## MATH 556: Mathematical Statistics I Hierarchical Models: Variance Components

Consider the three-level hierarchical model:
LEVEL 3: $\tau^{2}, \sigma^{2}>0$, fixed parameters;
LEVEL 2: $M_{1}, \ldots, M_{L} \sim \operatorname{Normal}\left(0, \tau^{2}\right)$ independent;
LEVEL 1: For $l=1, \ldots, L$

$$
X_{l 1}, \ldots, X_{l n_{l}} \mid M_{l}=m_{l} \sim \operatorname{Normal}\left(m_{l}, \sigma^{2}\right)
$$

where all the $X_{l j}$ are conditionally independent given $M_{1}, \ldots, M_{L}$.


In the following plot, we have $L=5$, with $n_{l}=1000$ for $l=1, \ldots, L$, with $\tau^{2}=2^{2}$ and $\sigma^{2}=0.1^{2}$.

```
set.seed(23984)
L<-5
nvec<-rep (1000,L)
tau<-2; sig<-0.1
M<-rnorm(L,0,tau)
mvec<-rep(M,nvec)
X<-rnorm(sum(nvec),mvec,sig)
par(mar=c (3, 3, 2, 1))
hist(X,breaks=seq( }-4,4,by=0.1),main='');box(
points(M,rep (0,L) ,pch=19,col='red', cex=0.5)
```



In the histogram,

- the red dots indicate the position of the sampled $m_{1}, \ldots, m_{5}$;
- the histograms represent the sampled $X_{l j}$ for $l=1, \ldots, 5$ and $j=1, \ldots, 1000$.

We can implement the same model with the variables having bivariate Normal distributions: for example

$$
\mathbf{M}_{l}=\left[\begin{array}{l}
M_{l 1} \\
M_{l 2}
\end{array}\right] \sim \operatorname{Normal}_{2}(\mathbf{0}, \mathbf{V})
$$

for $l=1, \ldots, L$, independently, with

$$
\mathbf{V}=\left[\begin{array}{ll}
2 & 3 \\
3 & 4
\end{array}\right]
$$

and, for $j=1, \ldots, n_{l}$

$$
\mathbf{X}_{l j} \mid \mathbf{M}_{l}=\mathbf{m}_{l} \sim \operatorname{Normal}_{2}\left(\mathbf{m}_{l}, \Sigma\right)
$$

conditionally independent, with the factorization of $\Sigma$ as

$$
\Sigma=\left[\begin{array}{ll}
0.50 & 0.00 \\
0.00 & 0.60
\end{array}\right]\left[\begin{array}{rr}
1.0 & -0.8 \\
-0.8 & 1.0
\end{array}\right]\left[\begin{array}{ll}
0.50 & 0.00 \\
0.00 & 0.60
\end{array}\right]=\left[\begin{array}{rr}
0.25 & -0.24 \\
-0.24 & 0.36
\end{array}\right] .
$$

In the following plot, we have $L=10$, with $n_{l}=100$ for $l=1, \ldots, L$

```
set.seed(23984)
library(mvnfast)
L<-10
nvec<-rep(100,L)
V<-matrix(c(4,3,3,4),2,2)
Sigma<-diag(c(0.5,0.60)) %*% matrix(c(1,-0.8,-0.8,1),2,2) %*% diag(c(0.5,0.60))
M<-rmvn(L,rep (0,2),V)
X<-numeric(length=2)
for(l in 1:L){
    Z<-rmvn(nvec [l],M[l,],Sigma)
    X<-rbind(X,Z)
}
```

```
par(mar=c(3,4,1,1))
```

plot $(X, p c h=19$, cex $=0.4, x \lim =r a n g e(-6,6)$, $y l i m=r a n g e(-6,6)$,
xlab=expression(X[lj1]),ylab=expression(X[lj2]))
points(M,pch=19, col='red', cex=0.5)


For each $l$, the $X_{l j}$ values for $j=1, \ldots, n_{l}$ are conditionally independent given $M_{l}=m_{l}$, but are not (unconditionally) independent. For the univariate case, the marginal distribution of $\mathbf{X}_{l}=\left(X_{l 1}, \ldots, X_{l n_{l}}\right)^{\top}$ is computed as
$f_{X_{l 1}, \ldots, X_{l n_{l}}}\left(x_{l 1}, \ldots, x_{l n_{l}} ; \tau^{2}, \sigma^{2}\right)=\int_{-\infty}^{\infty} \prod_{j=1}^{n_{l}} f_{X_{l j} \mid M_{l}}\left(x_{l j} \mid m_{l} ; \sigma^{2}\right) f_{M_{l}}\left(m_{l} ; \tau^{2}\right) d m_{l}$

