APPENDIX I

Figures representing component selection in IFS

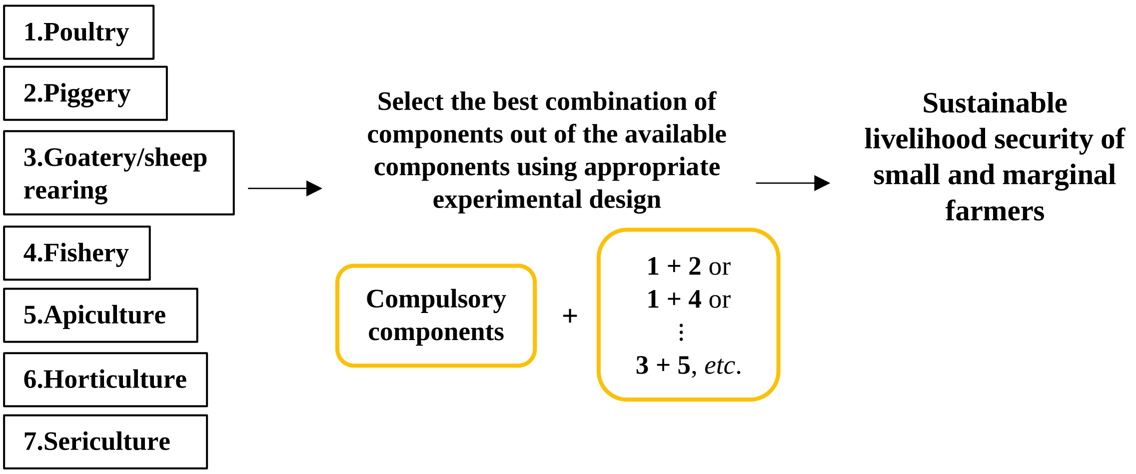
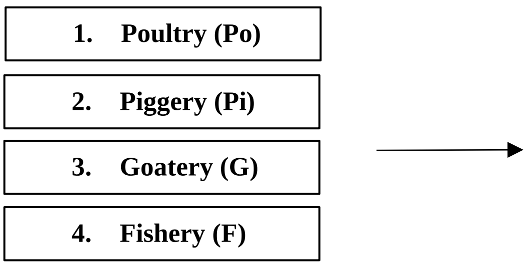


Figure 1: Steps for selecting best combination of components using experimental designs



Combinations	
Po + Pi	(1,2)
Po + G	(1,3)
Po + F	(1,4)
Pi + G	(2,3)
Pi + F	(2,4)
G + F	(3,4)

Figure 2: All possible 2-tuple combinations out of 4 available components

APPENDIX II

Derivation of Information (C) matrix

The model for a 2-part block design for v treatments, b blocks each of size k and each treatment being replicated r times as follows:

$$\mathbf{y} = \mu\mathbf{1} + \mathbf{D}_1'\boldsymbol{\tau} + \mathbf{D}_2'\boldsymbol{\beta} + \boldsymbol{\varepsilon} \qquad \cdots \quad (1)$$

where $\mathbf{y}$ is a $n \times 1$ vector of observations, μ is the general mean, $\mathbf{1}$ is the $n \times 1$ vector of ones, $\mathbf{D}_1'$ is a $n \times v$ design matrix of observations versus treatments, $\boldsymbol{\tau}$ is the $v \times 1$ vector of treatment effects, $\mathbf{D}_2'$ is the $n \times b$ design matrix of observations versus rows, $\boldsymbol{\beta}$ is the $b \times 1$ vector of column effects, and $\boldsymbol{\varepsilon}$ is a $n \times 1$ vector of random errors with $E(\boldsymbol{\varepsilon}) = 0$ and $D(\boldsymbol{\varepsilon}) = \sigma^2\mathbf{I}_n$.

