NOTES AND CORRESPONDENCE

On the Uniqueness of the Singular Value Decomposition in Meteorological Applications

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ABSTRACT

The author revisits the singular value decomposition (SVD) method and shows that the nonuniqueness of the left and right singular vectors related to SVD posts limitations on applications of the method. Caution should be observed when the heterogeneous and homogeneous correlation maps are applied to interpret the relationship between two meteorological data series.

1. Introduction

An application of the singular value decomposition (SVD) to pattern correlation analysis of meteorological data series was discussed by Bretherton et al. (1992).

In this note, we use Bretherton et al.'s notation and denote a time series by (t) and a vector by a boldface letter. Let $\mathbf{x}$(t) be a data series from a sequence of m observations of variable x over a number of p stations or grids (hence, an $m \times p$ matrix) and let $\mathbf{y}$(t) be another data series composed of n observations of variable y over q stations or grids (an $n \times q$ matrix) in the same area where observations of x are made. We call $\mathbf{x}$(t) the left data field and $\mathbf{y}$(t) the right data field. The SVD of the cross-covariance matrix of $\mathbf{x}$(t) and $\mathbf{y}$(t), defined by $\mathbf{C_{xy}} \in \mathbf{R}^{m \times n}$, yields

$$\mathbf{C_{xy}} = \mathbf{U\Sigma V}^{\mathrm{T}}, \tag{1}$$

where $\mathbf{U}$ is an $m \times p$ matrix and $\mathbf{V}^{\mathrm{T}}$ an $q \times n$ matrix. The column vectors of $\mathbf{U}$ and $\mathbf{V}^{\mathrm{T}}$ are the singular vectors and satisfy the orthogonal relation $\mathbf{u}_i\mathbf{u}_j^{\mathrm{T}} = \delta_{ij}$ and $\mathbf{v}_i\mathbf{v}_j^{\mathrm{T}} = \delta_{ij}$, where δ_{ij} is the Dirac delta function. The singular vectors $\mathbf{u}_i$ and $\mathbf{v}_i$ are also called left and right patterns, respectively (Bretherton et al. 1992). The matrix $\mathbf{\Sigma}$ is an $m \times n$ diagonal matrix holding the singular values. Each pair of singular vectors ($\mathbf{u}_i$, $\mathbf{v}_i$) corresponds to a singular value σ_i in $\mathbf{\Sigma}$.

The result from the SVD of $\mathbf{C_{xy}}$ may be used to evaluate the "closeness" of $\mathbf{x}$(t) and $\mathbf{y}$(t) because the leading singular value, σ_1, is also the 2-norm of $\mathbf{C_{xy}}$ and, hence, provides a measure of the covariance of $\mathbf{x}$(t) and $\mathbf{y}$(t). In other words, σ_1 may be used as a measure of cross correlation of the two data series. Furthermore, SVD guarantees that the linear combinations of the left data series and the left patterns and the right data series and right patterns, that is,

$$a_i(t) = \mathbf{u}_i^{\mathrm{T}}\,\mathbf{x}(t) \tag{2a}$$

and

$$b_i(t) = \mathbf{v}_i^{\mathrm{T}}\,\mathbf{y}(t), \tag{2b}$$

respectively, will have the maximum covariance. Therefore, applying SVD, not only may we measure closeness or correlation of two data series, but also the limit of this correlation.

Bretherton et al. (1992) extended the application of SVD results and introduced various correlation and covariance analysis tools used to gain additional information on correlations of the data series, $\mathbf{x}$(t) and $\mathbf{y}$(t). Among them are the homogeneous correlation map and the heterogeneous correlation map. The former is defined as correlations of a data field and its linear combination with corresponding patterns, that is, either $r[\mathbf{x}(t), a_i(t)]$ or $r[\mathbf{y}(t), b_i(t)]$; and the latter is defined in a similar way but in a cross-correlation form, $r[\mathbf{x}(t), b_i(t)]$ or $r[\mathbf{y}(t), a_i(t)]$. By the definition of heterogenous correlation map, a new $\mathbf{y}$(t) [or $\mathbf{x}$(t)] can be obtained from $b_i(t)$ [$a_i(t)$] if updated $\mathbf{x}$(t) [$\mathbf{y}$(t)] is known from observation, when the left and right patterns of the data series are known from an SVD analysis of historical data. This could be an attractive feature of the heterogeneous correlation map, and it would suggest a potential application of SVD for predictive purposes.