$$
\begin{aligned}
& =\int_{-\infty}^{\infty} \prod_{j=1}^{n_{l}}\left\{\left(\frac{1}{2 \pi \sigma^{2}}\right)^{1 / 2} \exp \left\{-\frac{1}{2 \sigma^{2}}\left(x_{l j}-m_{l}\right)^{2}\right\}\right\}\left(\frac{1}{2 \pi \tau^{2}}\right)^{1 / 2} \exp \left\{-\frac{1}{2 \tau^{2}} m_{l}^{2}\right\} d m_{l} \\
& =\left(\frac{1}{2 \pi}\right)^{\left(n_{l}+1\right) / 2}\left(\frac{1}{\sigma^{2}}\right)^{n_{l} / 2}\left(\frac{1}{\tau^{2}}\right)^{1 / 2} \int_{-\infty}^{\infty} \exp \left\{-\frac{1}{2}\left[\frac{1}{\sigma^{2}} \sum_{j=1}^{n}\left(x_{l j}-m_{l}\right)^{2}+\frac{1}{\tau^{2}} m_{l}^{2}\right]\right\} d m_{l}
\end{aligned}
$$

Completing the square gives

$$
\frac{1}{\sigma^{2}} \sum_{j=1}^{n}\left(x_{l j}-m_{l}\right)^{2}+\frac{1}{\tau^{2}} m_{l}^{2}=\frac{1}{\sigma^{2}} \sum_{j=1}^{n_{l}}\left(x_{l j}-\bar{x}_{l}\right)^{2}+\left(\frac{n_{l}}{\sigma^{2}}+\frac{1}{\tau^{2}}\right)\left(m_{l}-\frac{n_{l} \bar{x} / \sigma^{2}}{n / \sigma^{2}+1 / \tau^{2}}\right)^{2}+\frac{n / \sigma^{2}}{n / \sigma^{2}+1 / \tau^{2}} \bar{x}_{l}^{2}
$$

and thus integrating out $m_{l}$ yields

$$
\begin{aligned}
& f_{X_{l 1}, \ldots, X_{l n_{l}}}\left(x_{l 1}, \ldots, x_{l n_{l}} ; \tau^{2}, \sigma^{2}\right)=\left(\frac{1}{2 \pi}\right)^{n_{l} / 2}\left(\frac{1}{\sigma^{2}}\right)^{n_{l} / 2}\left(\frac{1}{\tau^{2}}\right)^{1 / 2}\left(\frac{n_{l}}{\sigma^{2}}+\frac{1}{\tau^{2}}\right)^{-1 / 2} \\
& \exp \left\{-\frac{1}{2}\left[\frac{1}{\sigma^{2}} \sum_{j=1}^{n_{l}}\left(x_{l j}-\bar{x}_{l}\right)^{2}+\frac{n / \sigma^{2}}{n / \sigma^{2}+1 / \tau^{2}} \bar{x}_{l}^{2}\right]\right\}
\end{aligned}
$$

This joint pdf does not factorize into a product of functions of the individual $x_{l j}$ values, and hence the random variables are not indepenent. We can compute the distribution more concisely using mgfs and iterated expectation. We have for the multivariate mgf

$$
\begin{array}{rlr}
M_{\mathbf{X}_{l}}(\mathbf{t})=\mathbb{E}_{\mathbf{X}}\left[\exp \left\{\mathbf{t}^{\top} \mathbf{X}\right\}\right] & =\mathbb{E}_{M_{l}}\left[\mathbb{E}_{\mathbf{X} \mid M_{l}}\left[\exp \left\{\mathbf{t}^{\top} \mathbf{X}\right\} \mid M_{l}\right]\right] & \text { by iterated expectation } \\
& =\mathbb{E}_{M_{l}}\left[\mathbb{E}_{\mathbf{X} \mid M_{l}}\left[\exp \left\{\sum_{j=1}^{n_{l}} t_{j} X_{l j}\right\} \mid M_{l}\right]\right] & \text { expanding the inner product } \\
& =\mathbb{E}_{M_{l}}\left[\prod_{j=1}^{n_{l}} \exp \left\{M_{l} t_{j}+\frac{t_{j}^{2} \sigma^{2}}{2}\right\}\right] & \text { using the Normal mgf for } X_{l j} \\
& =\exp \left\{\frac{\left(\mathbf{t}^{\top} \mathbf{t}\right) \sigma^{2}}{2}\right\} \mathbb{E}_{M_{l}}\left[\exp \left\{M_{l}\left(\mathbf{1}^{\top} \mathbf{t}\right)\right\}\right] & \\
& =\exp \left\{\frac{\left(\mathbf{t}^{\top} \mathbf{t}\right) \sigma^{2}}{2}\right\} \exp \left\{\frac{\left(\mathbf{1}^{\top} \mathbf{t}\right) \tau^{2}}{2}\right\} & \text { using the Normal mgf for } M_{l} \\
& =\exp \left\{\frac{\mathbf{t}^{\top} \mathbf{V} \mathbf{t}}{2}\right\} &
\end{array}
$$

where, by inspection, we have that

$$
\mathbf{V}=\sigma^{2} \mathbf{I}_{n_{l}}+\tau^{2} \mathbf{1 1}{ }^{\top}
$$

where, for the $(j, k)$ th element, we have

$$
[\mathbf{V}]_{j k}=\left\{\begin{array}{cc}
\sigma^{2}+\tau^{2} & j=k \\
\tau^{2} & j \neq k
\end{array}\right.
$$

