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APPENDICES

APPENDIX A

LISTING OF GAUSS PROGRAM FOR COMPARISON OF DIFFERENT ESTIMATORS IN THE MEASUREMENT-ERROR MODEL

A.1 MAIN PROGRAM

```
start:;
cls;
              Simulated comparison for measurement error model";
              _______;
print;
print;
                            David R. Fox";
print;
                        University of Wyoming";
                            January 1989";
print;
print;
count2=0;
cov=eye(2);
/* coeff=zeros(20,1); */;
"Enter parameter values :";
print;
     How many observations for each sample : ";;
nobs=con(1,1);
print;
     Length of simulation run : ";;
nrun=con(1,1);
errc=zeros(nrun,1);
erro=zeros(nrun,1);
errm=zeros(nrun,1);
errf=zeros(nrun,1);
print;
        How many correlation coefficients: ";;
ncoef=con(1,1);
print;
format /rd 2,0;
i=1;
do while i<=ncoef;</pre>
     Enter coefficient #";;i;;" : ";;
coeff[i,1] = con(1,1);
```

```
i=i+1;
endo; */;
      Enter correlation coefficient : ";;
rho=con(1,1);
print;
      Enter sigma-squared e : ";;
se=con(1,1);
print;
      Enter sigma-squared u : ";;
su=con(1,1);
print;
      Enter sigma-squared x : ";;
varx=con(1,1);
lamda=se/su;
repeat=0;
loop1:;
count2=0;
if repeat>0;
/* count=count+1;
if count>ncoef; */;
print;
print;
       Do you want to repeat for new parameters (y/n) : ";;
reply=cons;
if reply $=="Y" or reply $=="y";
goto start;
else;
format /rd 9,4;
stop;
endif;
endif:
/* endif;
rho=coeff[count,1]; */;
theta=rho*lamda^.5;
cov[1,1]=se;
cov[1,2]=rho*(se*su)^.5;
cov[2,1] = cov[1,2];
cov[2,2]=su;
{d,Q}=eigrs2(cov);
dd=diagrv(eye(2),d^.5);
a=q*dd;
loop2:;
repeat=1;
count2=count2+1;
if count2>nrun;
goto loop1;
endif:
"Iteration #";;count2;
z=rndn(nobs+1,2);
w=z*a';
/* w1=w[.,1]-meanc(w[.,1]); w2=w[.,2]-meanc(w[.,2]); ww=w1~w2; ww'ww/(nobs-
e=w[.,1];
u=w[.,2];
```

i=1;

if i<10:

do while i <= 81;

```
x=rndn(nobs+1,1)*varx^.5+ones(nobs+1,1)*10;
xx=x[1:nobs,1]+u[1:nobs,1];
y=0.5+xx+e[1:nobs,1];
x0=x[nobs+1,1];
y0=.5+x0+e[nobs+1,1];
sx=(xx)'(xx)-sumc(xx)^2/nobs;
sy=y'y-sumc(y)^2/nobs;
sxy=xx'y-sumc(xx)*sumc(y)/nobs;
beta1c=sxy/sx;
beta0c=(sumc(y)-beta1c*sumc(xx))/nobs;
format /rd 9,6;
/* beta0c;
beta1c; */;
errc[count2,1]=((y0-beta0c)/beta1c)-x0;
beta1o=(sy-sx+((sy-sx)^2+4*sxy^2)^.5)/2/sxy;
beta0o=(sumc(y)-beta1o*sumc(xx))/nobs;
erro[count2,1]=((y0-beta0o)/beta1o)-x0;
beta1m=(sy-lamda*sx+((sy-lamda*sx)^2-4*(sxy-theta*sx)*(theta*sy-lamda*sx
/2/(sxy-theta*sx);
beta0m=(sumc(y)-beta1m*sumc(xx))/nobs;
errm[count2,1]=((y0-beta0m)/beta1m)-x0;
lamda1=(sx-sxy^2/sy)/su;
if lamda1>1;
gamma1=((sx-su)*sxy+2*sxy*su/nobs)/(sxy^2+(sx*sy-sxy^2)/nobs);
gamma1=sxy/sy;
endif;
gamma0=(sumc(xx)-gamma1*sumc(y))/nobs;
errf[count2,1] = (gamma0+gamma1*y0) - x0;
goto loop2;
A.2 AUXILIARY ROUTINE :Q.ARC
proc (0)=aa;
meanc(errc); meanc(erro); meanc(errm); meanc(errf);
print;
print;
errc'errc/nobs;erro'erro/nobs;errm'errm/nobs;errf'errf/nobs;
q=errc~erro~errm~errf;
endp;
A.3 RESULTS.ARC
load path=d:\simul;
bias=zeros(81,4);
mse=zeros(81,4);
```

```
11=1;
else;
11=2;
endif;
j=1;
ext=ftos(i,"lf",11,0);
file="run" $+ ext;
file;
load q=^file;
do while j <= 4;
bias[i,j]=meanc(q[.,j]);
mse[i,j]=q[.,j]'q[.,j]/200;
j=j+1;
endo;
i=i+1;
endo;
```

A.4 PLOT.ARC

```
i=1;
qmajor=2;
library qgraph;
window(2,2);
beggraph;
do while i <=4;
{c,m,f}=hist(bias[.,i],12);
i=i+1;
endo;
endgraph;
beggraph;
i=1;
do while i <= 4;
{c,m,f}=hist(mse[.,i],12);
i=i+1;
endo;
endgraph;
```

APPENDIX B

LISTING OF GAUSS PROGRAM TO COMPUTE UNCONDITIONAL CONFIDENCE LEVELS FOR THE CSS PROCEDURE

```
start:;
cls;
            Experimentwise error rate for the CSS procedure";
            print;
print;
                         David R. Fox";
print;
                      University of Wyoming";
                         January 1989";
print;
print;
count2=1;
index=1;
"Enter parameter values :";
print;
     How many observations for each sample : ";;
nobs=con(1,1);
print;
     Length of each simulation run : ";;
nrun=con(1,1);
print;
            i=rows(cv);
j=rows(f);
k=rows(t);
alpha=zeros(i*j*k,4);
cvcount=1;
do while cvcount<=i;</pre>
fcount=1;
do while fcount<=j;</pre>
tcount=1;
do while tcount<=k;</pre>
tcrit=t[tcount,1];
fcrit=(2*f[fcount,1])^.5;
format /1d 6,3;
```

```
Current iteration : cv=";;cv[cvcount,1];;
" F=";;f[fcount,1];;" t=";;t[tcount,1];
ind=zeros(nrun,1);
count2=1:
do while count2<=nrun;
x=rndu(nobs+1,1);
e=cv[cvcount,1]*rndn(nobs+1,1);
y=x+e;
xbar=meanc(x);
x0=x[nobs+1,1];
y0=y[nobs+1,1];
xx=x[1:nobs,1];
sx=xx'xx-sumc(xx)^2/nobs;
yy=y[1:nobs,1];
xx=ones(nobs,1)~xx;
beta=inv(xx'xx)*xx'yy;
xhat=(y0-beta[1,1])/beta[2,1];
ehat=yy-xx*beta;
sigma=(ehat'ehat/(nobs-2))^.5;
delta=sigma*(tcrit+fcrit*(1/nobs+(xhat-xbar)^2/sx)^.5);
yupper=y0+delta;
ylower=y0-delta;
xupper=(yupper-beta[1,1])/beta[2,1];
xlower=(ylower-beta[1,1])/beta[2,1];
if x0>=xlower and x0<=xupper;
ind[count2,1]=1;
endif;
count2=count2+1;
endo;
format /rd 12,6;
alpha[index,1]=cv[cvcount,1];
alpha[index,2]=f[fcount,1];
alpha[index,3]=t[tcount,1];
alpha[index, 4] = 1 - sumc(ind) / nrun;
tcount=tcount+1;
index=index+1;
endo:
fcount=fcount+1;
endo:
cvcount=cvcount+1;
endo;
stop;
```

APPENDIX C

LISTING OF GAUSS PROGRAM FOR CONFIDENCE INTERVAL SIMULATION

```
start:;
bell=chrs(7);
cls;
             Confidence interval simulation for calibration";
             print;
print;
                            David R. Fox";
print;
                        University of Wyoming";
                            January 1989";
print;
print;
count2=1;
"Enter parameter values :";
print;
     How many observations for each sample : ";;
nobs=con(1,1);
print;
     Length of each simulation run : ";;
nrun=con(1,1);
print;
     Enter coefficient of variation: ";;
cv=con(1,1);
print;
     Enter F-value for CSS procedure : ";;
f=con(1,1);
print;
     Enter T-value for CSS procedure : ";;
tcss=con(1,1);
print;
     Enter T-value for all other procedures : ";;
tcrit=con(1,1);
fcrit=(2*f)^.5;
alpha=zeros(1,5);
length=zeros(nrun,5);
format /1d 4,0;
ind=zeros(nrun,5);
count2=1;
```

```
timeO=hsec/100;
do while count2<=nrun;
timen=hsec/100;
format /ld 3,0;
if timen-time0>30;
             Still working . . . ";;count2/nrun*100;;"% completed";
timeO=timen;
endif:
x=rndu(nobs+1,1);
e=cv*rndn(nobs+1,1);
y=x+e;
x0=x[nobs+1,1];
v0=v[nobs+1,1];
xx=x[1:nobs,1];
sx=xx'xx-sumc(xx)^2/nobs;
yy=y[1:nobs,1];
xbar=meanc(xx);
ybar=meanc(yy);
sy=yy'yy-sumc(yy)^2/nobs;
sxy=xx'yy-sumc(xx)*sumc(yy)/nobs;
xx=ones(nobs,1)~xx;
beta=inv(xx'xx)*xx'yy;
xhatc=(y0-beta[1,1])/beta[2,1];
ehatc=yy-xx*beta;
sigmac=(ehatc'ehatc/(nobs-2))^.5;
           CSS PROCEDURE #4
delta=sigmac*(tcss+fcrit*(1/nobs+(xhatc-xbar)^2/sx)^.5);
yupper=y0+delta;
ylower=y0-delta;
xupper=(yupper-beta[1,1])/beta[2,1];
xlower=(vlower-beta[1,1])/beta[2,1];
length[count2,4]=xupper-xlower;
if x0>=xlower and x0<=xupper;
ind[count2,4]=1;
endif;
           CLASSICAL PROCEDURE #2
/*
                                      */;
delta=tcrit*sigmac*(1+1/nobs+(xhatc-xbar)^2/sx)^.5;
yupper=y0+delta;
ylower=y0-delta;
xupper=(yupper-beta[1,1])/beta[2,1];
xlower=(ylower-beta[1,1])/beta[2,1];
length[count2,2]=xupper-xlower;
if x0>=xlower and x0<=xupper;
ind[count2,2]=1;
endif;
/*
                                       */;
           INVERSE PROCEDURE #1
gamma1=beta[2,1]*sx/sy;
gamma0=xbar-gamma1*ybar;
xhati=gamma0+gamma1*y0;
ehati=x[1:nobs]-(gamma0+gamma1*yy);
sigmai=(ehati'ehati/(nobs-2))^.5;
delta=tcrit*sigmai*(1+1/nobs+(y0-ybar)^2/sy)^.5;
xupper=xhati+delta;
```

```
xlower=xhati-delta:
length[count2,1]=xupper-xlower;
if x0>=xlower and x0<=xupper;
ind[count2,1]=1;
endif;
            CLASSICAL (GRAYBILL) PROCEDURE
                                              #3
                                                        */;
/*
a=beta[2,1]^2-sigmac^2*tcrit^2/sx;
b=xbar+beta[2,1]*(y0-ybar)/a;
delta=(sigmac/a)*tcrit*(a*(1+1/nobs)+(y0-ybar)^2/sx)^.5;
xupper=b+delta;
xlower=b-delta;
length[count2,3]=xupper-xlower;
if x0>=xlower and x0<=xupper;
ind[count2,3]=1;
endif:
             ORTHOGONAL PROCEDURE
                                                     */:
/*
b1=(sy-sx+((sy-sx)^2+4*sxy^2)^.5)/2/sxy;
b0=ybar-b1*xbar;
xhato=(y0-b0)/b1;
theta=arctan(b1);
ehato=yy-(b0+b1*x[1:nobs,1]);
/* sigmao=((ehato'ehato/(nobs-2))^.5); */;
sigmao=cos(theta)^2*sigmac+sin(theta)^2*sigmai;
delta=tcrit*sigmao*(1+1/nobs+(xhato-xbar)^2/sx)^.5;
yupper=y0+delta;
ylower=y0-delta;
xupper=(yupper-b0)/b1;
xlower=(ylower-b0)/b1;
length[count2,5]=xupper-xlower;
if x0>=xlower and x0<=xupper;
ind[count2,5]=1;
endif:
count2=count2+1;
endo:
format /rd 12,6;
alpha[1,1] = sumc(ind[.,1])/nrun;
alpha[1,2]=sumc(ind[.,2])/nrun;
alpha[1,3]=sumc(ind[.,3])/nrun;
alpha[1,4]=sumc(ind[.,4])/nrun;
alpha[1,5] = sumc(ind[.,5])/nrun;
print;
       Probability of interval capturing unknown x:";
alpha;
       Average interval length: ";
(meanc(length))';
bell;bell;bell;
stop;
```