With respect to applications in meteorology, the SVD method has been used in climatic data analyses and model-output interpretation of a wide variety of subjects (Wallace et al. 1992; Fang and Wallace 1994; Mantua and Battisti 1995).

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Although results from these applications of SVD appeared to be useful in identifying correlations of patterns and variations of two meteorological data series, restrictions on interpretation of SVD results have been cautioned. Newman and Sardeshmukh (1995) discussed the potential that SVD may result in unrealistic relations of two data series even though the calculated correlation between them may be high. They showed that if $\mathbf{x}(t)$ and $\mathbf{y}(t)$ are linearly related, for example, $\mathbf{y} = \mathbf{L}\mathbf{x}$, this relation can be correctly identified by the SVD of $\mathbf{C}_{\mathbf{xy}}$ only if the matrix $\mathbf{L}$, representing the relation or transformation between $\mathbf{x}$(t) and $\mathbf{y}$(t), is an orthogonal matrix. Newman and Sardeshmukh argued that it is difficult in reality to have such orthogonal mapping relations between two data series.

Another factor that exacerbates this difficulty is the data-sampling error rising from data collection and processing. Because the singular values of $\mathbf{C}_{\mathbf{xy}}$ are also eigenvalues of $(\mathbf{C}_{\mathbf{xy}}\mathbf{C}_{\mathbf{xy}}^{-1})$, sampling errors in $\mathbf{x}$(t) and $\mathbf{y}$(t) that can induce changes of the spacing between the eigenvalues of $(\mathbf{C}_{\mathbf{xy}}\mathbf{C}_{\mathbf{xy}}^{-1})$, as illustrated by North et al. (1982), may skew the property of $\mathbf{C}_{\mathbf{xy}}$. Even when the physical relation of the two data series is orthogonal, the skewness of $\mathbf{C}_{\mathbf{xy}}$ by the sampling errors may result in a relation $\mathbf{L}$ departing from being orthogonal.

Cherry (1996) extended Newman and Sardeshmukh's discussion to both spatial and temporal correlation structures. Using constructed examples, he showed that SVD analysis resulted in the highest correlation among the data series for a pair that have no temporal correlation at all. Cherry indicated that the spurious results of SVD resulted because ''there are, theoretically at least, an infinite number of processes with the same cross-covariance structure.'' These processes will, therefore, have the same sets of singular values and singular vectors.

In addition to the nonuniqueness of SVD discussed by Cherry (1996), there is another possibility for SVD to yield different sets of singular vectors for one same process in the data series. In this note, we will show that this nonuniqueness exists for a degenerated cross-covariance matrix and for normal matrices as well. Effects of this nonuniqueness of SVD on the heterogeneous correlation map and its potential application in prediction problems are discussed.

2. The nonuniqueness of the correlation maps

We first revisit some properties of the SVD and discuss the nonuniqueness of its singular vectors. The propagation of the nonuniqueness to the homogeneous and heterogeneous correlation maps is discussed in turn.

The primary application of SVD in linear algebra is to significantly simplify the construction of the pseudoinverse, $\mathbf{A}^+$, of a matrix $\mathbf{A} \in \mathbf{R}^{m\times n}$ (Strang 1976; Jiang et al. 1979). The usefulness of $\mathbf{A}^+$ is in the solution theory (Strang 1976). To derive $\mathbf{A}^+$ from $\mathbf{A}$, the SVD of $\mathbf{A}$ must exist. If $\mathbf{A} = \mathbf{E}\Lambda\mathbf{F}^T$, then $\mathbf{A}^+ = \mathbf{F}\Lambda^{-1}\mathbf{E}^T$. An important feature in constructing $\mathbf{A}^+$ is that $\mathbf{A}^+$ is solely determined by the singular values of $\mathbf{A}$, Λ. The fact that $\mathbf{A}^+$ does not depend on choices of $\mathbf{F}$ and $\mathbf{E}$ is because the singular vectors in $\mathbf{E}$ and $\mathbf{F}^T$ from the SVD of $\mathbf{A}$ are not unique.

