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Singular Value Decomposition for Multidimensional Matrices

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Abstract
Singular Value Decomposition (SVD) is of great significance in theory development of mathematics and statistics. In this paper we propose the SVD for 3-dimensional (3-D) matrices and extend it to the general Multidimensional Matrices (MM). We use the basic operations associated with MM introduced by Solo to define some additional aspects of MM. We achieve SVD for 3-D matrix through these MM operations. The proposed SVD has similar characterizations as for 2-D matrices. Further we summarize various characterizations of singular values obtained through the SVD of MM. We demonstrate our results with an example and compare them with the existing method. We also develop Matlab functions to perform SVD of MM and some related MM operations.
Keywords: Multidimensional Matrices, Multidimensional Matrix Algebra, Singular Value Decomposition.

I. Introduction

Solo introduces a new branch of mathematics called Multidimensional Matrix (MM) mathematics and its new subsets, MM algebra and MM calculus in series of papers Solo (2010 A-F). Solo (2010 A) introduces MM terminology, notations, representation etc. MM equality as well as the MM algebra operations like addition, subtraction, multiplication by a scalar and multiplication of two MM are defined by Solo (2010 B). Solo (2010 C) defines the multidimensional null matrix, identity matrix and other MM algebra operations for outer and inner products. MM algebra operations such as transpose, determinant, inverse, symmetry and anti-symmetry are defined by Solo (2010 D). Solo (2010 E) describes the commutative, associative and distributive laws of MM algebra. Dealing with system of linear equations through MM and solution of it has been discussed by Solo (2010 F).

The basic concept of the General Multidimensional Matrix and General Operation of Matrices is developed by Claude (2013). Claude refers an elementary matrix as the smallest matrix that has 1 or 2 dimensions (rows and columns which is similar to the traditional matrix) and defines the general MM that combines many elementary matrices into a single matrix which contains the same properties of all other combined matrices. The definition of MM by Claude is more general in the sense that each dimension of the MM is independent from other dimensions. Thus if the first elementary matrix has m_1 rows and n_1 columns then the second elementary matrix can have another number of rows and columns and the same is for other dimensions of the MM. According to Claude his concept of MM is more generalized than that introduced by Solo (2010).

Now we briefly review the literature on various generalizations of concept of SVD. Loan (1976) introduces two generalizations of singular value decomposition (SVD) by producing two matrix decompositions for a 2-D matrix. Paige and Saunders (1981) gave a constructive derivation of the generalized SVD of any two matrices having the same number of columns. An interesting survey on SVD is given by Stewart (1993). Mastorakis (1996) extends the method of SVD to multidimensional arrays by using indirect method. We discuss method by Mastorakis (1996) in detail in section 3. Leibovici (1998) establishes SVD of k-way array by employing tensorial approach. Lathauwer et al (2000) propose a multilinear generalization of the SVD based on unfolding the higher order tensor into 2-D matrix. This generalization of SVD is referred as higher order SVD (HOSVD) and is achieved through the concept of n-mode product of tensor by a matrix. Okuma et al (2009) compared third-order orthogonal tensor product expansion to HOSVD in terms of accuracy of calculation and computing time of resolution. Okuma et al (2010) propose improved algorithm for calculation of the third-order tensor product expansion by using SVD. The improvement in the method is in the sense of smaller residual as compared to their previous method.

In this paper we propose SVD of MM by using MM operations. For this we adopt the definition of MM and basic operations (addition, multiplication, transpose, inverse) on the MM as introduced by Solo (2010) and propose definition of multidimensional unitary matrix. In short the paper is organized as follows. In Section 2, we briefly review some basic MM operations given by Solo (2010) and introduce some more concepts for MM. In Section 3 we discuss the method of SVD of MM given by Mastorakis (1996), Lathauwer et al (2000) and propose our method of SVD based on MM operations. Various characterizations of singular values of MM are stated in Section 4. In Section 5 we demonstrate our method with the numerical example and compare with the existing methods. Finally in Section 6 we conclude our results.

II. Notations and basic operations on MM

Let A be d-dimensional matrix and the number of elements in the k^{th} dimension be m_k, $k = 1,2,\dots,d$, then the MM A is said to be of order $m_1 \times m_2 \times \dots \times m_d$. Let $a_{i_1 i_2 \dots i_d}$ be the $(i_1, i_2, \dots, i_d)^{th}$ element of the d-dimensional matrix A.

