SASᴿ Forum (Japan)# Users Group Academic Session 2004 (sugiJ2004)# PRESENTATION AID
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Rm 501, 5F, Tokyo Conference Center Shinagawa # | Revised: Finally, Feb. 04, 2007
Session Statistical Analysis, Chaired by Prof. Dr M. IWASAKI, Seikei University

Principles of determination of various sums of squares (SS's) in SAS/STATᴿ GLM procedure

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This PRESENTATION AID consists of the MAIN chapter and the REMI(nder) chapter*.

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*An excerpt of a SUGI-J2003 Presentation Aid "sugij03aidTadaoShibayama.doc" as supplemented and posted in the web folder 'ftp://ftp.sas.com/pub/webfiles/Japan/contrib/sugij03/shibayama.zip' by the courtesy of SAS Institute Japan Ltd. and SAS Institute Inc. It covers the parts **0**, **1**, **2**, **3**, '**An example of hypothesis testing**', '**A full estimable matrix**', '**Restoration matrix**', and **4**.

The MAIN chapter. Some notation should be referred to the REMI chapter.

ARTICLE **0** SAS/STATᴿ GLM procedure is familiar to

SAS professions

but may be not to **SAS beginner**s.

as it is based on the estimability principles of modern mathematical statistics that are, as detailed in this presentation later, a little different from the Fisher's classical principles of analysis of variance.

ARTICLE **1** SAS/STATᴿ GLM procedure employs

Estimable functions

as the basis of the analysis. That are defined by product of an

Estimable matrix Lu (full) or L (part) and

a true **Effect elements column vector cc** ,

as detailed in the REMI chapter (of this handout), PARTs **0**, **1** and **2** .

ARTICLE **2** SAS/STAT^R GLM procedure provides

Estimable functions

of the **Type I, II, III and IV**,

as detailed in Chapter 9, vol. 1, and Chapter 24, vol. 2, both SAS/STAT^R User's Guide, version 6.
Each defined of the # (Chapter 4, miswritten originally, revised after the presentation, to Chapter 9.)

Estimable matrix Lu (or L)

of the **Type I, II, III and IV**, respectively.

ARTICLE **2A** SAS^R Technical Report R-101, **Tests of Hypotheses in Fixed-Effects Linear Models,** SAS Institute Inc. (1978), demonstrates by an example that an

Estimable full matrix Lu of the **Type I**

is swept out, by Gauss-Jordan-Doolittle forward elimination, of

the **Coefficients matrix** $X'X$ **of the normal equation**.

Furthermore, the SAS^R Technical Report R-101 advocates that an

Estimable full matrix Lu of the **Type II**

is swept out of the **matrix** $X'X$, too, if the columns somewhat rearranged, and that an

Estimable full matrix Lu of the **Type III** or **IV**

is available if the rows of an estimable full matrix Lu are modified by orthogonality or balance.

ARTICLE **2B** The complete detail of the sweep or the modification for generation of

Estimable full matrix Lu of the **Type II**, **III** or **IV** is, however, not described at all. Furthermore, many other possibilities are not excluded even for generation of that of

the **Type I**, as found in **Output 24.3-6**, p. 932-936, SAS/STAT^R User's Guide, version 6, Volume 2, as of Type I, II, III or General (as defined). Cf. the REMI chapter of this handout, the PART, 'An example of hypothesis testing by SAS/STAT^R GLM procedure'.

ARTICLE **3** The detail should be left to a further study, but once an

Estimable matrix `Lu` (or `L`)

is found, the true value of estimable function or its estimate is defined or evaluated as follows.

`Lu.cc` or `Lu.cv`

in terms of a true or fitted effect elements column vector `cc` or `cv`. Then, tested is the

Testable hypothesis `L.cc = 0`

by the ratio of the **sum of squares (SS)** of the estimated response

`SS_yvP`, i.e., `(L.cv)′.[L(X′X)⁻L′]⁻¹.(L.cv)`,

to the sum of squared residues `SS_vy`, with the numbers of freedoms taken into account.

The sum of squares `SS_yvP` is of the **Type I**, **II**, **III** or **IV** according to the type of the estimable function `L.cc` (or `L.cv`) as employed.

