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Preface to the second version

As compared with the first version of January 2009 an example has been added (section 9) and some minor improvement have been made.

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The General Linear Model and the Generalized Singular Value Decomposition

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Abstract: The general linear model $y = X\beta + \varepsilon$ with correlated error variables can be transformed by means of the generalized singular value decomposition to a very simple model (canonical form) where the least squares solution is obvious. The method works also if *X* and the covariance matrix of the error variables do not have full rank or are nearly rank deficient (rank-k approximation). By backtransformation one obtains the solution for the original model.

Keywords
General linear model, canonical form, generalized singular value decomposition, CS-decomposition of an orthogonal matrix, multicollinearity, rank-k approximation.

1. Introduction and summary

The general linear model is given by

(1) $\quad y = X\beta + \varepsilon,\ \mathrm{E}(\varepsilon) = 0,\ \mathrm{var}(\varepsilon) = \sigma^2 W,\ X = (n \times p),\ W = (n \times n),\ n > p$.

$\sigma^2 W$ is the covariance matrix of ε and we assume that the matrix *W* is given (symmetric and positive semidefinite) while σ^2 is unknown. If $W = I_n$ we have the simple linear model with uncorrelated error variables $\varepsilon_1, \ldots, \varepsilon_n$. If $\mathrm{rk}(W) = k$ *W* can be written as $W = FF^\mathsf{T}$ where $F = (n \times k)$ and $\mathrm{rk}(F) = \mathrm{rk}(W) = k$. The random error ε can now be given in the form

(2) $\quad \varepsilon = Fu$ with $u \sim (0, \sigma^2 I_k)$ i.e. with $\mathrm{E}(u) = 0,\ \mathrm{var}(u) = \sigma^2 I_k$

as $\mathrm{E}(\varepsilon) = \mathrm{E}(Fu) = 0$ and $\mathrm{var}(\varepsilon) = \mathrm{E}(\varepsilon\varepsilon^\mathsf{T}) = F\,\mathrm{E}(uu^\mathsf{T})F^\mathsf{T} = \sigma^2 FF^\mathsf{T} = \sigma^2 W$. So the general linear model (1) can be written as

(3) $\quad y = X\beta + Fu,$ where $X = (n \times p),\ F = (n \times k)$ and $u \sim (0, \sigma^2 I_k)$,

and according to the method of least squares we have to determine $\beta = \hat\beta$ such that $u^\mathsf{T} u = \sum u_i^2 = \min$, where *u* must satisfy the equation (3). We want to state our estimation problem in other words. Consider for given y, X, F the set $M = \{(b,e) \mid y = Xb + Fe\}$. Now we are looking for the pair (b,e) with $e^\mathsf{T} e = \sum_{i=1}^k e_i^2 = \min$. Then $b = \hat\beta$ is the least squares estimator of β . If one is interested in the model with normally distributed error variables, one assumes that $u \sim N_k(0, \sigma^2 I_k)$, and then one has $\varepsilon = Fu \sim N_n(0, \sigma^2 W)$. Note that we do not make any assumptions on the rank of the matrices *X* and *W*.

By means of the generalized singular value decomposition we find linear transformations that transform (y, β, u) to ($\tilde{y}, \tilde{\beta}, \tilde{u}$), where again $\tilde{u} \sim (0, \sigma^2 I_k)$, and where $\tilde{y}$ can be decomposed in four subvectors $\tilde{y}_1,\ldots,\tilde{y}_4$, $\tilde{\beta}$ in three subvectors $\tilde{\beta}_1, \tilde{\beta}_2, \tilde{\beta}_3$ and $\tilde{u}$ in two subvectors $\tilde{u}_1, \tilde{u}_2$ such that model (3) becomes

$$
(4) \quad
\begin{array}{ll}
(a) & \tilde{y}_1 = \tilde{\beta}_1, \\
(b) & \tilde{y}_2 = C\tilde{\beta}_2 + S\tilde{u}_1, \text{ where } C \text{ and } S \text{ are diagonal with } C^2 + S^2 = I, \\
(c) & \tilde{y}_3 = \tilde{u}_2, \\
(d) & \tilde{y}_4 = 0.
\end{array}
$$

We call this the canonical form of the general linear model. We have four categories of observations ($\tilde{y}_1,\ldots,\tilde{y}_4$), three categories of parameters ($\tilde{\beta}_1, \tilde{\beta}_2, \tilde{\beta}_3$) and two categories of error variables ($\tilde{u}_1, \tilde{u}_2$).
The observations in (a) are completely fixed by the parameters $\tilde{\beta}_1$; they possess no random error.
The observations in (b) depend on $\tilde{\beta}_2$ and they have a random error $S\tilde{u}_1$.
The observations in (c) do not depend on the parameters, they are given by $\tilde{y}_3 = \tilde{u}_2$.
The observations in (d) are all zero; they are independent of the parameters and have no random error.
Note that the parameters in the third category $\tilde{\beta}_3$ do not appear in the canonical model (4); they can have arbitrary values and are not identifiable. As $\tilde{\beta} = U^\mathsf{T}\beta$ with orthogonal U the additional condition $\beta^\mathsf{T}\beta = \tilde{\beta}^\mathsf{T}\tilde{\beta} = \min$ (minimum length condition) entails $\tilde{\beta}_3 = 0$ and this way the whole parameter set $\tilde{\beta}$ as well as $\beta = U\tilde{\beta}$ becomes identifiable. Now it is very easy to find the least squares estimators in the canonical model and by backtransformation we obtain the estimators for the original parameters.
The basic ideas of this treatment of the general linear model are given in Kourouklis-Paige (1981) and Paige (1985). In this paper the derivations of Paige are simplified and we describe a clear computational procedure for finding the results; this procedure is demonstrated with a simple example. Some more examples are to be found in Knüsel (2009). Furthermore we demonstrate how the problem of near rank deficiency can be treated by means of the so-called rank-k-approximation.

Summary

In section 2 we describe the general linear model and in section 3 the generalized singular value decomposition. In section 4 the general linear model is reduced to the canonical model using the generalized singular value decomposition. The least squares estimators for the canonical and original model are derived in section 5. Section 6 deals with the special case $\mathrm{rk}(W) = n$ (correlation matrix with full rank) and $\mathrm{rk}(X) \le p$. If also X has full rank this case can be reduced to the classical linear model by the well-known method of Aitken (see Rao-Toutenburg et al., 2008, p. 151). In section 7 we show that the general linear model with linear restrictions can be extended to a general linear model without explicit restrictions according to a method of Rao (1971). Section 8 deals with the question what one can do if our matrices are nearly rank deficient (e.g. weak multicollinearity). The rank-k approximation of Golub-Van Loan (1996) is a wonderful means to overcome these problems. The example in section 9 deals with a general linear model with nearly rank deficient X and W. In a first step we demonstrate the application of the rank-k approximation to the given matrices and then our procedure leads to a numerically stable solution. Section 10 gives the conclusion. In the appendix a simplified derivation of the general singular value decomposition according to the ideas of Paige (1985) is presented.

2. The general linear model

The general linear model is given by

(5) $y = X\beta + \varepsilon,\ E(\varepsilon) = 0,\ \mathrm{var}(\varepsilon) = \sigma^2 W,\ X = (n \times p),\ W = (n \times n),\ n > p$.

$\sigma^2 W$ is the covariance matrix of ε, and we assume that the matrix W is given (symmetric and positive semidefinite) while σ^2 is unknown. If $W = I_n$ we have the simple linear model. W can be written as $W = FF^{\mathsf{T}}$ where $F = (n \times k)$ and $\mathrm{rk}(F) = \mathrm{rk}(W) = k$. This can be seen from the spectral decomposition of W

$$W = R\Lambda R^{\mathsf{T}},\ \text{where } R \text{ is orthogonal and } \Lambda = \mathrm{diag}(\lambda_1,\ldots,\lambda_k,0,\ldots,0),\ \lambda_i > 0.$$

Let $D = (n \times k) = \mathrm{diag}(\sqrt{\lambda_1},\ldots,\sqrt{\lambda_k})$ and $F = RD = (n \times k)$; then $DD^{\mathsf{T}} = (n \times n) = \Lambda$ and $FF^{\mathsf{T}} = R\,DD^{\mathsf{T}}R^{\mathsf{T}} = R\Lambda R^{\mathsf{T}} = W$. The random error ε can now be written in the form

(6) $\varepsilon = Fu$ with $u \sim (0,\sigma^2 I_k)$ i.e. with $\mathrm{E}(u) = 0,\ \mathrm{var}(u) = \sigma^2 I_k$,

as $\mathrm{E}(\varepsilon) = \mathrm{E}(Fu) = 0$ and $\mathrm{var}(\varepsilon) = \mathrm{E}(\varepsilon\varepsilon^{\mathsf{T}}) = F\,\mathrm{E}(uu^{\mathsf{T}})F^{\mathsf{T}} = \sigma^2 FF^{\mathsf{T}} = \sigma^2 W$. So model (5) can also be given as

(7) $y = X\beta + Fu,$ where $X = (n \times p),\ F = (n \times k),\ u \sim (0,\sigma^2 I_k)$,

and according to the method of least squares we have to determine $\beta = \hat{\beta}$ such that $u^{\mathsf{T}}u = \sum u_i^2 = \min$, where u must satisfy the equation (7). If one is interested in the model with normally distributed error variables, one assumes that $u \sim N_k(0,\sigma^2 I_k)$, and then we have $\varepsilon = Fu \sim N_n(0,\sigma^2 W)$. Let

$\mathfrak{R}_X =$ vector space of all column vectors of X (range of X),

$\mathfrak{R}_F =$ vector space of all column vectors of F (range of F).

Obviously $X\beta \in \mathfrak{R}_X$ for arbitrary β and $Fu \in \mathfrak{R}_F$ for arbitrary u, and so we derive from model (7) that $y \in \mathfrak{R}_X \cup \mathfrak{R}_F$. An observation $y \notin (\mathfrak{R}_X \cup \mathfrak{R}_F)$ is not admissible with model (7), it were an inconsistent observation.