If we express (1) in the form:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\varepsilon}$$

Then, $(\mathbf{X}'\mathbf{X})\boldsymbol{\theta} = \mathbf{X}'\mathbf{y}$ where,

$\mathbf{X} = [\mathbf{D}_1 \,\vert\, \mathbf{D}_2 \quad \mathbf{1}]$, $\boldsymbol{\theta} = \begin{bmatrix} \boldsymbol{\tau} \\ \hline \boldsymbol{\beta} \\ \mu \end{bmatrix} = \begin{bmatrix} \boldsymbol{\theta}_1 \\ \boldsymbol{\theta}_2 \end{bmatrix}$, where $\boldsymbol{\theta}_1$ consist of the parameter of interest ($\boldsymbol{\tau}$) and $\boldsymbol{\theta}_2$ includes the nuisance parameters ($\boldsymbol{\beta}, \mu$).

$$\mathbf{X}'\mathbf{X} = = \begin{bmatrix} \mathbf{X}_1'\mathbf{X}_1 & \mathbf{X}_1'\mathbf{X}_2 \\ \mathbf{X}_2'\mathbf{X}_1 & \mathbf{X}_2'\mathbf{X}_2 \end{bmatrix} = \left[\begin{array}{c|cc} v\mathbf{I}_v & \mathbf{N}_1 & v\mathbf{1}_v \\ \hline \mathbf{N}_1' & r_1\mathbf{I}_b & r_1\mathbf{1}_b \\ v\mathbf{1}_v' & r_1\mathbf{1}_b' & n \end{array}\right]$$

The generalized inverse of $\mathbf{X}_2'\mathbf{X}_2$ can be easily computed as:

$$(\mathbf{X}_2'\mathbf{X}_2)^- = \begin{bmatrix} \frac{1}{r_1}\mathbf{I}_b & \mathbf{0} \\ \mathbf{0} & 0 \end{bmatrix}_{(b+1)\times(b+1)}$$

Therefore, the information matrix under 2-part SI block design set-up is:

$$\mathbf{C} = \mathbf{X}_1'\mathbf{X}_1 - \mathbf{X}_1'\mathbf{X}_2(\mathbf{X}_2'\mathbf{X}_2)^-\mathbf{X}_2'\mathbf{X}_1 = v\mathbf{I}_v - \frac{1}{r_1}\mathbf{N}_1\mathbf{N}_1' \qquad \cdots \quad (2)$$

Now, if we add another source of variation in (1), we get the experimental model for 2-part RCDs for v treatments, each replicated r times arranged in ‘p’ rows and ‘q’ columns, can be represented in matrix notations as:

$$\mathbf{y} = \mathbf{D}_1'\boldsymbol{\tau} + \mathbf{D}_2'\boldsymbol{\alpha} + \mathbf{D}_3'\boldsymbol{\beta} + \mu\mathbf{1} + \boldsymbol{\varepsilon} \qquad \cdots \quad (3)$$

where $\mathbf{y}$ is a $\mathrm{n} \times 1$ vector of observations, $\mathbf{D}_1'$ is a $\mathrm{n} \times \mathrm{v}$ design matrix of observations versus treatments, $\boldsymbol{\tau}$ is the $\mathrm{v} \times 1$ vector of treatment effects, $\mathbf{D}_2'$ is the $\mathrm{n} \times \mathrm{p}$ design matrix of observations versus rows, $\boldsymbol{\alpha}$ is the $\mathrm{p} \times 1$ vector of row effects, $\mathbf{D}_3'$ is the $\mathrm{n} \times \mathrm{q}$ design matrix of observations versus columns, $\boldsymbol{\beta}$ is the $\mathrm{q} \times 1$ vector of column effects, μ is the general mean, $\mathbf{1}$ is the $\mathrm{n} \times 1$ vector of ones and $\boldsymbol{\varepsilon}$ is a $\mathrm{n} \times 1$ vector of random errors with $\mathrm{E}(\boldsymbol{\varepsilon}) = 0$ and $\mathrm{D}(\boldsymbol{\varepsilon}) = \sigma^2\mathbf{I}_\mathrm{n}$.