For simplicity of the development of results, we deal with 3-D matrices. A 3-D matrix A of order $m_1 \times m_2 \times m_3$ is an array of $m_1 m_2 m_3$ scalars arranged in m_1 rows, m_2 columns and m_3 layers. A 3-D matrix of dimension $m_1 \times m_2 \times m_3$ thus consists of 2-D matrices of dimension $m_1 \times m_2$ arranged in an array of size m_3. Thus A can be represented in the form of an array of matrices $A(:,:,i_3)$ of dimension $m_1 \times m_2$ and the elements of $A(:,:,i_3)$ are as follows.

$$A(:,:,i_3) = \begin{bmatrix} a_{11i_3} & a_{12i_3} & \cdots & a_{1m_2i_3} \\ a_{21i_3} & a_{22i_3} & \cdots & a_{2m_2i_3} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m_11i_3} & a_{m_12i_3} & \cdots & a_{m_1m_2i_3} \end{bmatrix}, i_3 = 1,2,\dots,m_3.$$

We describe the matrix A completely as $A = \left(\left(a_{i_1 i_2 i_3}\right)\right)$, with $i_j = 1,2,\dots,m_j$ and $j = 1,2,3$. Now we introduce some basic operations on MM.

Definition 2.1 If $A = \left(\left(a_{i_1 i_2 i_3}\right)\right)$ and $B = \left(\left(b_{i_1 i_2 i_3}\right)\right)$ are $m_1 \times m_2 \times m_3$ matrices then

i) αA is the $m_1 \times m_2 \times m_3$ matrix $\left(\left(\alpha a_{i_1 i_2 i_3}\right)\right)$,

ii) $A \pm B$ is the $m_1 \times m_2 \times m_3$ matrix $\left(\left(a_{i_1 i_2 i_3} \pm b_{i_1 i_2 i_3}\right)\right)$.

Definition 2.2 Let $A = \left(\left(a_{i_1 i_2 i_3}\right)\right)$ and $B = \left(\left(b_{i_1 i_2 i_3}\right)\right)$ be the 3-D matrices of dimension $m_1 \times m_2 \times m_3$ and $n_1 \times n_2 \times n_3$ respectively. Then multiplication of A and B is defined only if $m_2 = n_1$ and $m_3 = n_3$ and $C = AB$ is of dimension $m_1 \times n_2 \times n_3$. The elements of C matrix are given by,
$c_{i_1 i_2 i_3} = \sum_{l=1}^{m_2} a_{i_1 l i_3} b_{l i_2 i_3}$, $i_1 = 1,2,\dots,m_1$, $i_j = 1,2,\dots,n_j$, $j = 2,3$

The multiplication defined in the Definition 2.2 satisfies associative property (Solo (2010 E)). Note that, this multiplication is with respect to the third dimension and in this multiplication the first and second dimension of the MM are being multiplied. Solo (2010 B) defines multiplication of MM with respect to different dimensions. But multiplication defined with reference to other than first and second dimensions do not satisfy the associative property (Solo (2010 E)).

Definition 2.3 The matrix A of dimension $m_1 \times m_2 \times m_3$ is said to be square with respect to its first two dimensions if $m_1 = m_2$.

Definition 2.4 A square matrix A of dimension $m \times m \times m_3$ is an identity matrix if, for $i_3 = 1,2,\dots,m_3$,

$$a_{i_1 i_2 i_3} = \begin{cases} 1 & if\ i_1 = i_2, i_1, i_2 = 1,2,\dots,m \\ 0 & otherwise \end{cases}.$$

In general we denote the identity matrix of dimension $m \times m \times m_3 \times \dots \times m_d$ by $I_m^{(m_3 \times m_4 \times \dots \times m_d)}$, while the usual 2-D identity matrix of dimension $m \times m$ is denoted by I_m.

Definition 2.5 For the matrix A of dimension $m_1 \times m_2 \times m_3$, its transpose with respect to its first and second dimension is denoted by $A^T = B$(say) and is of dimension $m_2 \times m_1 \times m_3$ such that,
$b_{i_1 i_2 i_3} = a_{i_2 i_1 i_3}$, for $i_1 = 1,2,\dots,m_2, i_2 = 1,2,\dots,m_1, i_3 = 1,2,\dots,m_3$.

Definition 2.6 A square matrix A of dimension $m \times m \times m_3$ is said to be symmetric if $A^T = A$. That is, for $i_3 = 1,2,\dots,m_3$,

$$a_{i_1 i_2 i_3} = a_{i_2 i_1 i_3}, \quad i_1, i_2 = 1,2,\dots,m.$$

Solo (2010 B, D) defines transpose of MM with respect to different pairs of dimensions and prove various laws based on the proposed definition of transpose of MM.