ARTICLE **3A** The sum of squares `SS_yvP` of the **Type I** and **II** is defined, sometimes, by **Reduction** of the sum of squares `SS_yvP`, as denoted often in terms of the `R( )` **notation**. As fitted, for example,

`R(M)`, `R(M,A)`, `R(M,A,B)`, **...** for **Type I** case, and

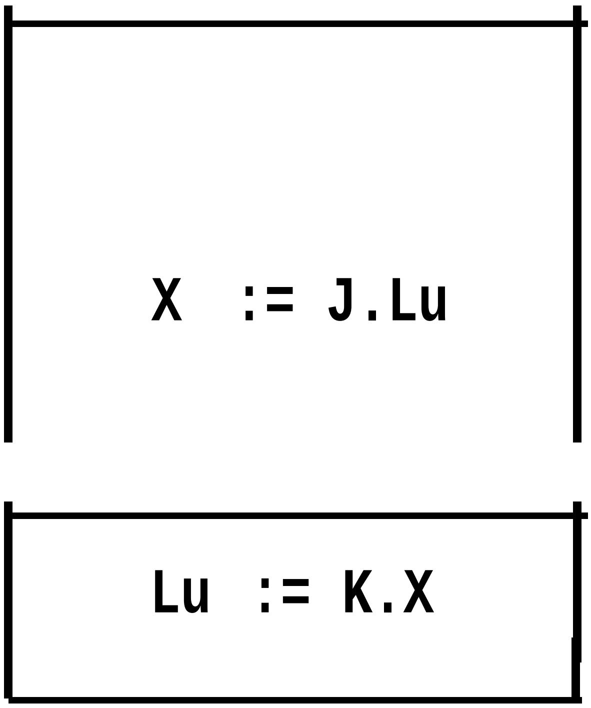
`R(A|B,C)`, `R(B|A,C)`, `R(C|A,B)` for **Type II** case.

The **Reduction** of the sum of squares is from that of the measured response, as to be remarked.

ARTICLE **3B** The definitions by the **Reductions** clarify meanings of those sums of squares of the **Type I** and **II** somehow, but it does not cover many other detail as mentioned above partly. Furthermore, it does not matter with those of the **Type III** or **IV**.

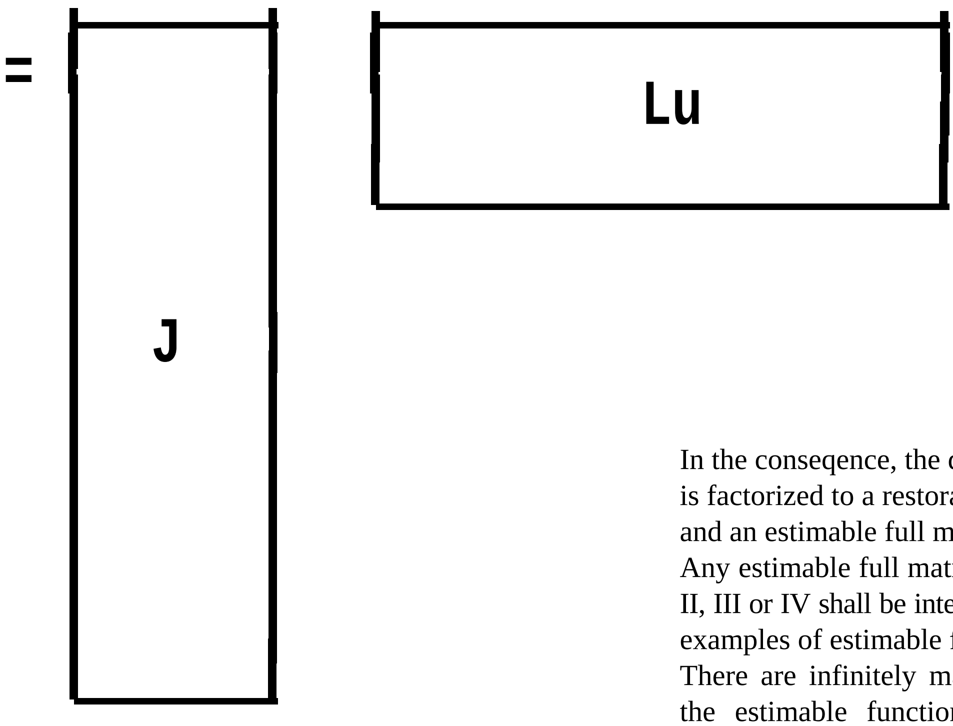
For beginners, some elementary consideration of estimable functions and hypotheses or of reduction may be helpful, such that covering detail of the estimable full and part matrices, and if possible, detail of solution of observation (and normal) equations on an actual arrangement in general.

ARTICLE 4 A restoration matrix(#) and.an estimable full matrix, derived of a design matrix.



The design matrix X may be reduced to an estimable full matrix Lu by operation of a contraction matrix K .

The design matrix X may be restored from an estimable full matrix Lu by operation of a restoration matrix J .



In the conseqence, the design matrix X is factorized to a restoration matrix J and an estimable full matrix Lu .
Any estimable full matrix Lu of Type I, II, III or IV shall be interpreted to be typical examples of estimable functions.
There are infinitely many possibilities of the estimable functions, not limited to those of the Type I, II, III or IV.
Those are only typical examples, any other possibilities should be never excluded.

