INTERNATIONAL JOURNAL OF CLIMATOLOGY
Int. J. Climatol. **20**: 1509–1516 (2000)

ORTHOGONALITY PROPERTIES OF ROTATED EMPIRICAL MODES

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Received 2 March 1999
Revised 21 January 2000
Accepted 26 January 2000

ABSTRACT

The properties (spatial orthogonality and temporal uncorrelatedness) of orthogonally rotated empirical modes depend on the normalization of the modes, prior to rotation. It is shown here that these properties also depend on how the empirical modes are formulated. The preferred convention is one that allows us to reconstruct the data from the unrotated or rotated modes. When the empirical modes are normalized so that the spatial eigenvectors are unit length (i.e. empirical orthogonal functions (EOFs)), the rotated modes preserve spatial orthogonality, but are no longer temporally uncorrelated. Relaxing the temporal orthogonality in this way does not prejudice conclusions that can be inferred regarding the temporal couplings of the rotated modes. Copyright © 2000 Royal Meteorological Society.

KEY WORDS: orthogonal rotation; principal component analysis; empirical orthogonal function analysis; eigenvector analysis; empirical modes; global mode(s); climate variable(s)

1. INTRODUCTION

Empirical orthogonal function (EOF) analysis and principal component analysis (PCA) have become standard statistical techniques in the geophysical sciences of meteorology and oceanography (e.g. Preisendorfer, 1988; Emery and Thomson, 1997), particularly in the area of climate research (Peixoto and Oort, 1992; von Storch and Zwiers, 1999). These eigentechniques allow us to represent the spatial and temporal variability of climate variables, such as temperature, as a number of 'empirical modes'. Because most of the variance in the data can generally be captured by a small number of modes, the decomposition may be useful in interpreting the variability in the data.

Each empirical mode is formed by a space pattern and a time series which are derived from the eigenvalues and eigenvectors of the covariance (or correlation) matrix. These functions are defined to be orthogonal in space and time. Because they are designed to describe the variance in the whole dataset efficiently, they usually do not represent a large fraction of the variance in a given spatial and temporal subdomain. Typically, as the space–time subdomain is expanded in comparison with the spatial and temporal scales of the dominant physical processes within the subdomain, one or more of the leading modes may capture significant features in different subdomains, but with less explained subdomain variance. In these circumstances, the temporal variability of the mode will not be highly representative of the dominant physical processes of such space–time subdomains, making those processes more difficult to assess.

The tendency of the empirical modes to extract poorly representative commonality among subdomains of large datasets can be remedied by grouping the variance through a rotation procedure. A variety of such procedures are available (Richman, 1986); however, the rotation technique most commonly used to group the variability in geophysical applications is the varimax orthogonal rotation. Rotations have been widely used in meteorology where long records of global scale observations are common, but not yet in oceanography.

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In general, a rotation is a linear transformation of the modes, that attempts to find a new location for the coordinate axis, such that projections of the variable onto those axes simplify the spatial or temporal structure of the modes. A detailed discussion of the advantages and disadvantages of rotated empirical modes is given by Richman (1986) (see also Jolliffe, 1987 and Richman, 1987). In most applications, the rotation is used to simplify the spatial structure by isolating regions with similar temporal variability (e.g. Horel, 1981; Barnston and Livezey, 1987; Kawamura, 1994; Mestas-Nuñez and Enfield, 1999). The resulting rotated space patterns are generally more robust (i.e. less sensitive to sampling errors) than their unrotated counterparts (Cheng *et al.*, 1995). Alternatively, the rotation can also be used to simplify the temporal structure by isolating time periods with similar space patterns (e.g. Fernández Mills, 1995).

An aspect of rotation that has lead to some apparent confusion in the literature concerns the orthogonality properties of orthogonally rotated empirical modes. This applies to varimax, as well as other orthogonal rotations. Jolliffe (1995) showed that it is impossible to preserve both spatial orthogonality and temporal uncorrelatedness of the modes after an orthogonal rotation–temporal uncorrelatedness is equivalent to temporal orthogonality when the temporal mean is removed from the data, which is generally the case. He pointed out that which of these properties is preserved depends on the choice of the normalization constraint imposed on the (unrotated) modes. Furthermore, he stated that the usual normalization which multiplies the unit length eigenvectors by the square root of the eigenvalues (i.e. PCA) leads to rotated modes that possess neither property. This seems to contradict the common concept that when this normalization is used, orthogonal rotations lead to modes that are temporally uncorrelated (orthogonal) (e.g. Horel, 1981; Walsh *et al.*, 1982; Easterling, 1991).