If we express (3) in the form:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\varepsilon}$$

Then, $(\mathbf{X}'\mathbf{X})\boldsymbol{\theta} = \mathbf{X}'\mathbf{y}$ where, $\mathbf{X} = [\mathbf{D}_1 \,\vdots\, \mathbf{D}_2 \quad \mathbf{D}_3 \quad \mathbf{1}] = [\mathbf{X}_1 \,\vdots\, \mathbf{X}_2]$, $\mathbf{X}_1$ and $\mathbf{X}_2$ are design matrices corresponding to the parameters of interest, $\boldsymbol{\theta} = \left[\begin{array}{c} \boldsymbol{\tau} \\ \hline \boldsymbol{\alpha} \\ \boldsymbol{\beta} \\ \mu \end{array}\right] = \begin{bmatrix} \boldsymbol{\theta}_1 \\ \boldsymbol{\theta}_2 \end{bmatrix}$, where $\boldsymbol{\theta}_1$ consist of the parameter of interest ($\boldsymbol{\tau}$) and $\boldsymbol{\theta}_2$ includes the nuisance parameters and

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} \mathbf{X}_1'\mathbf{X}_1 & \mathbf{X}_1'\mathbf{X}_2 \\ \mathbf{X}_2'\mathbf{X}_1 & \mathbf{X}_2'\mathbf{X}_2 \end{bmatrix} = \left[\begin{array}{c:ccc} \mathrm{q}\mathbf{I}_\mathrm{v} & \mathbf{N}_1 & \mathbf{J}_{(\mathrm{v}\times\mathrm{q})} & \mathrm{q}\mathbf{1}_\mathrm{v} \\ \hdashline \mathbf{N}_1' & (\mathrm{v}-1)\mathbf{I}_\mathrm{p} & \mathbf{N}_2 & (\mathrm{v}-1)\mathbf{1}_\mathrm{p} \\ \mathbf{J}_{(\mathrm{q}\times\mathrm{v})} & \mathbf{N}_2' & \mathrm{v}\mathbf{I}_\mathrm{q} & \mathrm{v}\mathbf{1}_\mathrm{q} \\ \mathrm{q}\mathbf{1}_\mathrm{v}' & (\mathrm{v}-1)\mathbf{1}_\mathrm{p}' & \mathrm{v}\mathbf{1}_\mathrm{q}' & \mathrm{n} \end{array}\right]$$

The reduced normal equation pertaining to treatment effects for this model is: $\mathbf{C}\hat{\boldsymbol{\tau}} = \mathbf{Q}$, where $\mathbf{C} = \mathbf{X}_1'\mathbf{X}_1 - \mathbf{X}_1'\mathbf{X}_2(\mathbf{X}_2'\mathbf{X}_2)^{-}\mathbf{X}_2'\mathbf{X}_1$, is the matrix of coefficients corresponding to the parameters of interest or information matrix and $\mathbf{Q}$ is the vector of adjusted treatment totals.

Upon simplification, the **C**- matrix can be obtained as:

So, $\mathbf{X}_2'\mathbf{X}_2$ can be written as:

$$\mathbf{X}_2'\mathbf{X}_2 = \begin{bmatrix} (\mathrm{v}-1)\mathbf{I}_\mathrm{p} & \mathbf{N}_2 & (\mathrm{v}-1)\mathbf{1}_\mathrm{p} \\ \mathbf{N}_2' & \mathrm{v}\mathbf{I}_\mathrm{q} & \mathrm{v}\mathbf{1}_\mathrm{q} \\ (\mathrm{v}-1)\mathbf{1}_\mathrm{p}' & \mathrm{v}\mathbf{1}_\mathrm{q}' & \mathrm{n} \end{bmatrix} = \begin{bmatrix} \mathbf{A_{11}} & \mathbf{A_{12}} \\ \mathbf{A_{21}} & \mathbf{A_{22}} \end{bmatrix}$$

$\mathbf{X}_2'\mathbf{X}_2$ is not of full rank. We find its generalized inverse by method of partitioning (Searle, 1982) as the condition rank($\mathbf{X}_2'\mathbf{X}_2$) = rank($\mathbf{A_{11}}$) + rank($\mathbf{A_{22}} - \mathbf{A_{21}}\mathbf{A_{11}^{-1}}\mathbf{A_{12}}$) is satisfied.