A special case of the nonuniqueness of $\mathbf{e}_i$ in $\mathbf{E}$ and $\mathbf{f}_i$ in $\mathbf{F}$ occurs when $\mathbf{A}$ is degenerate. This can happen because the singular values of the matrix $\mathbf{A}$ satisfy

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_k \geq \cdots \geq \lambda_n \geq 0, \tag{3}$$

where the equal signs indicate the potential for multiple singular values. If we suppose that the number of a multiple singular value, for example, λ_m, of $\mathbf{A}$ is m, because $\mathbf{E}$ and $\mathbf{F}$ are orthogonal, there must be m independent eigenvectors corresponding to the m multiplets of the singular value. Because any sets of m linearly independent vectors in the subspace spanned by the m eigenvectors can be used as an alternative set of the eigenvectors (Jiang et al. 1979), the singular vectors in $\mathbf{E}$ and $\mathbf{F}$ are nonunique. By the same token, the left and right singular vectors in $\mathbf{U}$ and $\mathbf{V}$ from the SVD of the cross-covariance matrix $\mathbf{C}_{\mathbf{xy}}$ of $\mathbf{x}(t)$ and $\mathbf{y}(t)$ are not unique.

The nonuniqueness of $\mathbf{E}$ and $\mathbf{F}$ from the SVD of $\mathbf{A}$ in generalized cases can be shown as follows. Again, if $\mathbf{A} = \mathbf{E}\Lambda\mathbf{F}^T$, noticing that $\mathbf{E}$ and $\mathbf{F}$ are orthogonal matrices, we can have

$$\mathbf{A}^T\mathbf{A} = \mathbf{F}\Lambda^T\mathbf{E}^T\,\mathbf{E}\Lambda\mathbf{F} = \mathbf{F}\Lambda^2\mathbf{F}^T$$

or

$$(\Lambda^2\mathbf{I} - \mathbf{A}^T\mathbf{A})\mathbf{F} = 0, \tag{4}$$

where $\mathbf{I}$ is the unit matrix. The above shows that Λ^2 contains eigenvalues of $(\mathbf{A}^T\mathbf{A})$, while $\mathbf{F}$ has the corresponding eigenvectors. Similarly, $\mathbf{E}$ has the eigenvectors of $(\mathbf{A}\mathbf{A}^T)$, which is algebraically similar to $(\mathbf{A}^T\mathbf{A})$.

Let us rewrite (4) as $(\Lambda'\mathbf{I} - \mathbf{A}')\mathbf{F} = 0$, where $\Lambda' = \Lambda^2$ and $\mathbf{A}' = \mathbf{A}^T\mathbf{A}$. It is known in linear algebra that for any eigenvalue, λ_k', of matrix $\mathbf{A}'$, there are an infinite number of eigenvectors, $\boldsymbol{\xi}_k$, satisfying $(\lambda_k'\mathbf{I} - \mathbf{A}')\boldsymbol{\xi}_k = 0$. However, the maximum number of linearly independent eigenvectors is finite for an eigenvalue. If corresponding to λ_k' there are a maximum of s $(s \geq 1)$ independent eigenvectors, this set of s eigenvectors form a vector base that spans a linear eigensubspace. In this subspace there exist other sets of s linearly independent vectors that can be expressed as linear transformations of the original set of eigenvectors. These sets of eigenvectors share the same eigenvalues. Hence, the eigenvectors corresponding to the eigenvalue λ_k' are not unique. In the special case when $\mathbf{A}'$ is orthogonal, there is only one eigenvector corresponding to each eigenvalue, and we will have number of rank $(\mathbf{A}')$ eigenvectors for the eigenvalue problem. For any $\boldsymbol{\xi}$ in this group of eigenvectors, a vector, $\boldsymbol{\xi}'$, which is linearly correlated with $\boldsymbol{\xi}$ and henceforth independent from the rest of the eigenvectors in the group, can replace $\boldsymbol{\xi}$ in the group and form a new group of eigenvectors corresponding to the same set of eigenvalues. Among the choices of $\boldsymbol{\xi}'$, there can be one with just an opposite sign to $\boldsymbol{\xi}$, because it is obvious that $\boldsymbol{\xi}' + \boldsymbol{\xi} = \mathbf{0}$. The eigenvectors of $\mathbf{A}'$ are therefore not unique when $\mathbf{A}'$ is an orthogonal and nondegenerate matrix. In the appendix, an example is presented to illustrate this nonuniqueness. This shows that the singular vectors of $\mathbf{C}_{xy}$ that are eigenvectors of $(\mathbf{C}_{xy}^{T}\mathbf{C}_{xy})$ or $(\mathbf{C}_{xy}\mathbf{C}_{xy}^{T})$ are not unique in general.

