Variance component estimation methods

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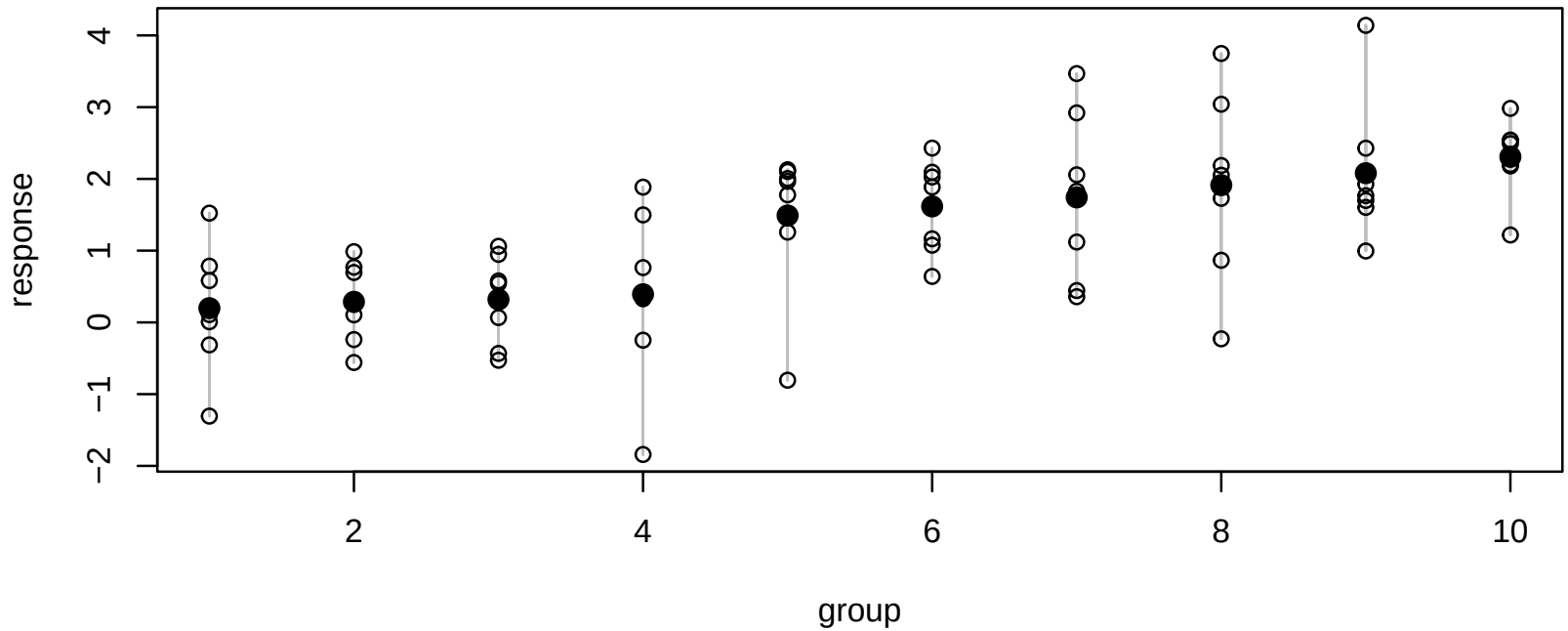
response
−2
−1
0
1
2
3
4
2
4
6
8
10
group

REML = TRUE

```
fitREML<-lmer( y ~ 1 + (1 | g) )

summary(fitREML)

## Linear mixed model fit by REML ['lmerMod']
## Formula: y ~ 1 + (1 | g)
##
## REML criterion at convergence: 208.2
##
## Scaled residuals:
##      Min       1Q   Median       3Q      Max
## -2.51361 -0.48196  0.09502  0.52383  2.33192
##
## Random effects:
##  Groups   Name        Variance Std.Dev.
##  g        (Intercept) 0.5727   0.7568
##  Residual             0.9026   0.9500
## Number of obs: 70, groups:  g, 10
##
## Fixed effects:
##             Estimate Std. Error t value
## (Intercept)   1.2346     0.2649   4.661
```

