $\theta \in [0,1]$
- The probability density is

$$\rho(y|\theta) = \left\{ \begin{array}{cc} (1-\theta) & \text{if } y = 0 \\ \theta & \text{if } y = 1 \end{array} \right.,$$

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Interpretation:

 $p(y|\theta)$ tells you how probable a given outcome is, for a particular θ .

```
Quiz: If n = 3 and \theta = 1/2, what is p(\{1,0,1\}|\theta)?

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$$L(\theta: \mathbf{y}) = p(\mathbf{y}|\theta)$$

Example (binomial model): If $y = \{0, 0, 0\}$, then

$$L(\frac{1}{2}:\{0,0,0\}) = \frac{1}{8} = 0.125$$

$$L(\frac{1}{3}:\{0,0,0\}) = \frac{8}{27} \approx 0.296$$

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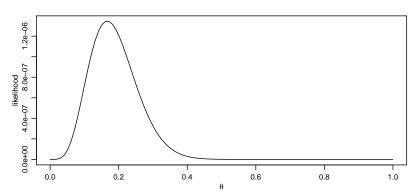
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Careful examination, or trial and error gives $\hat{\theta}=5/30=1/6=0.166\bar{6}.$

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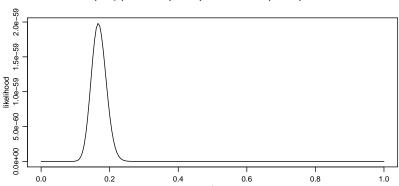
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Alternatively, we can make inference with the log-likelihood:

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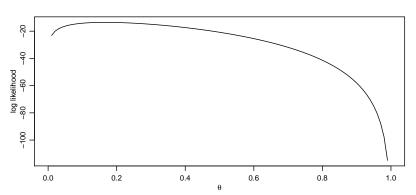
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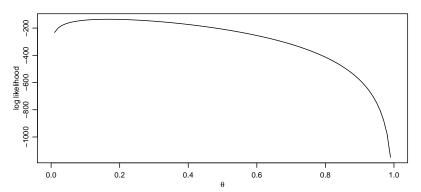
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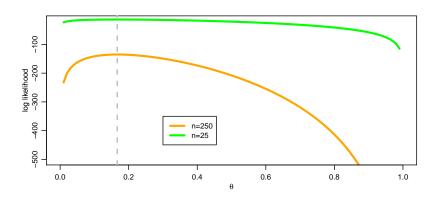
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Comparing log-likelihoods



As we've seen and discussed,

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Finding the MLE

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Let's try this for the binomial model. Recall that

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The derivative of the log-likelihood is

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

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

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

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

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

Therefore

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

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

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

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

For the binomial model, the second derivative is

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

Plugging in the MLE $\hat{\theta}$ for θ gives

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Parameters to estimate:

- Fixed effects: μ
- Variance components: σ^2 , τ^2
- Random effects: a1....am

Likelihood estimation focuses on estimation of $\theta = (\mu, \sigma^2, \tau^2)$

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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 $y_{i,i}$'s are normal with

- $E[y_{i,j}|\mu] = \mu$
- $\operatorname{Var}[y_{i,j}|\mu] = \sigma^2 + \tau^2$
- $Cov[y_{i_1,i_2},y_{i_2,i_3}]=\tau^2$

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

Likelihood contribution from a single group

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

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

- $\mathsf{E}[y_{i,j}|\mu] = \mu$
- $Var[y_{i,j}|\mu] = \sigma^2 + \tau^2$
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This means that y_i has a multivariate normal distribution.

The density of a general multivariate normal (μ, Σ) distribution is

$$p(y|\theta, \Sigma) = (2\pi)^{-p/2} |\Sigma|^{-1/2} \exp\{-(y-\theta)^T \Sigma^{-1} (y-\theta)/2\}$$

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{pmatrix} \quad \boldsymbol{\theta} = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_p \end{pmatrix} \quad \boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1^2 & \sigma_{1,2} & \cdots & \sigma_{1,p} \\ \sigma_{1,2} & \sigma_2^2 & \cdots & \sigma_{2,p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{1,p} & \sigma_{2,p} & \cdots & \sigma_p^2 \end{pmatrix}.$$

```
ldmvnorm<-function(y, theta, Sig)
{
    -.5*(
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MLEs of (μ, σ^2, τ^2) can be found by maximizing the log likelihood.

