The Use of PSVD and QSVD in Psychometrics[1]

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1. Introduction

Many multivariate analysis (MVA) techniques often used in psychometrics are based on singular value decomposition (SVD) of a certain matrix. In principal component analysis (PCA), for example, we obtain SVD of a data matrix, $\mathbf{Z}$, while in canonical correlation analysis (CANO) we obtain SVD of $\mathbf{P}_G\mathbf{P}_H$, where $\mathbf{P}_G$ and $\mathbf{P}_H$ are orthogonal projectors defined by two sets of variables, $\mathbf{G}$ and $\mathbf{H}$, respectively. Quite often, however, a matrix whose SVD we are to obtain is defined as a product (e.g., $\mathbf{AB}$) and/or a "quotient" (e.g., $\mathbf{AB}^-$, the product of $\mathbf{A}$ and $\mathbf{B}^-$, which is roughly analogous to the "quotient" of two numbers) of two or more matrices. For example, Takane & Koene (1997) have proposed a regularization technique for multi-layered back-propagation networks which involves SVD of $\mathbf{ZW}$, where $\mathbf{Z}$ is a matrix of input data, and $\mathbf{W}$ is a matrix of weights representing the strengths of connections between input neurons and output neurons. As another example, consider matrix $\mathbf{P}_G\mathbf{P}_H$ above. This matrix can be viewed as the product of six matrices, $\mathbf{G}$, $(\mathbf{G}'\mathbf{G})^-$, $\mathbf{G}'$, $\mathbf{H}$, $(\mathbf{H}'\mathbf{H})^-$, and $\mathbf{H}'$, which in turn can be viewed as the product of four matrices, $(\mathbf{G}_l^-)'$, $\mathbf{G}'$, $\mathbf{H}$ and $\mathbf{H}_l^-$, where $\mathbf{X}_l^-$ is a least squares g-inverse of $\mathbf{X}$. (Note that $\mathbf{G}_{lr}^- = (\mathbf{G}'\mathbf{G})^-\mathbf{G}'$, but $\mathbf{G}\mathbf{G}_{lr}^- = \mathbf{G}\mathbf{G}_l^-$, where $\mathbf{G}_{lr}^-$ is a least-squares reflexive inverse of $\mathbf{G}$. The same for $\mathbf{H}$.) In such cases, numerically more stable results can be obtained by applying the product SVD (PSVD; Fernando & Hammarling, 1988), the quotient SVD (QSVD; Van Loan, 1976), or combinations of them (De Moor, 1991), rather than forming a product first and then applying the ordinary SVD to the product. In this paper, we show how we can effectively use these new kinds of SVD in representative methods of multivariate analysis.

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2. PSVD

Let $\mathbf{A}$ $(m \times n)$ and $\mathbf{B}$ $(p \times n)$ be two matrices, and let $r = \text{rank}(\mathbf{A}) - \text{rank}(\mathbf{AB}')$, $t = \text{rank}(\mathbf{B}) - \text{rank}(\mathbf{AB}')$, $s = \text{rank}(\mathbf{AB}')$, and $k = s + r + t$. Then, the following pair of decompositions,

$$\mathbf{A} = \mathbf{UDX}^{-1}, \quad \text{and} \quad \mathbf{B}' = \mathbf{XJV}', \tag{1}$$

is called PSVD of the matrix pair, $\mathbf{A}$ and $\mathbf{B}'$, where $\mathbf{U}$ and $\mathbf{V}$ are orthogonal matrices of order m and p, respectively, $\mathbf{X}$ is a square nonsingular matrix of order n, and $\mathbf{D}$ and $\mathbf{J}$ are such that