Definition 2.7 For matrix A of dimension $m_1 \times m_2 \times m_3$, rank of A with respect to the third dimension is a m_3-dimensional vector of ranks of $A(:,:,i_3), i_3 = 1,3,\dots,m_3$. That is,

$$\rho(A) = [\rho_1 \quad \rho_2 \quad \cdots \quad \rho_{m_3}],$$

where $\rho_{i_3} = \rho\left(A(:,:,i_3)\right)$, $i_3 = 1,2,\dots,m_3$.

Along with the basic operations for MM, the other important concepts such as determinant, inverse of MM, commutative, associative, distributive laws of MM algebra, solution of system of linear equations with MM etc are also studied by Solo (2010 A-F).

We now introduce the concept of complex conjugate of MM, unitary matrices, orthogonal matrices and trace.

Definition 2.8 A square matrix $A^* = \left(\left(a^*_{i_1 i_2 i_3}\right)\right)$ of dimension $m_2 \times m_1 \times m_3$ is said to be complex conjugate of 3-D matrix A of dimension $m_1 \times m_2 \times m_3$ if, for $i_3 = 1,2,\dots,m_3$,

$$a^*_{i_1 i_2 i_3} = \bar{a}_{i_2 i_1 i_3}, \quad i_1 = 1,2,\dots,m_2, i_2 = 1,2,\dots,m_1,$$

where $\bar{z}$ is the complex conjugate of z. (Briefly complex conjugate A^* of A is $\overline{A}^T$ as in case of 2-D matrices)

Definition 2.9 A square matrix A of dimension $m \times m \times m_3$ is said to be unitary if,

$$AA^* = A^*A = I_m^{(m_3)}.$$

Particularly if A is a real matrix then the unitary matrix reduces to orthogonal matrix which has a property $AA^T = A^TA = I_m^{(m_3)}$.

Definition 2.10 For a square matrix A of dimension $m \times m \times m_3$, trace of A with respect to its third dimension is defined as,

$$trace(A) = \sum_{i_3=1}^{m_3} \sum_{i=1}^{m} a_{iii_3}.$$

Now with all the above notations and definitions, we proceed to develop SVD for 3-D matrix in the next section. The proposed theory can be easily extended to MM.

III. SVD for 3-dimensional matrix

A SVD of a $m_1 \times m_2$ matrix $B = \left(\left(b_{i_1 i_2}\right)\right)$ with rank r is a representation of B in the form,

$$B = U\Sigma V^T$$

where U and V are unitary matrices $\left(i.e. UU^* = I_{m_1}, VV^* = I_{m_2}\right)$ and Σ is a rectangular diagonal matrix of dimension $m_1 \times m_2$ with non-negative real numbers $\sigma_1, \sigma_2, \dots, \sigma_r$ on its diagonal which are known as singular values of A. We denote sum of squared singular values of B by $SS(B)$. That is $SS(B) = \sum_{s=1}^{r} \sigma_s^2$. The singular values of matrix have many interesting properties. Some of the properties are as follows.

i) $SS(B) = trace(B^T B)$

ii) $SS(B) = \sum_{i_1=1}^{m_1} \sum_{i_2=1}^{m_2} b_{i_1 i_2}^2$

iii) If B is partitioned (along each of its dimensions) in pq sub-matrices B_{ij} of dimension $p_i \times q_j$, $i = 1,2, \dots, p, j = 1,2, \dots, q$ (with $\sum_{i=1}^{p} p_i = m_1, \sum_{j=1}^{q} q_j = m_2$), then

$$\sum_{i=1}^{p} \sum_{j=1}^{q} SS(B_{ij}) = SS(B).$$

iv) Frobenius matrix norm $\|B\|$ is defined as,

$$\|B\| = \sqrt{\sum_{i_1=1}^{m_1} \sum_{i_2=1}^{m_2} b_{i_1 i_2}^2}.$$

v) If B_1 and B_2 are the matrices of same dimension, then the mapping $< B_1, B_2 >= trace(B_2^* B_1)$ forms an inner product on $\mathbb{C}^{m_1 \times m_2}$.

vi) The mapping $\|.\|: \mathbb{C}^{m \times m} \to \mathbb{R}$ defined as $\|B\| = \sqrt{\sum_{i_1, i_2=1}^{m} \left|b_{i_1 i_2}\right|^2}$ forms a norm on the vector space of all complex $m \times m$ matrices.

Extending the theory of usual 2-D matrices to MM is not an easy task. Solo (2010 A-E) has dealt with this problem. Mastorakis (1996) extends the method of SVD to MM. We summarize the method given by Mastorakis (1996) in the form of an algorithm in the following.