3. The generalized singular value decomposition

Let $X = (n \times p)$ and $F = (n \times k)$ be real matrices. Then there exist orthogonal matrices $P = (n \times n), U_1 = (p \times p), U_2 = (k \times k), V = (r_c \times r_c)$ such that

$$P^{\mathsf{T}}XU_1 = \begin{pmatrix} \Delta_0 V \\ 0 \end{pmatrix} D_1 \qquad (8)$$
$$P^{\mathsf{T}}FU_2 = \begin{pmatrix} \Delta_0 V \\ 0 \end{pmatrix} D_2$$

where

$$D_1 = (r_c \times p) = \left(\begin{array}{cc|c} I_{r_1} & 0 & 0 \\ 0 & C & 0 \\ \hline 0 & 0 & 0 \end{array}\right), \qquad D_2 = (r_c \times k) = \left(\begin{array}{c|cc} 0 & 0 & 0 \\ \hline 0 & S & 0 \\ 0 & 0 & I_{r_2} \end{array}\right),$$

$\Delta_0 = (r_c \times r_c) = \mathrm{diag}(\delta_1,\ldots,\delta_{r_c}),\ \delta_1 \ge \cdots \ge \delta_{r_c} > 0,\ \delta_1,\ldots\delta_{r_c}$ the positive singular values of $(X \mid F)$,

$C = (r \times r) = \mathrm{diag}(c_1,\ldots,c_r),\ 1 > c_1 \ge \cdots \ge c_r > 0,$

$S = (r \times r) = \mathrm{diag}(s_1,\ldots,s_r),\ 0 < s_1 \le \cdots \le s_r < 1,\ C^2 + S^2 = I,$

and where

$r_c = \mathrm{rk}(X \mid F),\ r_X = \mathrm{rk}(X),\ r_F = \mathrm{rk}(F),\ r = r_X + r_F - r_c,\ r_1 = r_X - r,\ r_2 = r_F - r$.

So the diagonal matrices D_1 and D_2 have the same rank as X and F. Note that

$$r_c = \dim(\mathfrak{R}_X \cup \mathfrak{R}_F),\ r = \dim(\mathfrak{R}_X \cap \mathfrak{R}_F),\ r_1 = \dim(\mathfrak{R}_X - \mathfrak{R}_F),\ r_2 = \dim(\mathfrak{R}_F - \mathfrak{R}_X).$$

The representation (8) is called the *generalized singular value decomposition of the pair* (X,F). A proof of this decomposition can be found in Paige (1985), and in the Appendix we give a sketch of this proof. All matrices in (8) are either orthogonal or diagonal (except X and F). Also note that D_1 and D_2 are diagonal matrices with a rectangular format the diagonal starting in the upper left and lower right corner, respectively.

In the general linear model (7) we have chosen $F = (n \times k)$ such that $\text{rk}(F) = r_2 + r = k$, and then the generalized singular value decomposition (8) of $(X \mid F)$ simplifies to

(9)

$$P^{\mathsf{T}} X U_1 = \left(\frac{\Delta_0 V}{0}\right) D_1,\quad D_1 = (r_c \times p) = \left(\begin{array}{cc|c} I_{r_1} & 0 & 0 \\ 0 & C & 0 \\ \hline 0 & 0 & 0 \end{array}\right) = \begin{array}{c|c|c|l} r_1 & r & p-r_X & \\ \hline \quad & \quad & \quad & r_1 \\ \hline \quad & \quad & \quad & r \\ \hline \quad & \quad & \quad & r_2 \end{array}$$

$$P^{\mathsf{T}} F U_2 = \left(\frac{\Delta_0 V}{0}\right) D_2,\quad D_2 = (r_c \times k) = \left(\begin{array}{cc} 0 & 0 \\ \hline S & 0 \\ 0 & I_{r_2} \end{array}\right) = \begin{array}{c|c|l} r & r_2 & \\ \hline \quad & \quad & r_1 \\ \hline \quad & \quad & r \\ \hline \quad & \quad & r_2 \end{array}$$

4. Reduction of the general linear model to the canonical model

Now we want to apply the decomposition (9) to the general linear model (7). We have

$$\begin{aligned} y &= X\beta + Fu, \quad \text{where } u \sim (0, \sigma^2 I_k) \\ &= XU_1 \underbrace{U_1^{\mathsf{T}}\beta}_{=\tilde{\beta}} + FU_2 \underbrace{U_2^{\mathsf{T}} u}_{=\tilde{u}} \end{aligned}$$

and multiplying the last equation by P^{T} we obtain

$$\underbrace{P^{\mathsf{T}} y}_{=\bar{y}} = P^{\mathsf{T}} X U_1 \tilde{\beta} + P^{\mathsf{T}} F U_2 \tilde{u}.$$

Applying the generalized singular value decomposition (9) we obtain

(10) $$\bar{y} = \left(\frac{\Delta_0 V}{0}\right)\left[D_1 \tilde{\beta} + D_2 \tilde{u}\right].$$

The last $n - r_c$ elements of $\bar{y}$ are zero and so we write $\bar{y} = \left(\frac{\bar{y}_0}{0}\right)$ where $\bar{y}_0$ denotes the vector of the first r_c elements of $\bar{y}$. Now we have from (10)

$$\bar{y}_0 = \Delta_0 V\left[D_1 \tilde{\beta} + D_2 \tilde{u}\right]$$

or

(11) $$\underbrace{V^{\mathsf{T}} \Delta_0^{-1} \bar{y}_0}_{=\tilde{y}_0} = D_1 \tilde{\beta} + D_2 \tilde{u}.$$

Thus the general linear model (7) can be transformed to

(12) $$\tilde{y} = \left(\frac{\tilde{y}_0}{0}\right) \quad \text{with } \tilde{y}_0 = (r_c \times 1) = D_1 \tilde{\beta} + D_2 \tilde{u}$$

where

$$\tilde\beta = U_1^{\mathsf T}\beta,$$
$$\tilde u = U_2^{\mathsf T}u,$$
$$\tilde y = \begin{pmatrix}\tilde y_0\\ \hline 0\end{pmatrix} = \left(\begin{array}{c|c} V^{\mathsf T}\Delta_0^{-1} & 0\\ \hline 0 & I\end{array}\right)P^{\mathsf T}y.$$

The transformed model (12) is very simple as D_1 and D_2 are diagonal matrices with the same ranks as X and F, and we call this representation the *canonical form* of the general linear model. Note that $r_1 + r + r_2 = r_c$ and so we write

$$\tilde y_0 = (r_c \times 1) = \begin{pmatrix}\tilde y_{01}\\ \tilde y_{02}\\ \tilde y_{03}\end{pmatrix} = \begin{array}{|c|}\hline \quad\\ \hline \quad\\ \hline \quad\\ \hline\end{array}\ \begin{array}{c} r_1\\ r\\ r_2\end{array}$$

and further

$$\tilde\beta = (p\times 1) = \begin{pmatrix}\tilde\beta_1\\ \tilde\beta_2\\ \tilde\beta_3\end{pmatrix} = \begin{array}{|c|}\hline \quad\\ \hline \quad\\ \hline \quad\\ \hline\end{array}\ \begin{array}{c} r_1\\ r\\ p-r_X\end{array}$$

$$\tilde u = (k\times 1) = \begin{pmatrix}\tilde u_1\\ \tilde u_2\end{pmatrix} = \begin{array}{|c|}\hline \quad\\ \hline \quad\\ \hline\end{array}\ \begin{array}{c} r\\ r_2\end{array}$$

and we obtain from (12)

$$\begin{pmatrix}\tilde y_{01}\\ \tilde y_{02}\\ \tilde y_{03}\end{pmatrix} = \left(\begin{array}{cc|c} I_{r_1} & 0 & 0\\ 0 & C & 0\\ \hline 0 & 0 & 0\end{array}\right)\begin{pmatrix}\tilde\beta_1\\ \tilde\beta_2\\ \tilde\beta_3\end{pmatrix} + \left(\begin{array}{cc} 0 & 0\\ \hline S & 0\\ 0 & I_{r_2}\end{array}\right)\begin{pmatrix}\tilde u_1\\ \tilde u_2\end{pmatrix}$$

i.e.

$$\begin{aligned}&\tilde y_{01} = \tilde\beta_1\\ (13)\quad &\tilde y_{02} = C\tilde\beta_2 + S\tilde u_1\\ &\tilde y_{03} = \tilde u_2.\end{aligned}$$

So we find the following four categories of observations

$$(14)\quad \begin{array}{ll}(a) & \tilde y_{01} = (r_1\times 1) = \tilde\beta_1\\ (b) & \tilde y_{02} = (r\times 1) = C\tilde\beta_2 + S\tilde u_1\\ (c) & \tilde y_{03} = (r_2\times 1) = \tilde u_2\\ (d) & \tilde y_1 = ((n-r_c)\times 1) = 0.\end{array}$$

The observations in (a) have no measurement errors and they are identical to the parameters in $\tilde\beta_1$. These observations can be described by the model $y = X\beta + Fu$, where $X = I$ and $F = 0$. The number of these observations is $r_1 = r_X - r$.

The observations in (b) depend on the parameter vector $\tilde\beta_2$ with a diagonal design matrix C; the distribution of the measurement errors is given by $S\tilde u_1 \sim (0, \sigma^2 S^2)$, where also S is diagonal. The observations in (b) can be described by the model $y = X\beta + Fu$, where both $X = C$ and $F = S$ are diagonal matrices with $C^2 + S^2 = I_r$. The number of these observations is $r = r_X + r_F - r_c$.

