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Notes on Singular Value Decomposition and Principal Strain Analysis

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1 BASIC UNDERSTANDING OF SVD

To understand the SVD, it's beneficial to start from its geometrical meaning. Taking the two-dimensional geometry transformation matrix as an example, given certain basis vectors, we accordingly have a certain grid of the 2D plane. Then operating the transformation matrix on such a grid will lead to the general shape changing (shearing) of the grid. Among all the grids, there will always exists a specific one, for which the application of the transformation matrix does not change the orthogonality of the grid. That's saying, the original basis vectors defining the grid are transformed to another set of orthogonal basis vectors, with respect to the changing of the orientation of the orthogonal basis vectors and their magnitudes.

A good and detailed mathematical derivation and explanation can be found in the following link: http://www.ams.org/publicoutreach/feature-column/fcarc-svd (also, a backup page clip has been saved to Evernote). Here following are some other links to the introduction of SVD, including the general mathematical procedure to carry out the SVD:

- https://blog.statsbot.co/singular-value-decomposition-tutorial-52c695315254, or alternative link to Evernote
- https://1drv.ms/b/s!AlZpbyasn9jtkMMOP0TOw71iaqluMQ
- https://1drv.ms/b/s!AlZpbyasn9jtkMMQDTOO4C5lDSUKzw
- https://1drv.ms/b/s!AlZpbyasn9jtkMMPgUwwOwDbm4-K3w

The SVD can be carried out for any general form of matrices, including both square and rectangular ones.

2 SVD AND PCA

Understanding the SVD from its geometrical representation is only the starting point, and in practice with the SVD tool in hand, we have very important application, such as the data compression, noise reduction and principal component analysis (PCA). Examples can be

found in the first link mentioned above. Since the diagonal matrix in the middle of each SVD component naturally represents the contribution from each single SVD component. Therefore the SVD can be naturally linked to the PCA, i.e. the bigger the diagonal element is, the more it contributes to the original matrix. Also, it should be kept in mind that each principal component corresponds to a coupled dual-space – **u** and **v** – between which the matrix transformation happens back and forth.

For a matrix B of general form, the SVD involves the eigenvalue problem for the BB^T matrix (which is symmetric). Specially, when the matrix A we want to carry out the SVD for is itself a symmetric matrix, it turns out the general form of the SVD becomes:

$$A = U\Lambda U^T \tag{2.1}$$

In this case, the eigenvalue problem for the SVD just becomes the eigenvalue of the symmetric matrix A itself, as demonstrated in this link:
https://1drv.ms/b/s!AlZpbyasn9jtkMMPgUwwOwDbm4-K3w.

Following the idea of the SVD and its PCA implication, the principal strain existing in crystals (e.g. as the result of the thermal effect) could be found. Detailed introduction can be found in A. Goodwin's paper: 10.1107/S0021889812043026. More detailed theoretical derivation used in that paper could be found in the book by C. Giacovazzo, et al. - *Fundamentals of crystallography* (Page-610, 1992). The derivation given there is quite clear, and there is only one thing to be specifically addressed here. In the context, it says *as fractional coordinates of points are not changed by a homogeneous deformation, then* $\bar{M}'x' = \bar{M}x$, where $\bar{M}$ means the transpose of the matrix M (similar for M'). The proof will be addressed as following:

$$\begin{bmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\Rightarrow$$

$$\begin{bmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{bmatrix} \begin{bmatrix} \mathbf{A}_1 \\ \mathbf{A}_2 \\ \mathbf{A}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \end{bmatrix} \tag{2.2}$$

where $\mathbf{A}_{i=1,2,3} = (A_{i1}, A_{i2}, A_{i3})$ is the representation of the lattice vector in the chosen orthogonal space, i.e. $\mathbf{A}_{i=1,2,3} = A_{i1}\mathbf{e}_1 + A_{i2}\mathbf{e}_2 + A_{i3}\mathbf{e}_3$. Then for any grid points in the crystal, we have its fractional coordination (x_1, x_2, x_3) in the orthogonal space, and therefore we can write:

$$\begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{bmatrix} \begin{bmatrix} \mathbf{A}_1 \\ \mathbf{A}_2 \\ \mathbf{A}_3 \end{bmatrix} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \end{bmatrix} \tag{2.3}$$

where

$$\begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{bmatrix} \tag{2.4}$$

gives the fractional coordinate in the lattice basis before the deformation, which in short could be written as $\bar{\mathbf{x}}M$ with $\bar{\mathbf{x}}$ as the row vector. Also, it could be written as $\bar{M}\mathbf{x}$ with $\mathbf{x}$ as the column vector. Therefore we have proved the statement given in the above statement mentioned in the book.