3.1 Review of SVD for MM proposed by Mastorakis (1996)

Mastorakis (1996) propose the SVD of MM by indirect method. Mastorakis transforms the 3-D array to 2-D array by unifying the two dimensions into one and apply SVD to it. Finally reforming the manipulated matrix, SVD for 3-D array is achieved. Thus SVD for MM is achieved indirectly through SVD of 2-D matrices. A systematic algorithm of SVD of 3-D matrix (by unifying second and third dimension) given by Mastorakis (1996) is as follows.

a) From 3-D matrix $A = \left(\left(a_{i_1 i_2 i_3}\right)\right)$ of dimension $m_1 \times m_2 \times m_3$, obtain a new equivalent 2-D matrix $B = \left(\left(b_{ij}\right)\right)$ of dimension $m_1 \times m_2 m_3$ by the following coordinate transformation. For $i = 1,2, \dots, m_1$ and $j = 1,2, \dots, m_2 m_3$,

$$b_{ij} = a_{i_1 i_2 i_3}, \text{ if } i = i_1 \text{ and } j = (i_2 - 1)m_3 + i_3.$$

(3.1)

where $i_k = 1,2, \dots, m_k, k = 1,2,3$. The inverse coordinate transformation required for the reconstruction of A from B is,

$a_{i_1 i_2 i_3} = b_{ij}$, if $i_1 = i, i_2 = j \; div \; m_3$ and $i_3 = j - \left((j \; div \; m_3) - 1\right)m_3$. (3.2)

Here $i \; div \; j$ denotes the quotient of the division of the integer i by integer j where $i = 1,2, \dots, m_1, j = 1,2, \dots, m_2 m_3$.

b) Obtain SVD of $m_1 \times m_2 m_3$ matrix B as follows.

$$B = U_B \Sigma_B V_B^T \quad (3.3)$$

where U_B (of dimension $m_1 \times m_1$) and V_B (of dimension $m_2 m_3 \times m_2 m_3$) are unitary matrices and Σ_B is a rectangular diagonal matrix of dimension $m_1 \times m_2 m_3$ with non-negative real numbers $\sigma_{1B}, \sigma_{2B}, \dots, \sigma_{r_B B}$ on its diagonal. Let $\underline{u}_{sB}$ and $\underline{v}_{sB}$ be the s^{th} column of U_B and V_B respectively, for $s = 1,2, \dots, r_B$.

c) Apply the inverse transformation in (3.2) to the s^{th} column of V_B (of length $m_2 m_3$) to get B^{sB} matrix of order $m_2 \times m_3$ for $s = 1,2, \dots, r_B$. Thus we have $B^{1B}, B^{2B}, \dots, B^{sB}$ matrices obtained from first r_B columns of V_B.

d) For $s = 1,2, \dots, r_B$ obtain SVD of B^{sB} as follows.

$$B^{sB} = V^{sB} \Sigma^{sB} (W^{sB})^T \quad (3.4)$$

Here Σ^{sB} is rectangular diagonal matrix of dimension $m_2 \times m_3$ with non-negative real numbers $\sigma_{s1}, \sigma_{s2}, \dots, \sigma_{s\tau_s}$ on its diagonal, $\underline{v}_{sj}$ and $\underline{w}_{sj}$ are the j^{th} columns of V^{sB} and W^{sB} respectively for $j = 1,2,\dots,\tau_s$.

e) SVD of A is achieved through the following representation. (Substituting B^{sB} for s^{th} column of V_B since s^{th} column of V_B is equivalent to B^{sB}).

$$A = \sigma_1 \underline{u}_1 \otimes \underline{v}_1 \otimes \underline{w}_1 + \sigma_2 \underline{u}_2 \otimes \underline{v}_2 \otimes \underline{w}_2 + \cdots + \sigma_r \underline{u}_r \otimes \underline{v}_r \otimes \underline{w}_r$$

where $\sigma_1, \sigma_2, \dots, \sigma_r$ are the non-negative singular values of 3-D matrix A,

$$r = \tau_1 + \tau_2 + \cdots + \tau_{r_B},$$

$$\sigma_t = \sigma_{tB}\sigma_{t\tau_s},$$

$t = 1,2,\dots,r$ and $s = 1,2,\dots,r_B$,

$\underline{u}_{j+\sum_{k=0}^{s-1}\tau_k} = \underline{u}_{sB}$, $j = 1,2,\dots,\tau_s$, $s = 1,2,\dots,r_B$, with $\tau_0 = 0$,

$\underline{v}_{j+\sum_{k=0}^{s-1}\tau_k} = \underline{v}_{sj}$, $j = 1,2,\dots,\tau_s$, $s = 1,2,\dots,r_B$,

$\underline{w}_{j+\sum_{k=0}^{s-1}\tau_k} = \underline{w}_{sj}$, $j = 1,2,\dots,\tau_s$, $s = 1,2,\dots,r_B$.