REML = FALSE

```
fitML<-lmer( y ~ 1 +  (1 | g), REML=FALSE )

summary(fitML)

## Linear mixed model fit by maximum likelihood  ['lmerMod']
## Formula: y ~ 1 + (1 | g)
##
##      AIC      BIC   logLik deviance df.resid
##    213.4    220.1   -103.7    207.4       67
##
## Scaled residuals:
##     Min      1Q  Median      3Q     Max
## -2.5317 -0.4807  0.1076  0.5275  2.3501
##
## Random effects:
##  Groups   Name        Variance Std.Dev.
##  g        (Intercept) 0.5025   0.7089
##  Residual             0.9026   0.9500
## Number of obs: 70, groups:  g, 10
##
## Fixed effects:
##             Estimate Std. Error t value
## (Intercept)   1.2346     0.2513   4.913
```

Estimator and calculation methods

$$y_{i,j} = \mu + a_j + \epsilon_{i,j}$$
$$a_1, \ldots, a_m \sim \text{ i.i.d. } N(0, \tau^2)$$
$$\{\epsilon_{i,j}\} \sim \text{ i.i.d. } N(0, \sigma^2)$$

Parameters: μ, σ^2, τ^2.

Variance component estimators: Estimators of σ^2, τ^2.

- Unbiased moment estimators (ANOVA).
- Maximum likelihood estimators.
- Restricted maximum likelihood estimators (?)

Moment estimators

Recall the unbiased ANOVA-based method of moments estimators for μ and σ^2:

$$\hat{\mu} = \bar{y} = \sum_j \sum_i y_{i,j}/(n \times m)$$

$$\hat{\sigma}^2 = \sum_j s_j^2/m.$$

We showed that $\mathrm{E}[\hat{\mu}] = \mu$ and $\mathrm{E}[\hat{\sigma}^2] = \sigma^2$. Also,

$$MSA = n \times \text{sample variance}(\bar{y}_1, \ldots, \bar{y}_m)$$

$$\mathrm{E}[MSA] = \sigma^2 + n \times \tau^2$$

This suggests we estimate τ^2 as

$$\hat{\tau}^2 = (MSA - \hat{\sigma}^2)/n,$$

in which case we have $\mathrm{E}[\hat{\tau}^2] = \tau^2$.

These are *moment-based estimators*. Normality not required for unbiasedness.

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These are *moment-based estimators*. Normality not required for unbiasedness.

```r
mean(y)
```

```
## [1] 1.234627
```

```r
anova(lm(y ~ as.factor(g)))
```

```
## Analysis of Variance Table
##
## Response: y
##              Df Sum Sq Mean Sq F value    Pr(>F)
## as.factor(g)  9 44.203  4.9115  5.4416 1.924e-05 ***
## Residuals    60 54.155  0.9026
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```r
MSA<-n*var( tapply(y,g,mean) )

MSW<-mean( tapply(y,g,var) )

MSA
```

```
## [1] 4.91148
```

```r
MSW
```

```
## [1] 0.9025845
```

```r
t2hat<-(MSA-MSW)/n

t2hat
```

```
## [1] 0.5726993
```

Maximum likelihood estimation

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

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

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

In vector form, we can express this as follows:

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

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Computing the log-likelihood

MLEs of (μ, σ^2, τ^2) can be found by maximizing the log likelihood.

Log likelihood:

$$
\begin{aligned}
L(\boldsymbol{y} : \mu, \sigma^2, \tau^2) &= p(\boldsymbol{y}_1, \ldots, \boldsymbol{y}_m | \mu, \sigma^2, \tau^2) \\
l(\boldsymbol{y} : \mu, \sigma^2, \tau^2) &= \log p(\boldsymbol{y}_1, \ldots, \boldsymbol{y}_m | \mu, \sigma^2, \tau^2) \\
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where $\log p(\boldsymbol{y}_j | \mu, \sigma^2, \tau^2)$ is the log of a multivariate normal density.