ARTICLE **4A** The sum of squared fitted response SS_yv is equal to

$$(Lu.cv)'.J'J.(Lu.cv)$$

as equivalent to

$$(Lu.cv)'.[Lu(X'X)^{-}Lu']^{-1}.(Lu.cv).$$

The columns of the matrix J may be orthogonalized to each other and normalized if a regular matrix GO is operated on the estimable full matrix Lu from the left side and the inverse matrix $GO*$ is operated on the restoration matrix J on the right side so that

$$JO = J.GO*,\quad LuO = GO.Lu \text{ and } X = JO.LuO.$$

Then, the sum of squared fitted response SS_yv is equal to

$$(LuO.cv)'.JO'JO.(LuO.cv)$$

$$= (LuO.cv)'.(LuO.cv) \quad \text{because} \quad JO'JO = 1 .$$

ARTICLE **4B** In singlet expressions eqns (14d) and (17b) in the Official Paper,

$$EOYV(qqJO) = \langle LuO(qqJO:\ ).cv(\ )\rangle$$

$$= \langle JO(qqJO:\ ).y(\ )\rangle \text{ for } qqJO \leqq lpLuO \text{ for the measured response.}$$

The inner product $\langle LuO(qqJO:\ ).cv(\ )\rangle$ is to be estimated in terms of the other inner product $\langle JO(qqJO:\ ).y(\ )\rangle$ of the measured response.

The estimate is compared to the fluctuations in eqn (17b), $EOVY(qqJO)$

$$= \langle JO(qqJO:\ ).y(\ )\rangle \text{ for } qqJO > lpLuO \text{ for fluctuations.}$$

Once the columns of the matrix J are orthogonalized to each other and normalized, giving the estimability full matrix LuO and the restoration matrix JO, these may be transformed to another pair LuW and JW by an arbitrary orthogonal matrix GW and the inverse $GW*$.

Under the transformation, is kept ever the equality $\langle JW(qqJW:\ ).y(\ )\rangle = \langle LuW(qqJW:\ ).cv(\ )\rangle$ exactly equivalent, any **indeterminacy** of the solution $cv(\ )$, too, if it is caused of any redundancy of the parametrization.

ARTICLE **5** In evaluation of **SAS sums of squares SSI, SSII, SSIII and SSIV**, also of the **reductions of sums of squares**, and of the **estimable functions E1, E2, E3 and E4**, consequently, in ordinary SAS analysis of variances or responses, and in ordinary hypothesis testing, the expression $[Lu(X'X)^{-}Lu']^{-1}$ is employed, often, instead of $J'J$, but the latter proves very legible for beginners, particularly if orthonormalized to $JO'JO$. Furthermore, it gives an interpretation very classic, just consistent to Fisher's original analysis of variance.

The analysis on the basis of the latter expression may be called **detached analysis** (say), contrasted to more modern **entailed analysis** (say) in professions employing the inverse of a general inverse that seemingly can meet problems without any artificial additional assumptions. Of course, a detached analysis may be convenient for removing some overcomplication.

REFERENCE

Shibayama, Tadao (2003): Indeterminacy of effect components of factorial experiments ··· (In Japanese), SAS Users Gp I'national Japan 22nd Ann. Conf. Official Papers (SAS Institute Japan Ltd.), p.151-158, with English handouts posted in 'ftp://ftp.sas.com/pub/webfiles/Japan/contrib/sugij03/shibayama.zip' by the courtesy of SAS Institute Japan Ltd. and SAS Institute Inc.

The REMI chapter - Attached below:

An excerpt of a SUGI-J2003 presentation aid "sugij03aidTadaoShibayama.doc" as supplemented and posted in the web folder 'ftp://ftp.sas.com/pub/webfiles/Japan/contrib/sugij03/shibayama.zip' by the courtesy of SAS Institute Japan Ltd. and SAS Institute Inc. It covers the

PART **0** Structure, observation and normal equations.
PART **1** Design, estimable, contraction and restoration matrices.
PART **2** Estimable functions.
PART **3** Sum of squared fitted responses.
PART **An example of hypothesis testing** by SAS/STAT^R GLM procedure, Version 6.
PART **A full estimable matrix** in SAS/STAT^R User's Guide, Version 6.
PART **Restoration matrix** for the full estimable matrix above.
PART **4** Another expression $[Lu(X'X)^{-}Lu']^{-1}$ for the matrix product $J'J$.