APPENDIX D

ELEMENTS OF THE GRADIENT VECTOR AND HESSIAN MATRIX

We give here the computing formulae required to determine the elements of the gradient vector and Hessian matrix for the components of variance estimation associated with the example given in $\S 2.7.2$.

We have :

$$\phi(\sigma_e^2; \sigma_u^2; \rho) = \sum_{i=1}^t (s_i^2 w_i - \ln w_i)$$

where

$$w_i = \frac{1}{\sigma_i^2}$$

and

$$\sigma_i^2 = \sigma_e^2 + \frac{c^2}{x_i^4} \sigma_u^2 - \frac{2c}{x_i} \rho \sigma_e \sigma_u$$

D.1 ELEMENTS OF THE GRADIENT VECTOR

From equation (2.59) we have

$$\mathbf{q}(\underline{\theta}) = \begin{bmatrix} \frac{\partial \Phi}{\partial \sigma_{\mathbf{e}}^2} & \frac{\partial \Phi}{\partial \sigma_{\mathbf{u}}^2} & \frac{\partial \Phi}{\partial \rho} \end{bmatrix}^{\mathsf{T}}$$

where

$$\frac{\partial \Phi}{\partial \sigma_{\mathbf{e}}^2} = \sum_{i=1}^{N} (\mathbf{w}_i - \mathbf{w}_i^2 \mathbf{s}_i^2) \frac{\partial \sigma_i^2}{\partial \sigma_{\mathbf{e}}^2}$$

$$\frac{\partial \Phi}{\partial \sigma_{\mathbf{u}}^2} = \sum_{i=1}^{\mathbf{N}} (\mathbf{w}_i - \mathbf{w}_i^2 \mathbf{s}_i^2) \frac{\partial \sigma_i^2}{\partial \sigma_{\mathbf{u}}^2}$$

$$\frac{\partial \Phi}{\partial \rho} = \sum_{i=1}^{N} (\mathbf{w}_i - \mathbf{w}_i^2 \mathbf{s}_i^2) \frac{\partial \sigma_i^2}{\partial \rho}$$

and

$$\frac{\partial \sigma_{i}^{2}}{\partial \sigma_{e}^{2}} = 1 - \frac{c \rho \sigma_{u}}{x_{i} \sigma_{e}}$$

$$\frac{\partial \sigma_i^2}{\partial \sigma_u^2} = \frac{c^2}{x_i^4} - \frac{c \rho \sigma_e}{x_i^2 \sigma_u}$$

$$\frac{\partial \sigma_{i}^{2}}{\partial \rho} = \frac{-2c\sigma_{u}\sigma_{e}}{x_{i}^{2}}$$

D.2 ELEMENTS OF THE HESSIAN MATRIX

 $\underline{\mathbf{H}}(\underline{\theta})$ is given in equation (2.60).

Elements of this matrix are :

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$$\frac{\partial^2 \Phi}{\partial \sigma_e^4} = \sum_{i=1}^{N} \left[\left[\left(\mathbf{w}_i^2 - 2 \mathbf{s}_i^2 \mathbf{w}_i^3 \right) \right] \left[1 - \frac{c \rho \sigma_u}{\mathbf{x}_i^2 \sigma_e} \right]^2 + \frac{1}{2} \left[\mathbf{s}_i^2 \mathbf{w}_i^2 - \mathbf{w}_i \right] \left[\frac{c \rho \sigma_u}{\mathbf{x}_i^2 \sigma_e} \right] \right]$$

$$\frac{\partial^2 \Phi}{\partial \sigma_{\mathbf{u}}^2 \partial \sigma_{\mathbf{e}}^2} = \sum_{i=1}^{N} \left[\left[\left(\mathbf{w}_i^2 - 2 \mathbf{s}_i^2 \mathbf{w}_i^3 \right) \right] \left[\frac{\mathbf{c}^2}{\mathbf{x}_i^4} - \frac{\mathbf{c} \rho \sigma_{\mathbf{e}}}{\mathbf{x}_i^2 \sigma_{\mathbf{u}}} \right]^2 - \frac{1}{2} \left[\mathbf{s}_i^2 \mathbf{w}_i^2 - \mathbf{w}_i \right] \left[\frac{\mathbf{c} \rho}{\sigma_{\mathbf{e}} \sigma_{\mathbf{u}} \mathbf{x}_i^2} \right] \right]$$

$$\frac{\partial^2 \Phi}{\partial \rho \partial \sigma_e^2} = \sum_{i=1}^{N} \left[\left[\left(\mathbf{w}_i^2 - 2 \mathbf{s}_i^2 \mathbf{w}_i^3 \right) \right] \left[\frac{-2 \mathbf{c} \sigma_{\mathbf{u}} \sigma_e}{\mathbf{x}_i^2} \right] \left[1 - \frac{\mathbf{c} \rho \sigma_{\mathbf{u}}}{\mathbf{x}_i^2 \sigma_e} \right] - \left[\mathbf{s}_i^2 \mathbf{w}_i^2 - \mathbf{w}_i \right] \left[\frac{\mathbf{c} \sigma_{\mathbf{u}}}{\sigma_e \mathbf{x}_i^2} \right] \right]$$

$$\frac{\partial^2 \Phi}{\partial \rho \partial \sigma_{\mathbf{u}}^2} = \sum_{i=1}^{N} \left[\left[\left(\mathbf{w}_{i}^2 - 2 \mathbf{s}_{i}^2 \mathbf{w}_{i}^3 \right) \right] \left[\frac{-2 \mathbf{c} \sigma_{\mathbf{u}} \sigma_{\mathbf{e}}}{\mathbf{x}_{i}^2} \right] \left[\frac{\mathbf{c}^2}{\mathbf{x}_{i}^4} - \frac{\mathbf{c} \rho \sigma_{\mathbf{e}}}{\mathbf{x}_{i}^2 \sigma_{\mathbf{u}}} \right] - \left[\mathbf{s}_{i}^2 \mathbf{w}_{i}^2 - \mathbf{w}_{i} \right] \left[\frac{\mathbf{c} \sigma_{\mathbf{e}}}{\sigma_{\mathbf{u}} \mathbf{x}_{i}^2} \right] \right]$$

$$\frac{\partial^2 \Phi}{\partial \sigma_{\mathbf{u}}^4} = \sum_{i=1}^{N} \left[\left[\left(\mathbf{w}_i^2 - 2 \mathbf{s}_i^2 \mathbf{w}_i^3 \right) \right] \left[\frac{\mathbf{c}^2}{\mathbf{x}_i^4} - \frac{\mathbf{c} \rho \sigma_{\mathbf{e}}}{\mathbf{x}_i^2 \sigma_{\mathbf{u}}} \right] + \frac{1}{2} \left[\mathbf{s}_i^2 \mathbf{w}_i^2 - \mathbf{w}_i \right] \left[\frac{\mathbf{c} \rho \sigma_{\mathbf{e}}}{\mathbf{x}_i^2 \sigma_{\mathbf{u}}} \right] \right]$$

$$\frac{\partial^2 \Phi}{\partial \rho^2} = \sum_{i=1}^{N} \left[\left[\left(\mathbf{w}_i^2 - 2 \mathbf{s}_i^2 \mathbf{w}_i^3 \right) \right] \left[\frac{-2 \mathbf{c} \sigma_{\mathbf{u}} \sigma_{\mathbf{e}}}{\mathbf{x}_i^2} \right]^2 \right]$$