The goal of this study is to clarify the apparent confusion found in the literature regarding the orthogonality properties of the rotated empirical modes. It is shown that this confusion arises from not realizing that the properties of the rotated modes depend not only on the normalization constraint imposed on the unrotated modes, as noted by Jolliffe (1995), but also on the way in which the modes are formulated.

Section 2 reviews the formalism and presents two common formulations of the empirical modal decomposition. The normalized and orthogonally rotated versions of these two modal formulations are introduced in Sections 3 and 4, respectively. In Section 5, we show the effect of three different normalizations on the orthogonality properties of the rotated modes using the two modal formulations. In Section 6, we give an example that illustrates the usefulness of rotation in relaxing the temporal orthogonality constraint of the unrotated modes. The paper ends with a summary, and a discussion of other applications in Section 7.

2. FORMALISM

The formalism of the empirical modes can be written using the singular value decomposition (SVD) of a matrix (Rasmusson *et al.*, 1981; Kelly, 1988). Let us consider a set of time series of length N at P different locations, and with the temporal mean removed at every grid point. These time series can be combined to form an $N \times P$ matrix of data X, whose number of rows N is the number of temporal points and the number of columns P is the number of spatial points. The SVD of X (e.g. Lawson and Hanson, 1995; Golub and Van Loan, 1996) is given by

$$X = USA^T \tag{1}$$

The matrices U and A are both orthonormal because they satisfy the following orthogonality properties $U^TU = I$ and $A^TA = I$, where I is the identity matrix. The diagonal matrix S is formed with the singular values, which are the square root of the eigenvalues of the coupled eigenvalue problems $XX^TU = US^2$ and $X^TXA = AS^2$. Thus, A and U are the eigenvectors of the scatter matrix X^TX (Preisendorfer, 1988) and its transpose XX^T, respectively—the scatter matrix X^TX is proportional to the covariance matrix C (i.e. $X^TX = NC$).

Equation (1) allows us to formulate the modal decomposition as (e.g. Jolliffe, 1995)

$$Z = XA \qquad \text{(analysis)} \tag{2}$$

or equivalently (e.g. Richman, 1986)

$$X = ZA^T \qquad \text{(synthesis)} \tag{3}$$

where A are the space patterns and $Z = US$ are the time series. Equations (2) and (3) are, respectively, the 'analysis' and 'synthesis' formulas of Preisendorfer (1988).

The orthogonality properties of the unrotated modes in Equations (2) and (3) follow from the properties of U and A. The modal space patterns (A) and time series (Z) are, respectively, orthogonal in space and time because A^TA ($= I$) and Z^TZ ($= S^2$) are both diagonal. Furthermore, the modes are also temporally uncorrelated because they are orthogonal in time and have zero temporal mean. The modes have zero temporal mean because the temporal mean of the data was removed before forming X (see Section 2). The scatter ($= N \times$ variance) of the modes are given by the square singular values, which are the eigenvalues of the scatter matrix (or its transpose) derived from Equation (1).

3. NORMALIZATION

It is clear from Equation (1) that there is not a unique way of constructing the space patterns and time series of the empirical modes. In fact, there are an infinite number of possibilities depending on how S is combined with U and A. In Equations (2) and (3), the singular values were grouped with the temporal eigenvectors (i.e. US). However, one could have combined the singular values with the spatial eigenvectors (i.e. SA^T), or even with both spatial and temporal eigenvectors simultaneously (e.g. $US^{1/2}$ and $S^{1/2}A^T$). When U and/or A are multiplied by a diagonal matrix (e.g. $S \neq I$) the resulting matrix is no longer orthonormal. Therefore, the different ways in which the orthogonal modes can be constructed result in different normalizations, and in different orthogonality properties.