The nonuniqueness of the singular vectors in $\mathbf{U}$ and $\mathbf{V}^{T}$ in the SVD of $\mathbf{C}_{xy}$ poses restrictions on applications of both the homogeneous and the heterogeneous correlation maps. This is because the sign of the heterogeneous correlation map can be reversed when signs of singular vectors or patterns from SVD reverse. We notice that in (2) a sign reverse of a singular vector $\mathbf{u}_i$ or $\mathbf{v}_i$ will affect the sign of the linear combination a_i or b_i. Because the data series, either $\mathbf{x}(t)$ or $\mathbf{y}(t)$, is fixed, this sign change of a pattern will flip the sign of the heterogeneous or homogeneous correlation maps. This nonuniqueness is not a problem in the principal component analysis or the empirical orthogonal function (EOF) analysis in which we are interested in the behavior of a single data series.

In the following, we use an example to illustrate the nonuniqueness of the sign of the heterogeneous correlation map that resulted from an SVD analysis. This example is from an analysis originally designed to use SVD to identify the relationship between spring–summer season anomalies of precipitation amount and anomalies of previous winter season deep soil temperature in the central Unites States. This analysis was motivated by studies that have suggested that regional surface heat and moisture fluxes can have a significant effect on precipitation development in the central United States (e.g., Paegle et al. 1996).

The data used in this analysis are 12-yr (1982–93) station precipitation records and soil temperatures at different depths in the Great Plains. The data are from the National Climatic Data Center. The quality controls on both the precipitation and soil temperature data were discussed by Reek and Crowe (1991). Precipitation data at each station are first averaged over each of the spring seasons (February–April) over the 12-yr period. After normalization, the precipitation values are interpolated to a mesh system of 50 km $\times$ 50 km covering the area shown in Fig. 1. Soil temperatures at 1-m depth for previous winter seasons (December–February) over the 12 yr are analyzed in a similar manner, and normalized soil temperature distributions are obtained. The two gridded fields are then analyzed using the SVD method to examine their relation. Two SVD solution methods were applied to decompose the cross-covariance matrix of the two fields and to construct the heterogeneous correlation map. The first method is the one described by Nash (1990), and the second one is the method of an ICEPACK routine, ''svd.f.''