APPENDIX E

FORTRAN PROGRAM LISTING FOR NEWTON-RAPHSON COMPONENTS OF VARIANCE ESTIMATION

E.1 MAIN PROGRAM

```
double precision x(3), f, g(3), w(30), b1(3), bu(3), y(30), s(30)
     common k,y,s
     integer iw(5)
     open(unit=21,file='varcomp.dat',status='old',readonly)
     do 1 i=1,30
     read(21,210,end=98)y(i),s(i)
1
    write(6,699)y(i),s(i)
699 format(2x,2(1x,f12.6))
98 k=i-1
210 format(f6.0,2x,f12.0)
    n=3
     liw=5
    1w = 30
     ifail=1
     ibound=0
     b1(1)=1e-6
    b1(2)=1e-6
    b1(3) = -0.99
    bu(1) = 1e6
    bu(2)=1e6
    bu(3)=0.99
    write(6,610)
610 format(//2x,'Enter initial estimates: ')
    write(6,650)
650 format(//2x,'Sigma-squared V=',$)
    read(5,500)x(1)
    write(6,651)
651 format(//2x, 'Sigma-squared U=',$)
    read(5,500)x(2)
    write(6,652)
652 format(//2x,'Rho=',$)
    read(5,500)x(3)
500 format(f12.0)
     call e04laf(n,ibound,bl,bu,x,f,g,iw,liw,w,lw,ifail)
```

```
if(ifail.ne.0) write(6,600)ifail
   if(ifail.eq.1) go to 99
600 format(//2x,'Error exit type ',i3,'see NAG documentation')
   write(6,601)f
   write(6,602)(x(j),j=1,n)
   write(6,603)(g(j),j=1,n)
601 format(//2x,'Function value on exit is ',f12.6)
602 format(//2x,'at the point ',3f9.4)
603 format(//2x,'The corresponding gradient is' /15x,3f12.4)
99 stop
   end
```

E.2 SUBROUTINE FUNCT2: FUNCTION AND GRADIENT VECTOR EVALUATION

```
subroutine funct2(n,xc,fc,gc)
    common k,y,s
    double precision gc(n),xc(n),fc,y(30),s(30),w,z,x1,x2,x3,x4
    fc=0
    gc(1)=0
    gc(2) = 0
    gc(3)=0
    do 1 i=1,k
    z=y(1)**2
    w=xc(1)+xc(2)*(1800/z)**2-(3600/z)*xc(3)*(xc(1)*xc(2))**0.5
    W=1/W
    fc=fc+s(i)*w-log(w)
    x1=1-xc(3)*1800*((xc(2)/xc(1))**0.5)/z
    x2=(1800/z)**2-xc(3)*1800*((xc(1)/xc(2))**0.5)/z
    x3=-(3600/z)*(xc(1)*xc(2))**0.5
    x4=w-s(i)*w**2
    gc(1) = gc(1) + x1 * x4
    gc(2) = gc(2) + x2 \times x4
    gc(3) = gc(3) + x3 \times x4
1
    continue
    return
    end
```

E.3 SUBROUTINE HESS2: EVALUATION OF HESSIAN MATRIX

```
subroutine hess2(n,xc,heslc,lh,hesdc)
common k,y,s
double precision xc(n),heslc(lh),hesdc(n),x1,x2,x3,x4,x5
double precision x6,x7,x8,x9,x10,x11,y(30),s(30),w,z
heslc(1)=0
heslc(2)=0
heslc(3)=0
hesdc(1)=0
hesdc(2)=0
```

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```
hesdc(2)=0
    do 1 i=1,k
    z=y(i)**2
    w=xc(1)+xc(2)*(1800/z)**2-(3600/z)*xc(3)*(xc(1)*xc(2))**0.5
    w=1/w
    x1=2*(w**3)*s(i)-w**2
    x2=w-s(i)*w**2
    x3=(1800/z)**2-((xc(1)/xc(2))**0.5)*1800*xc(3)/z
    x4=1-(1800*xc(3)/z*(xc(2)/xc(1))**0.5)
    x5=-1800*xc(3)/((xc(1)*xc(2)**0.5)*z)
    x6=-(3600/z)*(xc(1)*xc(2))**0.5
    x8=-1800/z*(xc(2)/xc(1))**0.5
    x7=x8
    x9=-1800/z*(xc(1)/xc(2))**0.5
    heslc(1) = heslc(1) + (x1*x3*x4+0.5*x2*x5)
    heslc(2) = heslc(2) + (x1*x6*x4+x2*x7)
    heslc(3) = heslc(3) + (x1*x6*x3+x2*x9)
    x10=-(1800*xc(3)*xc(2)**0.5)/(z*xc(1)**1.5)
    x11=-(1800*xc(3)*xc(1)**0.5)/(z*xc(2)**1.5)
    hesdc(1) = hesdc(1) + (x1*x4**2-0.5*x2*x10)
    hesdc(2) = hesdc(2) + (x1*x3**2-0.5*x2*x11)
    hesdc(3) = hesdc(3) + (x1*x6**2)
1
    continue
    return
    end
```

APPENDIX F

DERIVATION OF (y^*-y) and (x^*-x) for orthogonal least-squares estimation

$$y_{i}^{*} - y_{i}$$

Using equation (3.25) it can be established that

$$y_{i}^{*} = \frac{1}{1 + \sum_{k=1}^{p} \beta_{k}^{2}} \left[\beta_{i} x_{1 i} + \beta_{2} x_{2 i} + \dots + \beta_{p} x_{p i} + \sum_{j=1}^{p} \beta_{j}^{2} \right]$$

and thus

$$(y_{i}^{*} - y_{i}) = \frac{\left[\sum_{j=1}^{p} \beta_{j} x_{ji} + y_{i} \sum_{j=1}^{p} \beta_{j}^{2}\right] - \left[1 + \sum_{j=1}^{p} \beta_{j}^{2}\right] y_{i}}{1 + \sum_{k=1}^{p} \beta_{k}^{2}}$$

$$= \frac{\sum_{j=1}^{P} \beta_j x_{ji} - y_i}{1 + \sum_{k=1}^{P} \beta_k^2}$$

F.2
$$(x_{ji}^* - x_{ji})$$

Again using equation (3.25) we have that the projection of $x_{j\,i}$ is $x_{i\,i}^*$ where :

$$\mathbf{x}_{j\,i}^{*} = \frac{1}{1 + \sum_{k=1}^{p} \beta_{k}^{2}} \left[1 + \beta_{1}^{2} + \beta_{2}^{2} + \ldots + \beta_{j-1}^{2} + \beta_{j+1}^{2} + \beta_{p}^{2} - \sum_{\substack{k=1 \ k \neq j}}^{p} \beta_{k} \beta_{j} \mathbf{x}_{k} \right]$$

$$= \frac{1}{1 + \sum_{k=1}^{p} \beta_{k}^{2}} \left[\left[1 + \sum_{k=1}^{p} \beta_{k}^{2} \right] x_{ji} - \sum_{k=1}^{p} \beta_{k} \beta_{j} x_{ki} \right]$$

and

$$(x_{ji}^{*} - x_{ji}) = \frac{\left[1 + \sum_{k=1}^{p} \beta_{k}^{2}\right] x_{ji} - \sum_{k=1}^{p} \beta_{j} \beta_{k} x_{ki} - x_{ji} \left[1 + \sum_{k=1}^{p} \beta_{k}^{2}\right]}{1 + \sum_{k=1}^{p} \beta_{k}^{2}}$$

thus

$$(x_{ji}^* - x_{ji}) = \frac{-\sum_{k=1}^{p} \beta_j \beta_k x_{ki}}{1 + \sum_{k=1}^{p} \beta_k^2}$$

APPENDIX G

DERIVATION OF ORTHOGONAL LEAST-SQUARES ESTIMATES

The orthogonal least-squares criterion of equation (3.28) is given as:

We differentiate $I\!\!I$ with respect to eta_{j} and set the result to zero. Thus :

$$\frac{\partial \mathbf{Z}}{\partial \beta_{i}} = 0 \quad \Rightarrow \quad$$

$$\sum_{i=1}^{n} \left[\frac{\partial}{\partial \beta_{j}} \left[\frac{\sum_{i=1}^{p} \beta_{j} x_{ji} - y_{i}}{1 + \sum_{k=1}^{p} \beta_{k}^{2}} \right]^{2} + \frac{\partial}{\partial \beta_{j}} \sum_{j=1}^{p} \left[\frac{-\sum_{k=1}^{p} \beta_{j} \beta_{k} x_{ki}}{1 + \sum_{k=1}^{p} \beta_{k}^{2}} \right]^{2} \right] = 0$$

$$\Rightarrow \sum_{i=1}^{n} \left[2 \left[\frac{\sum_{i=1}^{p} \beta_{j} x_{ji} - y_{i}}{1 + \sum_{k=1}^{p} \beta_{k}^{2}} \right] \left[\frac{x_{ji} \left[1 + \sum_{k=1}^{p} \beta_{k}^{2} \right] - 2\beta_{j} \left[\sum_{k=1}^{p} \beta_{k} x_{ki} - y_{i} \right]}{\left[1 + \sum_{k=1}^{p} \beta_{k}^{2} \right]^{2}} \right] + 2 \sum_{\substack{m=1 \\ m \neq j}}^{p} \left[\frac{\sum_{k=1}^{p} \beta_{m} \beta_{k} x_{ki}}{1 + \sum_{k=1}^{p} \beta_{k}^{2}} \right] \frac{\partial}{\partial \beta_{j}} \left[\frac{\beta_{m} \beta_{k} x_{ki}}{1 + \sum_{k=1}^{p} \beta_{k}^{2}} \right] + 2 \left[\frac{\sum_{k=1}^{p} \beta_{j} \beta_{k} x_{ki}}{1 + \sum_{k=1}^{p} \beta_{k}^{2}} \right] \left[\sum_{k\neq j}^{p} \frac{\partial}{\partial \beta_{j}} \left[\frac{\beta_{m} \beta_{k} x_{ki}}{1 + \sum_{k=1}^{p} \beta_{k}^{2}} \right] + \frac{\partial}{\partial \beta_{j}} \left[\frac{\beta_{j}^{2} x_{ji}}{1 + \sum_{k=1}^{p} \beta_{k}^{2}} \right] \right] \right] = 0$$

After some algebraic manipulation we obtain

$$\frac{\partial \overline{Z}}{\partial \beta_{j}} = 0 \Rightarrow$$

$$\sum_{i=1}^{n} \left[2 \left[\frac{\sum_{k=1}^{p} \beta_{k} \mathbf{x}_{ki} - \mathbf{y}_{i}}{1 + \sum_{k=1}^{p} \beta_{k}^{2}} \right] \left[\frac{\mathbf{x}_{ji} \left[\mathbf{1} + \sum_{k=1}^{p} \beta_{k}^{2} \right] - 2\beta_{j} \left[\sum_{k=1}^{p} \beta_{k} \mathbf{x}_{ki} - \mathbf{y}_{i} \right]}{\left[\mathbf{1} + \sum_{k=1}^{p} \beta_{k}^{2} \right]^{2}} \right]$$

$$+ 2 \left[\begin{array}{c} \sum_{k=1}^{p} \beta_{j} \beta_{k} x_{k i} \\ 1 + \sum_{k=1}^{p} \beta_{k}^{2} \end{array} \right] \left[\sum_{k=1}^{p} \beta_{k} x_{k i} \left[\begin{array}{c} 1 + \sum_{k=1}^{p} \beta_{k}^{2} \\ \end{array} \right] - 2 \beta_{j}^{2} \beta_{k} x_{k i} \end{array} \right]^{2} = 0$$

$$\Rightarrow \sum_{i=1}^{n} \left[\sum_{k=1}^{p} \beta_{k} x_{ki} - y_{i} \right] \left[x_{ji} \left[1 + \sum_{k=1}^{p} \beta_{k}^{2} \right] - 2\beta_{j} \left[\sum_{k=1}^{p} \beta_{k} x_{ki} - y_{i} \right] \right]$$

$$+ \left[\sum_{k=1}^{p} \beta_{j} \beta_{k} x_{k i} \right] \left[\sum_{k=1}^{p} \beta_{k} x_{k i} \left[1 + \sum_{k=1}^{p} \beta_{k}^{2} \right] - 2 \beta_{j} \beta_{k} x_{k i} \right] = 0$$

For simplicity, let $\lambda = 1 + \sum_{k=1}^p \beta_k^2$ and $\hat{y}_i = \sum_{k=1}^p \beta_k x_{ki}$, thus the last expression can be written as :

$$\sum_{i=1}^{n} \left[\hat{\mathbf{y}}_{i} - \mathbf{y}_{i} \right] \left[\lambda \mathbf{x}_{ji} - 2\beta_{j} \hat{\mathbf{y}}_{i} - \mathbf{y}_{i} \right] + \beta_{j} \hat{\mathbf{y}}_{i} \left[\sum_{\substack{k=1 \ k \neq j}}^{p} \beta_{k} \mathbf{x}_{ki} \left[\lambda - 2\beta_{j}^{2} \right] \right] = 0$$

After further algebraic manipulation this reduces to

$$2\beta_{i}^{4}\hat{y}_{i}x_{ii} - 2\beta_{i}^{3}\hat{y}_{i}^{2} - \lambda\beta_{i}^{2}\hat{y}_{i}x_{ii} + \beta_{i}[\lambda\hat{y}_{i}^{2} - 2(y_{i}^{2} + \hat{y}_{i}^{2})] + \lambda x_{ii}(\hat{y}_{i} - y_{i})$$

which is a quartic in eta_j . This has no closed-form solution since the coefficients of the eta_j terms involve \hat{y}_i 's which themselves depend on eta_j .

APPENDIX H

PROGRAM LISTING FOR MULTIVARIATE ORTHOGONAL PARAMETER ESTIMATION

H.1 MAIN PROGRAM

