1. $Y = X\beta + Zu + \epsilon$

(a)
$$\begin{bmatrix} y_{11} \\ y_{12} \\ y_{13} \\ y_{21} \\ y_{22} \\ y_{23} \\ y_{31} \\ y_{32} \\ y_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 4 \\ 1 & 0 \\ 1 & 1 \\ 1 & 4 \\ 1 & 0 \\ 1 & 1 \\ 1 & 4 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 4 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 4 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ \delta_1 \\ \delta_2 \\ \delta_3 \end{bmatrix} + \begin{bmatrix} \epsilon_{11} \\ \epsilon_{12} \\ \epsilon_{13} \\ \epsilon_{21} \\ \epsilon_{22} \\ \epsilon_{23} \\ \epsilon_{31} \\ \epsilon_{32} \\ \epsilon_{33} \end{bmatrix}$$

(b)
$$E(Y) = X\beta = \begin{bmatrix} \alpha \\ \alpha+\beta \\ \alpha+4\beta \\ \alpha \\ \alpha+\beta \\ \alpha+4\beta \\ \alpha \\ \alpha+\beta \\ \alpha+4\beta \end{bmatrix} \text{ and } Var(Y) = \begin{bmatrix} A & 0 & 0 \\ 0 & A & 0 \\ 0 & 0 & A \end{bmatrix} \text{ where } A = \begin{bmatrix} \sigma^2_\gamma + \sigma^2 & \sigma^2_\gamma & \sigma^2_\gamma \\ \sigma^2_\gamma & \sigma^2_\gamma + \sigma^2_\delta + \sigma^2 & \sigma^2_\gamma + 4\sigma^2_\delta \\ \sigma^2_\gamma & \sigma^2_\gamma + 4\sigma^2_\delta & \sigma^2_\gamma + 16\sigma^2_\delta + \sigma^2 \end{bmatrix}$$

That is, $Var(Y) = \sigma^2_\gamma I_{3\times 3} \otimes J_{3\times 3} + \sigma^2_\delta I_{3\times 3} \otimes (t_1,t_2,t_3)'(t_1,t_2,t_3) + \sigma^2 I_{9\times 9}$.

(c) $\widehat{\alpha} = 99.4551$ and $\widehat{\beta} = 9.7936$ in both cases. Note that in both cases the variance components have the same proportional relation.

```
X <- matrix(c(rep(1,9),rep(c(0,1,4),3)),9,2)
Y <- matrix(c(99.8,108.1,136.0,100.3,109.5,137.7,98.3,110.1,142.2),9,1)
sg <- 1; sd <- 1; s <- 0.25     # case 1
sg <- 4; sd <- 4; s <- 1        # case 2 (times sigma^2)
A <- matrix(c(sg+s,sg,sg,sg,sg+sd+s,sg+4*sd,sg,sg+4*sd,sg+16*sd+s),3,3)
V <- matrix(0,9,9); V[1:3,1:3] <- A; V[4:6,4:6] <- A; V[7:9,7:9] <- A
b <- solve(t(X)%*%solve(V)%*%X)%*%t(X)%*%solve(V)%*%Y
```

(d) The BLUE for (α,β) are the same as those obtained in (c). (Use `sg <- 1; sd <- 1; s <- 1` and follow steps in (c)).

(e) For each V compute Y^* and $L^*(\sigma^2)$.

$\sigma^2_\gamma = 1, \sigma^2_\delta = 1, \sigma^2 = 0.25$ $\quad \log L^*(\sigma^2) = -14.30018$ larger value of profile loglikelihood
$\sigma^2_\gamma = 1, \sigma^2_\delta = 1, \sigma^2 = 1$ $\quad \log L^*(\sigma^2) = -15.55036$

```
Ystar <- X%*%ginv(t(X)%*%solve(V)%*%X)%*%t(X)%*%solve(V)%*%Y
logLstar <- (-9/2)*log(2*pi)-.5*log (det(V))-.5*(t(Y-Ystar)%*%solve(V)%*%(Y-Ystar))
```

(f) Results match those obtained in 1(e). The ML estimates are: $\widehat{\sigma}^2_\gamma = 0.0629$, $\widehat{\sigma}^2_\delta = 0.4441$ and $\widehat{\sigma}^2 = 0.3733$.