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Indeterminacy of effect components of factorial experiments arising from the ways of expression

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FORMULAS: PART **0**

(A1) $y = X.cc + vv = yy + vv$

provided that $yy = X.cc$

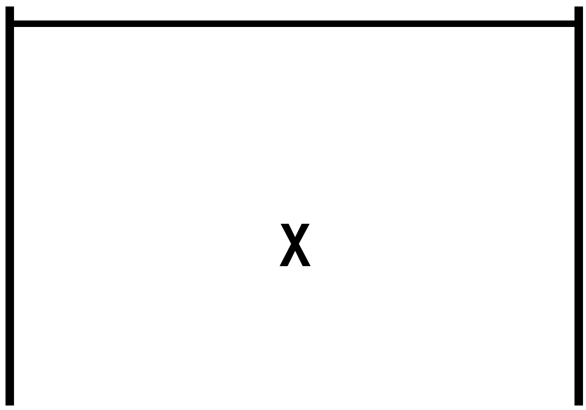
(A2) $y = X.cv + vy = yv + vy$

provided that $yv = X.cv$

(A3) $X'X.cv = X'.y$ so

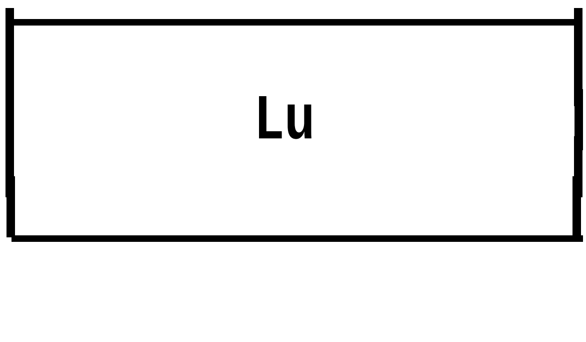
a solution $cv = (X'X)^{-}.X'.y$

PART **1**



(A4)

$Lu = K.X$



(A5)

$J.Lu = X$

PART **2**

(A6)

$$Lu^{-}o = Lu\_1.Lu^{-}1 + Lu\_2.Lu^{-}2 + \dots + Lu\_qu.Lu^{-}qu$$

(A7)

$$Lu^{-}o.cc$$
$$Lu^{-}o.cv$$

(A′1) $y = Xp.ccP + vvP = yyP + vvP$

provided that $yyP = Xp.ccP$

(A′2) $y = Xp.cvP + vyP = yvP + vyP$

provided that $yvP = Xp.cvP$

(A′3) $Xp'Xp.cvP = Xp'.y$ so

a solution $cvP = (Xp'Xp)^{-}.Xp'.y$

PART **3**

(A8) $SS\_yv = yv'.yv = cv'.X'X.cv$
$= (Lu.cv)'.J'J.(Lu.cv)$

(A′8) $SS\_yvP = yvP'.yvP = cvP'.Xp'Xp.cvP$
$= (L.cvP)'.J'J.(L.cvP)$

An example of hypothesis testing by SAS/STAT^{R} GLM procedure.
Cf. SAS/STAT^{R} User's Guide, version 6, Volume 2, Chap. 24, p. 932-936,
and Volume 1, Chap. 9, p. 109-110, and around as it may concern.
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The structure equation of a model. `y = yy + vv = X.cc + vv`
The response column vector, with the element for the treatment-run `AaBb.r` of the `r`-th run of the level `a` of the factor `A` and the level `b` of the factor `B` such as follows

`A1B1.1  A1B1.2  A1B2  A2B1  A2B2.1  A2B2.2  A3B1.1  A3B1.2  A3B2.1  A3B2.2 :`

- as observed `y = ( y1,  y2,  y3,  y4,  y5,  y6,  y7,  y8,  y9,  y10)'`
- of the true values `yy = (yy1, yy2, yy3, yy4, yy5, yy6, yy7, yy8, yy9, yy10)'`

The error column vector
of the true samples `vv = (vv1, vv2, vv3, vv4, vv5, vv6, vv7, vv8, vv9, vv10)'`
The effect elements column vector, of the true values, `cc := (ccM, ccA1, ccA2, ccA3, ccB1, ccB2, ccAB11, ccAB12, ccAB21, ccAB22, ccAB31, ccAB32)'`
The design matrix.

$$\begin{array}{rc} & \begin{array}{cccccc} \text{ccM} & \text{ccA1,2,3} & \text{ccB1,2} & \text{ccAB11, 12, 21, 22, 31, 32} \end{array} \\ X = \begin{array}{r} \text{A1B1.1} \\ \text{A1B1.2} \\ \text{A1B2} \\ \text{A2B1} \\ \text{A2B2.1} \\ \text{A2B2.2} \\ \text{A3B1.1} \\ \text{A3B1.2} \\ \text{A3B2.1} \\ \text{A3B2.2} \end{array} & \left[\begin{array}{cccccccccccc} 1 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right] \end{array}$$

The arid design matrix (`X*` of p.110, The Volume 1), with the duplicate rows deleted:

$$XX = \left[\begin{array}{cccccccccccc} 1 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right] \begin{array}{l} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array}$$

The full estimable matrix, with the linearly independent rows arbitrarily extracted:

$$Lu = \left[\begin{array}{cccccccccccc} 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & -1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 \end{array}\right] \begin{array}{l} 6 \\ 2\text{-}6 \\ 4\text{-}6 \\ 5\text{-}6 \\ 1\text{-}2\text{-}5\text{+}6 \\ 3\text{-}4\text{-}5\text{+}6 \end{array}$$

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$$J = \left[\begin{array}{cccccc} -1 & 1 & 0 & -1 & 1 & 0 \\ -1 & 1 & 0 & -1 & 1 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{array}\right]$$

The restoration matrix.