A SVD of 3-D matrix obtained by unifying any other two dimensions instead of second and third dimension will lead to other form of decomposition of the matrix.

The difficulty of Mastorakis (1996) method is to unify any two dimensions of the 3-D matrix into one and to arrange it an equivalent 2-D matrix. To achieve SVD of original matrix, one has to obtain the SVD of unified equivalent 2-D matrix and then reform the 3-D matrix from this SVD. We propose SVD of 3-D matrix based on MM operations and this proposed SVD have similar characterizations as the SVD of 2-D matrices have.

3.2 HOSVD proposed by Lathauwer et al (2000)

Lathauwer et al (2000) propose the multilinear SVD based on n-mode product of tensors. For every complex $(I_1 \times I_2 \times \dots \times I_N)$-tensor $\mathcal{A}$ proposed by Lathauwer et al (2000) is written as the product

$$\mathcal{A} = \mathcal{S} \times_1 U^{(1)} \times_2 U^{(2)} \times_3 \dots \times_N U^{(N)}$$

where,

$U^{(n)}: (I_n \times I_n)$ unitary matrix obtained by applying SVD to n-mode unfolding matrix $A_{(n)}, n = 1,2,\dots,N$,

$\mathcal{S}$: a complex $(I_1 \times I_2 \times \dots \times I_N)$-tensor which is called as a core tensor,

$\times_n$: n-mode product of a tensor.

Here the core tensor is ordered and has a characterization of all-orthogonality. The Frobenius-norms of sub-tensors obtained from the core tensor $\mathcal{S}$ by fixing the n^{th} index are the n-mode singular values of $\mathcal{A}$.

The n-mode product of a tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ by a matrix $U \in \mathbb{C}^{J_n \times I_n}$ is an $(I_1 \times I_2 \times \dots \times I_{n-1} \times J_n \times I_{n+1} \times \dots \times I_N)$ tensor with entries given by,

$$(\mathcal{A} \times_n U)_{i_1 i_2 \dots i_{n-1} j_n i_{n+1} \dots i_N} = \sum a_{i_1 i_2 \dots i_{n-1} j_n i_{n+1} \dots i_N} u_{j_n i_n}.$$

The concept of n-mode product used to propose the above HOSVD of a tensor is quite complicated. Further the HOSVD of $(I_1 \times I_2 \times \dots \times I_N)$-tensor $\mathcal{A}$ gives only I_n n-mode singular values and it will be very difficult to give proper interpretations to these singular values.

3.3 SVD based on MM operations

Our method for SVD of MM is based on the basic MM operations and the concept of multidimensional unitary matrix. Through this method, we decompose the matrix A of dimension $m_1 \times m_2 \times m_3$ as follows.

$$A = U\Sigma V^T, \tag{3.5}$$

where

Σ is rectangular diagonal matrix of singular values of dimension $m_1 \times m_2 \times m_3$,

U is unitary matrix of dimension $m_1 \times m_1 \times m_3$ and

V is unitary matrix of dimension $m_2 \times m_2 \times m_3$.

We refer the SVD proposed in (3.5) as SVD of A along the first and second dimension and to achieve this SVD, we now give a step by step procedure.

a) Obtain the SVD of $m_1 \times m_2$ submatrix $A(:,:,i_3)$, of A as follows.

$$A(:,:,i_3) = U_{i_3}\Sigma_{i_3}V_{i_3}^T, \quad i_3 = 1,2,\dots,m_3,$$

where U_{i_3} and V_{i_3} are unitary matrices $\left(i.e. U_{i_3}U_{i_3}^* = I_{m_1}, V_{i_3}V_{i_3}^* = I_{m_2}\right)$ and σ_{i_3} is rectangular diagonal matrix of dimension $m_1 \times m_2$ with non-negative singular values $\sigma_{i_3 s}$, $s = 1,2,\dots,r_{i_3}$ for $i_3 = 1,2,\dots,m_3$.

b) Construct 3-D square matrices U and V of dimension $m_1 \times m_1 \times m_3$ and $m_2 \times m_2 \times m_3$ respectively as follows.

$$U(:,:,i_3) = U_{i_3},$$
$$V(:,:,i_3) = V_{i_3}, \; i_3 = 1,2,\dots,m_3.$$

c) Also construct 3-D rectangular diagonal matrix Σ of dimension $m_1 \times m_2 \times m_3$ as follows.

$$\Sigma(:,:,i_3) = \Sigma_{i_3}, \quad i_3 = 1,2,\dots,m_3.$$

d) To achieve SVD of A, observe that with reference to 3-D matrix operations,

$$U\Sigma V^T = A,$$

where $UU^* = I_{m_1}^{m_3}$,
$VV^* = I_{m_2}^{m_3}$.