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

(g) The REML estimates are: $\widehat{\sigma}^2_\gamma = 0.3438$, $\widehat{\sigma}^2_\delta = 0.8087$, and $\widehat{\sigma}^2 = 0.2848$. REML estimates for σ^2_γ and σ^2_δ 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)$rank
[1] 7
> optim(c(.07,.45,.37),minuslLstar2,Y=Y,B=B,hessian=TRUE)$par
[1] 0.3437852 0.8087115 0.2848388
```

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

```
s2 <- optim(c(.07,.45,.37),minuslLstar,Y=Y,hessian=TRUE)$par       # ML estimates
s2 <- optim(c(.07,.45,.37),minuslLstar2,Y=Y,B=B,hessian=TRUE)$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
```

(i)
```
Var <- C%*%ginv(t(X)%*%solve(Vhat)%*%X)%*%t(C); stderr <- sqrt(diag(Var))
> stderr                         # for ML estimates
[1] 0.3198840 0.4029905
> stderr                         # for REML estimates
[1] 0.4203276 0.5296469
```

(j)
```
G <- diag(c(rep(s2[1],3),rep(s2[2],3)))
Z <- matrix(c(rep(1,3),rep(0,9),rep(1,3),rep(0,9),rep(1,3),0,1,4,rep(0,9),0,1,4,rep(0,9),0,1,4),9,6)
B <- X%*%ginv(t(X)%*%solve(Vhat)%*%X)%*%t(X)%*%solve(Vhat)
P <- solve(Vhat)%*%(diag(rep(1,9))-B)
uhathat <- G%*%t(Z)%*%P%*%Y
```

	γ_1	γ_2	γ_3	δ_1	δ_2	δ_3
$\hat{\hat{u}}_{MLE}$	-0.02172176	0.1511162	-0.1293945	-0.6478563	-0.2366669	0.8845232
$\hat{\hat{u}}_{REMLE}$	-0.02999012	0.4881394	-0.4581493	-0.6637030	-0.3404386	1.0041420

(k)
```
Var <- G - G%*%t(Z)%*%P%*%Z%*%G; stderr <- sqrt(diag(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
```

(l) ML BLUPs for α_1 and β_1 are $\widehat{\alpha}_{MLE} + \widehat{\widehat{u}}_{MLE}[1]$ and $\widehat{\beta}_{MLE} + \widehat{\widehat{u}}_{MLE}[4]$, respectively. REML BLUPs are obtained similarly.

```
cvector <- matrix(c(1,0),2,1); svector <- matrix(c(1,0,0,0,0,0),6,1)   # alpha1
cvector <- matrix(c(0,1),2,1); svector <- matrix(c(0,0,0,1,0,0),6,1)   # beta1
l <- t(cvector)%*%b+t(svector)%*%uhathat
at <- t(cvector)%*%t(X)%*%ginv(X%*%t(X))
Var <- t(cvector)%*%ginv(t(X)%*%solve(Vhat)%*%X)%*%cvector+
       t(svector)%*%G%*%t(Z)%*%P%*%Z%*%G%*%svector - 2*at%*%B%*%Z%*%G%*%svector
stderr <- sqrt(diag(Var))
```

	ML	std error	REML	std error
α_1	99.4334	0.2632	99.4251	0.3117
β_1	9.1457	0.3819	9.1299	0.5128

(m)
```
thermo <- read.table("hw07.data1.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(h)
(Intercept)        temp
   99.45513     9.79359
```