`X = J.Lu`

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A full estimable matrix, `LuI`, `LuII`, `LuIII` or `Lu` (above), each in SAS/STAT^R User's Guide, version 6, Volume 2, p. 932-936, **Output 24.3-6**, as of Type I, II, III, or General, respectively, and the sweep operator (`LL`'s) such that `LuI=LLI.Lu`, `LuII=LLII.Lu` or `LuIII=LLIII.Lu`.

****

$$\mathrm{LuI} = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & -1 & 1/6 & -1/6 & 2/3 & 1/3 & 0 & 0 & -1/2 & -1/2 \\ 0 & 0 & 1 & -1 & -1/6 & 1/6 & 0 & 0 & 1/3 & 2/3 & -1/2 & -1/2 \\ 0 & 0 & 0 & 0 & 1 & -1 & 2/7 & -2/7 & 2/7 & -2/7 & 3/7 & -3/7 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 \end{bmatrix}$$

$$\mathrm{LuII} = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & -1 & 0 & 0 & 13/21 & 8/21 & -1/21 & 1/21 & -4/7 & -3/7 \\ 0 & 0 & 1 & -1 & 0 & 0 & 1/21 & -1/21 & 8/21 & 13/21 & -3/7 & -4/7 \\ 0 & 0 & 0 & 0 & 1 & -1 & 2/7 & -2/7 & 2/7 & -2/7 & 3/7 & -3/7 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 \end{bmatrix}$$

$$\mathrm{LuIII} = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & -1 & 0 & 0 & 1/2 & 1/2 & 0 & 0 & -1/2 & -1/2 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1/2 & 1/2 & -1/2 & -1/2 \\ 0 & 0 & 0 & 0 & 1 & -1 & 1/3 & -1/3 & 1/3 & -1/3 & 1/3 & -1/3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 \end{bmatrix}$$

****

$$\mathrm{LLI} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/6 & 2/3 & 0 \\ 0 & 0 & 1 & -1/6 & 0 & 1/3 \\ 0 & 0 & 0 & 1 & 2/7 & 2/7 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\mathrm{LLII} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 13/21 & -1/21 \\ 0 & 0 & 1 & 0 & 1/21 & 8/21 \\ 0 & 0 & 0 & 1 & 2/7 & 2/7 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\mathrm{LLIII} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1/2 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1/2 \\ 0 & 0 & 0 & 1 & 1/3 & 1/3 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

****

-1. The sweep operators should be derived on the basis of descriptions of Chap. 9, Volume 1, p.109-124, though explicit and complete descriptions of the steps are often not so popular.

-2. Construction of rows of any particular full or part estimable matrix (`Lu` or `L`) for estimation of Type I, II, III etc., respectively, from that of Type General is important. It is, perhaps, done by part estimable matrices (`L`) built of the full matrix (`Lu`) with rows zeroed. And, if necessary, done by 'curt' estimable matrices (`Lv`), too, built of the full matrix (`Lu`) with columns zeroed.

-3. Many estimable functions are formed arbitrarily (by linear transformation or so) of rows of the full estimable matrix (`Lu`) yet all governed by the linear independence and the estimability. It secures general applicability of the scheme but with complication by the indeterminacy of the effect elements, to be relieved perhaps by the usual constraints on the basis of isolability.

****

Restoration matrix, JI, JII or JIII, for the full estimable matrix (above), LuI, LuII or LuIII, of Type I, II or III, respectively, such as built of the restoration matrix J of the General type by the inverse sweep operator (KK's) such that JI=J.KKI, JII=J.KKII or JIII=J.KKIII.

****

$$JI = \begin{bmatrix} -1 & 1 & 0 & -7/6 & 2/21 & 3/7 \\ -1 & 1 & 0 & -7/6 & 2/21 & 3/7 \\ -1 & 1 & 0 & -1/6 & -13/21 & 1/21 \\ 1 & 0 & 1 & 1/6 & -1/3 & 1/3 \\ 1 & 0 & 1 & 1/6 & -13/21 & -8/21 \\ 1 & 0 & 1 & 1/6 & -13/21 & -8/21 \\ 1 & 0 & 0 & 1 & 2/7 & -2/7 \\ 1 & 0 & 0 & 1 & 2/7 & -2/7 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The restoration matrix.