Let $(\mathbf{X}_2'\mathbf{X}_2)^- = \begin{bmatrix} \mathbf{B_{11}} & \mathbf{B_{12}} \\ \mathbf{B_{21}} & \mathbf{B_{22}} \end{bmatrix}$

where, $\mathbf{B}_{22} = \boldsymbol{\xi}^-$ where $\boldsymbol{\xi} = \mathbf{A_{22}} - \mathbf{A_{21}}\mathbf{A_{11}^{-1}}\mathbf{A_{21}}$

$$\boldsymbol{\xi} = \begin{bmatrix} \mathrm{v}\mathbf{I}_\mathrm{q} & \mathrm{v}\mathbf{1}_\mathrm{q} \\ \mathrm{v}\mathbf{1}_\mathrm{q}' & \mathrm{n} \end{bmatrix} - \begin{bmatrix} \mathbf{N}_2' \\ (\mathrm{v}-1)\mathbf{1}_\mathrm{p}' \end{bmatrix} \frac{1}{(\mathrm{v}-1)} \mathbf{I}_\mathrm{p} [\mathbf{N}_2 \quad (\mathrm{v}-1)\mathbf{1}_\mathrm{p}]$$

$$= \begin{bmatrix} \mathrm{v}\mathbf{I}_\mathrm{q} - \frac{\mathbf{N}_2'\mathbf{N}_2}{(\mathrm{v}-1)} & \mathbf{0} \\ \mathbf{0} & \mathrm{n} - \mathrm{p}(\mathrm{v}-1)^2 \end{bmatrix}_{(\mathrm{q}+1)\times(\mathrm{q}+1)}$$

The generalized inverse of $\boldsymbol{\xi}$ is given as:

$$\therefore \boldsymbol{\xi}^- = \begin{bmatrix} \left(\mathrm{v}\mathbf{I}_{\mathrm{q}-1} - \frac{\mathbf{N}_2'^{*}\mathbf{N}_2^{*}}{(\mathrm{v}-1)}\right)^{-1} & \mathbf{0} \\ \mathbf{0} & 0 \end{bmatrix} = \mathbf{B}_{22},$$ where $\mathbf{N}_2'^{*}\mathbf{N}_2^{*}$ is a full rank sub-matrix of $\mathbf{N}_2'\mathbf{N}_2$.

$$\mathbf{B}_{12} = -(\mathbf{A}_{11}^{-1}\mathbf{A}_{12})\boldsymbol{\xi}^- = \begin{bmatrix} \frac{\mathbf{N}_2^{*}}{\mathrm{v}-1}\left(\mathrm{v}\mathbf{I}_{\mathrm{q}-1} - \frac{\mathbf{N}_2'^{*}\mathbf{N}_2^{*}}{(\mathrm{v}-1)}\right)^{-1} & \mathbf{0} \end{bmatrix}_{\mathrm{p}\times(\mathrm{q}+1)}$$, where $\mathbf{N}_2$ is further partitioned into $\mathbf{N}_2^{*}$ of order p × (q-1) so that it will be conformable for multiplication.