```
> random.effects(fm3)        # ML results in 1(j)
  (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(l) 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(f). (e.g., `sd((Intercept))` $= \sqrt{\widehat{\sigma}^2_\gamma} = \sqrt{0.0629} \approx 0.2516$). 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
attr(,"label")
[1] "Fixed effects:"

 Random Effects:
  Level: group
                       lower      est.       upper
sd((Intercept)) 5.173841e-05 0.2516244 1223.749260
sd(temp)        2.287991e-01 0.6666714    1.942537

 Within-group standard error:
    lower      est.     upper
0.1459462 0.6106299 2.5548378
```

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

2. Part III from MS Exam Spring 2003.

   (a)

$$Z\underline{u} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \delta_1 \\ \delta_2 \\ \delta_3 \\ \delta_4 \end{bmatrix}$$

   (b) From R output provided, an approximate 95% confidence interval for σ_δ is $(2.004, 13.018)$.

```
> lmout <- lme(y~1+flow+ratio+temp,random=~1|day)
> intervals(lmout)
Approximate 95% confidence intervals
 Random Effects:
  Level: day
                   lower     est.    upper
sd((Intercept)) 2.003549 5.107096 13.01812
```

(c) Using estimates from `summary()`, the BLUE is $\widehat{\beta}_0 + 50\widehat{\beta}_1 + 4\widehat{\beta}_2 + 470\widehat{\beta}_3 = 86.208$. Notice that `Run` = 2 has this set of conditions (see Table). Hence, you could get this estimate from `predict()` under the column "predict.fixed", also provided. [The second column is the approximate BLUP of $\beta_0 + 50\beta_1 + 4\beta_2 + 470\beta_3 + \delta_1$].

```
> summary(lmout)
Fixed effects: y ~ 1 + flow + ratio + temp
                 Value Std.Error DF   t-value p-value
(Intercept) -109.14936 25.504194  5 -4.279663  0.0079
flow          -0.17885  0.019403  5 -9.217415  0.0003
ratio         -3.56250  0.630600  5 -5.649384  0.0024
temp           0.46500  0.050448  5  9.217415  0.0003

> predict(lmout,level=0:1)
   day predict.fixed predict.day
1    1      79.08333    82.16544
2    1      86.20833    89.29044
3    1      71.95833    75.04044
4    2     109.45833   102.79239
5    2      48.70833    42.04239
6    2      79.08333    72.41739
7    3      95.20833    95.13666
8    3      62.95833    62.88666
9    3      79.08333    79.01166
10   4      71.95833    75.61385
11   4      86.20833    89.86385
12   4      79.08333    82.73885
```

The standard error for this estimate can be obtained with $\sqrt{(1,50,4,470)\texttt{vcov(lmout)}(1,50,4,470)'}$. [Final numerical value was not required in the exam.]

```
> sqrt(c(1,50,4,470)%*%vcov(lmout)%*%c(1,50,4,470))    # vcov(lmout) from R output provided
  [1,] 3.514669
```

(d) i. The sample variance of these four observations estimates the common variance of these iid observations, namely $\sigma_\delta + \sigma$.

ii. A REML estimate of this is $\widehat{\sigma}_\delta^2 + \widehat{\sigma}^2 = 5.107^2 + 3.567^2 = 38.8$.

```
> summary(lmout)
Linear mixed-effects model fit by REML
 Data: NULL
       AIC      BIC    logLik
  85.84857 86.32522 -36.92429

Random effects:
 Formula: ~1 | day
        (Intercept) Residual
StdDev:    5.107096 3.567211
```

iii. The sample variance of these four observations $y = (82, 77, 81, 82)$ is 5.67. Our REML estimate is substantially different from 5.67.

iv. "Given the uncertainty evident in the `R` intervals for σ_δ and σ, perhaps this isn't cause to get too upset about poor model fit." [It also helps to notice the uncertainty calculated in part I(b) of this MS Exam.]

3. See Prof. Vardeman's solutions posted on the 2003 Stat 511 Web page.