$$\mathbf{D} = \begin{bmatrix} {}_s\mathbf{S}_s & {}_s\mathbf{0}_r & {}_s\mathbf{0}_t & {}_s\mathbf{0}_{n-k} \\ {}_r\mathbf{0}_s & {}_r\mathbf{I}_r & {}_r\mathbf{0}_t & {}_r\mathbf{0}_{n-k} \\ {}_q\mathbf{0}_s & {}_q\mathbf{0}_r & {}_q\mathbf{0}_t & {}_q\mathbf{0}_{n-k} \end{bmatrix}, \quad \text{and} \quad \mathbf{J} = \begin{bmatrix} {}_s\mathbf{I}_s & {}_s\mathbf{0}_t & {}_s\mathbf{0}_j \\ {}_r\mathbf{0}_s & {}_r\mathbf{0}_t & {}_r\mathbf{0}_j \\ {}_t\mathbf{0}_s & {}_t\mathbf{I}_t & {}_t\mathbf{0}_j \\ {}_{n-k}\mathbf{0}_s & {}_{n-k}\mathbf{0}_t & {}_{n-k}\mathbf{0}_j \end{bmatrix},$$

where $\mathbf{S}$ is a *pd* diagonal matrix, and $q = m-(s+r)$ and $j = p-(s+t)$. SVD($\mathbf{AB}'$) follows from $\mathbf{AB}' = \mathbf{U}(\mathbf{DJ})\mathbf{V}'$, where $\mathbf{DJ} = \text{diag}(\mathbf{S}, \mathbf{0}, \mathbf{0})$. $\mathbf{S}$ contains nonzero singular values of $\mathbf{AB}'$ in its diagonal.

PSVD of matrix pair $(\mathbf{A}, \mathbf{B}')$ is denoted as PSVD$(\mathbf{A}, \mathbf{B}')$. The PSVD can easily be generalized to more than two matrices.

3. QSVD

Let $\mathbf{A}$ and $\mathbf{B}$ be as defined in the previous section. Let $s = \dim(\text{Sp}(\mathbf{A}') \cap \text{Sp}(\mathbf{B}')) = \text{rank}(\mathbf{A}) + \text{rank}(\mathbf{B}) - k$, $r = k - \text{rank}(\mathbf{B})$, and $t = k - \text{rank}(\mathbf{A})$, where $k = \text{rank}\begin{pmatrix} \mathbf{A} \\ \mathbf{B} \end{pmatrix} = s + r + t = \dim(\text{Sp}(\mathbf{A}') \cup \text{Sp}(\mathbf{B}'))$. Then, the following pair of decompositions,

$$\mathbf{A} = \mathbf{UDX}^{-1}, \quad \text{and} \quad \mathbf{B} = \mathbf{VJX}^{-1}, \tag{2}$$

is called QSVD of the matrix pair, $\mathbf{A}$ and $\mathbf{B}$, where $\mathbf{U}$, $\mathbf{V}$ and $\mathbf{X}$ are the same as defind in the previous section, and $\mathbf{D}$ and $\mathbf{J}$ are such that

$$\mathbf{D} = \begin{bmatrix} {}_s\mathbf{T}_s & {}_s\mathbf{0}_r & {}_s\mathbf{0}_t & {}_s\mathbf{0}_{n-k} \\ {}_r\mathbf{0}_s & {}_r\mathbf{I}_r & {}_r\mathbf{0}_t & {}_r\mathbf{0}_{n-k} \\ {}_q\mathbf{0}_s & {}_q\mathbf{0}_r & {}_q\mathbf{0}_t & {}_q\mathbf{0}_{n-k} \end{bmatrix}, \quad \text{and} \quad \mathbf{J} = \begin{bmatrix} {}_s\mathbf{I}_s & {}_s\mathbf{0}_r & {}_s\mathbf{0}_t & {}_s\mathbf{0}_{n-k} \\ {}_t\mathbf{0}_s & {}_t\mathbf{0}_r & {}_t\mathbf{I}_t & {}_t\mathbf{0}_{n-k} \\ {}_j\mathbf{0}_s & {}_j\mathbf{0}_r & {}_j\mathbf{0}_t & {}_j\mathbf{0}_{n-k} \end{bmatrix},$$

where $\mathbf{T}$ is a *pd* diagonal matrix, and $q = m - (s + r)$ and $j = p - (s + t)$. QSVD of matrix pair $(\mathbf{A}, \mathbf{B})$ is denoted as QSVD$(\mathbf{A}, \mathbf{B})$.