Similarly, $$\mathbf{B}_{21} = -\boldsymbol{\xi}^-(\mathbf{A}_{21}\mathbf{A}_{11}^{-1}) = \begin{bmatrix} \left(\mathrm{v}\mathbf{I}_{\mathrm{q}-1} - \frac{\mathbf{N}_2'^{*}\mathbf{N}_2^{*}}{(\mathrm{v}-1)}\right)^{-1} \cdot \frac{\mathbf{N}_2'^{*}}{\mathrm{v}-1} \\ \mathbf{0} \end{bmatrix}_{(\mathrm{q}+1)\times\mathrm{p}}$$

Further, $\mathbf{B}_{11} = \mathbf{A}_{11}^{-1} + (\mathbf{A}_{11}^{-1}\mathbf{A}_{12})\boldsymbol{\xi}^-(\mathbf{A}_{21}\mathbf{A}_{11}^{-1})$

$$= \frac{1}{\mathrm{v}-1}\mathbf{I}_\mathrm{p} + \left[\frac{\mathbf{N}_2^{*}}{\mathrm{v}-1}\left(\mathrm{v}\mathbf{I}_{\mathrm{q}-1} - \frac{\mathbf{N}_2'^{*}\mathbf{N}_2^{*}}{(\mathrm{v}-1)}\right)^{-1} \frac{\mathbf{N}_2'^{*}}{\mathrm{v}-1}\right]_{\mathrm{p}\times\mathrm{p}}.$$

$$\therefore (\mathbf{X}_2'\mathbf{X}_2)^- = \begin{bmatrix} \frac{1}{v-1}\mathbf{I}_p + \left[\frac{\mathbf{N}_2^*}{(v-1)^2}\left(v\mathbf{I}_{q-1} - \frac{\mathbf{N}_2'^*\mathbf{N}_2^*}{(v-1)}\right)^{-1}\frac{\mathbf{N}_2'^*}{v-1}\right] & \frac{\mathbf{N}_2^*}{v-1}\left(v\mathbf{I}_{q-1} - \frac{\mathbf{N}_2'^*\mathbf{N}_2^*}{(v-1)}\right)^{-1} & \mathbf{0} \\ \left(v\mathbf{I}_{q-1} - \frac{\mathbf{N}_2'^*\mathbf{N}_2^*}{(v-1)}\right)^{-1}.\frac{\mathbf{N}_2'^*}{v-1} & \left(v\mathbf{I}_{q-1} - \frac{\mathbf{N}_2'^*\mathbf{N}_2^*}{(v-1)}\right)^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & 0 \end{bmatrix}$$

C-matrix for the estimation of treatment contrasts pertaining to 2-part row-column design can be derived as:

$$\mathbf{C} = \mathbf{q}\mathbf{I}_v - [\mathbf{N}_1 \quad \mathbf{J}_{(v\times q)} \quad q\mathbf{1}_v](\mathbf{X}_2'\mathbf{X}_2)^- \begin{bmatrix} \mathbf{N}_1' \\ \mathbf{J}_{(q\times v)} \\ q\mathbf{1}_v' \end{bmatrix}$$

$$= q\mathbf{I}_v - [\mathbf{N}_1 \quad \mathbf{J}_{(v\times q-1)} \quad \mathbf{Z}_{v\times 2}](\mathbf{X}_2'\mathbf{X}_2)^- \begin{bmatrix} \mathbf{N}_1' \\ \mathbf{J}_{(q-1\times v)} \\ \mathbf{Z}_{2\times v}' \end{bmatrix},$$

to ensure the conformability of matrix multiplication, the last column of $\mathbf{J}_{(v\times q)}$ is combined with $q\mathbf{I}_v$ to form $\mathbf{Z}_{v\times 2}$

$$= q\mathbf{I}_v - \frac{\mathbf{N}_1\mathbf{N}_1'}{(v-1)}\mathbf{I}_p - \frac{\mathbf{N}_1\mathbf{N}_2^*}{(v-1)^2}\left(v\mathbf{I}_{q-1} - \frac{\mathbf{N}_2'^*\mathbf{N}_2^*}{(v-1)}\right)^{-1}\frac{\mathbf{N}_2^{*\prime}\mathbf{N}_1'}{(v-1)} - \mathbf{J}_{v\times(q-1)}\left(v\mathbf{I}_{q-1} - \frac{\mathbf{N}_2'^*\mathbf{N}_2^*}{(v-1)}\right)^{-1}\frac{\mathbf{N}_2^{*\prime}\mathbf{N}_1'}{(v-1)} -$$

