

1. Use (mixed model) thermocouple calibration problem of HW8.

(a) Results match those obtained in 3(e) of HW8. The ML estimates are: $\hat{\sigma}_\gamma^2 = 0.0629$, $\hat{\sigma}_\delta^2 = 0.4441$ and $\hat{\sigma}^2 = 0.3733$.

```
> minusLstar(c(1,1,1),Y)
[1,] 15.55036
> minusLstar(c(1,1,.25),Y)
[1,] 14.30018
> optim(c(.07,.45,.37),minusLstar,Y=Y,hessian=TRUE)$par
[1] 0.06291014 0.44413348 0.37327909
```

(b) The REML estimates are: $\hat{\sigma}_\gamma^2 = 0.3438$, $\hat{\sigma}_\delta^2 = 0.8087$, and $\hat{\sigma}^2 = 0.2848$. REML estimates for σ_γ^2 and σ_δ^2 are bigger than ML estimates.

```
Px <- X%ginv(t(X)%X)%t(X)
N <- diag(rep(1,9))-Px
B <- N[1:7,]
> qr(B)$rank
[1] 7
> optim(c(.07,.45,.37),minusLstar2,Y=Y,B=B,hessian=TRUE)$par
[1] 0.3437852 0.8087115 0.2848388
```

(c) $C\hat{\beta}_{MLE} = C\hat{\beta}_{REMLE} = (\hat{\alpha} = 99.4551, \hat{\beta} = 9.7936)$

```
s2 <- optim(c(.07,.45,.37),minusLstar,Y=Y,hessian=TRUE)$par # ML estimates
s2 <- optim(c(.07,.45,.37),minusLstar2,Y=Y,B=B,hessian=TRUE)$par # REML estimates
Vhat <- kronecker(I3,((s2[1]*J3)+(s2[2]*M)+(s2[3]*I3)))
C <- diag(c(1,1)); b <- ginv(t(X)%solve(Vhat)%X)%t(X)%solve(Vhat)%Y
Cb <- C%b
```

(d) $\text{Var} <- C\text{ginv}(t(X)\text{solve}(Vhat)X)t(C)$; $\text{stderr} <- \text{sqrt}(\text{diag}(\text{Var}))$

```
> stderr # for ML estimates
[1] 0.3198840 0.4029905
> stderr # for REML estimates
[1] 0.4203276 0.5296469
```

(e) $G <- \text{diag}(c(\text{rep}(s2[1],3),\text{rep}(s2[2],3)))$
 $Z <- \text{matrix}(c(\text{rep}(1,3),\text{rep}(0,9),\text{rep}(1,3),\text{rep}(0,9),\text{rep}(1,3),0,1,4,\text{rep}(0,9),0,1,4,\text{rep}(0,9),0,1,4),9,6)$
 $B <- X\text{ginv}(t(X)\text{solve}(Vhat)X)t(X)\text{solve}(Vhat)$
 $P <- \text{solve}(Vhat)\text{diag}(\text{rep}(1,9))-B$
 $uhathat <- G\text{t}(Z)P\text{Y}$

```
      û_MLE      -0.02172176  0.1511162  -0.1293945  -0.6478563  -0.2366669  0.8845232
      û_REMLE     -0.02999012  0.4881394  -0.4581493  -0.6637030  -0.3404386  1.0041420
```

(f) $\text{Var} <- G - G\text{t}(Z)P\text{Z}G$; $\text{stderr} <- \text{sqrt}(\text{diag}(\text{Var}))$

```
> stderr # for ML estimates
[1] 0.2323972 0.2323972 0.2323972 0.4056949 0.4056949 0.4056949
> stderr # for REML estimates
[1] 0.4405919 0.4405919 0.4405919 0.5358329 0.5358329 0.5358329
```

(g) $\text{cvector} <- \text{matrix}(c(1,0),2,1)$; $\text{svector} <- \text{matrix}(c(1,0,0,0,0),6,1)$ # alpha1
 $\text{cvector} <- \text{matrix}(c(0,1),2,1)$; $\text{svector} <- \text{matrix}(c(0,0,0,1,0,0),6,1)$ # beta1
 $l <- t(\text{cvector})\text{b}+t(\text{svector})\text{uhathat}$
 $\text{at} <- t(\text{cvector})\text{t}(X)\text{ginv}(X)\text{t}(X)$
 $\text{Var} <- t(\text{cvector})\text{ginv}(t(X)\text{solve}(Vhat)X)\text{cvector}+$
 $t(\text{svector})\text{G}\text{t}(Z)P\text{Z}\text{G}\text{svector} - 2\text{at}\text{B}\text{Z}\text{G}\text{svector}$
 $\text{stderr} <- \text{sqrt}(\text{diag}(\text{Var}))$

	MLE	std error	REMLE	std error
α_1	99.4334	0.2632	99.4251	0.3117
β_1	9.1457	0.3819	9.1299	0.5128

```

2. thermo <- read.table("hw09.txt",header=T)
gd <- groupedData(y~temp|group,data=thermo)
fm1 <- lme(y~temp,data=gd,random=~1+temp|group,method="ML")
fm2 <- lme(y~temp,data=gd,random=~1+temp|group,method="REML")
fm3 <- update(fm1,random=pdDiag(~1+temp),method="ML")
fm4 <- update(fm2,random=pdDiag(~1+temp),method="REML")

> fixed.effects(fm3)          # ML results in 1(c)
(Intercept)      temp
  99.45513      9.79359
> random.effects(fm3)       # ML results in 1(e)
(Intercept)      temp
1 -0.02181365 -0.6478858
2  0.15202592 -0.2369421
3 -0.13021227  0.8848279
> coefficients(fm3)
(Intercept)      temp
1   99.43331  9.145704    # This row was obtained in 1(g) using ML
2   99.60715  9.556648
3   99.32492 10.678418

```

In the function `intervals()` the point estimates for the variance components correspond to the square root of the estimates obtained in 1(a). (e.g., $\text{sd}(\text{Intercept}) = \sqrt{\hat{\sigma}_\gamma^2} = \sqrt{0.0629} \approx 0.2516$). Note that given the size of the data, the confidence intervals for the ML estimates of the variance components are very wide.

```

> intervals(fm3)
Approximate 95% confidence intervals
Fixed effects:
              lower      est.      upper
(Intercept) 98.632658 99.45513 100.27760
temp         8.757383  9.79359  10.82980

Random Effects:
Level: group
              lower      est.      upper
sd((Intercept)) 4.895553e-05 0.2516244 1293.313462
sd(temp)        2.272768e-01 0.6666714   1.955548

Within-group standard error:
              lower      est.      upper
0.1449576 0.6106299 2.5722616

```

Results for REML estimates are obtained using the same functions with the model stored in `fm4`.