X = JI.LLI

$$JII = \begin{bmatrix} -1 & 1 & 0 & -1 & 2/3 & 0 \\ -1 & 1 & 0 & -1 & 2/3 & 1/3 \\ -1 & 1 & 0 & 0 & -13/21 & 1/21 \\ 1 & 0 & 1 & 1 & -1/3 & 1/3 \\ 1 & 0 & 1 & 0 & -1/21 & -8/21 \\ 1 & 0 & 1 & 0 & -1/21 & -8/21 \\ 1 & 0 & 0 & 1 & -2/7 & -2/7 \\ 1 & 0 & 0 & 1 & -2/7 & -2/7 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The restoration matrix.

X = JII.LLII

$$JIII = \begin{bmatrix} -1 & 1 & 0 & -1 & 5/6 & 0 \\ -1 & 1 & 0 & -1 & 5/6 & 0 \\ -1 & 1 & 0 & 0 & -1/2 & 0 \\ 1 & 0 & 1 & 1 & -1/3 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1/6 \\ 1 & 0 & 1 & 0 & 0 & 1/6 \\ 1 & 0 & 0 & 1 & -1/3 & -1/2 \\ 1 & 0 & 0 & 1 & -1/3 & -1/2 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The restoration matrix.

X = JIII.LLIII

****

$$KKI = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1/6 & -13/21 & 1/21 \\ 0 & 0 & 1 & 1/6 & -1/21 & -8/21 \\ 0 & 0 & 0 & 1 & -2/7 & -2/7 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$KKII = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -13/21 & 1/21 \\ 0 & 0 & 1 & 0 & -1/21 & -8/21 \\ 0 & 0 & 0 & 1 & -2/7 & -2/7 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$KKIII = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1/2 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1/2 \\ 0 & 0 & 0 & 1 & -1/3 & -1/3 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

****

PART **4** **Cf.** PART **3**

Another expression of eqn (A8) or (A′8)

$$SS\_yv = yv'.yv = cv'.X'X.cv$$
$$= (Lu.cv)'.J'J.(Lu.cv) \quad (A8)$$

$$(A14)\quad X'X.cv = X'.y = (J.Lu)'.y :$$
$$cv = (X'X)^{-}.(J.Lu)'.y = (X'X)^{-}Lu'.J'y$$
$$(A15)\quad Lu.cv = Lu(X'X)^{-}Lu'.J'y$$
$$(A16)\quad J'y = (Lu(X'X)^{-}Lu')^{-1}.(Lu.cv)$$
$$(A17)\quad (Lu.cv)'.J'y = (J.Lu.cv)'.y$$
$$= (Lu.cv)'.(Lu(X'X)^{-}Lu')^{-1}.(Lu.cv)$$
$$= (X.cv)'.y = cv'.X'y = cv'.(X'X).cv$$
$$= (X.cv)'(X.cv) = yv'.yv = SS\_yv$$

$$(A18)\quad SS\_yv$$
$$= (Lu.cv)'.[Lu(X'X)^{-}Lu']^{-1}.(Lu.cv)$$

$(A'18)\ SS\_yvP$ **similarly with** eqn $(A'8)$
$$= (L.cvP)'.[L(Xp'Xp)^{-}L']^{-1}.(L.cvP)$$

****

-4. The equation (A18) or (A’18) is identical with that at the end of the section **ESTIMABILITY** in Chap. 9, Volume 1, p.109-110, the last line of the section just around the middle of p.110.
-5. The matrix $[Lu(X'X)^{-}Lu]^{-1}$ in eqn (A18) or $[L(Xp'Xp)^{-}L']^{-1}$ in eqn (A’18) may be replaced consistently by the matrix $J'J$ in eqn (A11) or (A’11) in PART **B** as shown.
-6. The full estimable matrix LuI, LuII or LuIII and the sweep operator LLI, LLII or LLIII reflect the procedure of solution of the normal equation by Type I, II or III estimation, respectively. A‘full’estimable matrix may be linearly transformed to another, so an estimable function Lu¯o.cvP (cf. expn (A7)) may be generated in a ‘part’ estimable matrix arbitrarily.
-7. Each sum of squares SS_yvP shall be tesed of a null hypothesis. If necessary, columns of the restoration matrix J should be orthogonalized to each other by an inverse sweep operator KK, with rows of the estimable matrix transformed by a sweep operator LL ($=KK^{-1}$). Such the test might be an approximation only, without the orthogonality of the columns.
-8. Often the effect components are too much flexible under the conception of estimability and reduction. A more specific formulation may be preferable and possible, sometimes.

SAS® Forum (Japan)[#] Users Group Academic Session 2004 REMARKS ON THE PRESENTATION

Principles of determination of various sums of squares (SS's) in SAS/STAT® GLM procedure

Tadao SHIBAYAMA 1430-1500, July 30, 2004 Session Statistical Analysis

Prof. Dr Iwasaki,M. (Chair): In the scheme, linear algebra plays an important role on the one hand, though loaded heavy by matrices. On the other hand, theory of samples of normal population.