$$\frac{\mathbf{N}_1\mathbf{N}_2^*}{(v-1)}\left(v\mathbf{I}_{q-1} - \frac{\mathbf{N}_2'^*\mathbf{N}_2^*}{(v-1)}\right)^{-1}\mathbf{J}_{q\times v} - \mathbf{J}_{v\times(q-1)}\left(v\mathbf{I}_{q-1} - \frac{\mathbf{N}_2'^*\mathbf{N}_2^*}{(v-1)}\right)^{-1}\mathbf{J}_{q\times v} \qquad \cdots \quad (4)$$

Now, for Example 4.1, the **C**-matrix given in (2) is simplified as:

$$\mathbf{C} = 4.5\mathbf{I}_6 - 0.75\mathbf{A}_6 - 1.5\mathbf{B}_6$$

Here, $\mathbf{I}_6$ is an identity matrix of order $v = 6$, $\mathbf{A}_6$, $\mathbf{B}_6$ and $\mathbf{C}_6$ are called association matrices and are defined as follows: $\mathbf{A}_v = \{a_{jl}\}$ is a symmetric matrix of order v with elements 0's and 1's where $a_{jl} = 1$ if the j^{th} and l^{th} combinations are first associates and $a_{jl} = 0$ otherwise and $\mathbf{B}_v = \{b_{jl}\}$ is a symmetric matrix of order v with elements 0's and 1's where $b_{jl} = 1$ if the j^{th} and l^{th} combinations are second associates and $b_{jl} = 0$ otherwise.

The treatment combinations of the design obtained in Example 4.1 follow a Group Divisible association scheme as shown:

1,2	3,4
1,3	2,4
1,4	2,3

The association scheme is as follows: Treatment combinations in the same row are first associates and rest are second associates.

For Example 4.2, the **C**-matrix given in (4) is simplified as:

$$\mathbf{C} = 7.967\mathbf{I}_6 - 1.583\mathbf{A}_6 - 1.583\mathbf{B}_6 - 1.608\mathbf{C}_6$$

to clearly indicate the underlying partial variance balance property of the treatments in the design. Here, $\mathbf{I}_6$ is an identity matrix of order v = 6, $\mathbf{A}_6$, $\mathbf{B}_6$ and $\mathbf{C}_6$ are called association matrices and are defined as follows: $\mathbf{A}_\mathrm{v} = \{a_{jl}\}$ is a symmetric matrix of order v with elements 0's and 1's where $a_{jl} = 1$ if the j^{th} and l^{th} combinations are first associates and $a_{jl} = 0$ otherwise, $\mathbf{B}_\mathrm{v} = \{b_{jl}\}$ is a symmetric matrix of order v with elements 0's and 1's where $b_{jl} = 1$ if the j^{th} and l^{th} combinations are second associates and $b_{jl} = 0$ otherwise, and $\mathbf{C}_\mathrm{v} = \{c_{jl}\}$ is a symmetric matrix of order v with elements 0's and 1's where $c_{jl} = 1$ if the j^{th} and l^{th} combinations are third associates and $c_{jl} = 0$ otherwise.

The treatment combinations follow a rectangular association scheme as shown:

1,2	1,4	2,4
1,3	2,3	3,4

Treatment combinations in the same row are first associates, in the same column are second associates and rest are third associates.

For Example 4.3, the **C**-matrix given in (4) is simplified as:

$$\mathbf{C} = 4.33\mathbf{I}_6 - 0.667\mathbf{A}_6 - 1.667\mathbf{B}_6,$$

where, $\mathbf{I}_6$, $\mathbf{A}_6$ and $\mathbf{B}_6$ are as defined earlier in Example 4.1.