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Maximum likelihood estimates

```
fitML<-lmer(y ~ 1 + (1|g), REML=FALSE )

fixef(fitML)

## (Intercept)
##    1.234627

as.data.frame( VarCorr(fitML) )

##        grp        var1 var2      vcov     sdcor
## 1        g (Intercept) <NA> 0.5025353 0.7088973
## 2 Residual        <NA> <NA> 0.9025845 0.9500445
```

Notice:

- The estimate of μ is the same as the unbiased moment estimator.
- The estimate of τ^2 is different.

In fact, the MLE is *biased* for this variance components:

$$\mathrm{E}[\hat{\tau}^2_{MLE}] \neq \tau^2.$$

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Restricted maximum likelihood

The default estimates in `lme4` are the REML estimates.

```
fit0<-lmer(y ~ 1 + (1|g) )

fixef(fit0)

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as.data.frame( VarCorr(fit0) )

##        grp        var1 var2      vcov     sdcor
## 1        g (Intercept) <NA> 0.5726994 0.7567690
## 2 Residual        <NA> <NA> 0.9025845 0.9500445
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Notice that for this model, the estimates are the same as the unbiased moment estimates we got from ANOVA:

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mean(y)

## [1] 1.234627

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REML

REML estimates maximize an alternative "restricted" likelihood function.

- In some cases they are equivalent to unbiased moment estimators.
- In others they are different, but generally have lower bias than MLEs.

The main idea:

- Bias in MLEs of variances arise from "plugging in" the mean estimates.
- Restricted likelihoods don't involve mean parameters, so avoid "plug-in" bias.

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Simplest REML example

One sample normal model

$$y_1, \ldots, y_n \sim \text{ i.i.d. } N(\mu, \sigma^2)$$

MLEs

$$p(\mathbf{y}|\mu, \sigma^2) = (2\pi\sigma^2)^{-n/2} \exp(-\sum (y_i - \mu)^2/[2\sigma^2])$$

$$-2 \times \log p(y|\mu, \sigma^2) + c = n \log \sigma^2 + \sum (y_i - \mu)^2/\sigma^2$$

Exercise: Show that the MLEs $(\hat{\mu}_{MLE}, \hat{\sigma}^2_{MLE})$ of (μ, σ^2) are

- $\hat{\mu}_{MLE} = \bar{y}$;
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Bias of MLE variance estimates

Exercise: Show that

$$\mathsf{E}[\hat{\mu}_{MLE}] = \mu$$
$$\mathsf{E}[\hat{\sigma}^2_{MLE}] = \frac{(n-1)}{n}\sigma^2.$$

- The MLE of σ^2 is biased.
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Plug-in bias

Note that

$$\mathrm{E}[\sum_i (y_i - \bar{y})^2/n] = \sigma^2(n-1)/n$$

$$\mathrm{E}[\sum_i (y_i - \mu)^2/n] = \sigma^2$$

So the bias in the MLE can be thought of as "plug-in" bias:

- If we knew μ, then we would use the second equation to estimate σ^2.
- We don't know μ, so we simply "plug-in" an estimate $\bar{y}$.
- But $\bar{y}$ is closer to $(y_1, \ldots, y_n)$ than μ is.
- The MLE underestimates the variance.

Restricted likelihood

REML:

- Obtain an estimate of σ^2 where there is no plug-in bias.
- We need a "likelihood" that doesn't depend on μ.
- Such a likelihood can be obtained from a transformed data set.

Centering to eliminate fixed effects

The model $y_1, \ldots, y_n \sim$ i.i.d. $N(\mu, \sigma^2)$ can be written

$$\mathbf{y} = \mu\mathbf{1} + \mathbf{e}$$
$$\mathbf{e} \sim N(0, \sigma^2\mathbf{I}_n)$$

Let $\mathbf{C} = \mathbf{I} - \mathbf{1}\mathbf{1}^\top/n$. Then

$$\mathbf{C}\mathbf{1} = \mathbf{0}$$
$$\mathbf{C}\mathbf{y} = \mathbf{0} + \mathbf{C}\mathbf{e}.$$

Letting $\check{\mathbf{y}} = \mathbf{C}\mathbf{y}$, we have

$$\check{\mathbf{y}} \sim N(\mathbf{0}, \sigma^2\mathbf{C}).$$

Idea: Estimate σ^2 as the MLE of σ^2 based on $\check{\mathbf{y}}$.

Problem: $\mathbf{C}$ is a singular matrix ($\text{rank}(\mathbf{C}) = n - 1$).

Centering to eliminate fixed effects

The model $y_1, \ldots, y_n \sim$ i.i.d. $N(\mu, \sigma^2)$ can be written

$$\mathbf{y} = \mu\mathbf{1} + \mathbf{e}$$
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Let $\mathbf{C} = \mathbf{I} - \mathbf{1}\mathbf{1}^\top/n$. Then

$$\mathbf{C1} = \mathbf{0}$$
$$\mathbf{Cy} = \mathbf{0} + \mathbf{Ce}.$$

Letting $\check{\mathbf{y}} = \mathbf{Cy}$, we have

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Dimension-reduced data

The matrix $\mathbf{C}$ can be represented as $\mathbf{C} = \mathbf{N}\mathbf{N}^\top$ where

- $\mathbf{N} \in \mathbb{R}^{n \times (n-1)}$;
- $\mathbf{N}^\top \mathbf{N} = \mathbf{I}_{n-1}$;
- $\mathbf{N}^\top \mathbf{1} = \mathbf{0}$.

Dimension-reduced data

The columns of **N** are the eigenvectors of **C** having nonzero eigenvalues.