The observations in (c) do not depend on the parameter vector $\tilde\beta$; their distribution is given by $\tilde y_{03} = \tilde u_2 \sim (0, \sigma^2 I_{r_2})$. These observations can be described by the model $y = X\beta + Fu$, where $X = 0$ and $F = I$. The number of these observations is $r_2 = r_F - r$.

The observations in (d) have no measurement errors and do not depend on the parameter vector $\tilde{\beta}$, they are all identical to zero. These observations can be described by the model $y = X\beta + Fu$, where $X = 0$ and $F = 0$. The number of these observations is $n - r_c$.

The total number of the observations in category (a) and (d) which possess no random error is $r_1 + n - r_c = n - r_F = n - r_W$. The parameter vector $\tilde{\beta}_3$ does not show up in the canonical model (13); these parameters can have arbitrary values, they can all be chosen as zero. Then $\tilde{\beta}^\mathsf{T}\tilde{\beta} = \beta^\mathsf{T}\beta = \min$ (minimum length solution).

5. Least squares estimators

Now we want to estimate the unknown parameters in the canonical model (13) according to the method of least squares. $\tilde{\beta}_1 = (r_1 \times 1)$ is completely fixed by the equation $\tilde{y}_{01} = \tilde{\beta}_1$; the observations in $\tilde{y}_{01}$ have no measurement errors. $\tilde{\beta}_3 = (r_2 \times 1)$ has no effect in model (13); these parameters can have arbitrary values. If we are interested in the minimal length solution with $\tilde{\beta}^\mathsf{T}\tilde{\beta} = \min$ we have to set $\tilde{\beta}_3 = \hat{\tilde{\beta}}_3 = 0$. $\tilde{\beta}_2 = (r \times 1)$ has to be determined from the equations $\tilde{y}_{02} = C\tilde{\beta}_2 + S\tilde{u}_1$. We can choose $\tilde{\beta}_2$ such that $\tilde{u}_1 = 0$ namely $\tilde{\beta}_2 = \hat{\tilde{\beta}}_2 = C^{-1}\tilde{y}_{02}$ and this is obviously the least squares estimator. The variance of the estimator $\hat{\tilde{\beta}}_2$ is given by

$$\operatorname{var}(\hat{\tilde{\beta}}_2) = \operatorname{var}\left(C^{-1}\tilde{y}_{12}\right) = \operatorname{var}\left(C^{-1}S\tilde{u}_1\right) = \sigma^2 C^{-2} S^2 .$$

If we set $\tilde{\beta}_3 = \hat{\tilde{\beta}}_3 = 0$ we have

$$\operatorname{var}(\hat{\tilde{\beta}}) = (p \times p) = \sigma^2 \left(\begin{array}{c|c|c} 0 & 0 & 0 \\ \hline 0 & C^{-2}S^2 & 0 \\ \hline 0 & 0 & 0 \end{array}\right) =$$

	r_1	r	$p-r_X$
r_1			
r			
$p-r_X$			

An unbiased estimator of σ^2 is found from the equation $\tilde{y}_{03} = (r_2 \times 1) = \tilde{u}_2$ as $\tilde{u}_2 \sim (0, \sigma^2 I_{r_2})$:

(15) $\quad \hat{\sigma}^2 = \dfrac{1}{r_2}(\tilde{y}_{03})^\mathsf{T}(\tilde{y}_{03}) = \dfrac{1}{r_2}\tilde{u}_2^\mathsf{T}\tilde{u}_2 = \dfrac{1}{r_2}\sum_{i=1}^{r_2}\tilde{u}_{2i}^2$ as obviously $E\left(\hat{\sigma}^2\right) = \sigma^2$.

From equation (12) we now have

$$\tilde{y}_0 = D_1\hat{\tilde{\beta}} + D_2\tilde{e}, \text{ where } \tilde{e} = \begin{pmatrix} \tilde{e}_1 \\ \hline \tilde{e}_2 \end{pmatrix} = \begin{pmatrix} r \times 1 \\ \hline r_2 \times 1 \end{pmatrix} \text{ denotes the residual vector}.$$

The least squares estimator has been chosen such that $\tilde{e}_1 = 0$ and $\tilde{e}_2 = \tilde{u}_2$. So the estimator $\hat{\sigma}^2$ in (15) can also be written as

$$\hat{\sigma}^2 = \frac{1}{r_2}\tilde{e}^\mathsf{T}\tilde{e} = \frac{1}{r_2}(\text{sum of all squared residuals}).$$

Backtransformation to the original parameters

The estimators for the original parameters $\beta = (p \times 1)$ are found by backtransformation. We have

$\tilde{\beta} = U_1^\mathsf{T}\beta$ and so $\beta = U_1\tilde{\beta}, \ \hat{\beta} = U_1\hat{\tilde{\beta}}$,

$\tilde{u} = U_2^\mathsf{T}u$ and so $u = U_2\,\tilde{u}, \ e = U_2\,\tilde{e}$

$\tilde{y} = \left(\begin{array}{c|c} V^\mathsf{T}\Delta_0^{-1} & 0 \\ \hline 0 & I \end{array}\right)P^\mathsf{T}y$ and so $y = P\left(\begin{array}{c|c} \Delta_0^{-1}V & 0 \\ \hline 0 & I \end{array}\right)\tilde{y}.$

Note that the residuals in the original model are found from $e = U_2\,\tilde{e}$ and as U_2 is orthogonal we have $e^\top e = \tilde{e}^\top \tilde{e}$, and so the parameters $\hat{\beta} = U_1 \hat{\tilde{\beta}}$ are indeed the least squares estimators in the original model and

$$\hat{\sigma}^2 = \frac{1}{r_2}\tilde{e}^\top \tilde{e} = \frac{1}{r_2} e^\top e = \frac{1}{r_2}(\text{sum of all squared residuals})\,.$$

The variance-covariance matrix of $\hat{\beta}$ is

$$\operatorname{var}(\hat{\beta}) = \operatorname{var}\left(U_1\hat{\tilde{\beta}}\right) = U_1 \operatorname{var}\left(\hat{\tilde{\beta}}\right) U_1^\top = \sigma^2 U_1 \left(\begin{array}{c|c|c} 0 & 0 & 0 \\ \hline 0 & C^{-2}S^2 & 0 \\ \hline 0 & 0 & 0 \end{array}\right) U_1^\top\,.$$

How can we prevent the diagonal matrices Δ_0, C, S from becoming nearly singular such that the computation of the inverse becomes numerically unstable? This question will be answered in the section 8 (rank-k approximation).

6. Special case with rk(*W*) = *n*

If $rk(W) = n$ we can apply three different procedures to find the least squares solution, the classical method of Aitken, the method with the simple singular values decomposition and the method with the generalized singular value decomposition.

A) Classical procedure of Aitken

As $\operatorname{rk}(W) = n$ and $W = FF^\top$ we also have $\operatorname{rk}(F) = r_F = n$ and thus the matrix F is regular; F can also be chosen as a symmetric matrix e.g. using the spectral decomposition of W; W can be written as

$W = R\Lambda R^\top$ where R is orthogonal and $\Lambda = \operatorname{diag}(\lambda_1,\ldots,\lambda_n),\ \lambda_i > 0$.

We set

$F = R\Lambda^{1/2}R^\top$ where $\Lambda^{1/2} = \operatorname{diag}\left(\sqrt{\lambda_1},\ldots,\sqrt{\lambda_n}\right)$;

then F is symmetric and $F^2 = FF^\top = R\Lambda R^\top = W$. So model (7)

$y = X\beta + Fu$

can be written as

$$\underbrace{F^{-1}y}_{=\bar{y}} = \underbrace{F^{-1}X}_{=\bar{X}}\beta + u, \text{ where } u \sim (0, \sigma^2 I_n)$$

i.e.

(16) $\bar{y} = \bar{X}\beta + u$, where $u \sim (0,\sigma^2 I_n)$.

This is the simple linear model and thus the least squares estimator is given by

$$\text{(17)}\quad \begin{aligned} \hat{\beta} &= (\bar{X}^\top \bar{X})^{-1}\bar{X}^\top \bar{y} = (X^\top F^{-2}X)^{-1}X^\top F^{-2}y = (X^\top W^{-1}X)^{-1}X^\top W^{-1}y \\ \operatorname{var}(\hat{\beta}) &= \sigma^2(\bar{X}^\top \bar{X})^{-1} = \sigma^2(X^\top W^{-1}X)^{-1} \end{aligned}\,.$$

This representation is only possible if $\operatorname{rk}(X) = p$; if $\operatorname{rk}(X) < p$ the inverse $(\bar{X}^\top \bar{X})^{-1}$ in (17) does not exist. The solution (17) is the so-called Aitken estimator (see Rao-Toutenburg et al., 2008, p. 151).

B) Procedure with (simple) singular value decomposition

The singular value decomposition of $\bar{X}$ in (16) gives $\bar{X} = UDV^{\top}$, where $U = (n \times n)$ and $V = (p \times p)$ are orthogonal matrices and $D = (n \times p) = \text{diag}(\sigma_1, \ldots, \sigma_p)$; $\sigma_1 \geq \ldots \geq \sigma_p \geq 0$ are the singular values of $\bar{X}$. So we obtain from (16)

$$\bar{y} = UDV^{\top}\beta + u, \text{ where } u \sim (0, \sigma^2 I_n)$$

or

$$\underbrace{U^{\top}\bar{y}}_{=\tilde{y}} = D\underbrace{V^{\top}\beta}_{=\tilde{\beta}} + \underbrace{U^{\top}u}_{=\tilde{u}},$$

i.e.

(18) $\tilde{y} = D\tilde{\beta} + \tilde{u}$, and as $\tilde{u} = U^{\top}u$ we have again $\tilde{u} \sim (0, \sigma^2 I_n)$.