Here, the treatment combinations follow a Group Divisible association scheme as shown:

1,2	1,3
1,4	2,3
2,4	3,4

For the association scheme given above, treatment combinations in the same row are first associates and the rest are second associates.

APPENDIX III

SAS code for generating C-matrix and computing Canonical efficiency factors of 2-part designs

```
proc iml;
/*design*/
a={
1  2  0  0  1  3  2  3  1  4  0  0  0  0  0  0  2  4  0  0,
0  0  1  3  0  0  2  4  2  3  3  4  0  0  0  0  0  0  1  4,
.
.
.
3  4  1  2  2  4  0  0  0  0  0  0  1  3  0  0  0  0  2  3
};
/*cell sizes*/
b={2  0     2     2     2     0     0     0     2     0,
0     2     0     2     2     2     0     0     0     2,
.
.
.
2     2     2     0     0     0     2     0     0     2
};
a1=ncol(loc(b));
*print a1;
m1=j(a1,1,1);/*mean vector*/
/*print m1;*/
dir1=j(nrow(a)*ncol(a),max(a),0);/*design matrix -obs VS direct treatment*/
k=1;
do i=1 to nrow(a);
do j=1 to ncol(b);
do l=1 to b[i,j];
if a[i,(b[i,j]*(j-1))+l]>0
then do;
dir1[k,a[i,(b[i,j]*(j-1))+l]]=1;
end;
end;
k=k+1;
end;
end;
*print dir1;
```

```
*dir=j(a1,max(a),0);
count = dir1[,+];            /* add across rows */
keepIdx = loc(count>0);  /* rows where all elements are in [0,1] */
*print keepIdx;
if ncol(keepIdx)>0 then dir = dir1[keepIdx,];
*print dir;
row1=j(nrow(b)*ncol(b),nrow(b),0);/*design matrix -obs VS row*/
k=1;
do i=1 to nrow(b);
do j=1 to ncol(b);
if b[i,j]>0
then row1[k,i]=1;
k=k+1;
end;
end;
*print row1;
count = row1[,+];            /* add across rows */
keepIdx = loc(count>0);  /* rows where all elements are in [0,1] */
*print keepIdx;
if ncol(keepIdx)>0 then row = row1[keepIdx,];
*print row;
column1=j(nrow(b)*ncol(b),ncol(b),0);/*design matrix-obs VS row*/
k=1;
do i=1 to nrow(b);
do j=1 to ncol(b);
if b[i,j]>0
then column1[k,j]=1;
k=k+1;
end;
end;
*print column1;
count = column1[,+];            /* add across rows */
keepIdx = loc(count>0);  /* rows where all elements are in [0,1] */
*print keepIdx;
if ncol(keepIdx)>0 then column = column1[keepIdx,];
*print row;
/*For row-column set-up*/
x=m1||dir||row||column;/*design matrix*/
print x[format=3.0];
x1=dir;
x2=m1||row||column;
```

```
c_mat=(x1`*x1)-(x1`*x2*(ginv(x2`*x2))*x2`*x1)/*C matrix*/;
print c_mat;
/*For block set-up*/
x=m1||dir||column;/*design matrix
print x[format=3.0];
x1=dir;
x2=m1||column;
c_mat=(x1`*x1)-(x1`*x2*(ginv(x2`*x2))*x2`*x1)/*C matrix;
print c_mat;
rep=dir`*dir;
*print rep;
eig=eigval(c_mat);
print eig;
eig1=eig[loc(eig>0.0000001),];/*positive eigen values*/
rep=dir`*dir;
eig2=eig1/(rep[1,1]);/*assuming same replications*/
eig3=1/eig2;
CanEffFactor=nrow(eig3)/sum(eig3);
print CanEffFactor;
quit;
```

For block set-up, row may be excluded in x2 and column is treated as block