To investigate the effect of various normalizations on the properties of the rotated orthogonal modes, a diagonal normalization matrix K is introduced. This allows us to write normalized versions of Equations (2) and (3). The normalized analysis equation is constructed by right multiplying Equation (2) with the diagonal matrix K to obtain

$$\hat{Z} = X\hat{A} \qquad \text{(analysis)} \tag{4}$$

where $\hat{Z} = ZK = USK$ and $\hat{A} = AK$. Right multiplying Z in Equation (3) with the identity matrix $I = K^{-1}K$ gives the normalized synthesis equation

$$X = \tilde{Z}\tilde{A}^T \qquad \text{(synthesis)} \tag{5}$$

where $\tilde{Z} = ZK^{-1} = USK^{-1}$ and $\tilde{A} = \hat{A} = AK$. An advantage of Equation (5) is that allows us to recover the data matrix by straightforward multiplication of the normalized modes.

4. ROTATION

The rotated modes are a linear transformation of the unrotated modes defined by an orthogonal, square matrix T also referred to as the rotation matrix. Because T is orthogonal and square it satisfies

$$T^TT = TT^T = I$$

Using the rotation matrix T, one can write rotated versions of Equations (4) and (5). The rotated form of Equation (4) is obtained by right multiplying it by T to get

$$\hat{Z}^* = X\hat{A}^* \qquad \text{(analysis)} \tag{6}$$

where $\hat{A}^* = \hat{A}T$ are the rotated spatial patterns and $\hat{Z}^* = \hat{Z}T$ are the rotated time series—note that commonly T is applied only to a subset of the leading empirical modes.

Right multiplying $\tilde{Z}$ in Equation (5) by the identity matrix $I = TT^T$ gives the rotated form of Equation (5)

$$X = \tilde{Z}^* \tilde{A}^{*T} \qquad \text{(synthesis)} \tag{7}$$

where $\tilde{Z}^* = \tilde{Z}T$ and $\tilde{A}^* = \tilde{A}T$. Equation (7) shows that in this case, as in Equation (5), the data matrix can also be reconstructed by simple matrix multiplication of the rotated modes.

5. ORTHOGONALITY

The orthogonality properties of the normalized modes in the analysis (Equation (4)) and synthesis (Equation (5)) formulations (see Appendix for derivation) are $\hat{A}^T\hat{A} = K^2, \hat{Z}^T\hat{Z} = KS^2K$ and $\tilde{A}^T\tilde{A} = K^2, \tilde{Z}^T\tilde{Z} = K^{-1}S^2K^{-1}$, respectively. Similarly, the orthogonality properties of the rotated modes in both formulations (Equations (6) and (7)) are $\hat{A}^{*T}\hat{A}^* = T^TK^2T, \hat{Z}^{*T}\hat{Z}^* = T^TKS^2KT$ and $\tilde{A}^{*T}\tilde{A}^* = T^TK^2T, \tilde{Z}^{*T}\tilde{Z}^* = T^TK^{-1}S^2K^{-1}T$, respectively.

The orthogonality properties of the unrotated and rotated modes for the normalized forms of the analysis and synthesis formulations and three cases of the normalization matrix K (i.e. $K = S$, $K = I$ and $K = S^{-1}$) are summarized in Table I. The cases $K = S$ and $K = I$ (columns 1 and 2) are the most common choices for K in meteorology and oceanography (e.g. Preisendorfer, 1988). The case $K = S^{-1}$ defines the PCA model, which weights the eigenvectors with the singular values—in the PCA model the space patterns represent covariances (correlations) between each variable and each empirical mode. Similarly, the case $K = I$ defines the EOF or unit length eigenvector model. Note that in this paper, the EOF and PCA models arise through particular choices of the normalizations as in Jolliffe (1987). The more unusual $K = S^{-1}$ case (column 3), in which all the time series for the normalized form of Equation (2) ($\hat{Z}$) have unit scatter (see row 2), is included for comparison with the results of Jolliffe (1995).

Rows 1–4 show that the normalization (Equations (4) and (5)) of the analysis and synthesis formulations (Equations (2) and (3)) do not alter the properties of the modes described in Section 2. Therefore, the normalized modes are orthogonal in space and uncorrelated in time.

Rows 5 and 6 summarize the orthogonality properties of the rotated modes for the analysis formulation given by Equation (2), and in normalized form by Equation (4), for the three choices of the normalization matrix. These results correspond to the three cases discussed by Jolliffe (1995). Column 1 shows that for $K = S$, which is the default option in some computer packages, neither spatial orthogonality nor temporal uncorrelatedness are preserved by an orthogonal rotation. Columns 2 and 3 show that K can be chosen so that an orthogonal rotation preserves orthogonality in space ($K = I$, column 3) or uncorrelatedness in time ($K = S^{-1}$, column 4), but not both simultaneously.