Log likelihood

$$L(\mathbf{y} : \mu, \sigma^{2}, \tau^{2}) = p(\mathbf{y}_{1}, \dots, \mathbf{y}_{m} | \mu, \sigma^{2}, \tau^{2})$$

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$$\begin{split} L(\mathbf{y}: \mu, \sigma^2, \tau^2) &= p(\mathbf{y}_1, \dots, \mathbf{y}_m | \mu, \sigma^2, \tau^2) \\ I(\mathbf{y}: \mu, \sigma^2, \tau^2) &= \log p(\mathbf{y}_1, \dots, \mathbf{y}_m | \mu, \sigma^2, \tau^2) \\ &= \log \prod_{j=1}^m p(\mathbf{y}_j | \mu, \sigma^2, \tau^2) \\ &= \sum_{j=1}^m \log p(\mathbf{y}_j | \mu, \sigma^2, \tau^2), \end{split}$$

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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==gj],mu,S)
##
##
##
     }
##
## -11
##
## }
```

Example: Wheat data

```
mll.oneway( c(16.3, 1.787, 0.384 ), y,g)
         [,1]
##
## [1,] 88.6121
mll.oneway( c(15, 1.787, 0.384 ), y,g)
## [,1]
## [1,] 100.1217
mll.oneway( c(16.3, 2, 0.384 ), y,g)
## [,1]
## [1,] 88.76881
mll.oneway( c(16.3, 1.787, 0.3), y,g)
## [,1]
## [1,] 88.58599
mll.oneway( c(16.3, 1.787, 0.2), y,g)
## [,1]
## [1,] 88.67161
```

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
               Γ.17
                    [,2] [,3]
##
## [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 MI Fs 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);
- $\hat{\theta} \stackrel{.}{\sim} \text{normal}(\theta, \text{Var}[\hat{\theta}])$, where
- $Var[\hat{\theta}] \approx -[d^2I(\theta|y)/d\theta^2]^{-1}$ for large sample sizes.

For our hierarchical normal model, this means that approximate 95% confidence intervals for (μ, τ^2, σ^2) can be obtained from the curvature of the log likelihood.

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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):

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

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

$$\operatorname{\mathsf{Var}}[\hat{ heta}:y] pprox I_n^{-1}(\hat{ heta}:y)$$

From this, we can get confidence intervals

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

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

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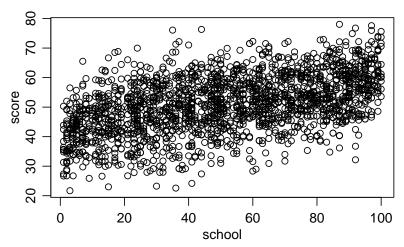
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```
theta.wheat <- fit.ml $par
theta.wheat
## [1] 16.3063995 1.7872063 0.3099255
I<-fit.ml$hessian
V.wheat<-solve(I)
V.wheat
##
                [,1] [,2]
                                           [.3]
## [1.] 6.673668e-02 -5.694851e-11 -6.482475e-08
## [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
```

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 = mscores, g = schools, lower = c(-Inf, 0, 0), m
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: Wheat

```
fit.wheat<-lmer(yield~1+(1|region),REML=FALSE)
summary(fit.wheat)
## Linear mixed model fit by maximum likelihood ['lmerMod']
## Formula: yield ~ 1 + (1 | region)
##
##
       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.
## region (Intercept) 0.3099 0.5567
## Residual
                     1.7872 1.3369
## Number of obs: 50, groups: region, 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
```

Fitting via 1me4: Schools

```
fit.nels<-lmer(mscores~1+(1|schools),REML=FALSE)
summary(fit.nels)
## Linear mixed model fit by maximum likelihood ['lmerMod']
## Formula: mscores ~ 1 + (1 | schools)
##
       AIC BIC logLik deviance df.resid
##
## 93919.3 93941.7 -46956.6 93913.3 12971
##
## Scaled residuals:
    Min 1Q Median 3Q Max
## -3.8112 -0.6534 0.0093 0.6732 4.6999
##
## Random effects:
## Groups Name Variance Std.Dev.
## schools (Intercept) 23.63 4.861
## Residual
                      73.71 8.585
## Number of obs: 12974, groups: schools, 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 $\hat{\mu}, \hat{\sigma}^2, \hat{\tau}^2$)
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What about estimation of a_j or μ_j 's \bar{a}_j

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We will consider two types of estimates of the μ_i 's:

Unbiased sample mean estimates:

$$\hat{\mu}_j = \bar{y}_j$$

Biased shrinkage estimates:

$$\hat{\mu}_{j} = \frac{n_{j}/\hat{\sigma}^{2}}{n_{j}/\hat{\sigma}^{2} + \hat{\tau}^{2}} \bar{y}_{j} + \frac{1/\hat{1}/\tau^{2}}{n_{j}/\hat{\sigma}^{2} + 1/\hat{\tau}^{2}} \bar{y}$$

The latter will be preferable when au^2 is small compared to σ^2/n_j

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