```
cls;
count=1;
pcount=1;
               Orthogonal Least-Squares for Multivariate Calibration";
               _______;
print;
                               David R. Fox";
print;
                          University of Wyoming";
                              February 1989.";
print;
print;
" Input requirements: ";
" ===========;
print;
                   Matrix Y (nxp) of dependent variable values";
print;
                   Matrix X (nxq) of independent variable values";
print;
print;
" Output : ";
" ======";
print;
                   Matrix B (qxp) of paramter estimates which minimize
                   generalized distance.";
print;
dos pause;
cls;
print;
       Enter epsilon for convergence : ";;
epsilon=con(1,1);
cls;
/*
       Determine p , q and n
                                */;
p=cols(y);
q=cols(x);
n=rows(y);
borthog=zeros(q,p);
```

```
Obtain OLS estimate for b */;
b=inv(x'x)*x'y;
do while pcount<=p;</pre>
        Extract current components of Y and B */;
yc=y[.,pcount];
bc=b[.,pcount];
        Perform Newton-Raphson iteration
        Note: Projection matrix is computed in Proc calc */;
kk=1;
inc=999999;
format /ld 4,0;
do while inc>epsilon;
h=hessp(&calc,bc);
g=gradp(&calc,bc);
delta=inv(h)*g';
inc=delta'delta;
bc=bc-delta;
"Iteration # ";;kk;
kk=kk+1;
format /rd 12,6;
bc;
endo:
print;
format /ld 4,0;
      Convergence established at iteration ";;kk;;" for column ";;pcount
print;
borthog[.,pcount]=bc;
pcount=pcount+1;
endo;
print;
                                 DONE !! ";
print;
     Orthogonal matrix is :";
format /rd 12,6;
borthog;
print;
     OLS matrix is : ";
b;
stop;
```

H.2 SUBROUTINE FOR CALCULATION OF ELEMENTS OF HESSIAN MATRIX.

```
proc calc(bc);
local w;
/* Form matrix Q */;
Qc=eye(q)-inv(1+bc'bc)*bc*bc';
/* Form matrix Z */;
Zc=x~yc;
/* Construct projection matrix P */;
```

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APPENDIX I

PROGRAM LISTING FOR MULTIVARIATE BIAS/MSE SIMULATION

I.1 MAIN PROGRAM

```
cls;
count=1;
pcount=1;
               Simulation of multivariate calibration estimators";
               print;
                               David R. Fox";
print;
                           University of Wyoming";
11
                              February 1989.";
print;
print;
print;
print;
       This program simulates multivariate X and Y data having";
       a specified covariance structure. X is 2-dimensional and";
       Y is 4-dimensional.";
print;
print;
                   means and variances for X1 and X2";
/* "
                coefficients of variation for Y1, Y2, Y3, and Y4.";
                correlation between errors in X1 and X2";
11
                correlation between errors in Y's";
          *
                correlation between errors in X's and errors in Y's";
**
                measurement error variances for X1 and X2";
print;
dos pause;
cls;
                                DATA ENTRY";
                                _____";
print;
print; */;
dos pause;
loop1:;
dos e:input;
cls:
load data[15,1]=e:mvc.dat;
```

```
load beta[2,4] = e: beta.dat;
rhox=data[11,1];rhoy=data[12,1];rhoxy=data[13,1];nsamp=data[14,1];
nsim=data[15,1];
cy=data[7:10,1]; varx=data[3:4,1]; mux=data[1:2,1]; varu=data[5:6,1];
print;
print;
print;
print;
              Do you want to change any of the input data (y/n) ? : ";;
reply=cons;
if reply $=="Y" or reply $=="y";
goto loop1;
endif;
ncount=1;
biasi=zeros(nsim, 2);
biasc=zeros(nsim, 2);
biaso=zeros(nsim,2);
do while ncount<=nsim;</pre>
print;
format /ld 3,0;
" Simulation run # ";;ncount;
format /rd 9,4;
                                                  */;
/*
                         construct sigmax
s12=rhox*(varx[1,1]*varx[2,1])^.5;
sigmax=varx[1,1]~s12|s12~varx[2,1];
                                                                   */;
                         spectral decomposition of sigmax
{va,p}=eigrs2(sigmax);
va=va^.5;
d1=eye(2);
d1=diagrv(d1,va);
a=p*d1;
                         generate (n+1) observations from N2(0,1)
/*
z1=rndn(nsamp+1,2);
                         compute matrix of xs
                                                  */;
m1=ones(nsamp+1,1)*mux[1,1];
m2=ones(nsamp+1,1)*mux[2,1];
m=m1^m2;
x=z1*a+m;
                                          */;
/*
                         compute muY
muy=mux'*beta;
                                                  */;
                         assemble sigmae
sigmae=zeros(4,4);
i=1;
j=1;
do while i <= 4;</pre>
j=1;
do while j <= 4;
if i==j;
sigmae[i,i]=(cv[i,1]*muy[1,i])^2;
sigmae[i,j]=rhoy*cv[i,1]*muy[1,i]*cv[j,1]*muy[1,j];
endif;
j=j+1;
```

```
endo;
i=i+1;
endo:
                        assemble sigmaeu
                                                */;
/*
sigmaeu=zeros(4,2);
i=1;
j=1:
do while i <= 4;
j=1;
do while j \le 2;
sigmaeu[i,j]=rhoxy*(cv[i,1]*muy[1,i]*varx[j,1])^.5;
j=j+1;
endo;
i=i+1;
endo;
                        assemble sigmau
                                                */;
/*
s12=rhox*(varu[1,1]*varu[2,1])^.5;
sigmau=varu[1,1]~s12|s12~varu[2,1];
                                                */;
                        assemble sigma
sigma=sigmae~sigmaeu |sigmaeu'~sigmau;
                                                              */;
                        spectral decomposition of sigma
{var, vai, p, vei} = eigrg2(sigma);
k=1;
do while k < =6;
if var[k,1]<0;
var[k,1]=0;
endif;
k=k+1;
endo;
var=var^.5;
d2=eye(6);
d2=diagrv(d2, var);
b=p*d2;
                        generate (n+1) observations from N6(0,1)
/*
z2=rndn(nsamp+1,6);
er=z2*b;
e=er[.,1:4];
u=er[.,5:6];
capx=x+u;
capy=x*beta+e;
x0=x[nsamp+1,.];
y0=capy[nsamp+1,.];
capx=capx[1:nsamp,.];
capy=capy[1:nsamp,.];
                    /*
/*
*/;
                                                        */;
                                Inverse estimation
ghat=inv(capy'capy)*capy'capx;
biasi[ncount,.]=x0-y0*ghat;
                                                        */;
                                Classical estimation
/*
bhat=inv(capx'capx)*capx'capy;
```

```
resid=capy-capx*bhat;
shat=resid'resid/nsamp;
shat=inv(shat);
biasc[ncount,.]=x0-(inv(bhat*shat*bhat')*bhat*shat*y0')';
/* Orthogonal estimator */;
borthog=orthog;
resid=capy-capx*borthog;
shat=resid'resid/nsamp;
shat=inv(shat);
biaso[ncount,.]=x0-(inv(borthog*shat*borthog')*borthog*shat*y0')';
ncount=ncount+1;
endo;
format /rd 9,4;
stop;
```

1.2 INITIALIZATION SUBROUTINE.

```
capx=zeros(nsamp+1,2);
capy=zeros(nsamp+1,4);
bhat=zeros(2,4);
bc=zeros(2,1);
p=4;
q=2;
qc=zeros(q,q);
zc=zeros(nsamp,q+1);
p2=zeros(q,1);
p4=zeros(1,1);
pc=zeros(q+1,q+1);
zp=zc;
xp=zeros(nsamp,q);
yp=zeros(nsamp,1);
yc=zeros(nsamp,1);
run e:mvccalc.arc;
run gradp.g;
run hessp.g;
```

I.3 ITERATIVE PROCEDURE FOR CALCULATION OF ORTHOGONAL ESTIMATES.