The non-negative singular values collected together in a vector, $\underline{\sigma} = (\underline{\sigma_1} \quad \underline{\sigma_2} \quad \cdots \quad \underline{\sigma_{m_3}})$ where $\underline{\sigma_{i_3}} = (\sigma_{i_3 1} \quad \sigma_{i_3 2} \quad \cdots \quad \sigma_{i_3 r_{i_3}}), i_3 = 1,2,\dots,m_3$ are collectively referred as singular values of 3-D matrix A.

The proposed SVD can be easily extended to the MM by using the MM operations introduced by Solo and extending the concept of unitary matrices to MM.

IV. Characterizations of Singular Values of 3-D matrices

In this Section we develop some interesting characterizations of singular values of 3-D matrix. Let A be a 3-D matrix of dimension $m_1 \times m_2 \times m_3$ with rank $\underline{\rho} = (\rho_1 \quad \rho_2 \quad \cdots \quad \rho_{m_3})$ and singular values $\underline{\sigma} = (\underline{\sigma_1} \quad \underline{\sigma_2} \quad \cdots \quad \underline{\sigma_{m_3}})$ where $\underline{\sigma_{i_3}} = (\sigma_{i_3 1} \quad \sigma_{i_3 2} \quad \cdots \quad \sigma_{i_3 r_{i_3}}), i_3 = 1,2,\dots,m_3$. . Let $SS(A) = \sum_{i_3=1}^{m_3} \sum_{s=1}^{\rho_k} \sigma_{i_3 s}^2$. Now we state the characterizations of singular values of A as follows.

i) $SS(A) = trace(A^T A)$.

ii) $SS(A) = \sum_{i_1=1}^{m_1} \sum_{i_2=1}^{m_2} \sum_{i_3=1}^{m_3} a_{i_1 i_2 i_3}^2$.

iii) Let the matrix A be partitioned (along each of the three dimensions in two parts) so that we get 8 sub-matrices A_{ijk} of dimensions $p_i \times q_j \times r_k$ for $i,j,k = 1,2$ such that $p_1 + p_2 = m_1, q_1 + q_2 = m_2$ and $r_1 + r_2 = m_3$. Then,

$$\sum_{i,j,k=1}^{2} SS(A_{ijk}) = SS(A).$$

iv) The matrix norm $\|A\|$ of A is given as,

$$\|A\| = \sqrt{\sum_{i_1=1}^{m_1} \sum_{i_2=1}^{m_2} \sum_{i_3=1}^{m_3} a_{i_1 i_2 i_3}^2},$$

It can be also seen that $\|A\| = \sqrt{SS(A)}$.

To look at to some other characterizations, we define the following elementary layer operations on the MM.

- $E_{k_1 k_2}$: Interchange of k_1^{th} layer with k_2^{th} layer of A, $k_1, k_2 = 1,2,\dots,m_3$ and $k_1 \neq k_2$.
- $\alpha(E_{k_1})$: Multiplying k_1^{th} layer of A by scalar $\alpha \in \mathbb{R}$, $k_1 = 1,2,\dots,m_3$.
- $E_{k_1 k_2}(\beta)$: Adding β-multiple of k_2^{th} layer to k_1^{th} layer of A where $k_1 \neq k_2, \beta \in \mathbb{R}$.

With reference to the above elementary operations we continue with the next characterizations of singular values.

v) The $SS(A)$, Sum of squared singular values of A is invariant to the first elementary layer operation. That is if matrix B is obtained by performing $E_{k_1 k_2}$ on A then sum of squared singular values of B are same as $SS(A)$.

vi) If matrix B is obtained by performing second elementary layer operation $\alpha(E_{k_1})$ on A then,

$$SS(B) = SS(A) + (\alpha^2 - 1) \sum_{s=1}^{\rho_{k_1}} \sigma_{k_1 s}^2.$$

vii) If matrix C is obtained by performing third elementary layer operation $E_{k_1 k_2}(\beta)$ on A then,

$$SS(C) \leq SS(A) + |\beta| (\sum_{s=1}^{\rho_{k_2}} \sigma_{k_2 s}^2)$$

viii) If D is the matrix of same dimension as of A, then $< A, D >= trace(D^* A)$ forms an inner product on $\mathbb{C}^{m_1 \times m_2 \times m_3}$.

ix) The mapping $\|.\|: \mathbb{C}^{m \times m \times m_3} \to \mathbb{R}$ defined as $\|A\| = \sqrt{\sum_{i_1,i_2=1}^{m} \sum_{i_3=1}^{m_3} |a_{i_1 i_2 i_3}|^2}$ forms a norm on the vector space of all complex matrices of dimension $m \times m \times m_3$.