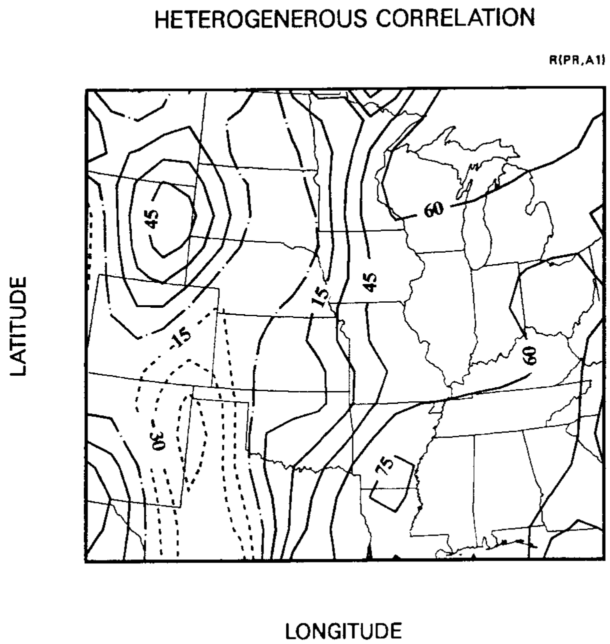

FIG. 1. Heterogeneous correlation map between spring season precipitation anomalies and previous winter season deep soil temperature anomalies. Positive correlations are shown by solid lines and negative correlations by dashed lines.

The heterogeneous correlation between the spring season precipitation and the leading expansion coefficient of previous winter season soil temperature is shown in Fig. 1, using Nash's method. The correlation coefficient between the leading expansion coefficients of the two fields is 83%, from both methods. The solid lines in Fig. 1 indicate positive correlation, and the dashed lines show negative correlation. Away from the mountainous regions in the west, the Great Plains show high positive correlation between the two fields. This correlation is also suggested by the relations of the three leading expansion coefficients of the two data series shown in Fig. 2. These results suggest that a positive anomaly in winter season deep soil temperature corresponds to a positive anomaly of precipitation in the following spring season in the region. This positive correlation of the two fields was also identified by Tang and Reiter (1986) using a different method. This relation is what we planned to look for. However, when we were further evaluating this relation an ambiguity in the results arose. When applying the svd.f routine in calculation we obtained results similar to that in Fig. 1 except that the sign of the correlation was now reversed. In accordance, the three leading coefficients all have an opposite relation compared to that shown in Fig. 2. The results now suggest that negative anomalies of precipitation occur in spring seasons corresponding to positive anomalies in deep soil temperature in the previous winter seasons. These contrary results indicate that