```
proc orthog;
local n,kk,pcount,inc,h,g,delta,borthog,newstart,mss;
newstart=0;
pcount=1;
/* Determine p , q and n */;
p=cols(capy);
q=cols(capx);
n=rows(capy);
borthog=zeros(q,p);
```

```
format /1d 2,0;
do while pcount <= p;</pre>
        Orthogonal estimate: Iterating on column ";;pcount;;
/*
        Extract current components of Y and B */;
yc=capy[.,pcount];
bc=bhat[.,pcount];
        Perform Newton-Raphson iteration
        Note: Projection matrix is computed in Proc calc */;
kk=1:
inc=999999;
do while inc>.00001;
if kk>15;
if newstart>4;
print:
" No convergence after 5 restarts - giving up !!";
borthog=zeros(q,p);
mss=zeros(1,p);
borthog=miss(borthog, mss);
retp(borthog);
endif;
print;
" Convergence not obtained after 15 iterations - trying new initial esti
newstart=newstart+1;
bc=rndu(q,1)*10;
kk=1;
endif;
h=hessp(&calc,bc);
g=gradp(&calc,bc);
delta=inv(h)*g';
inc=delta'delta;
bc=bc-delta;
kk=kk+1;
endo;
"(";;kk;;")";
borthog[.,pcount]=bc;
pcount=pcount+1;
endo;
retp(borthog);
endp;
```

1.4 SUBROUTINE FOR GRADIENT AND HESSIAN ELEMENTS.

```
proc calc(bc);
local w;
/* Form matrix Q */;
Qc=eye(q)-inv(1+bc'bc)*bc*bc';
/* Form matrix Z */;
Zc=capx~yc;
/* Construct projection matrix P */;
P2=Qc*bc;
```

```
P4=bc'qc*bc;
Pc=(Qc^P2) | (P2'^P4);
/* Obtain X and Y projections , store into xp and yp */;
Zp=zc*Pc;
xp=zp[.,1:q];
yp=zp[.,q+1];
w=(yp-yc)'(yp-yc)+sumc(diag((xp-capx)'(xp-capx)));
retp(w);
endp;
```

I.5 DBASEIII SUBROUTINE FOR DATA ENTRY.

```
set talk off
set exact on
set confirm on
clear memory
store chr(7) to bell
store '' to fn
clear
use e:mvc.dbf
@1,1 say date()
@1,20 say 'MULTIVARIATE CALIBRATION SIMULATION'
@1,70 say 'DATA ENTRY'
@2,20 say '=========='
@2,72 say time()
@5,10 say 'The following information is required:'
@7,5 say '* Mean of X1'
@8,5 say '*
              Variance of X1'
@9,5 say '*
              Mean of X2'
             Variance of X2'
@10,5 say '*
@11,5 say '* Measurement error variance for X1'
@12,5 say '* Measurement error variance for X2'
@13,5 say '* Coefficients of variation for Y1, Y2, Y3, and Y4'
@14,5 say '*
               Correlation between Xs'
               Correlation between Ys'
@15,5 say '*
@16,5 say '*
               Corrrelation between Xs and Ys'
@22,25 say 'Press Q to exit procedure'
                           Press any other key to continue to continue
wait '
if continue="Q".or.continue="q"
quit
endif
store '' to fn
store .f. to flag3
clear
@1,1 say date()
@1,20 say 'MULTIVARIATE CALIBRATION SIMULATION'
@1,70 say 'DATA ENTRY'
@2,20 say '================================
@2,72 say time()
@3,5 say 'Mean X1 : ' get mux1
```