Shibayama,T. (Presenter): Yes, really. Thanks. (And, after the conference, wrote:)

PARAGRAPH **1.** `---` Consequently, at the inception of the scheme, the responses `y` as measured are generally looked as if to be samples of a normal population with the population mean `mm` (=0) and the population standard deviation `ss`, as the basis and control in spite of the actual nature.

2. `---` On the other hand, each response `y` is related to each row of the design matrix `X`, one by one, identified by the identification number `ppX` (=1,···,`lpX`) of the row of the design matrix `X` from 1 to the total number of the rows `lpX`. The responses `y(ppX)` as identified build a column vector

(R1) `y> = y(-ppX-)> = y(ppX)>`

as denoted by a Dirac ket `>` (and a row vector `<y` by a Dirac bra `<`). Two short hyphens (that may be omitted) emphasize that the variable in between is an indefinite element floating and running.

3. `---` A response `y` as measured is assumed generally to be a sum of the true response `yy` and a true sample `vv` of fluctuation, and the true response vector `yy>` is defined by the design matrix `X` that is operated on the true effect vector `cc(-qqX-)>` . So, **the structure equation** follows

(R2) `y> = yy> + vv> = yy(-ppX-)> + vv(-ppX-)>`

(R2a) `yy(-ppX-)> = X.cc(-qqX-)>`

The true effect vector `cc(-qqX-)>` is built of the true effect elements `cc(qqX)`, each related to each column of the design matrix `X`, one by one, and identified by the identification number `ppX` (=1,···,`lpX`) of the column of the design matrix `X` running from 1 to the total number of the columns `lpX`.

3a. `---` In a form similar to the equations (R2) and (R2a), **the observation equation** is to follow

(R3) `y> = yv> + vy> = yv(-ppX-)> + vy(-ppX-)>`

(R3a) `yv(-ppX-)> = X.cv(-qqX-)>`

The measured response vector `y>` is decomposed to a sum of the fitted response vector `yv>` and the fitted residue vector `vy>` both to make the sum of squared residues `<vy.vy>` least so that

(R3b) `X'.yv(-ppX-)> = X'X.cv(-qqX-)> = X'.y(-ppX-)>` and

(R3c) `X'.vy(-ppX-)> = 0` `---` **the normal equation**.

4. `---` As mentioned in the section **ESTIMABILITY** of SAS/STAT® User's Guide, version 6, Volume 1, Chap. 9, p.109-110, and in the subsection **General Form of an Estimable Function** as it follows, and sketched in p.110-124 and in SAS® Technical Reports R101 and R106, a set of linearly independent rows of the design matrix `X` may be extracted arbitrarily by the procedures such as

Type I procedure by Gauss-Jordan-Doolittle forward (sequential) elimination,
Type II procedure by Gauss-Jordan-Doolittle forward (partial) elimination,
Type III procedure by Type I, II or other procedure and adjustment by orthogonality of rows,
Type IV procedure by Type I, II or other procedure and adjustment by balance of rows,

or by other possible procedures, each detailed precisely or not, to form an estimable full matrix `Lu`.

To be regretted, any the procedure is complicate, not to be described so concisely, and hardly tractable even in the well readable SAS/STAT® User's Guide. Furthermore, if some different conceptions are amalgamated in a software, the internal consistency may be established only to a limited extent.

4a. `---` Though an estimable full matrix `Lu` is extracted by any procedure, any row of the original design matrix `X` is to be a linear combination of the rows of the estimable full matrix `Lu`. Consequently, the design matrix `X` is to be decomposed to a product of a restoration matrix `J` and the estimable full matrix `Lu`. The restoration matrix `J` is operated on the estimable full matrix `Lu` from the left:

(R4)(R4a) `X = J.Lu` , as the inverse of `Lu = K.X`

that mentioned in the section **ESTIMABILITY** of SAS/STAT® User's Guide, version 6, Volume 1, Chap. 9, p.109-110, and in the section ESTIMABILITY of SAS® Technical Report R101.

A row of the restoration matrix `J` is related to a row of the design matrix `X`, one by one, and identified by the identification number `ppJ` (=1, ···,`lpX`) just like the rows of the design matrix `X`. On the other hand, a column is related to a row of the estimable full matrix Lu, and identified by the identification number qqJ (=1,···,lpLu) that is related to the rows of the estimable full matrix Lu, therefore running from 1 to the total number lpLu of the rows of the estimable full matrix Lu.