Thus we can conclude that $\mathbf{X}_{l} \sim \operatorname{Normal}_{n_{l}}(\mathbf{0}, \mathbf{V})$.
We can verify this by direct calculation: we have that

$$
\mathbb{E}_{X_{l j}}\left[X_{l j}\right]=\mathbb{E}_{M_{l}}\left[\mathbb{E}_{X_{l j} \mid M_{l}}\left[X_{l j} \mid M_{l}\right]\right]=\mathbb{E}_{M_{l}}\left[M_{l}\right]=0
$$

and

$$
\mathbb{E}_{X_{l j}}\left[X_{l j}^{2}\right]=\mathbb{E}_{M_{l}}\left[\mathbb{E}_{X_{l j} \mid M_{l}}\left[X_{l j}^{2} \mid M_{l}\right]\right]=\mathbb{E}_{M_{l}}\left[M_{l}^{2}+\tau^{2}\right]=\sigma^{2}+\tau^{2}
$$

so $\operatorname{Var}_{X_{l j}}\left[X_{l j}\right]=\sigma^{2}+\tau^{2}$. Finally, for $j \neq k$,

$$
\mathbb{E}_{X_{l j}, X_{l k}}\left[X_{l j} X_{l k}\right]=\mathbb{E}_{M_{l}}\left[\mathbb{E}_{X_{l j}, X_{l k} \mid M_{l}}\left[X_{l j} X_{l k} \mid M_{l}\right]\right]=\mathbb{E}_{M_{l}}\left[M_{l}^{2}\right]=\tau^{2}
$$

as $X_{l j}$ and $X_{l k}$ are conditionally independent given $M_{l}$, each with mean $M_{l}$. We therefore conclude that

$$
\operatorname{Corr}_{X_{l j}, X_{l k}}\left[X_{l j}, X_{l k}\right]=\frac{\operatorname{Cov}_{X_{l j}, X_{l k}}\left[X_{l j}, X_{l k}\right]}{\operatorname{Var}_{X_{l j}}\left[X_{l j}\right]}=\frac{\tau^{2}}{\sigma^{2}+\tau^{2}}
$$

Note that

- this correlation is always positive;
- if $\tau^{2} \longrightarrow 0$, the correlation converges to zero, and we have reverted to the iid $\operatorname{Normal}\left(0, \sigma^{2}\right)$ case;
- as $\sigma^{2} \longrightarrow 0$, the correlation converges to one.
- In this model, $l_{1} \neq l_{2}$, the $X_{l_{1} j_{1}}$ and $X_{l_{2} j_{2}}$ are unconditionally independent for all $j_{1}$ and $j_{2}$.

In the following simulation, we have $L=2$ and $n_{1}=n_{2}=3$, with $\tau=2$ and $\sigma=1$, yielding a within-cluster correlation of

$$
\frac{\tau^{2}}{\sigma^{2}+\tau^{2}}=0.8
$$

```
tau<-2;sig<-1
X<-t(replicate(1000,c(rnorm(3,rnorm(1,0,tau),sig),c(rnorm(3,rnorm(1,0,tau),sig)))))
par(mar=c(3,3,0,1))
pairs(X,cex=0.5,pch=19,labels=c(expression(X[11]), expression(X[12]), expression(X[13]),
                            expression(X[21]), expression(X[22]), expression(X[23])))
```


round $(\operatorname{cor}(X), 4)$

| + | $[, 1]$ | $[, 2]$ | $[, 3]$ | $[, 4]$ | $[, 5]$ | $[, 6]$ |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: |
| + | $[1]$, | 1.0000 | 0.8106 | 0.8059 | 0.0099 | 0.0209 |
| 0.0394 |  |  |  |  |  |  |
| $+[2]$, | 0.8106 | 1.0000 | 0.8075 | -0.0003 | 0.0158 | 0.0190 |
| $+[3]$, | 0.8059 | 0.8075 | 1.0000 | -0.0013 | 0.0181 | 0.0281 |
| $+[4]$, | 0.0099 | -0.0003 | -0.0013 | 1.0000 | 0.8191 | 0.8070 |
| $+[5]$, | 0.0209 | 0.0158 | 0.0181 | 0.8191 | 1.0000 | 0.8203 |
| $+[6]$, | 0.0394 | 0.0190 | 0.0281 | 0.8070 | 0.8203 | 1.0000 |