This is the canonical form of the original model (16). If $\text{rk}(X) = \text{rk}(\bar{X}) = r_X$ we have

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{r_X} > \sigma_{r_X+1} = \cdots = \sigma_p = 0.$$

Then the parameters $\tilde{\beta}_{r_X+1}, \ldots, \tilde{\beta}_p$ do not show up in the canonical model, they can have arbitrary values; they are not identifiable and can all be chosen as zero such that $\tilde{\beta}^{\top}\tilde{\beta} = \beta^{\top}\beta = \sum \beta_i^2 = \min$ (minimum length definition). According to the method of least squares we have to choose the vector $\tilde{\beta} = \hat{\tilde{\beta}}$ in (18) such that $\tilde{e}^{\top}\tilde{e} = \sum \tilde{e}_i^2 = \min$, where $\tilde{e} = \tilde{y} - D\tilde{\beta}$ From (18) we have

(19)
$$\tilde{y}_i = d_i\tilde{\beta}_i + \tilde{u}_i \text{ for } i = 1, \ldots, r_X,$$
$$\tilde{y}_i = \tilde{u}_i \text{ for } i = r_X + 1, \ldots, n,$$

and thus

$$\tilde{e}_i = \tilde{y}_i - d_i\tilde{\beta}_i \quad \text{for } i = 1, \ldots, r_X,$$
$$\tilde{e}_i = \tilde{y}_i \quad \text{for } i = r_X + 1, \ldots, n.$$

Obviously $\sum \tilde{e}_i^2$ becomes minimal for $\tilde{e}_1 = \cdots = \tilde{e}_{r_X} = 0$ i.e. for

$$\tilde{\beta}_i = \hat{\tilde{\beta}}_i = \tilde{y}_i / d_i \quad \text{for } i = 1, \ldots, r_X$$
$$\tilde{\beta}_i \text{ arbitrary} \quad \text{for } i = r_X + 1, \ldots, p.$$

If we are interested in the minimum length solution $\sum \tilde{\beta}_i^2 = \min$, we have to choose $\tilde{\beta}_i = \hat{\tilde{\beta}}_i = 0$ for $i = r_X + 1, \ldots, p$, and then the solution can be written as

(20) $\tilde{\beta} = \hat{\tilde{\beta}} = D^{+}\tilde{y}$, where $D^{+} = (p \times n) = diag(1/\sigma_1, \ldots, 1/\sigma_{r_X}, 0, \ldots, 0)$.

The variance-covariance matrix of $\hat{\tilde{\beta}}$ is given by

$$\text{var}(\hat{\tilde{\beta}}) = \text{var}(D^{+}\tilde{y}) = \text{var}(D^{+}\tilde{u}) = \sigma^2\left(D^{+}(D^{+})^{\top}\right) = \sigma^2(D^{\top}D)^{+} = \sigma^2 \,\text{diag}\left(\frac{1}{\sigma_1^2}, \ldots, \frac{1}{\sigma_{r_X}^2}, 0 \ldots, 0\right).$$

As $\tilde{y} = U^{\top}\bar{y} = U^{\top}F^{-1}y$ the estimator for the original parameters is

(21) $\hat{\beta} = V\hat{\tilde{\beta}} = VD^{+}\tilde{y} = VD^{+}U^{\top}F^{-1}y = \bar{X}^{+}F^{-1}y$.

If $rk(X) = p$ i.e. if X has full rank this solution is equivalent to the classical Aitken estimator (17) as

$$\bar{X} = UDV^{\top}, \quad \bar{X}^{\top} = VD^{\top}U^{\top}$$
$$\bar{X}^{\top}\bar{X} = VD^{\top}DV^{\top}$$
$$(\bar{X}^{\top}\bar{X})^{-1} = V(D^{\top}D)^{-1}V^{\top}$$
$$(\bar{X}^{\top}\bar{X})^{-1}\bar{X}^{\top}\bar{y} = V(D^{\top}D)^{-1}V^{\top}VD^{\top}U^{\top}F^{-1}y = VD^{+}U^{\top}F^{-1}y = \bar{X}^{+}F^{-1}y.$$

The representation (21) is correct also if $\text{rk}(X) < p$ i.e. if multicollinearity is present.

Remark

From (19) we see that in the canonical model we find observations falling in only two of the categories described in (4):

$(b)\quad \tilde{y}_i = d_i\tilde{\beta}_i + \tilde{u}_i$ for $i = 1,\ldots,r_X$;

$(c)\quad \tilde{y}_i = \tilde{u}_i$ for $i = r_X + 1,\ldots,n$.

Observations in category (a) and (d) that have no measurement errors do not arise when $\mathrm{rk}(W) = n$.

C) Procedure with generalized singular value decomposition

We consider the generalized singular value decomposition of $(X \mid F)$ in (9). As $\mathrm{rk}(F) = r_F = n$ we have $\mathrm{rk}(X \mid F) = r_c = n$, $r = r_X + r_F - r_c = r_X \le p$, and $r_1 = r_X - r = 0$. So we obtain from (9)

(22) $P^{\mathsf{T}} X U_1 = \Delta_0 V D_1$ and $P^{\mathsf{T}} F U_2 = \Delta_0 V D_2$

where

$$D_1 = (n \times p) = \begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix}, \quad D_2 = (n \times k) = \begin{pmatrix} S & 0 \\ 0 & I \end{pmatrix}.$$

Equation (10) gives

$$\bar{y} = \Delta_0 V \left[D_1 \tilde{\beta} + D_2 \tilde{u} \right]$$

or

$$V^{\mathsf{T}} \Delta_0^{-1} \bar{y} = D_1 \tilde{\beta} + D_2 \tilde{u}.$$

Multiplying this equation by D_2^{-1} gives

$$\underbrace{D_2^{-1} V^{\mathsf{T}} \Delta_0^{-1} \bar{y}}_{=\tilde{y}} = D_2^{-1} D_1 \tilde{\beta} + \tilde{u} = \begin{pmatrix} S^{-1}C & 0 \\ 0 & 0 \end{pmatrix} \tilde{\beta} + \tilde{u},$$

and this equation is equivalent to (18); the matrix $D_2^{-1} D_1$ is identical to the diagonal matrix D in (18) as according to (22) $\bar{X} = F^{-1} X = U_2 D_2^{-1} D_1 U_1^{\mathsf{T}}$, and this corresponds to the singular value decomposition of $\bar{X}$ in procedure B.

7. General linear model with linear restrictions

According to Rao (1971) a general linear model (5)

$$y = X\beta + \varepsilon,\ E(\varepsilon) = 0,\ \mathrm{var}(\varepsilon) = \sigma^2 W,\ X = (n \times p),\ W = (n \times n),\ n > p$$

with linear restrictions $R\beta = c$ where $R = (r \times p)$, can be extended to a linear model (without explicit restrictions)

(23) $y_e = X_e \beta + \varepsilon_e,\ \mathrm{E}(\varepsilon_e) = 0,\ \mathrm{var}(\varepsilon_e) = \sigma^2 W_e$,

with

$$y_e = \begin{pmatrix} y \\ c \end{pmatrix},\ X_e = \begin{pmatrix} X \\ R \end{pmatrix},\ \varepsilon_e = \begin{pmatrix} \varepsilon \\ 0 \end{pmatrix},\ W_e = \left(\begin{array}{c|c} W & 0 \\ \hline 0 & 0 \end{array}\right).$$

The general linear model (23) is obviously equivalent to model (5) with the restrictions $R\beta = c$, and so the least squares estimators can be found by the methods in the above sections.

8. Rank-k approximation

a) A useful inequality

Let $A=(a_{ij})=(m\times n)$ be an arbitrary real matrix and $\sigma_{\max}$ its largest singular value. Then $\max|a_{ij}| \le \sigma_{\max}$ (cf. Rao-Rao, 1998, P 11.2.5, p. 365; the parameter θ has the value 1).

b) Optimal rank-k approximation of a real matrix (see Golub-Van Loan, 1996, p. 72)

Let $A=(a_{ij})=(m\times n)$ be an arbitrary real matrix with $m\ge n$. We want to approximate *A* by a matrix $B=(m\times n)$ with $\text{rk}(B)=k<r=\text{rk}(A)$. Let $A=UDV^{\mathsf{T}}$ be the singular value decomposition of *A* where $D=(m\times n)=\text{diag}(\sigma_1,\ldots,\sigma_n)$ with $\sigma_1\ge\cdots\ge\sigma_r>\sigma_{r+1}=\cdots=\sigma_n=0$. Now let $D_k=(m\times n)=\text{diag}(\sigma_1,\ldots,\sigma_k,0,\ldots,0)$ and $A_k=UD_kV^{\mathsf{T}}$. Then

$$\min_{\text{rk}(B)=k}\|A-B\|=\|A-A_k\|=\sigma_{k+1}$$

where $\|A\|$ denotes the supreme norm (spectral norm) corresponding to the Euclidian vector norm. As the largest singular value of $\Delta=A-A_k=(\delta_{ij})$ is σ_{k+1} we have $\max|\delta_{ij}| \le \sigma_{k+1}$.

So if the rounding errors of a_{ij} are within the range $\pm\varepsilon$ and if there are singular values $<\varepsilon$, then it is sensible to use the rank-k approximation $A_k=(\tilde{a}_{ij})$ of *A* where $\sigma_k\ge\varepsilon>\sigma_{k+1}$ as then $\tilde{a}_{ij}-a_{ij}$ will also be within the range of $\pm\varepsilon$ (for some examples see Knüsel, 2009).

c) Rank-k approximation and the general linear model

We consider again the general linear model (5)

$$y=X\beta+\varepsilon,\ E(\varepsilon)=0,\ \text{var}(\varepsilon)=\sigma^2W,\ X=(n\times p),\ W=(n\times n),\ n>p\,.$$

We assume that the matrices *X* and *W* are found empirically and possess rounding errors. Let us assume that $X_0=(n\times p)$ is a matrix with $\text{rk}(X_0)<p$ and let $X=X_0+\Delta$ where $\Delta=(\delta_{ij})$ is a matrix of small perturbations (rounding errors). Even if $\max|\delta_{ij}|$ is very small *X* will usually have full rank *p*. So if an empirical matrix *X* has full rank our question is to find an approximation X_1 to *X* with a numerically stable rank in the sense that the rank of X_1 cannot be made *smaller* by small perturbations of *X*. The approximation procedure with the general linear model works as follows:

(i) *Rank-k approximation and factorization of W*

In a first step we perform a rank-k approximation W_1 of *W* so that the rank of W_1 becomes numerically stable. Then we perform the factorization of $W_1=F_1F_1^{\mathsf{T}}$.