Table I. Orthogonality properties of unrotated and rotated empirical modes from the analysis and synthesis formulations for three different values of the normalization matrix K

	$K = S$ (PCA)	$K = I$ (EOF)	$K = S^{-1}$
$\hat{A}^T\hat{A}$	S^2	I	S^{-2}
$\hat{Z}^T\hat{Z}$	S^4	S^2	I
$\tilde{A}^T\tilde{A}$	S^2	I	S^{-2}
$\tilde{Z}^T\tilde{Z}$	I	S^2	S^4
$\hat{A}^{*T}\hat{A}^*$	T^TS^2T	I	$T^TS^{-2}T$
$\hat{Z}^{*T}\hat{Z}^*$	T^TS^4T	T^TS^2T	I
$\tilde{A}^{*T}\tilde{A}^*$	T^TS^2T	I	$T^TS^{-2}T$
$\tilde{Z}^{*T}\tilde{Z}^*$	I	T^TS^2T	T^TS^4T

The last two rows (7 and 8) show the orthogonality properties for the synthesis formulation given by Equation (3), and in normalized form by Equation (5), for the three choices of the normalization matrix. As noted in Sections 3 and 4, this convention is preferred because the data matrix can be reconstructed directly from the unrotated or rotated modes (Equations (5) and (7)). With this convention, the most common choices of the normalization matrix ($K = S$ and $K = I$) preserve at least one of the properties of the unrotated modes after an orthogonal rotation. The choice $K = S$ (PCA) preserves orthogonality in time, but not in space (column 1). The choice $K = I$ (EOF analysis), which is the most common in oceanography (e.g. Emery and Thomson, 1997), preserves orthogonality in space but not in time (column 2). Finally, the more unusual $K = S^{-1}$ case does not preserve either property (column 3).

6. EXAMPLE

In the following example, we compare rotated PC (RPC) and rotated EOF (REOF) analyses, focusing on the relaxation of the temporal orthogonality constraint of the unrotated modes. The dataset used is the global monthly reconstruction of 1856–1991 sea surface temperature (SST) anomalies generated by Kaplan *et al.* (1998) in a 5° × 5° grid. Enfield and Mestas-Nuñez (1999) used this dataset to estimate and remove a global El Niño–Southern Oscillation (ENSO) mode based on a complex EOF representation which allowed for phase propagation. The variability of the non-ENSO residual data, with scales shorter than 1.5 years and a linear trend removed at every grid point, was then studied using EOFs (Enfield and Mestas-Nuñez, 1999) and REOFs (Mestas-Nuñez and Enfield, 1999). Here we compare some of the Mestas-Nuñez and Enfield REOF results with the results of a RPC analysis applied to the same dataset.

We first calculated the empirical modes of the low-passed and detrended non-ENSO SST anomalies using the synthesis formulation of the PC model. This was done by decomposing the data as in Equation (5) using a SVD routine and a normalization matrix $K = S$. We then rotated the first ten normalized spatial eigenvectors using a varimax orthogonal rotation. The space patterns and the time series of the resulting RPCs will therefore satisfy Equation (7). The modal distribution of global (low-passed and detrended) non-ENSO SST anomaly variance explained by the RPCs is shown in the right column of Table II. For comparison, we also show the distribution of variance of the unrotated modes (left column) and of the REOFs (centre column), as shown in Table I of Mestas-Nuñez and Enfield (1999). Table II shows that the distributions of variance explained by the REOFs and RPCs, which is proportional to the eigenvalues or square singular values, are very similar.