```
@3,42 say 'Mean X2 : ' get mux2
@5,1 say 'Variance X1 : ' get varx1
@5,38 say 'Variance X2 : ' get varx2
@7,25 say 'Measurement-error variances :'
@8,25 say '-----'
@10,12 say 'For X1 : ' get varu1
@10,45 say 'For X2 : ' get varu2
@12,25 say 'Coefficients of Variation : '
@13,25 say '-----'
@15,15 say 'For Y1 : ' get cy1
@15,45 say 'For Y2 : ' get cy2
@17,15 say 'For Y3 : ' get cy3
@17,45 say 'For Y4 : ' get cy4
@19,15 say 'Correlation coefficients for error components :'
@20,15 say '-----'
@21,5 say 'Between Xs : ' get rhox
@21,27 say 'Between Ys : ' get rhoy
@21,50 say 'Between Xs and Ys : ' get rhoxy
@23,10 say 'Sample size : ' get nsamp
@23,40 say 'Length of simulation run : ' get nsim
read
                                                                   fields
                                         e:mvc.dat
сору
                     to
mux1, mux2, varx1, varx2, varu1, varu2, cy1, cy2, cy3, cy4, rhox, rhoy, rhoxy, nsamp,
clear
go top
@1,1 say date()
@1,20 say 'MULTIVARIATE CALIBRATION SIMULATION'
@1,70 say 'DATA ENTRY'
@2,20 say '============'
@2,72 say time()
@5,25 say 'ENTER ELEMENTS OF B MATRIX'
@10,5 say 'B11 : ' get b11
@10,23 say 'B12 : ' get b12
@10,43 say 'B13 : ' get b13
@10,63 say 'B14 : ' get b14
@12,5 say 'B21 : ' get b21
@12,23 say 'B22 : ' get b22
@12,43 say 'B23 : ' get b23
@12,63 say 'B24 : ' get b24
copy to e:beta.dat fields b11,b12,b13,b14,b21,b22,b23,b24 sdf
```

APPENDIX J

DERIVATION OF CONDITIONAL MULTIVARIATE NORMAL P.D.F.

Let X and Y be two random vectors and $\left[\begin{array}{c} X \\ Y \end{array} \right]$ be multivariate normally distributed with mean vector

$$\mathbb{E}\left[\begin{array}{c} X \\ Y \end{array}\right] = \left[\begin{array}{c} \mu_X \\ \mu_Y \end{array}\right]$$

and non-singular covariance matrix

$$\operatorname{Cov}\left[\begin{array}{c} \mathbf{X} \\ \mathbf{Y} \end{array}\right] = \left[\begin{array}{ccc} \mathbf{C}_{11} & \mathbf{C}_{12} \\ \mathbf{C}_{12}^{\mathsf{T}} & \mathbf{C}_{22} \end{array}\right].$$

Define \widetilde{Y} as the random vector Y given X = x, where x is a vector of deterministic scalars. Then \widetilde{Y} has the multivariate normal distribution with mean

$$\mathbb{E}[\widetilde{\mathbf{Y}}] = \mathbf{C}_{12}^{\mathsf{T}} \mathbf{C}_{11}^{-1} (\mathbf{x} - \boldsymbol{\mu}_{\mathbf{x}}) + \boldsymbol{\mu}_{\mathbf{y}}$$

and covariance matrix

$$Cov[\tilde{Y}] = C_{22} - C_{12}^{T}C_{11}^{-1}C_{12}$$
.

Proof:

$$\mathbf{f}_{X,Y}(x,y) = \frac{\exp\left[-\frac{1}{2}(X^{\mathsf{T}} - \mu_{X}^{\mathsf{T}}, Y^{\mathsf{T}} - \mu_{y}^{\mathsf{T}}) \begin{bmatrix} c_{11} & c_{12} \\ c_{12}^{\mathsf{T}} & c_{22} \end{bmatrix}^{-1} \begin{bmatrix} X - \mu_{X} \\ Y - \mu_{Y} \end{bmatrix} \right]}{(2\pi)^{\frac{\nu_{1} + \nu_{2}}{2}} \begin{bmatrix} c_{11} & c_{12} \\ c_{12}^{\mathsf{T}} & c_{22} \end{bmatrix}^{\frac{1}{2}}}$$

where

 $\nu_{_{\rm I}}$ is the dimension of X

and

 $\boldsymbol{\nu}_2$ is the dimension of Y .

The marginal density for X is

$$f_{X}(x) = \frac{\exp\left[-\frac{1}{2}(X^{T} - \mu_{X}^{T}) C_{11}^{-1} (X - \mu_{X})\right]}{(2\pi)^{\nu_{1}/2} |C_{11}|^{\frac{1}{2}}}$$

The conditional density for $\tilde{Y} = (Y \mid X = x)$ is :

$$f_{\widetilde{Y}}(y) = f_{Y|X=x}(y) = f_{X,Y}(x,y)/f_{X}(x)$$

$$= \kappa \exp \left[\frac{1}{2} (\mathbf{x} - \mu_{\mathbf{x}})^{\mathsf{T}} C_{11}^{-1} (\mathbf{x} - \mu_{\mathbf{x}})^{-\frac{1}{2}} (\mathbf{x} - \mu_{\mathbf{x}}, \mathbf{y} - \mu_{\mathbf{y}})^{\mathsf{T}} \begin{bmatrix} \mathbf{M}_{11} & \mathbf{M}_{12} \\ \mathbf{M}_{12}^{\mathsf{T}} & \mathbf{M}_{22} \end{bmatrix} \begin{bmatrix} \mathbf{x} - \mu_{\mathbf{x}} \\ \mathbf{y} - \mu_{\mathbf{y}} \end{bmatrix} \right]$$

where

$$\kappa = \frac{\left| C_{11} \right|^{\frac{1}{2}}}{\left(2\pi \right)^{\nu_2/2} \left| \begin{matrix} C_{11} & C_{12} \\ C_{12}^{\mathsf{T}} & C_{22} \end{matrix} \right|^{\frac{1}{2}}}$$

and

$$\begin{bmatrix} \mathbf{M}_{11} & \mathbf{M}_{12} \\ \mathbf{M}_{12}^{\mathsf{T}} & \mathbf{M}_{22} \end{bmatrix} = \begin{bmatrix} \mathbf{C}_{11} & \mathbf{C}_{12} \\ \mathbf{C}_{12}^{\mathsf{T}} & \mathbf{C}_{22} \end{bmatrix}^{-1} .$$

Furthermore, it can be shown that

$$\begin{aligned} \mathbf{M}_{11} &= \left(\mathbf{C}_{11} - \mathbf{C}_{12} \mathbf{C}_{22}^{-1} \mathbf{C}_{12}^{\mathsf{T}} \right)^{-1} ; \\ \mathbf{M}_{22} &= \left(\mathbf{C}_{22} - \mathbf{C}_{12}^{\mathsf{T}} \mathbf{C}_{11}^{-1} \mathbf{C}_{12} \right)^{-1} ; \\ \mathbf{M}_{12} &= -\mathbf{C}_{11}^{-1} \mathbf{C}_{12} \mathbf{M}_{22} \\ &= -\mathbf{C}_{11}^{-1} \mathbf{C}_{12} \left(\mathbf{C}_{22} - \mathbf{C}_{12}^{\mathsf{T}} \mathbf{C}_{11}^{-1} \mathbf{C}_{12} \right)^{-1} . \end{aligned}$$

Thus $f_{\widetilde{Y}}(y) =$

where

$$\kappa \exp \left[\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_{x})^{\top} (C_{11}^{-1} - \mathbf{M}_{11}) (\mathbf{x} - \boldsymbol{\mu}_{x})\right] \exp \left[-\frac{1}{2}\left[(\mathbf{y} - \boldsymbol{\mu}_{y})^{\top} \mathbf{M}_{22} (\mathbf{y} - \boldsymbol{\mu}_{y}) + 2(\mathbf{x} - \boldsymbol{\mu}_{x})^{\top} \mathbf{M}_{12} (\mathbf{y} - \boldsymbol{\mu}_{y})\right]\right]$$

The last exponent of the previous expression can be written as

$$(\mathbf{y} - \boldsymbol{\mu}_{\mathbf{y}})^{\mathsf{T}} \mathbf{M}_{22} (\mathbf{y} - \boldsymbol{\mu}_{\mathbf{y}}) + 2(\mathbf{x} - \boldsymbol{\mu}_{\mathbf{x}})^{\mathsf{T}} \mathbf{M}_{12} (\mathbf{y} - \boldsymbol{\mu}_{\mathbf{y}}) =$$

$$(\mathbf{y} - \boldsymbol{\mu}_{\mathbf{y}} - \mathbf{m})^{\mathsf{T}} \mathbf{M}_{22} (\mathbf{y} - \boldsymbol{\mu}_{\mathbf{y}} - \mathbf{m}) - (\mathbf{x} - \boldsymbol{\mu}_{\mathbf{x}})^{\mathsf{T}} \mathbf{M}_{12} \mathbf{M}_{22}^{-1} \mathbf{M}_{12}^{\mathsf{T}} (\mathbf{x} - \boldsymbol{\mu}_{\mathbf{x}})$$

$$\mathbf{m} = -\mathbf{M}_{22}^{-1} \mathbf{M}_{12}^{\mathsf{T}} (\mathbf{x} - \boldsymbol{\mu}_{\mathbf{x}}) .$$

After some algebraic manipulation we obtain

 $= \mu_{y} + C_{12}^{T}C_{11}^{-1}(x - \mu_{x})$.

$$f_{\widetilde{\mathbf{Y}}}(\mathbf{y}) = \kappa \exp[(\mathbf{y} - \boldsymbol{\mu}_{\mathbf{y}} - \mathbf{m})^{\mathsf{T}} \mathbf{M}_{22}(\mathbf{y} - \boldsymbol{\mu}_{\mathbf{y}} - \mathbf{m})]$$
.

This is the multivariate normal density with mean vector $\pmb{\mu}_{\rm y}$ + ${\bf m}$ and covariance matrix ${\rm M}_{2\,2}^{-1}$.

Thus:

$$\begin{split} \mathbb{E}[\widetilde{Y}] &= \mu_{y} + \mathbf{m} = \mu_{y} - \mathbf{M}_{22}^{-1} \mathbf{M}_{12}^{\mathsf{T}} (\mathbf{x} - \mu_{x}) \\ &= \mu_{y} - (\mathbf{C}_{22} - \mathbf{C}_{12}^{\mathsf{T}} \mathbf{C}_{11}^{-1} \mathbf{C}_{12}) \left[-\mathbf{C}_{11}^{-1} \mathbf{C}_{12} (\mathbf{C}_{22} - \mathbf{C}_{12}^{\mathsf{T}} \mathbf{C}_{11}^{-1} \mathbf{C}_{12})^{-1} \right]^{\mathsf{T}} (\mathbf{x} - \mu_{x}) \\ &= \mu_{y} + (\mathbf{C}_{22} - \mathbf{C}_{12}^{\mathsf{T}} \mathbf{C}_{11}^{-1} \mathbf{C}_{12}) (\mathbf{C}_{22} - \mathbf{C}_{12}^{\mathsf{T}} \mathbf{C}_{11}^{-1} \mathbf{C}_{12})^{-1} \mathbf{C}_{12}^{\mathsf{T}} \mathbf{C}_{11}^{-1} (\mathbf{x} - \mu_{x}) \end{split}$$

and

$$Cov[\widetilde{Y}] = M_{22}^{-1} = C_{22} - C_{12}^{T}C_{11}^{-1}C_{12}$$
 QED.

APPENDIX K

DELETION STATISTICS: REVISED PARAMETER AND COVARIANCE ESTIMATES

K.1 REVISED PARAMETER ESTIMATES

The derivation of equation (3.61) is as follows:

Without loss of generality, we can partition X as $\left[\frac{X_{(I)}}{X_{I}}\right]$ where $X_{(I)}$ is a (n-m) x p matrix and X_{I} is m x p.

Thus

$$\mathbf{X}^{\mathsf{T}}\mathbf{X} = \begin{bmatrix} \mathbf{X}_{(1)}^{\mathsf{T}} & \mathbf{X}_{1}^{\mathsf{T}} \end{bmatrix} \begin{bmatrix} \mathbf{X}_{(1)}^{\mathsf{T}} \\ \mathbf{X}_{1} \end{bmatrix} = \mathbf{X}_{(1)}^{\mathsf{T}}\mathbf{X}_{(1)} + \mathbf{X}_{1}^{\mathsf{T}}\mathbf{X}_{1}$$

and

$$\mathbf{X}_{(\mathtt{I})}^{\mathsf{T}}\mathbf{X}_{(\mathtt{I})} = \mathbf{X}^{\mathsf{T}}\mathbf{X} - \mathbf{X}_{\mathtt{I}}^{\mathsf{T}}\mathbf{X}_{\mathtt{I}}$$

$$\Rightarrow \left[\mathbf{X}_{(\mathtt{I})}^{\mathsf{T}}\mathbf{X}_{(\mathtt{I})}\right]^{-1} = \left[\mathbf{X}^{\mathsf{T}}\mathbf{X} - \mathbf{X}_{\mathtt{I}}^{\mathsf{T}}\mathbf{X}_{\mathtt{I}}\right]^{-1}$$

Using the fact that $(A - UV^{\mathsf{T}})^{-1} = A^{-1} + A^{-1}U(I - V^{\mathsf{T}}A^{-1}U)^{-1}V^{\mathsf{T}}A^{-1}$ with $A = (X^{\mathsf{T}}X)$, $U = X_{\mathsf{I}}^{\mathsf{T}}$ and $V = X_{\mathsf{I}}$ we have

$$[X^{\mathsf{T}}X - X_{\mathtt{I}}^{\mathsf{T}}X_{\mathtt{I}}]^{-1} = (X^{\mathsf{T}}X)^{-1} + (X^{\mathsf{T}}X)^{-1}X_{\mathtt{I}}^{\mathsf{T}}[I - X_{\mathtt{I}}(X^{\mathsf{T}}X)^{-1}X_{\mathtt{I}}^{\mathsf{T}}]^{-1}X_{\mathtt{I}}(X^{\mathsf{T}}X)^{-1}$$
.

We identify the hat matrix: $H_{I} = X_{I}(X^{T}X)^{-1}X_{I}^{T}$ and therfore

$$[x_{(1)}^{\mathsf{T}}x_{(1)}]^{-1} = (x^{\mathsf{T}}x)^{-1} + (x^{\mathsf{T}}x)^{-1}x_{1}^{\mathsf{T}}[1 - H_{1}]^{-1}x_{1}(x^{\mathsf{T}}x)^{-1}$$