(ii) *Rank-k approximation of X*

Then we compute the rank-k approximation X_1 of *X*.

(iii) *Rank-k approximation of* $(X_1\,|\,F_1)$

We also need a numerically stable rank of $(X_1\,|\,F_1)$ which is not yet guaranteed by step (i) and (ii). So we determine the rank-k approximation of $(X_1\,|\,F_1)$ and obtain $(X_2\,|\,F_2)$. Although X_2 will differ only little from X_1 one must expect that the numerically stable rank of X_1 goes lost with X_2. But against our expectations this is not true. Our numerous examples (cf. Knüsel, 2009) confirm the following *Conjecture:* If $(X_2\,|\,F_2)$ is a rank-k approximation of $(X_1\,|\,F_1)$ and if $\sigma_1\ge\sigma_2\ge\cdots$ and $\tau_1\ge\tau_2\ge\cdots$ are the singular values of X_1 and X_2, respectively, then $\tau_i\le\sigma_i, i=1,2,\ldots$. If $\sigma_i=0$ then also $\tau_i=0$, and so the rank of X_2 cannot become larger than the rank of X_1. A mathematical proof of this conjecture is not yet known to the author.

9. Example: General linear model with nearly rank deficient *X* and *W*

In this example we consider the general linear model

(24) $y = X\beta + \varepsilon$, where $X = (n \times p)$ and $\varepsilon \sim \left(0, \sigma^2 W\right)$,

and where both matrices *X* and *W* are nearly rank deficient (*X* with weak multicollinearity). Let

$$X_0 = (x_1, x_2, x_3) = (5\times 3) = \sqrt{2}\begin{pmatrix} 3 & 2 & 4 \\ 1 & 9 & -7 \\ 4 & 1 & 7 \\ 7 & 2 & 12 \\ 5 & 6 & 4 \end{pmatrix} \approx \begin{pmatrix} 4.243 & 2.828 & 5.657 \\ 1.414 & 12.728 & -9.899 \\ 5.657 & 1.414 & 9.899 \\ 9.899 & 2.828 & 16.971 \\ 7.071 & 8.485 & 5.657 \end{pmatrix} = X\,.$$

We have $x_3 = 2x_1 - x_2$, i.e. the third column of X_0 is a linear combination of the first two columns, and so the matrix X_0 has rank 2, but the matrix $X\,(=X_0$ rounded to three decimal places) has full rank 3 as all three singular values of *X* are positive (see Table 1). Let

$$F_0 = (5\times 4) = \begin{pmatrix} -7 & -8 & -5 & 9 \\ -8 & -2 & 7 & 6 \\ 0 & -1 & 5 & -1 \\ 7 & -7 & -2 & -8 \\ 4 & -9 & -2 & 0 \end{pmatrix},$$

$$W_0 = (5\times 5) = \frac{\sqrt{3}}{20} F_0 F_0^{\mathsf{T}} \approx \begin{pmatrix} 18.966 & 7.881 & -2.252 & -4.763 & 4.667 \\ * & 13.250 & 2.685 & -9.007 & -2.425 \\ * & * & 2.338 & 0.433 & -0.087 \\ * & * & * & 14.376 & 8.227 \\ * & * & * & * & 8.747 \end{pmatrix} = W\,.$$

$F_0 = (5\times 4)$ has rank 4, and so $W_0 = (5\times 5)$ is a symmetric and positive semidefinite matrix with rank 4. But the matrix $W\,(=W_0$ rounded to three decimal places) has full rank 5 as all five singular values of *W* are positive (see Table 1). In addition *W* has become an indefinite matrix as one of the eigenvalues is negative (see Table 2). So both *X* and *W* are nearly rank deficient. Now we consider the general linear model (24) with $X = (n\times p)$ and $W = (n \times n)$ as given above.

Table 1: Singular values of X_0, X, W_0, W

	$X_0 = (5\times 3)$	$X = (5\times 3)$	$W_0 = (5\times 5)$	$W = (5\times 5)$
Singular values	$\begin{pmatrix} 26.590 \\ 17.117 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 26.590 \\ 17.116 \\ 0.000\,748 \end{pmatrix}$	$\begin{pmatrix} 30.513 \\ 19.825 \\ 6.877 \\ 0.463 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 30.513 \\ 19.825 \\ 6.876 \\ 0.463 \\ 0.000\,644 \end{pmatrix}$

Table 2: Eigenvalues of W_0, W

	$W_0 = (5\times 5)$	$W = (5\times 5)$
Eigenvalues	$\begin{pmatrix} 30.513 \\ 19.825 \\ 6.877 \\ 0.463 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 30.513 \\ 19.825 \\ 6.876 \\ 0.463 \\ -0.000\,644 \end{pmatrix}$

(i) *Rank-k approximation and factorization of W*

The elements of *W* are given with three decimal places and the smallest singular value $\sigma_5 = 0.000\,644$ is about the size of the maximal rounding error. The rank-4-approximation of W will give an approximation $W_1 = (w_{ij}^{(1)})$ of $W = (w_{ij})$ with $rk(W_1) = 4$ and with $\max|w_{ij} - w_{ij}^{(1)}| \le \sigma_5 = 0.000\,644$. The singular value decomposition of *W* is given by $W = UDV^{\mathsf{T}}$ where $U = (5\times5)$ and $V = (5\times5)$ are orthogonal and $D = (5\times5) = \mathrm{diag}(\sigma_1,\ldots,\sigma_5)$; $\sigma_1,\ldots,\sigma_5$ are the singular values of *W*. Now we define W_1 as

(25) $W_1 = UD_1V^{\mathsf{T}}$ $(= UD_1U^{\mathsf{T}})$ where $D_1 = (5\times5) = \mathrm{diag}(\sigma_1,\sigma_2,\sigma_3,\sigma_4,0)$.

Obviously $\mathrm{rk}(W_1) = 4$ and we obtain $\max|w_{ij} - w_{ij}^{(1)}| = 0.000\,427 < \sigma_5 = 0.000\,644$; so $W_1 \approx W$. The rank of W_1 is numerically stable in the sense that it cannot be reduced by small perturbations of the matrix elements $w_{ij}^{(1)}$.

In a second step we factorize W_1 such that $W_1 = F_1F_1^{\mathsf{T}}$ with $F_1 = (5\times4)$. Let

(26) $F_1 = UD_2$ where $D_2 = (5\times4) = \mathrm{diag}\left(\sqrt{\sigma_1},\sqrt{\sigma_2},\sqrt{\sigma_3},\sqrt{\sigma_4}\right)$.

As $D_2D_2^{\mathsf{T}} = \mathrm{diag}(\sigma_1,\ldots,\sigma_4,0) = D_1$ we have $F_1F_1^{\mathsf{T}} = UD_2D_2^{\mathsf{T}}U^{\mathsf{T}} = UD_1U^{\mathsf{T}} = W_1$. So $W_1 = F_1F_1^{\mathsf{T}}$ and W_1 is positive semidefinite as W_0.

(ii) *Rank-k approximation of* $X = (n\times p)$

The elements of *X* are given with three decimal places and the smallest singular value $\sigma_3 = 0.000\,748$ is about the size of the maximal rounding error. The rank-2 approximation of *X* will give an approximation $X_1 = (x_{ij}^{(1)})$ with $\mathrm{rk}(X_1) = 2$ and with $\max|x_{ij} - x_{ij}^{(1)}| \le \sigma_3 = 0.000\,748$. The singular value decomposition of $X = (5\times3)$ is given by $X = UDV^{\mathsf{T}}$ where $U = (5\times5)$ and $V = (3\times3)$ are orthogonal and $D = (5\times3) = \mathrm{diag}(\sigma_1,\sigma_2,\sigma_3)$; $\sigma_1,\sigma_2,\sigma_3$ are the singular values of *X*. Now define X_1 as

(27) $X_1 = UD_1V^{\mathsf{T}}$ where $D_1 = (5\times3) = \mathrm{diag}\left(\sigma_1,\sigma_2,0\right)$.

Obviously $\mathrm{rk}(X_1) = 2$ and we obtain $\max|x_{ij} - x_{ij}^{(1)}| = 0.000\,379 < \sigma_3 = 0.000\,748$; so $X_1 \approx X$. The rank of X_1 is numerically stable in the sense that it cannot be reduced by small perturbations of the matrix elements $x_{ij}^{(1)}$.

(iii) *Rank-k approximation of* $(X_1\,|\,F_1)$

We have $X_1 = (n\times p) = (5\times3)$ and $F_1 = (n\times k) = (5\times4)$ and so $(X_1\,|\,F_1) = (n\times m) = (5\times7)$, where $m = p + k = 7$. The matrices X_1 and F_1 possess numerically stable ranks, but this does not necessarily mean that also the rank of the combined matrix $(X_1\,|\,F_1)$ is numerically stable. It could be that the smallest singular value of $(X_1\,|\,F_1)$ is very small or even zero (see the examples in Knüsel, 2009b). As a rank-k-approximation $(X_2\,|\,F_2)$ of $(X_1\,|\,F_1)$ changes both X_1 and F_1 one must expect that X_2 will again have full rank 3 and will again be nearly rank deficient, and so it would have been in vain to compute the rank-2 approximation X_1 of *X*. But surprisingly this is not true. To demonstrate this in teresting fact we compute the rank-4 approximation of $(X_1 \mid F_1)$. The singular value decomposition of $(X_1 \mid F_1)$ is given by

(28) $(X_1 \mid F_1) = P\Delta Q^{\mathsf{T}}$,

where $P = (5\times 5)$ and $Q = (7\times 7)$ are orthogonal and $\Delta = (5\times 7) = \operatorname{diag}(\sigma_1,\dots,\sigma_5)$.