V. Numerical Work

In this section we demonstrate the SVD of 3-D matrices through an example. To compare the method of SVD based on MM operation as proposed in this paper with Mastorakis's method we consider the same matrix as in Mastorakis (1996) in the following example.

Consider the 3-D matrix \$A\$ of dimension \$2\times 3\times 4\$ which can be expressed in the form of array of matrices as follows with the notations introduced in Section 2.

$$A(:,:,1) = \begin{bmatrix} 6.6 & 9 & 11.6 \\ 11.4 & 19 & 23 \end{bmatrix},$$
$$A(:,:,2) = \begin{bmatrix} -2 & -3 & -4 \\ -3.7 & -6.1 & -8 \end{bmatrix},$$
$$A(:,:,3) = \begin{bmatrix} 4.1 & 6.5 & 7.8 \\ 8.2 & 12.5 & 15.5 \end{bmatrix},$$
$$A(:,:,4) = \begin{bmatrix} 2.13 & 2.9 & 3.8 \\ 4 & 5.6 & 8.2 \end{bmatrix}$$

By performing SVD on \$A\$ along the first and second dimension, we have the representation of \$A\$ as follows.

$$A = U\Sigma V^T$$

Where, U and V are unitary matrices of dimension $2 \times 2 \times 4$ and $3 \times 3 \times 4$ respectively, and Σ is matrix of singular values of dimension $2 \times 3 \times 4$.

The matrices U, V and Σ are obtained using algorithm in Section 3.2 and are as follows.

$$U(:,:,1) = \begin{bmatrix} -0.4497 & -0.8932 \\ -0.8932 & 0.4497 \end{bmatrix},$$
$$U(:,:,2) = \begin{bmatrix} -0.4488 & -0.8936 \\ -0.8936 & 0.4488 \end{bmatrix},$$

$$U(:,:,3) = \begin{bmatrix} -0.4532 & -0.8914 \\ -0.8914 & 0.4532 \end{bmatrix}, \quad U(:,:,4) = \begin{bmatrix} -0.4388 & -0.8986 \\ -0.8986 & 0.4388 \end{bmatrix}$$

$$V(:,:,1) = \begin{bmatrix} -0.3678 & -0.8359 & -0.4074 \\ -0.5879 & 0.5485 & -0.5946 \\ -0.7205 & -0.0208 & 0.6931 \end{bmatrix}, \quad V(:,:,2) = \begin{bmatrix} 0.3505 & 0.9057 & -0.2386 \\ 0.5667 & -0.4079 & -0.7159 \\ 0.7457 & -0.1157 & 0.6562 \end{bmatrix}$$

$$V(:,:,3) = \begin{bmatrix} -0.3795 & 0.3856 & -0.8410 \\ -0.5832 & -0.8054 & -0.1061 \\ -0.7183 & 0.4502 & 0.5305 \end{bmatrix}, \quad V(:,:,4) = \begin{bmatrix} -0.3802 & -0.5582 & -0.7375 \\ -0.5292 & -0.5226 & 0.6684 \\ -0.7585 & 0.6444 & -0.0968 \end{bmatrix}$$

$$\Sigma(:,:,1) = \begin{bmatrix} 35.7524 & 0 & 0 \\ 0 & 0.9200 & 0 \end{bmatrix}, \quad \Sigma(:,:,2) = \begin{bmatrix} 11.9950 & 0 & 0 \\ 0 & 0.1398 & 0 \end{bmatrix}$$

$$\Sigma(:,:,3) = \begin{bmatrix} 24.1581 & 0 & 0 \\ 0 & 0.1600 & 0 \end{bmatrix}, \quad \Sigma(:,:,4) = \begin{bmatrix} 11.9124 & 0 & 0 \\ 0 & 0.2846 & 0 \end{bmatrix}$$

The singular values obtained by this SVD can be summarized as follows by using notations introduced.

$$\underline{\sigma} = (\underline{\sigma}_1 \quad \underline{\sigma}_2 \quad \underline{\sigma}_3 \quad \underline{\sigma}_4),$$

where, $\underline{\sigma}_1 = (35.7524 \quad 0.9200)$, $\underline{\sigma}_2 = (11.9950 \quad 0.1398)$,

$\underline{\sigma}_3 = (24.1581 \quad 0.1600)$, $\underline{\sigma}_4 = (11.9124 \quad 0.2846)$.