.

Now, the matrix of revised parameter estimates $\hat{m{\beta}}_{(1)}$ is

$$\hat{\beta}_{(1)} = [X_{(1)}^{T} X_{(1)}]^{-1} X_{(1)}^{T} Y_{(1)}$$

Furthermore

$$X = \begin{bmatrix} X_{(1)} \\ \overline{X_{1}} \end{bmatrix}$$
 and $Y = \begin{bmatrix} Y_{(1)} \\ \overline{Y_{1}} \end{bmatrix}$

thus

$$\mathbf{X}^{\mathsf{T}}\mathbf{Y} = \begin{bmatrix} \mathbf{X}_{(1)}^{\mathsf{T}} & \mathbf{X}_{1}^{\mathsf{T}} \end{bmatrix} \begin{bmatrix} \mathbf{Y}_{(1)}^{\mathsf{T}} \\ \mathbf{Y}_{1} \end{bmatrix} = \mathbf{X}_{(1)}^{\mathsf{T}}\mathbf{Y}_{(1)}^{\mathsf{T}} + \mathbf{X}_{1}^{\mathsf{T}}\mathbf{Y}_{1}^{\mathsf{T}}$$

$$\Rightarrow \qquad \mathbf{X}_{(\mathbf{I})}^{\mathsf{T}}\mathbf{Y}_{(\mathbf{I})} = \mathbf{X}^{\mathsf{T}}\mathbf{Y} - \mathbf{X}_{\mathbf{I}}^{\mathsf{T}}\mathbf{Y}_{\mathbf{I}} .$$

Hence

$$\hat{\beta}_{(I)} = [X_{(I)}^{T}X_{(I)}]^{-1}[X^{T}Y - X_{I}^{T}Y_{I}]$$

$$= \{(X^{T}X)^{-1} + (X^{T}X)^{-1}X_{I}^{T}[I - H_{I}]^{-1}X_{I}(X^{T}X)^{-1}\}[X^{T}Y - X_{I}^{T}Y_{I}]$$

$$= (X^{T}X)^{-1}X^{T}Y + (X^{T}X)^{-1}X_{I}^{T}[I - H_{I}]^{-1}X_{I}(X^{T}X)^{-1}X^{T}Y - (X^{T}X)^{-1}X_{I}^{T}Y_{I}$$

$$- (X^{T}X)^{-1}X_{I}^{T}[I - H_{I}]^{-1}X_{I}(X^{T}X)^{-1}X_{I}^{T}Y_{I}$$

$$= \hat{\beta} + (X^{T}X)^{-1}X_{I}^{T}[I - H_{I}]^{-1}X_{I}\hat{\beta} - (X^{T}X)^{-1}X_{I}^{T}Y_{I}$$

$$- (X^{T}X)^{-1}X_{I}^{T}[I - H_{I}]^{-1}X_{I}(X^{T}X)^{-1}X_{I}^{T}Y_{I}$$

$$= \hat{\beta} + (X^{T}X)^{-1}X_{I}^{T}[I - H_{I}]^{-1}\hat{\gamma}_{I} - (X^{T}X)^{-1}X_{I}^{T}Y_{I} - (X^{T}X)^{-1}X_{I}^{T}Y_{I}$$

Thus
$$\hat{\boldsymbol{\beta}}_{(1)} - \hat{\boldsymbol{\beta}} = (\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1}\mathbf{X}_{1}^{\mathsf{T}}\{[\mathbf{I} - \mathbf{H}_{1}]^{-1}\hat{\mathbf{Y}}_{1} - \mathbf{Y}_{1} - [\mathbf{I} - \mathbf{H}_{1}]^{-1}\mathbf{H}_{1}\mathbf{Y}_{1}\}$$

$$= (\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1}\mathbf{X}_{1}^{\mathsf{T}}\{-\mathbf{Y}_{1} - [\mathbf{I} - \mathbf{H}_{1}]^{-1}\mathbf{H}_{1}\mathbf{Y}_{1} + [\mathbf{I} - \mathbf{H}_{1}]^{-1}\hat{\mathbf{Y}}_{1}\}$$

Now,
$$-Y_{I} - [I - H_{I}]^{-1}H_{I}Y_{I} = -[I + (I - H_{I})^{-1}H_{I}]Y_{I}$$
.

Next consider the term $I + (I - H_I)^{-1}H_I$ and again use $(A - UV^T)^{-1} = A^{-1} + A^{-1}U(I - V^TA^{-1}U)^{-1}V^TA^{-1}$ with A = I; U = I; and $V^T = H_I$ thus

$$(I - H_I)^{-1} = I + (I - H_I)^{-1}H_I$$

and therefore

$$-Y_{I} - [I - H_{I}]^{-1}H_{I}Y_{I} = -(I - H_{I})^{-1}Y_{I}$$

and so

$$\hat{\beta}_{(I)} - \hat{\beta} = (X^{T}X)^{-1}X_{I}^{T}\{-(I - H_{I})^{-1}Y_{I} + (I - H_{I})^{-1}\hat{Y}_{I}\}$$

$$= (X^{T}X)^{-1}X_{I}^{T}(I - H_{I})^{-1}[\hat{Y}_{I} - Y_{I}]$$

Letting $R_I = \hat{Y}_I - Y_I$ we thus obtain

$$\hat{\boldsymbol{\beta}}_{(I)} - \hat{\boldsymbol{\beta}} = (\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1}\mathbf{X}_{\mathsf{T}}^{\mathsf{T}}(\mathbf{I} - \mathbf{H}_{\mathsf{T}})^{-1}\mathbf{R}_{\mathsf{T}}$$

K.2 REVISED RESIDUAL SUM OF SQUARES

Prior to deletion our estimate of the error-covariance matrix Σ is

$$(\mathbf{n}-\mathbf{p})\,\hat{\Sigma} = \mathbf{Y}^{\mathsf{T}}\mathbf{Y} - \hat{\boldsymbol{\beta}}^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}\mathbf{Y}$$

After deletion of the ith observation this becomes:

$$(n-m-p)\hat{\Sigma}_{(1)} = Y^{T}Y - Y_{1}^{T}Y_{1} - \hat{\beta}_{(1)}^{T}(X^{T}Y - X_{1}^{T}Y_{1})$$

$$\Rightarrow (n-m-p)\hat{\Sigma}_{(1)} = (n-p)\hat{\Sigma} + \hat{\beta}X^{T}Y - Y_{1}^{T}Y_{1} - \hat{\beta}_{(1)}^{T}(X^{T}Y - X_{1}^{T}Y_{1})$$

$$= (n-p)\hat{\Sigma} - \{R_{1}^{T}(I - H_{1})^{-1}X_{1}(X^{T}X)^{-1}\}X^{T}Y - Y_{1}^{T}Y_{1} + \hat{\beta}_{(1)}^{T}X_{1}^{T}Y_{1}$$

$$= (n-p)\hat{\Sigma} - R_{I}^{T}(I - H_{I})^{-1}X_{I}\hat{\beta} - Y_{I}^{T}Y_{I} + \hat{\beta}_{(I)}^{T}X_{I}^{T}Y_{I}$$

$$= (n-p)\hat{\Sigma} - R_{I}^{T}(I - H_{I})^{-1}\hat{Y}_{I} - Y_{I}^{T}Y_{I} + \hat{\beta}_{(I)}^{T}X_{I}^{T}Y_{I}$$

$$= (n-p)\hat{\Sigma} - R_{I}^{T}(I - H_{I})^{-1}\hat{Y}_{I} - \{Y_{I}^{T}Y_{I} - \hat{\beta}_{(I)}^{T}X_{I}^{T}Y_{I}\}$$

Consider the expression inside the braces {}:

$$\mathbf{Y}_{\mathbf{I}}^{\mathsf{T}}\mathbf{Y}_{\mathbf{I}} - \hat{\boldsymbol{\beta}}_{(\mathbf{I})}^{\mathsf{T}}\mathbf{X}_{\mathbf{I}}^{\mathsf{T}}\mathbf{Y}_{\mathbf{I}} = (\mathbf{Y}_{\mathbf{I}}^{\mathsf{T}} - \hat{\boldsymbol{\beta}}_{(\mathbf{I})}^{\mathsf{T}}\mathbf{X}_{\mathbf{I}}^{\mathsf{T}})\mathbf{Y}_{\mathbf{I}} = (\mathbf{Y}_{\mathbf{I}} - \mathbf{X}_{\mathbf{I}}\hat{\boldsymbol{\beta}}_{(\mathbf{I})})^{\mathsf{T}}\mathbf{Y}_{\mathbf{I}}$$

Now,

$$\begin{aligned} \mathbf{Y}_{1} - \mathbf{X}_{1} \hat{\boldsymbol{\beta}}_{(1)} &= \mathbf{Y}_{1} - \mathbf{X}_{1} \{ [\mathbf{X}_{(1)}^{\mathsf{T}} \mathbf{X}_{(1)}]^{-1} [\mathbf{X}^{\mathsf{T}} \mathbf{Y} - \mathbf{X}_{1}^{\mathsf{T}} \mathbf{Y}_{1}] \} \\ &= \mathbf{Y}_{1} - \mathbf{X}_{1} \{ [(\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} + (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}_{1}^{\mathsf{T}} (\mathbf{I} - \mathbf{H}_{1})^{-1} \mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1}] (\mathbf{X}^{\mathsf{T}} \mathbf{Y} - \mathbf{X}_{1}^{\mathsf{T}} \mathbf{Y}_{1}) \} \\ &= \mathbf{Y}_{1} - \{ [\mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} + \mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}_{1}^{\mathsf{T}} (\mathbf{I} - \mathbf{H}_{1})^{-1} \mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1}] (\mathbf{X}^{\mathsf{T}} \mathbf{Y} - \mathbf{X}_{1}^{\mathsf{T}} \mathbf{Y}_{1}) \} \\ &= \mathbf{Y}_{1} - \{ \mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}^{\mathsf{T}} \mathbf{Y} + \mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}_{1}^{\mathsf{T}} (\mathbf{I} - \mathbf{H}_{1})^{-1} \mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}^{\mathsf{T}} \mathbf{Y} \\ &- \mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}_{1}^{\mathsf{T}} \mathbf{Y}_{1} - \mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}_{1}^{\mathsf{T}} (\mathbf{I} - \mathbf{H}_{1})^{-1} \mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}_{1}^{\mathsf{T}} \mathbf{Y}_{1} \} \\ &= \mathbf{Y}_{1} - \mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}^{\mathsf{T}} \mathbf{Y} - \mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}_{1}^{\mathsf{T}} (\mathbf{I} - \mathbf{H}_{1})^{-1} \mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}_{1}^{\mathsf{T}} \mathbf{Y}_{1} \\ &+ \mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}_{1}^{\mathsf{T}} \mathbf{Y}_{1} + \mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}_{1}^{\mathsf{T}} (\mathbf{I} - \mathbf{H}_{1})^{-1} \mathbf{X}_{1} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}_{1}^{\mathsf{T}} \mathbf{Y}_{1} \end{aligned}$$

Recall that $H_I = X_I (X^T X)^{-1} X_I^T$; $R_I = \hat{Y}_I - Y_I$; and $\hat{Y}_I = X_I \hat{\beta}$, thus the right hand side of the previous expression becomes

$$=Y_{1} - \hat{Y}_{1} - H_{1}(I - H_{1})^{-1}\hat{Y}_{1} + H_{1}Y_{1} + H_{1}(I - H_{1})^{-1}H_{1}Y_{1}$$

Now,

$$H_{1}Y_{1} + H_{1}(I - H_{1})^{-1}H_{1}Y_{1} = [I + H_{1}(I - H_{1})^{-1}]H_{1}Y_{1}$$

and since both $H_{\scriptscriptstyle \rm I}$ and $\left(I - H_{\scriptscriptstyle \rm I}\right)^{-1}$ are symmetric their product is commutative and hence

$$H_{I}Y_{I} + H_{I}(I - H_{I})^{-1}H_{I}Y_{I} = [I + (I - H_{I})^{-1}H_{I}]H_{I}Y_{I}$$

Finally,

$$\mathbf{Y}_{I} - \hat{\mathbf{Y}}_{I} - \mathbf{H}_{I} (\mathbf{I} - \mathbf{H}_{I})^{-1} \hat{\mathbf{Y}}_{I} + (\mathbf{I} - \mathbf{H}_{I})^{-1} \mathbf{H}_{I} \mathbf{Y}_{I}
= \mathbf{Y}_{I} - \hat{\mathbf{Y}}_{I} + (\mathbf{I} - \mathbf{H}_{I})^{-1} \mathbf{H}_{I} \{ \mathbf{Y}_{I} - \hat{\mathbf{Y}}_{I} \}
= \mathbf{Y}_{I} - \hat{\mathbf{Y}}_{I} \{ \mathbf{I} + (\mathbf{I} - \mathbf{H}_{I})^{-1} \mathbf{H}_{I} \}
= \mathbf{Y}_{I} - \hat{\mathbf{Y}}_{I} (\mathbf{I} - \mathbf{H}_{I})^{-1}
= -\mathbf{R}_{I} (\mathbf{I} - \mathbf{H}_{I})^{-1}$$

Therefore:
$$\mathbf{Y}_{\mathbf{I}}^{\mathsf{T}}\mathbf{Y}_{\mathbf{I}} - \hat{\boldsymbol{\beta}}_{(\mathbf{I})}^{\mathsf{T}}\mathbf{X}_{\mathbf{I}}^{\mathsf{T}}\mathbf{Y}_{\mathbf{I}} = (\mathbf{Y}_{\mathbf{I}} - \mathbf{X}_{\mathbf{I}}\hat{\boldsymbol{\beta}}_{(\mathbf{I})})^{\mathsf{T}}\mathbf{Y}_{\mathbf{I}}$$

$$= -[\mathbf{R}_{\mathbf{I}}(\mathbf{I} - \mathbf{H}_{\mathbf{I}})^{-1}]^{\mathsf{T}}\mathbf{Y}_{\mathbf{I}}$$

$$= -(\mathbf{I} - \mathbf{H}_{\mathbf{I}})^{-1}\mathbf{R}_{\mathbf{I}}^{\mathsf{T}}\mathbf{Y}_{\mathbf{I}}$$

and

$$(n-m-p)\hat{\Sigma}_{(r)} = (n-p)\hat{\Sigma} - R_{r}^{T}(I - H_{r})^{-1}\hat{Y}_{r} + R_{r}^{T}(I - H_{r})^{-1}Y_{r}$$

$$= (n-p)\hat{\Sigma} - R_{r}^{T}(I - H_{r})^{-1}[\hat{Y}_{r} - Y_{r}].$$

Thus

$$(n-m-p)\hat{\Sigma}_{(I)} = (n-p)\hat{\Sigma} - R_{I}^{T}(I-H_{I})^{-1}R_{I}$$
 QED.

APPENDIX L

PROGRAM LISTING FOR CALIBRATION IN A NON-STATIONARY FIELD

L.1 MAIN PROGRAM