The singular values of $(X_1 \mid F_1)$ are given in Table 3. Now the rank-4-approximation of $(X_1 \mid F_1)$ is given by

$$(X_2 \mid F_2) = P\Delta_1 Q^{\mathsf{T}}, \text{ where } \Delta_1 = (5\times 7) = \operatorname{diag}(\sigma_1,\dots,\sigma_4,0).$$

We find obtain $\max|x_{ij}^{(2)} - x_{ij}^{(1)}| = 0.014$ and $\max|f_{ij}^{(2)} - f_{ij}^{(1)}| = 0.373 < \sigma_5 = 0.641$, and the singular values of $X_2, F_2, (X_2 \mid F_2)$ are given in Table 4. By comparison of Table 3 and 4 we see that the rank-4 approximation of $(X_1 \mid F_1)$ did not increase any singular values, and in particular the rank of X_2 has not become larger than the rank of X_1. A general proof of this interesting and very useful property of the rank-k approximation is not known to the author, but I could not find any counterexample up to now. As the difference between $(X_1 \mid F_1)$ and $(X_2 \mid F_2)$ is too large as compared with the maximal rounding error of *X* and *W* we will do without the rank-4 approximation $(X_2 \mid F_2)$. Instead of the original linear model (24) we now consider the model

(29) $y = X_1\beta + F_1 u$, where $X_1 = (n\times p)$, F_1=$(n\times k)$ and $u \sim \left(0, \sigma^2 I_k\right)$.

For the error term $\varepsilon = F_1 u$ we have $\mathrm{E}(\varepsilon) = 0$ and $\operatorname{var}(\varepsilon) = \mathrm{E}(\varepsilon\varepsilon^{\mathsf{T}}) = \sigma^2 F_1 F_1^{\mathsf{T}} = \sigma^2 W_1$, and as we have seen above $X_1 \approx X$ and $W_1 \approx W$. So model (29) is an approximation to the original model (24) but now the three matrices X_1, F_1 and $(X_1 \mid F_1)$ possess all numerically stable ranks.

Table 3: Singular values of $X_1, F_1, (X_1 \mid F_1)$

	$X_1 = (5\times 3)$	$F_1 = (5\times 4)$	$(X_1 \mid F_1)$
singular values	$\begin{pmatrix}26.590\\17.116\\0\end{pmatrix}$	$\begin{pmatrix}5.524\\4.453\\2.622\\0.680\end{pmatrix}$	$\begin{pmatrix}26.905\\17.488\\4.355\\2.926\\0.641\end{pmatrix}$

Table 4: Singular values of $X_2, F_2, (X_2 \mid F_2)$

	$X_2 = (5\times 3)$	$F_2 = (5\times 4)$	$(X_2 \mid F_2)$
singular values	$\begin{pmatrix}26.590\\17.116\\0\end{pmatrix}$	$\begin{pmatrix}5.524\\4.452\\2.619\\0.268\end{pmatrix}$	$\begin{pmatrix}26.905\\17.488\\4.355\\2.926\\0\end{pmatrix}$

(iv) *CS-decomposition of Q*

As $r_c = \text{rk}(X_1 \mid F_1) = n = 5$ we have to determine the CS-decomposition of $Q = (m \times m) = (7 \times 7)$ with the format

$$Q = \left(\begin{array}{c|c} Q_{11} & Q_{12} \\ \hline Q_{21} & Q_{22} \end{array}\right) = \left(\begin{array}{c|c} (p \times n) & (p \times (m-n)) \\ \hline (k \times n) & (k \times (m-n)) \end{array}\right) = \left(\begin{array}{c|c} (3 \times 5) & (3 \times 2) \\ \hline (4 \times 5) & (4 \times 2) \end{array}\right).$$

We obtain orthogonal matrices

$$U = (7 \times 7) = \left(\begin{array}{c|c} U_1 & 0 \\ \hline 0 & U_2 \end{array}\right) = \left(\begin{array}{c|c} (3 \times 3) & * \\ \hline * & (4 \times 4) \end{array}\right)$$

$$V = (8 \times 8) = \left(\begin{array}{c|c} V_1 & 0 \\ \hline 0 & V_2 \end{array}\right) = \left(\begin{array}{c|c} (5 \times 5) & * \\ \hline * & (2 \times 2) \end{array}\right)$$

with

$$U_1 = \begin{pmatrix} 0.229 & -0.530 & -0.817 \\ -0.420 & -0.810 & 0.408 \\ 0.878 & -0.250 & 0.408 \end{pmatrix}, \quad U_2 = \begin{pmatrix} -0.008 & 0 & 0 & 1.000 \\ -0.521 & -0.295 & -0.801 & -0.004 \\ 0.826 & 0.064 & -0.561 & 0.006 \\ 0.217 & -0.953 & 0.210 & 0.002 \end{pmatrix}$$

$$V_1 = \begin{pmatrix} 0.800 & -0.587 & -0.032 & -0.076 & 0.095 \\ 0.572 & 0.802 & 0.036 & 0.012 & 0.166 \\ 0.120 & 0.099 & -0.089 & -0.514 & -0.839 \\ -0.136 & 0.015 & -0.248 & -0.814 & 0.507 \\ -0.019 & -0.036 & 0.964 & -0.260 & 0.050 \end{pmatrix}, \quad V_2 = \begin{pmatrix} -0.778 & -0.629 \\ -0.629 & 0.778 \end{pmatrix}$$

such that

$$(30) \quad U^{\mathsf{T}} Q V = D = \left(\begin{array}{c|c} D_{11} & D_{12} \\ \hline D_{21} & D_{22} \end{array}\right) = \left(\begin{array}{c|c} (3 \times 5) & (3 \times 2) \\ \hline (4 \times 5) & (4 \times 2) \end{array}\right)$$

where

$$D = \left(\begin{array}{ccccc|cc} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & c_1 & 0 & 0 & 0 & s_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ \hline 0 & s_1 & 0 & 0 & 0 & -c_1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{array}\right).$$

The diagonal elements c_1 and s_1 are given in Table 2. Note that $c_1^2 + s_1^2 = 1$, and so the matrix D is orthogonal, too. Also note that D_{12} and D_{21} are not classical diagonal matrices as the diagonal starts in the lower right corner and not in the upper left one.

Table 5: Diagonal elements c_1, s_1

i	c_i	s_i
1	0.988 642	0.150 288

(v) *Generalized singular value decomposition and canonical model*

According to (28) and (30) we have

$$(X_1 \mid F_1) = P\Delta Q^{\mathsf{T}} \quad \text{and} \quad Q = UDV^{\mathsf{T}},$$

and from this we find the so-called *generalized singular value decomposition* of the pair X_1, F_1

$$\text{(31)} \quad \begin{aligned} P^{\mathsf{T}} X_1 U_1 &= \Delta_0 V_1 D_{11}^{\mathsf{T}}, \\ P^{\mathsf{T}} F_1 U_2 &= \Delta_0 V_1 D_{21}^{\mathsf{T}}, \end{aligned}$$

where $\Delta_0 = (5\times 5) = \operatorname{diag}(\sigma_1,\ldots,\sigma_5)$ and where $\sigma_1,\ldots,\sigma_5$ are the singular values of $(X_1 \mid F_1)$ as given above in Table 3. Our model can now be written in the canonical form

$$\text{(32)} \quad \tilde{y} = D_1\tilde{\beta} + D_2\tilde{u},$$

where

$$\tilde{y} = M_1 y \quad \text{with} \quad M_1 = V_1^{\mathsf{T}}\Delta_0^{-1}P^{\mathsf{T}}$$

$$\tilde{\beta} = U_1^{\mathsf{T}}\beta,$$

$$\tilde{u} = U_2^{\mathsf{T}}u,$$

$$M_1 = (5\times 5) = \begin{pmatrix} 0.023 & -0.034 & 0.062 & -0.007 & -0.015 \\ 0.002 & -0.055 & 0.011 & -0.056 & 0.005 \\ 0.155 & 0.463 & -0.602 & 0.883 & -0.940 \\ -0.174 & -0.027 & 0.402 & -0.228 & 0.107 \\ -0.164 & -0.017 & -0.165 & 0.119 & 0.068 \end{pmatrix},$$

$$D_1 = D_{11}^{\mathsf{T}} = (5\times 3) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$D_2 = D_{21}^{\mathsf{T}} = (5\times 4) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ s_1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

From (31) we can see that $\operatorname{rk}(X_1) = \operatorname{rk}(D_{11}) = \operatorname{rk}(D_1) = 2$ and $\operatorname{rk}(F_1) = \operatorname{rk}(D_{21}) = \operatorname{rk}(D_2) = 4$. The canonical model (32) explicitly written has the form

$$\text{(33)} \quad \begin{aligned} \tilde{y}_1 &= \tilde{\beta}_1, \\ \tilde{y}_2 &= c_1\tilde{\beta}_2 + s_1\tilde{u}_1, \\ \tilde{y}_3 &= \tilde{u}_2, \\ \tilde{y}_4 &= \tilde{u}_3, \\ \tilde{y}_5 &= \tilde{u}_4. \end{aligned}$$