Just as SVD($\mathbf{A}$) is the SVD counterpart of the eigenvalue-vector decomposition of $\mathbf{A}'\mathbf{A}$, SVD($\mathbf{AB}^{-}_{N/A'A}$) is the SVD counterpart of the generalized eigenvalue-vector decomposition of $\mathbf{A}'\mathbf{A}$ with respect to $\mathbf{B}'\mathbf{B}$. Here, $\mathbf{B}^-_{N/A'A} = \mathbf{Q}_{N/A'A}\mathbf{B}^-_l$, where $\mathbf{Q}_{N/A'A} = \mathbf{I} - \mathbf{N}(\mathbf{N}'\mathbf{A}'\mathbf{A}\mathbf{N})^-\mathbf{N}'\mathbf{A}'\mathbf{A}$ and $\mathbf{N}$ is such that $\mathrm{Ker}(\mathbf{B}) = \mathrm{Sp}(\mathbf{N})$, satisfies

1. $\mathbf{B}\mathbf{B}^-_{N/A'A}\mathbf{B} = \mathbf{B}$.

2. $(\mathbf{B}\mathbf{B}^-_{N/A'A})' = \mathbf{B}\mathbf{B}^-_{N/A'A}$.

3. $(\mathbf{A}'\mathbf{A}\mathbf{B}^-_{N/A'A}\mathbf{B})' = \mathbf{A}'\mathbf{A}\mathbf{B}^-_{N/A'A}\mathbf{B}$.

SVD$(\mathbf{A}\mathbf{B}^-_{N/A'A})$ can be derived from QSVD$(\mathbf{A},\mathbf{B})$ by

$$\begin{aligned}\mathbf{A}\mathbf{B}^-_{N/A'A} &= \mathbf{A}\mathbf{Q}_{N/A'A}\mathbf{B}^-_l \\ &= \mathbf{U}\mathbf{D}\mathbf{X}^{-1}\mathbf{Q}_{N/A'A}\mathbf{X}\mathbf{J}^-_l\mathbf{V}' \\ &= \mathbf{U}\mathbf{D}\mathbf{Q}_{N^*/D'D}\mathbf{J}^-_l\mathbf{V}' \\ &= \mathbf{U}(\mathbf{D}\mathbf{J}^-_{N^*/D'D})\mathbf{V}', \end{aligned} \tag{3}$$

where $\mathbf{N}^* = \mathbf{X}^{-1}\mathbf{N}$ and $\mathbf{J}^-_{N^*/D'D} = \mathbf{Q}_{N^*/D'D}\mathbf{J}^-_l$. The latter has a property similar to that of $\mathbf{B}^-_{N/A'A}$ mentioned above. Note that $\mathbf{A}'\mathbf{A} = (\mathbf{X}^{-1})'\mathbf{D}'\mathbf{D}\mathbf{X}^{-1}$, and $\mathbf{Q}_{N/A'A} = \mathbf{I} - \mathbf{X}\mathbf{N}^*(\mathbf{N}^{*\prime}\mathbf{D}'\mathbf{D}\mathbf{N}^*)^-\mathbf{N}^{*\prime}\mathbf{D}'\mathbf{D}\mathbf{X}^{-1}$. Note also that

$$\mathbf{J}^-_l = \begin{bmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{Z}_1 & \mathbf{Z}_2 & \mathbf{Z}_3 \\ \mathbf{0} & \mathbf{I} & \mathbf{0} \\ \mathbf{E}_1 & \mathbf{E}_2 & \mathbf{E}_3 \end{bmatrix}, \quad \text{but} \quad \mathbf{J}^-_{N^*/D'D} = \begin{bmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} & \mathbf{0} \\ \mathbf{E}^*_1 & \mathbf{E}^*_2 & \mathbf{E}^*_3 \end{bmatrix},$$

where $\mathbf{Z}_i$'s and $\mathbf{E}_i$'s are arbitrary.

$\mathbf{D}\mathbf{J}^-_{N^*/D'D} = \mathrm{diag}(\mathbf{T},\mathbf{0},\mathbf{0})$, where $\mathbf{T}$ contains nonzero finite singular values of $\mathbf{A}$ with respect to $\mathbf{B}$ in its diagonal. (All improper (infinite and indeterminate) singular values of $\mathbf{A}$ with respect to $\mathbf{B}$ become 0 in SVD$(\mathbf{A}\mathbf{B}^-_{N/A'A})$.)