4b. --- All of infinitely many possible pairs of the estimable full matrices Lu ('s) and the restoration matrix J are exhausted by eqn (R4), as an identity matrix Ɪ of size lpLu may be inserted in between the matrices J and Lu and factorized to a product of a regular matrix G and the inverse G* so that

(R4b)(R4c) Ɪ = G*.G and therefore X = J.Lu = J.G*.G.Lu

Any estimable full matrix LuB is got as equal to the product G.LuA from any original estimable full matrix LuA, and the restoration matrix JB is got as equal to the product JA.G* from the original JA.

5. --- From the observation and the normal equations, eqns (R3),(R3a),(R3b) and (R3c), it follows that sum of the squared measured response SS_y (=<y.y>) is composed of i) sum of the squared fitted response SS_yv (=<yv.yv>) and ii) sum of the squared fitted response SS_vy (=<vy.vy>).

The sum of the squared fitted response SS_yv is represented as follows

(R5) SS_yv = <yv.yv> = <cv.X'X.cv> = <cv.Lu'.J'J.Lu.cv>

If an estimable full matrix Lu is transformed to another matrix Lu0 appropriately by eqn (R4c), the restoration matrix J can be transformed to the other J0 such that the columns are orthogonal to each other and normalized. Then, the sum of squares SS_yv is represented as follows:

(R5a) SS_yv = <cv.Lu0'.Lu0.cv> because J'J = Ɪ

The expression is reduced very simple by the orthonormalized columns of the restoration matrix J0.

5a. --- Each of the orthonormalized columns of a restoration matrix J0 may be identified by the identification number qqJ0 (=1,···,lpLu0) and interpreted as a column vector J0(qqJ0:-ppJ0-)> as denoted. The running variable ppJ0 is the identification number of the elements and also of rows of the restoration matrix J0. That is running from 1 to the total number of the rows, lpJ0 (=lpX).

So, a new set of orthonormal column vectors J0(qqJ0:-ppJ0-)> may be defined arbitrarily as to be identified by the identification number qqJ0 (=lpLu0+1, ···, lpX) so that each is orthogonal to each other and to each of the orthonormal column vectors J0(qqJ0:-ppJ0-)> (qqJ0 =1,···,lpLu0).

5b. --- The newly defined orthonormal column vectors J0(qqJ0:-ppJ0-)> (qqJ0 =lpLu0+1, ···, lpX) build a complementary matrix JV for the restoration matrix J0. The restoration matrix J0 and the complementary matrix JV, if joined directly, form an orthonormal matrix Ɉ0 such that

(R5b) I = Ɉ0'.Ɉ0 = Ɉ0.Ɉ0' = I0 + IV , I0 = J0.J0' , IV = JV.JV' ;
Ɪ = J0'.J0 , ⅠV = JV'.JV , J0'.JV = 0 , JV'.J0 = 0 ;
I , Ɪ , ⅠV : an identity matrix of size lpX , lpLu or lpV (=lpX-lpLu) , respectively.

6. --- Columns of the design matrix X may be replaced by that of the restoration matrix J0, and the product J0'.J0 (= Ɪ) omitted, the normal equation (eqns (R3b) and (R3c)) is rewritten as follows:

(R6)(R6a) Lu0.cv(-qqX-)> = J0'.y(-ppX-)> and J0'.vy(-ppX-)> = 0 .

Each row of the estimable full matrix Lu0 may be looked as a row vector <Lu0(ppLu0:-qqLu0-) that corresponding to the column vector J0(qqJ0:-ppJ0-)> (qqJ0 =1,···,lpLu0), with the identification number ppLu0 of that replaced by qqJ0, i.e., that of the column vector J0(qqJ0:-ppJ0-)>. Then,

(R6b) <Lu0(qqJ0:).cv> = <J0(qqJ0:).y> provided that <J0(qqJ0:) = (J0(qqJ0:)>)'

6a. --- An estimable function <Lu0(qqJ0:).cv> is equal to a contrast <J0(qqJ0:).y> related to a column of the restoration matrix J0, defining the elements cv with some algebraic indeterminacy.

Each contrast <J0(qqJ0:).y> is a true sample of the normal population (PAR. **1.**), if the true response yy> is zero. (Basis for chi-square tests of hypotheses and of the significance of effects.)

6b. --- The pair of the restoration matrix J0 and the estimable full matrix Lu0 may be transformed by any orthonormal matrix GW and the inverse GW* (=GW') to another pair (PAR. **4b.**) but the normal equation and the solution are essentially invariant, and the algebraic indeterminacy as well.

7. --- If a design matrix X is factorized to a restoration matrix J and an estimable full matrix Lu, and if columns of the restoration matrix are orthonormalized, the estimable functions of the fitted effect elements are detached simple and defined uniquely. Sums of squares, etc., too, of course.

If the columns not orthonormalized, the matrix product J'.J entails non-diagonal elements to the equations as to be tractable necessarily by many-sided means of analysis of various 'Type'(s) as known.