The observation $\tilde{y}_1$ is identical to the parameter $\tilde{\beta}_1$, this observation has no random error. The parameter $\tilde{\beta}_3$ can have arbitrary values as it does not show up in the canonical model, and we set this parameter to zero (minimum length definition). The least squares estimators are given by

$$\hat{\tilde{\beta}}_1 = \tilde{y}_1,$$

$$\hat{\tilde{\beta}}_2 = \tilde{y}_2 / c_1,$$

$$\hat{\tilde{\beta}}_3 = 0.$$

In matrix notation we can write

$$\hat{\tilde{\beta}} = D_1^+ \tilde{y} \quad \text{as} \quad D_1^+ = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1/c_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\operatorname{var}(\tilde{y}) = \sigma^2 D_2 D_2^\mathsf{T} = \sigma^2 \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & s_1^2 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\operatorname{var}(\hat{\tilde{\beta}}) = D_1^+ \operatorname{var}(\tilde{y})(D_1^+)^\mathsf{T} = \sigma^2 D_1^+ D_2 D_2^\mathsf{T} (D_1^+)^\mathsf{T} = \sigma^2 \begin{pmatrix} 0 & 0 & 0 \\ 0 & s_1^2/c_1^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \sigma^2 D_0 .$$

For the original parameters we obtain

$$\hat{\beta} = U_1 \hat{\tilde{\beta}} = U_1 D_1^+ \tilde{y} = M_2 y$$

where

$$M_2 = U_1 D_1^+ V_1^\mathsf{T} \Delta_0^{-1} P^\mathsf{T} = \begin{pmatrix} 0.00\,423 & 0.02\,198 & 0.00\,803 & 0.02\,832 & -0.00\,587 \\ -0.01\,146 & 0.05\,958 & -0.03\,536 & 0.04\,859 & 0.00\,236 \\ 0.01\,991 & -0.01\,562 & 0.05\,142 & 0.00\,806 & -0.01\,410 \end{pmatrix}$$

and

$$\operatorname{var}(\hat{\beta}) = U_1 \operatorname{var}(\hat{\tilde{\beta}}) U_1^\mathsf{T} = \sigma^2 U_1 D_0 U_1^\mathsf{T} = \sigma^2 \begin{pmatrix} 0.00\,649 & 0.00\,993 & 0.00\,306 \\ * & 0.01\,517 & 0.00\,468 \\ * & * & 0.00\,144 \end{pmatrix}.$$

The unknown variance σ^2 is estimated by

$$\hat{\sigma}^2 = \tfrac{1}{3}(\tilde{y}_3^2 + \tilde{y}_4^2 + \tilde{y}_5^2).$$

Remark

In our example we have $n = 5$, $p = 3$, $r_c = \operatorname{rk}(X_1 \mid F_1) = n = 5$ and

$$\begin{aligned} r_X &= \operatorname{rk}(X_1) = 2 && < p = 3, \\ r_F &= \operatorname{rk}(F_1) = \operatorname{rk}(W_1) = k = 4 && < n = 5, \\ r &= r_X + r_F - r_c = 1 && > 0. \end{aligned}$$

In the canonical model (33) we have three categories of observations:

(a) observations with no random error, that are identical to a parameter ($\tilde{y}_1$ in the example); number of these observations: $r_X - r = n - r_F = n - r_W = 5 - 4 = 1$;

(b) "classical" observations, that depend on the parameters and possess a random error ($\tilde{y}_2$ in the example); number of these observations: $r = 1$;

(c) observations, that do not depend on the parameters and possess a random error ($\tilde{y}_3$, $\tilde{y}_4$, and $\tilde{y}_5$ in the example); number of these observations: $r_F - r = 4 - 1 = 3$.

Furthermore we have three categories of parameters:

(α) parameters, that are completely fixed by the observations ($\tilde{\beta}_1$ in the example); number of these parameters: $r_X - r = 2 - 1 = 1$;

(β) "classical" parameters, that can be estimated with a random error ($\tilde{\beta}_2$ in the example); number of these parameters: $r = 1$;

(γ) parameters that do not show up in the canonical model ($\tilde{\beta}_3$ in the example); these parameters can have arbitrary values and they can be set to zero in order to make all parameters identifiable (minimum length definition); number of these parameters: $p - r_X = 3 - 2 = 1$.

Final remarks

a) If we replace in the general linear model (29) the matrices X_1 and F_1 by X_0 and F_0 (with 15 significant digits) we obtain essentially the same results.

b) The computations in the example are done with Matlab (2008) and Maple (2006). Matlab offers a procedure *gsvd* (generalized singular value decomposition) that includes a subfunction *csd* (CS-decomposition), and this subfunction is used for computing the CS-decomposition of an orthogonal matrix.

10. Conclusion

With the aid of the generalized singular value decomposition the general linear model $y = X\beta + Fu$ can be transformed to a very simple *canonical form*. The canonical form exhibits the basic structure of the linear model, four categories of observations, three categories of parameters and two categories of random errors. For this canonical form the least squares estimators can be found easily and by back-transformation the estimators for the original parameters are found. The basic ideas of this procedure are found in Kourouklis and Paige (1981) and Paige (1985). In Rao-Toutenburg et al. (2008) a unified theory of the general linear model is presented being based on Rao (1971,1972,1973), but the clear structure of the linear model shown by the canonical form is not found there. The general linear model with linear restrictions can be extended to a general linear model without explicit restrictions as shown by Rao (1971), and so this case offers no new problems. The generalized singular value decomposition can be made numerically stable by using the rank-k approximation of Golub-Van Loan (1996).

Appendix: The generalized singular value decomposition

A1 Lemma 2.1 of Paige, 1985, page 272

Let A and B be $(n \times p)$ matrices with $\mathrm{rk}(A) = \mathrm{rk}(B) = p$ and with $\mathfrak{R}_A = \mathfrak{R}_B$ i.e. with identical column spaces. Then there exist two orthogonal matrices U and V and two positive diagonal matrices S and C all four with format $(p \times p)$ such that

$$AUS = BVC \text{ where } S^2 + C^2 = I .$$

So the matrices AU and BV possess parallel columns, i.e. column i of AU is a multiple of column i of BV.

Proof:

As $\mathfrak{R}_A = \mathfrak{R}_B$ there exists a matrix $G = (p \times p)$ such that $A = BG$ i.e. such that $Bg_i = a_i$ where $A = (a_1, \ldots, a_p)$ and $G = (g_1, \ldots, g_p)$. The singular value decomposition of G has the form $G = VDU^\top$, where U and V are orthogonal and D is diagonal with positive diagonal elements. Now we have

$$A = BG = BVDU^\top \text{ or } AU = BVD .$$

We set

$$S^2 = (D^2 + I)^{-1} \text{ and } C = DS ,$$

and obtain from $AU = BVD$

$$AUS = BVDS = BVC$$

where

$$C^2 + S^2 = D^2 S^2 + S^2 = S^2(D^2 + I) = I .$$

A2 CS Decomposition (cf. Paige-Wei, 1994)

If

$$Q = (n \times n) = \left(\begin{array}{c|c} Q_{11} & Q_{12} \\ \hline Q_{21} & Q_{22} \end{array}\right) = \left(\begin{array}{c|c} p \times k & p \times \ell \\ \hline q \times k & q \times \ell \end{array}\right), \; p + q = k + \ell = n$$

is an arbitrary 2×2 partitioning of the orthogonal matrix Q, then there exist two orthogonal matrices

$$U = \left(\begin{array}{c|c} U_1 & 0 \\ \hline 0 & U_2 \end{array}\right) = \left(\begin{array}{c|c} p \times p & p \times q \\ \hline q \times p & q \times q \end{array}\right) \text{ and } V = \left(\begin{array}{c|c} V_1 & 0 \\ \hline 0 & V_2 \end{array}\right) = \left(\begin{array}{c|c} k \times k & k \times \ell \\ \hline \ell \times k & \ell \times \ell \end{array}\right)$$

such that

$$(34) \quad U^\top Q V = \left(\begin{array}{ccc|ccc} I & 0 & 0 & 0 & 0 & 0 \\ 0 & C & 0 & 0 & S & 0 \\ 0 & 0 & 0 & 0 & 0 & I \\ \hline 0 & 0 & 0 & -I & 0 & 0 \\ 0 & S & 0 & 0 & -C & 0 \\ 0 & 0 & I & 0 & 0 & 0 \end{array}\right) = \left(\begin{array}{c|c} p \times k & p \times \ell \\ \hline q \times k & q \times \ell \end{array}\right) = \left(\begin{array}{c|c} D_{11} & D_{12} \\ \hline D_{21} & D_{22} \end{array}\right) = D$$

where

$$C = (r \times r) = \mathrm{diag}(c_1, \ldots, c_r), \; 1 > c_1 \geq \cdots \geq c_r > 0,$$
$$S = (r \times r) = \mathrm{diag}(s_1, \ldots, s_r), \; 0 < s_1 \leq \cdots \leq s_r < 1,$$
$$C^2 + S^2 = I.$$

Note that D_{11} and D_{22} are rectangular diagonal matrices the diagonal starting at the upper left corner whereas D_{12} and D_{21} are rectangular diagonal matrices the diagonal starting at the lower right corner.

Also note that D is again an orthogonal matrix as

$$D^{\mathsf{T}}D=\left(\begin{array}{ccc|ccc} I & 0 & 0 & 0 & 0 & 0 \\ 0 & C^2+S^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & I & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & I & 0 & 0 \\ 0 & 0 & 0 & 0 & C^2+S^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & I \end{array}\right)$$

and $C^2+S^2=I$. As U and V are orthogonal also U_1,U_2,V_1,V_2 must be orthogonal. According to (34) we have $Q=UDV^{\mathsf{T}}$ and from this we derive $Q_{ij}=U_i D_{ij} V_j^{\mathsf{T}}$; this is essentially the singular value decomposition of Q_{ij} ($i,j=1,2$) as the sign and the order of the singular values can be changed by changing the order and sign of the columns of U_i and V_j . The CS-decomposition is also called the cosine-sine-decomposition as $c_i=\cos(\varphi_i)$ and $s_i=\sin(\varphi_i)$, $0<\varphi_i<\pi/2$, $\sin^2(\varphi_i)+\cos^2(\varphi_i)=1$.