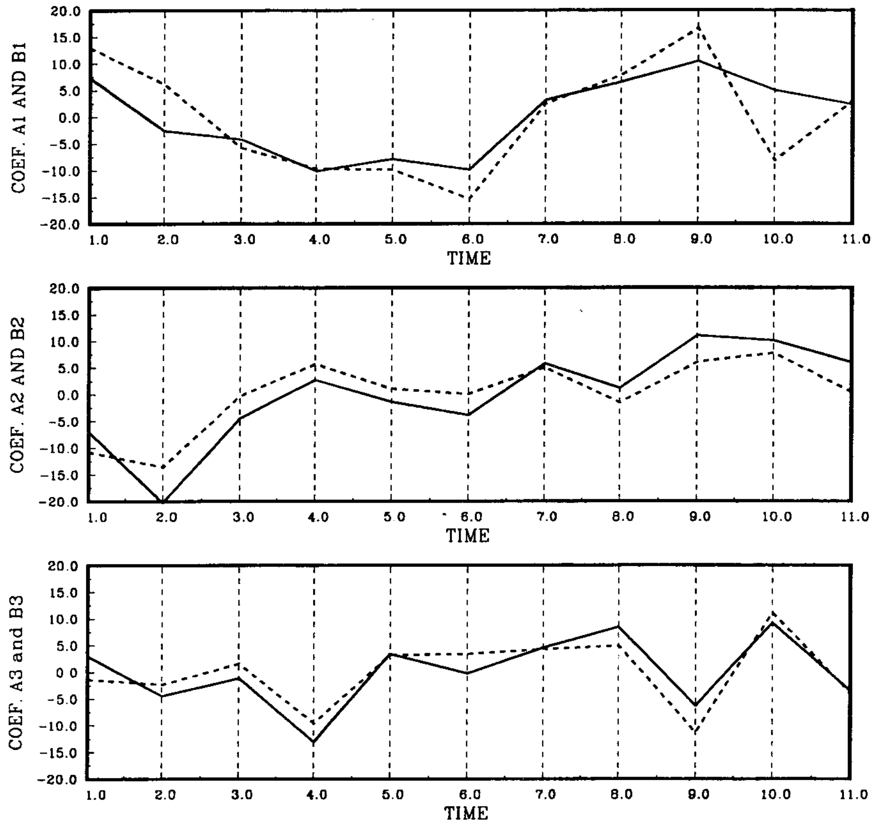

FIG. 2. Temporal variations of the three leading expansion coefficients of spring season precipitation anomalies (solid) and previous winter season deep soil temperature anomalies (dashed). The abscissa shows time in years from 1983 to 1993.

the nonuniqueness of the heterogeneous correlation map, related to the nonuniqueness of the singular vectors of SVD, limits the application of the heterogeneous correlation map.

To summarize, this note shows that because of the nonuniqueness of the signs of both the left and right singular vectors in the SVD of a cross-covariance matrix of two data series, the signs of both the heterogeneous and homogeneous correlation maps calculated using these vectors cannot be uniquely determined. This ambiguity means caution is required when these correlation maps are used to interpret data relations and structures. It seems that the SVD results can be used to assist us in gaining information about correlation and covariance structure of two data series *after* their physical relation is known. A solo use of SVD in detecting physical relations between two data series is beyond the SVD's ability.

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APPENDIX

An Example of Nonuniqueness of Singular Vectors

In this example, we assume the cross-covariance matrix from two data series $\mathbf{x}(t)$ and $\mathbf{y}(t)$ to be

$$\mathbf{C}_{xy} = \begin{pmatrix} 5.0 & 1.0e^{-6} & 1.0 \\ 6.0 & 0.999999 & 1.0 \\ 7.0 & 2.00001 & 1.0 \\ 8.0 & 2.9999 & 1.0 \end{pmatrix}.$$

Nash (1990) used this matrix to demonstrate the sensitivity of $\mathbf{C}_{xy}^{+}$ to singular values of $\mathbf{C}_{xy}$.

If the SVD method described by Nash (1990) is used, the decomposition yields

$$\mathbf{C_{xy}} = \mathbf{U\Sigma V}^{\mathrm{T}},$$

where

$$\mathbf{\Sigma} = \begin{pmatrix} 13.7530 & 0.0 & 0.0 \\ 0.0 & 1.68961 & 0.0 \\ 0.0 & 0.0 & 1.18853e^{-5} \end{pmatrix},$$

$$\mathbf{U} = \begin{pmatrix} 0.358943 & -0.755762 & -0.328687 \\ 0.446526 & -0.317194 & 0.111741 \\ 0.534110 & 0.121383 & 0.762674 \\ 0.621692 & 0.559891 & -0.545716 \end{pmatrix},$$

and

$$\mathbf{V} = \begin{pmatrix} 0.958786 & -0.209025 & -0.192451 \\ 0.245748 & 0.950036 & 0.192456 \\ 0.142607 & -0.231819 & 0.962249 \end{pmatrix}.$$

It can be easily shown that if we reverse the signs of the first and second singular vectors in both $\mathbf{U}$ and $\mathbf{V}$, which correspond to the two nontrivial singular values in $\mathbf{\Sigma}$, and define the new matrices as $\hat{\mathbf{U}}$ and $\hat{\mathbf{V}}$, respectively, $\hat{\mathbf{U}}$ and $\hat{\mathbf{V}}$ will still satisfy $\mathbf{C_{xy}} = \hat{\mathbf{U}}\mathbf{\Sigma}\hat{\mathbf{V}}^{\mathrm{T}}$. In other words, the vectors in $\hat{\mathbf{U}}$ and $\hat{\mathbf{V}}$ also hold, respectively, the left and right singular vectors of $\mathbf{C_{xy}}$.

When the left and right patterns of SVD corresponding to the nontrivial singular values change their signs, the linear combinations in (2) reverse their signs also. This sign change will be observed in both the heterogeneous and homogeneous correlation maps, as may be seen in their definitions.

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