Mastorakis (1996) perform the SVD of the same matrix using indirect method and obtains the vector of singular values of A as follows.

$$\underline{\sigma} = (46.3329 \quad 0.8475 \quad 0.3853 \quad 0.9395 \quad 0.3243 \quad 0.1221)$$

The singular values obtained by Mastorakis (1996) and by our method are different but the $SS(A)$ based on both methods is same and is 2148.6.

If we perform SVD along the first and third/second and third dimension we get the different decompositions of A. Thus SVD with reference to all the three pairs of dimensions leads to different singular values but in all the three cases $SS(A)$ is same which coincides with $\|A\|^2$.

The matrix of singular values of A when SVD is performed along the first and third dimension are as follows.

$$\Sigma(1,:,:) = \begin{bmatrix} 20.8602 & 0 & 0 \\ 0 & 0.4658 & 0 \\ 0 & 0 & 0.2016 \\ 0 & 0 & 0 \end{bmatrix}, \quad \Sigma(2,:,:) = \begin{bmatrix} 41.3776 & 0 & 0 \\ 0 & 0.9199 & 0 \\ 0 & 0 & 0.4943 \\ 0 & 0 & 0 \end{bmatrix}.$$

Similarly the 3-D matrix of singular values of A when SVD is performed along the second and third dimension are as follows.

$$\Sigma(:,1,:) = \begin{bmatrix} 17.1924 & 0 & 0 & 0 \\ 0 & 0.4662 & 0 & 0 \end{bmatrix}, \quad \Sigma(:,2,:) = \begin{bmatrix} 26.9494 & 0 & 0 & 0 \\ 0 & 0.4589 & 0 & 0 \end{bmatrix},$$

$$\Sigma(:,3,:) = \begin{bmatrix} 33.5596 & 0 & 0 & 0 \\ 0 & 0.2857 & 0 & 0 \end{bmatrix}.$$

To obtain the SVD of MM, we developed a Matlab function $svdm(.,.)$ which needs two arguments, a d-D matrix A and an integer r (representing the dimension with respect to which SVD is to be obtained, $r = 1,2,\ldots,d$). The function returns the d-D matrices U, Σ and V as in (3.5). We also developed the other Matlab functions for MM operations such as transpose, multiplication, trace, norm, complex conjugate of a matrix etc which helped us to verify the characterizations of SVD. Briefly we extended some Matlab functions for 2-D matrices to MM.

VI. Conclusions

In this paper we propose SVD of MM through MM operations. Using the MM operations, MM algebra and MM calculus introduced by Solo (2010 A-F) we propose the concept of multidimensional unitary matrices. We achieve the SVD of MM based on MM operations which has the similar characterizations as in case of 2-D matrices. We developed Matlab functions to deal with MM and to give SVD of MM. We bring out some interesting characterizations of proposed SVD. All these characterizations will lead to many interesting applications in theory of Mathematics as well as in Statistics.

Our proposed method of SVD can be performed along any pairs of dimension of MM. The SVD of $m_1 \times m_2 \times m_3$ matrix A, obtained along the first and second dimension gives $m_3 \times \min(m_1 m_2)$ singular values while that of along second and third dimension gives $m_1 \times \min(m_2 m_3)$ singular values and so on. The SVD of 3-D matrix A proposed by Mastorakis (1996) unifying any pair of dimension leads to the same number of singular values as in our case. While the SVD proposed by Lathauwer et al (2000) leads to m_n n-mode singular values when the MM is unfolded along the n^{th} dimension. In statistics singular values have the special interpretations in terms of variation/inertia contributed by the pairs of attributes associated with rows/columns/layers corresponding to MM. Hence more the number of singular values, more are the components of total variation/inertia. The SVD of MM proposed in this paper gives more number of singular values as compared to Lathauwer et al (2000). Further since we are applying SVD to MM through MM operations, the singular values can be given specific meanings. While since Mastorakis (1996) unifies dimensions of MM and Lathauwer et al (2000) unfolds the MM, the singular values obtained through these methods may not be given proper interpretations. Specifically the proposed SVD for MM will give very promising results in Correspondence Analysis and Principle Component Analysis in Statistics. We will come up with its applications.

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