```
cls;
count=1:
mseold=9999999999;
note="":
loadp gradp=c:\gauss\cp\gradp;
loadp hessp=c:\gauss\cp\hessp;
format /rd 3,0;
                    Calibration in a correlated field";
                    ------:::
                    (Generalized Least-Squares Version)";
print;
                             David R. Fox";
print;
                         University of Wyoming";
                            November 1988";
print;
print;
                         It is assumed there are k locations for which
   Input requirements:
                         following data is available at each location:
  _____
print;
         Xi : (v x 1) position vector for ith. location.";
**
         Wi: (n x p) matrix of n observations on p independent variab
         Vi : (n x 1) vector of observations on dependent variable.";
print;
  Given the linear model: Vi=Xi*Bi + Ei where Bi is a (p x 1) vector
   (unknown) parameters, the program will estimate using a least-squares
  procedure, the matrix A (p x v) where it is further assumed that :";
print;
                         Bi = A*Xi";
print;
dos pause;
cls;
print;
print;
print;
print;
                      HAVE YOU LOADED THE GLSCALC PROGRAM (y/n) ? : ";
```

```
reply=cons;
if reply $/="Y" and reply $/="y";
stop;
endif;
start:;
cls;
                               DATA ENTRY";
11
                               =======";
print;
print;
loop1:;
          Is data to come from keyboard or file (k/f): ";;
device=cons;
if device $/="K" and device $/="k" and device $/="F" and device $/="f";
print;
                * * * ERROR - MUST BE EITHER K OR T !";
11
                         Please reenter";
                      ";;
11
dos pause;
goto start;
elseif device $=="f" or device $=="F";
          Enter drive and (optionally) a path for stored matrices: ";;
source=cons;
load path=^source;
loadm w:
loadm v;
loadm x;
nu=rows(x);
k=cols(x);
n=rows(w)/k;
p=cols(w);
goto flag1;
endif;
          How many locations are there ? : ";;
k=con(1,1);
k=floor(k);
if k \le 0;
          < NOT A VALID SELECTION - REENTER >";
goto loop1;
endif;
print;
loop2:;
          How many observations at each of these locations ? : ";;
n=con(1,1);
n=floor(n);
if n \le 0;
          < NOT A VALID SELECTION - REENTER >";
goto loop2;
endif;
print;
loop3:;
          How many INDEPENDENT variables are there (Wi's) ? :";;
```

```
p=con(1,1);
p=floor(p);
if p \le 0;
          < NOT A VALID SELECTION - REENTER >";
goto loop3;
endif;
          Is a constant (B0) term to be included in the model (y/n): ";
reply1=cons;
if reply1 $=="Y" or reply1 $=="y";
note="(First value corresponds to B0 term)";
endif;
if p>n;
print;
                  * * * ERROR IN INPUT DATA * * *";
PRINT;
                  There are more parameters than observations";
print;
                       Please reenter from the beginning";
dos pause;
goto start;
endif;
print;
loop4:;
print;
          What is the DIMENSION of the field (1,2,or 3): ";;
nu=con(1,1);
if nu/=1 and nu/=2 and nu/=3;
print;
                 * * * ERROR - MUST BE 1,2, OR 3 ! * * *";
goto loop4;
endif;
nu1=nu;
cls;
if reply1$=="Y" or reply1$=="y";
nu=nu+1;
endif;
                          SUMMARY OF DESIGN PARAMETERS";
                          print;
print;
format /ld 3,0;
                        You have specified the following: ";
print;
print;
      At each of ";;k;;" locations in ";;nu1;;"dimensional space";
      there are ";;p-1;;" independent variables.";
print;
      The number of observations on each variable at each location is ";
print;
print;
print;
               Is this information correct (y/n): ";;
```

```
reply=cons;
if reply $/= "Y" and reply $/="y";
print;
print;
dos pause;
goto start;
endif;
i=1;
do while i<=k;</pre>
cls;
j=1;
                              DATA ENTRY";
                              ========";
print;
print;
"LOCATION ";;i;
print;
"Enter the ";;nu;;"POSITION coordinates : "$+note;
x1=con(nu,1);
if i==1;
x=x1;
else;
x=x^x1;
endif;
do while j <= n;
print;
"INDEPENDENT variable information (LOCATION ";;i;;")";
"-----------;
"Enter the ";;p;;"values for observation ";;j;;note;
w1=con(1,p);
print;
"Enter the value of the DEPENDENT variable : ";;
v1=con(1,1);
if j==1 and i==1;
w=w1;
v=v1;
goto jump1;
endif;
w=w | w1;
v=v | v1;
jump1:;
j=j+1;
endo;
i=i+1;
endo;
print;
print;
      Do you want to save these matrices to a file (y/n): ";;
reply=cons;
if reply $=="Y" or reply $== "y";
print;
      Enter drive (and optionally a path ) : ";;
destn=cons;
```

```
save path=^destn;
save w;
      File ";;destn;;"W.FMT successfully saved";
save x;
      File ";;destn;;"X.FMT successfully saved";
save v;
      File ";;destn;;"V.FMT successfully saved";
endif:
/* loadp gradp=c:\gauss\cp\gradp; */
/*" Matrix W";
W;
" Matrix V";
v;
" Matrix X";
x: */
/* loadp fcalc=c:\gauss\cp\fcalc; */;
aold=zeros(p*nu,1);
print;
print;
       Do you want OLS estimation or GLS estimation (Type O or G): ";;
olsgls=cons;
if olsgls $=="G" or olsgls $=="g";
vv=reshape(v,k,n);vv=vv';
kk=1;
do while kk<=k;
vv[.,kk]=vv[.,kk]-meanc(vv[.,kk]);
kk=kk+1;
endo;
cov=vv'*vv/n;
print;
        Are observations WITHIN a location independent (y/n) : ";;
reply=cons;
jump8:;
if reply $=="y" or reply$=="Y";
psi=cov.*.eye(n);
else;
psi=cov.*.ones(n,n);
loadexe path=c:\gauss\gxe;
loadp pinv=c:\gauss\cp\pinv;
psi=pinv(psi);
goto jump9;
endif;
if n<k and reply $=="y" or reply $=="Y";
print;
print;
       NOTE: Since the number of observations WITHIN each location";
              is less than the number of locations, will have to ";
11
              compute the Moore-Penrose inverse of the psi matrix.";
loadexe path=c:\gauss\gxe;
loadp pinv=c:\gauss\cp\pinv;
psi=pinv(psi);
else;
```

```
psi=inv(psi);
endif;
else;
psi=eye(k*n);
endif;
jump9:;
if count>1;
goto jump7;
endif;
z=zeros(k*n,k*p);
kk=1;
do while kk<=k;</pre>
kk1 = (kk-1)*n+1;
kk2=kk*n;
kk3 = (kk-1) * p+1;
kk4=kk*p;
w1=w[kk1:kk2,1:p];
z[kk1:kk2,kk3:kk4]=w1;
kk=kk+1:
endo;
/* z; */
jump7:;
itern=1;
kk=1;
inc=9999;
/* a0=ones(p*nu,1); */
gamhat=inv(z'*psi*z)*z'*psi*v;
gamhat=reshape(gamhat,k,p);gamhat=gamhat';
a0=gamhat*x'*inv(x*x');
format /rd 9,4;
print;
print;
"Two-stage regression estimate of matrix A: ";;a0;
dos pause;
a0=ones(p*nu,1);
cls;
if count>1;
goto jump6;
endif;
       Enter tolerance for determining stopping criterion : ";;
epsilon=con(1,1);
jump6:;
do while inc>epsilon;
"Iteration ";;kk;
pp=gradp(&glscalc,a0);
ph=hessp(&glscalc,a0);
delta=inv(ph)*pp';
inc=delta'delta;
a0=a0-delta;
kk=kk+1;
a0;
endo;
cls;
```

```
print;
print;
a0=reshape(a0,p,nu);
                     Convergence established at iteration ";;kk;
print;
print;
format /rd 9,4;
                     Matrix A = ";
a0;
print;
print;
       Will now compute the predicted values of dependent variable";
       using this A matrix . . . ";
print;
                        ";;dos pause;
i=1;
do while i <= k;
i1=(i-1)*n;
x1=x[.,i];
i2=1;
do while i2<=n;
if i2==1;
w1=w[i1+i2,.];
else;
w1=w1 | w[i1+i2,.];
endif;
i2=i2+1;
endo;
if i==1;
vhat=w1*a0*x1;
else;
vhat=vhat |w1*a0*x1;
endif;
i=i+1;
endo;
print;
    V and Vhat . . . ";
v~vhat;
resid=v-vhat;
mse=resid'resid;
mse=mse/k/n;
print;
format /re 15,9;
            Mean Square Error is ";;mse;
print;
format /rd 9,4;
if olsgls $=="o" or olsgls $=="0";
stop;
else;
print;
            Do you want to continue iterating on psi matrix (y/n): ";;
cont=cons;
if cont $=="n" or cont $=="N";
```

stop;

```
endif;
if abs(mseold-mse) >= epsilon;
aold=a0:
mseold=mse;
resid=(reshape(resid,k,n))';
cov=(resid'resid)/n;
count=count+1;
goto jump8;
endif;
endif;
L.2 AUXILIARY PROCEDURE FOR COMPUTATION OF EQUATION (4.29)
proc glscalc(arg);
local q,i,i1,i2,w1,v1,x1,f,f1,gn,a1,b1;
a1=reshape(arg,p,nu);
/* i=1;
do while i <= k;</pre>
i1=(i-1)*n;
i2=1;
do while i2<=n;
if i2==1;
w1=w[i1+i2,.];
v1=v[i1+i2,1];
else;
w1=w1 | w[i1+i2,.];
v1=v1 |v[i1+i2,1];
endif;
i2=i2+1;
endo;
x1=x[.,i];
f1=(v1-w1*a1*x1)'psi*(v1-w1*a1*x1);
if i==1;
f=f1;
else;
f=f+f1;
endif;
i=i+1;
endo; */
b1=vec(a1*x);
f=v-z*b1;
q=f'*psi*f;
retp(q);
endp;
```

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