QSVD has been generalized to apply to three matrices, $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$, simultaneously, which obtains SVD$((\mathbf{C}^-_{M/AA'})'\mathbf{A}\mathbf{B}^-_{N/A'A})$, where $\mathbf{M}$ is such that $\mathrm{Ker}(\mathbf{C}) = \mathrm{Sp}(\mathbf{M})$. This is called restricted SVD (RSVD; Zha, 1991; De Moor & Golub, 1991).

4. Applications

How can we effectively use PSVD and QSVD (RSVD) in representative methods of MVA? Let us take constrained PCA (CPCA; Takane & Shibayama, 1991) as an example. CPCA of data matrix $\mathbf{Z}$ with two external constraint matrices, $\mathbf{G}$ and $\mathbf{H}$, and two metric matrices, $\mathbf{K}$ and $\mathbf{L}$, is denoted by CPCA$(\mathbf{Z},\mathbf{G},\mathbf{H})_{K,L}$. This method subsumes a number of existing MVA techniques as special cases, so that discussing the use of PSVD and QSVD in this context entails their relationships to a host of other techniques. For example, canonical correlation analysis (CANO) between $\mathbf{G}$ and $\mathbf{H}$ follows from CPCA when $\mathbf{Z} = \mathbf{I}$, $\mathbf{K} = \mathbf{I}$ and $\mathbf{L} = \mathbf{I}$, while constrained CANO (CANOLC; Yanai & Takane, 1992) between $\mathbf{X}$ and $\mathbf{Y}$ with constraints $\mathbf{G}$ and $\mathbf{H}$ by setting $\mathbf{Z} = \mathbf{X}'\mathbf{Y}$, $\mathbf{K} = \mathbf{I}$ and $\mathbf{L} = \mathbf{I}$.

For simplicity, we temporarily assume that $\mathbf{K} = \mathbf{I}$ and $\mathbf{L} = \mathbf{I}$. Then, CPCA amounts to SVD($\mathbf{P}_G\mathbf{Z}\mathbf{P}_H$). One way to obtain this is via PSVD($\mathbf{G}, (\mathbf{G}'\mathbf{G})^-, \mathbf{G}', \mathbf{Z}, \mathbf{H}, (\mathbf{H}'\mathbf{H})^-, \mathbf{H}'$). A little more elegant way is via RSVD($\mathbf{G}'\mathbf{Z}\mathbf{H}, \mathbf{G}, \mathbf{H}$). Note that in this case both $\mathbf{Q}_{N/A'A} = \mathbf{I}$ and $\mathbf{Q}_{M/AA'} = \mathbf{I}$, so that $\mathbf{H}^-_{N/H'Z'GG'ZH} = \mathbf{H}^-_l$ and $\mathbf{G}^-_{M/G'ZHH'Z'G} = \mathbf{G}^-_l$. This is equivalent to PSVD($(\mathbf{G}^-_l)', \mathbf{G}', \mathbf{Z}, \mathbf{H}, \mathbf{H}^-_l$). Perhaps the most elegent way is to combine PSVD and RSVD into RSVD(PSVD($\mathbf{G}', \mathbf{Z}, \mathbf{H}$), $\mathbf{G}', \mathbf{H}$), which De Moor (1991) calls QPPQ-SVD.

With non-identity metric matrices, $\mathbf{K}$ and $\mathbf{L}$, let $\mathbf{R}_K$ and $\mathbf{R}_L$ be square-root factors of $\mathbf{K}$ and $\mathbf{L}$. We then obtain RSVD(PSVD($\mathbf{G}', \mathbf{K}, \mathbf{Z}, \mathbf{L}, \mathbf{H}$), PSVD($\mathbf{R}'_K, \mathbf{G}$), PSVD($\mathbf{R}'_L, \mathbf{H}$)).

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SUMMARY

Many multivariate analysis techniques are based on singular value decomposition (SVD) of a matrix product or quotient. This paper discussed basic properties of the product SVD (PSVD) and the quotient SVD (QSVD) that obtain SVD of a matrix product and a matrix quotient, respectively, without explicitly forming them. It was shown how they could effectively be used in representative MVA techniques such as constrained PCA (CPCA).