```
n<-5
C<-diag(n) - matrix(1/n,n,n)

eC<-eigen(C)
eC$val
```

```
## [1] 1.000000e+00 1.000000e+00 1.000000e+00 1.000000e+00 8.881784e-16
```

```
N<-eC$vec[,1:(n-1)]

t(N)%*%N
```

```
##               [,1]          [,2]          [,3]          [,4]
## [1,]  1.000000e+00 -1.220637e-16 -4.507497e-17 -2.922069e-17
## [2,] -1.220637e-16  1.000000e+00  1.665335e-16 -1.387779e-17
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REML

$\mathbf{N}$ can be used to transform an

- n-dimensional normal vector $\mathbf{y}$ with mean $\mu\mathbf{1}$ to an
- $(n-1)$-dimensional normal vector $\tilde{\mathbf{y}}$ with mean $\mathbf{0}$.

$$\begin{aligned} \mathbf{N}^\top \mathbf{y} = \tilde{\mathbf{y}} &= \mu \mathbf{N}^\top \mathbf{1} + \mathbf{N}^\top \mathbf{e} \\ \tilde{\mathbf{y}} &= \mathbf{0} + \tilde{\mathbf{e}} \end{aligned}$$

where $\tilde{\mathbf{e}} \sim N_{n-1}(\mathbf{0}, \sigma^2 \mathbf{N}^\top \mathbf{N}) = N_{n-1}(\mathbf{0}, \sigma^2 \mathbf{I}_{n-1})$.

The -2 log likelihood $-2 \log p(\tilde{\mathbf{y}}|\sigma^2)$ is

$$-2 \log p(\tilde{\mathbf{y}}|\sigma^2) = (n-1)\sigma^2 + \sum_{i=1}^{n-1} \tilde{y}_i^2 .$$

This is the "restricted likelihood." The (R)MLE of σ^2 based on $\tilde{\mathbf{y}}$ is

$$\hat{\sigma}^2_{REML} = \sum_i \tilde{y}_i^2 / (n-1).$$

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The final step

$$\begin{aligned}
\hat{\sigma}^2_{REML} &= \sum_i \tilde{y}_i^2/(n-1) \\
&= \tilde{\mathbf{y}}^\top \tilde{\mathbf{y}}/(n-1) \\
&= \mathbf{y}^\top C^\top C\mathbf{y}/(n-1) \\
&= \sum_{i=1}^{n} (y_i - \bar{y})^2/(n-1) = s^2.
\end{aligned}$$

So in this case,

- the REML estimate of σ^2 based $\tilde{\mathbf{y}}$ is equal to
- the (unbiased) sample variance estimate s^2.

REML for normal linear regression