A3 Generalized singular value decomposition

Let $X=(n\times p)$, $F=(n\times k)$, and $r_c=rk(X\,|\,F)$. Obviously $r_c\le p+k=m$. Now we consider the singular value decomposition of $(X\,|\,F)$

(35) $(X\,|\,F)=P\Delta Q^{\mathsf{T}}$,

where $P=(n\times n)$ and $Q=(m\times m)$ are orthogonal and

$$\Delta=(n\times m)=\left(\begin{array}{c|c}\Delta_0 & 0 \\ \hline 0 & 0\end{array}\right), \text{ with } \Delta_0=(r_c\times r_c)=\operatorname{diag}(\delta_1,\ldots,\delta_{r_c}),\ \delta_1\ge\cdots\ge\delta_{r_c}>0\,.$$

$\Delta_0=(r_c\times r_c)$ is the reduced form of $\Delta=(m\times n)$; it is square and regular. From (35) we derive

(36) $(X\,|\,F)Q=P\Delta=(P_1\Delta_0\,|\,0)$, where $P=(P_1\,|\,P_2)$ with $P_1=(n\times r_c)$. Now we consider the CS-decomposition of

$$Q=(m\times m)=\left(\begin{array}{c|c} p\times r_c & p\times(m-r_c) \\ \hline k\times r_c & k\times(m-r_c)\end{array}\right)=\left(\begin{array}{c|c} Q_{11} & Q_{12} \\ \hline Q_{21} & Q_{22}\end{array}\right);$$

there exist orthogonal matrices

$$U=(m\times m)=\left(\begin{array}{c|c} U_1 & 0 \\ \hline 0 & U_2\end{array}\right)=\left(\begin{array}{c|c} p\times p & p\times k \\ \hline k\times p & k\times k\end{array}\right)$$

$$V=(m\times m)=\left(\begin{array}{c|c} V_1 & 0 \\ \hline 0 & V_2\end{array}\right)=\left(\begin{array}{c|c} r_c\times r_c & r_c\times(m-r_c) \\ \hline (m-r_c)\times r_c & (m-r_c)\times(m-r_c)\end{array}\right)$$

such that

$$\text{(37)}\quad U^{\mathsf{T}}QV=(m\times m)=\left(\begin{array}{c|c} p\times r_c & p\times(m-r_c) \\ \hline k\times r_c & k\times(m-r_c)\end{array}\right)=\left(\begin{array}{ccc|ccc} I & 0 & 0 & 0 & 0 & 0 \\ 0 & C & 0 & 0 & S & 0 \\ 0 & 0 & 0 & 0 & 0 & I \\ \hline 0 & 0 & 0 & -I & 0 & 0 \\ 0 & S & 0 & 0 & -C & 0 \\ 0 & 0 & I & 0 & 0 & 0 \end{array}\right)=\left(\begin{array}{c|c} D_{11} & D_{12} \\ \hline D_{21} & D_{22}\end{array}\right)=D$$

where

$$C=(r\times r)=\operatorname{diag}(c_1,\ldots,c_r),\ 1>c_1\ge\cdots\ge c_r>0,$$
$$S=(r\times r)=\operatorname{diag}(s_1,\ldots,s_r),\ 0<s_1\le\cdots\le s_r<1,$$
$$c_i^2+s_i^2=1,\ i=1,\ldots,r.$$

From (37) we have

(38) $QV=UD$

where

$$QV = \left(\begin{array}{c|c} Q_{11}V_1 & Q_{12}V_1 \\ \hline Q_{21}V_2 & Q_{22}V_2 \end{array}\right) \quad \text{and} \quad UD = \left(\begin{array}{c|c} U_1D_{11} & U_1D_{12} \\ \hline U_2D_{21} & U_2D_{22} \end{array}\right).$$

From (36) we have

$$(X \mid F)QV = P\Delta V = \left(P_1\Delta_0 V_1 \mid 0\right)$$

and together with (38) we obtain

(39) $(X \mid F)UD = P\Delta V = \left(P_1\Delta_0 V_1 \mid 0\right)$.

Now

$$(X \mid F)UD = (X \mid F)\left(\begin{array}{c|c} U_1D_{11} & U_1D_{12} \\ \hline U_2D_{21} & U_2D_{22} \end{array}\right) = \left(XU_1D_{11} + FU_2D_{21} \mid XU_1D_{12} + FU_2D_{22}\right)$$

and according to (39) we obtain

$$XU_1D_{12} + FU_2D_{22} = 0, \text{ i.e. } XU_1D_{12} = -FU_2D_{22}.$$

Thus we have proved the following result.

Result 1

There exist orthogonal matrices $U\,(=U_1)$ and $V\,(=U_2)$ such that

$$XU\left(\begin{array}{c|cc} 0 & 0 & 0 \\ \hline 0 & S & 0 \\ 0 & 0 & I \end{array}\right) = FV\left(\begin{array}{cc|c} I & 0 & 0 \\ 0 & C & 0 \\ \hline 0 & 0 & 0 \end{array}\right).$$

This is formula (2.5) of Paige (1985) on page 273 (with interchanged *X* and *F*).

From (39) we derive further

(40) $$P^{\mathsf{T}}(X \mid F)U = \Delta V D^{\mathsf{T}} = \left(\begin{array}{c|c} \Delta_0 V_1 & 0 \\ \hline 0 & 0 \end{array}\right)D^{\mathsf{T}} = \left(\begin{array}{c} \Delta_0 V_1 \\ \hline 0 \end{array}\right)\left(D_{11}^{\mathsf{T}} \mid D_{21}^{\mathsf{T}}\right)$$

or

(41) $$P^{\mathsf{T}}XU_1 = \left(\begin{array}{c} \Delta_0 V_1 \\ \hline 0 \end{array}\right)D_{11}^{\mathsf{T}}, \qquad P^{\mathsf{T}}FU_2 = \left(\begin{array}{c} \Delta_0 V_1 \\ \hline 0 \end{array}\right)D_{21}^{\mathsf{T}}.$$

Thus we have proved the following result.

Result 2

There exist orthogonal matrices $P = (n \times n), U_1 = (p \times p), U_2 = (k \times k), V\,(=V_1) = (r_c \times r_c)$ such that

(42) $$P^{\mathsf{T}}XU_1 = \left(\begin{array}{c} \Delta_0 V \\ \hline 0 \end{array}\right)D_1 \qquad P^{\mathsf{T}}FU_2 = \left(\begin{array}{c} \Delta_0 V \\ \hline 0 \end{array}\right)D_2$$

where

$$D_1\,(=D_{11}^{\mathsf{T}}) = (r_c \times p) = \left(\begin{array}{cc|c} I & 0 & 0 \\ 0 & C & 0 \\ \hline 0 & 0 & 0 \end{array}\right), \qquad D_2\,(=D_{21}^{\mathsf{T}}) = (r_c \times k) = \left(\begin{array}{c|cc} 0 & 0 & 0 \\ \hline 0 & S & 0 \\ 0 & 0 & I \end{array}\right),$$

$\Delta_0 = (r_c \times r_c) = \operatorname{diag}(\delta_1, \ldots, \delta_{r_c}),\ \delta_1, \ldots \delta_{r_c}$ the positive singular values of $(X \mid F)$.

(40) corresponds to formula (2.8) of Paige (1985) on page 274 (with interchanged *X* and *F*). The representation (40) or (42) is called the *generalized singular value decomposition* of $(X \mid F)$. Now we summarize our result.

Generalized singular value decomposition

Let $X = (n \times p)$ and $F = (n \times k)$ be real matrices. Then there exist orthogonal matrices $P = (n \times n), U_1 = (p \times p), U_2 = (k \times k), V = (r_c \times r_c)$ such that

$$(43) \quad \begin{aligned} P^{\mathsf{T}} X U_1 &= \begin{pmatrix} \Delta_0 V \\ \hline 0 \end{pmatrix} D_1 \\ P^{\mathsf{T}} F U_2 &= \begin{pmatrix} \Delta_0 V \\ \hline 0 \end{pmatrix} D_2 \end{aligned}$$

where

$$D_1 = (r_c \times p) = \left(\begin{array}{cc|c} I_{r_1} & 0 & 0 \\ 0 & C & 0 \\ \hline 0 & 0 & 0 \end{array}\right). \qquad D_2 = (r_c \times k) = \left(\begin{array}{c|cc} 0 & 0 & 0 \\ \hline 0 & S & 0 \\ 0 & 0 & I_{r_2} \end{array}\right)$$

$\Delta_0 = (r_c \times r_c) = \mathrm{diag}(\delta_1, \ldots, \delta_{r_c}), \delta_1, \ldots \delta_{r_c}$ the positive singular values of $(X \mid F)$, $\delta_1 \geq \cdots \geq \delta_{r_c} > 0$

$C = (r \times r) = \mathrm{diag}(c_1, \ldots, c_r),\ 1 > c_1 \geq \cdots \geq c_r > 0,$

$S = (r \times r) = \mathrm{diag}(s_1, \ldots, s_r),\ 0 < s_1 \leq \cdots \leq s_r < 1,$

$C^2 + S^2 = I,$

and where

$$r_c = \mathrm{rk}(X \mid F),\ r_X = \mathrm{rk}(X),\ r_F = \mathrm{rk}(F),\ r = r_X + r_F - r_c,\ r_1 = r_X - r,\ r_2 = r_F - r\,.$$

So the diagonal matrices D_1 and D_2 have the same rank as *X* and *F*. Note that

$$r_c = \dim(\mathfrak{R}_X \cup \mathfrak{R}_F),\ r = \dim(\mathfrak{R}_X \cap \mathfrak{R}_F),\ r_1 = \dim(\mathfrak{R}_X - \mathfrak{R}_F),\ r_2 = \dim(\mathfrak{R}_F - \mathfrak{R}_X)\,.$$

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