We found that every RPC mode has a corresponding REOF mode in the Mestas-Nuñez and Enfield study, but their order (i.e. in terms of the global variance explained in Table II) is slightly different: RPC1 (see Figure 1) is the North Atlantic multidecadal mode (REOF1), RPC2 is the eastern North Pacific

Table II. Percentage of low-passed and detrended SST anomaly variance explained by the first ten unrotated and rotated non-ENSO modes

Mode	Unrotated	REOFs	RPCs
1	12.6	7.3	7.8
2	11.1	7.1	7.3
3	7.2	6.9	7.2
4	5.3	6.9	6.8
5	5.0	6.1	5.9
6	4.2	5.5	5.8
7	3.9	5.2	5.1
8	3.3	5.2	4.8
9	3.0	4.3	4.1
10	2.9	4.2	3.9
Total	58.6	58.6	58.6

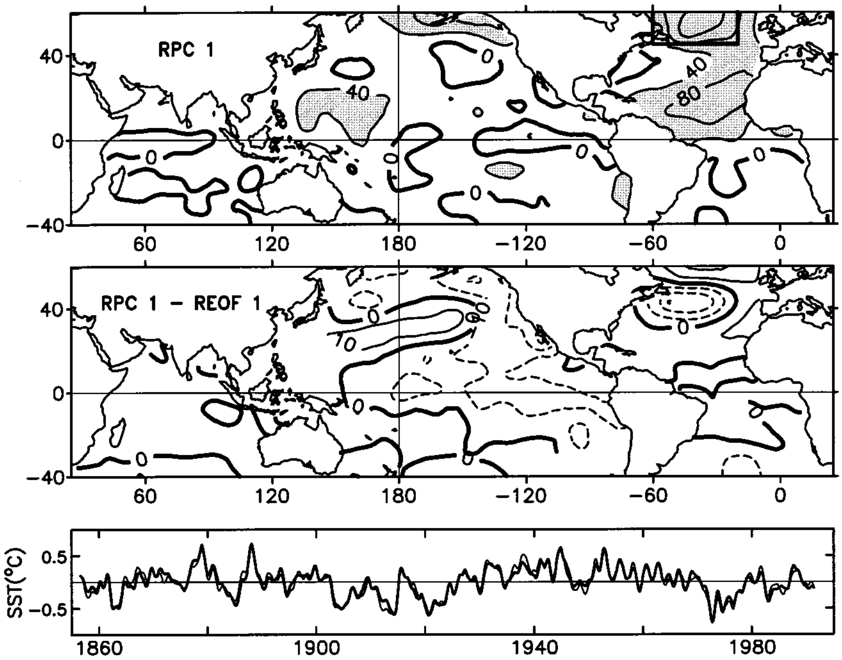

Figure 1. Comparison of the first mode of the rotated PC (RPC) and EOF (REOF) analyses of the non-ENSO residual data set, describing the North Atlantic multidecadal mode. Upper: Spatial distribution of the response with respect to the RPC modal reconstruction over the index region (rectangle): contour interval is 40, and a score of 100 is the average response over the index region. Regions with scores greater than 40 are shaded. Middle: Difference between the RPC1 space pattern (upper) minus the REOF1 space pattern (shown in Figure 1 of Mestas-Nuñez and Enfield, 1999); contour interval is 10 and negative contours are dashed. Lower: The thick (thin) line indicates the temporal reconstruction of the RPC1 (REOF1) mode related variability averaged over the index region

interdecadal mode (REOF2), RPC3 is the central tropical Pacific decadal mode (REOF4), RPC4 is the eastern tropical Pacific decadal mode (REOF3), RPC5 is the North Pacific multidecadal mode (REOF5), and RPC6 is the South Atlantic interannual mode (REOF6).

The spatial and temporal structures of REOF1 and RPC1, describing the North Atlantic multidecadal mode, are compared in Figure 1. The bottom panel shows that the temporal SST anomaly reconstructions in the index area (rectangular box) using RPC1 (thick) and REOFI (thin) are very similar—the correlation coefficient between the two time series is 0.96. The spatial structure of RPC1 (Figure 1, upper) is very similar to the space pattern of REOF1 of Mestas-Nuñez and Enfield (1999). The differences between the RPC and REOF space patterns (Figure 1, middle) are generally smaller than 30% of the average response in the index area. Similarly, we compared RPC and REOF modes 2–6 (not shown), and found very close agreement between their spatial and temporal structures.

Because the temporal orthogonality of the PCs is preserved by an orthogonal rotation, the cross-correlations between the RPC time series is zero. This suggests that the North Atlantic (RPC1) and South Atlantic (RPC6) modes, and the North Pacific (RPC5) and central tropical Pacific (RPC3) modes are temporally uncoupled. However, Table I shows that when the orthogonal rotation is applied to the EOFs (instead of the PCs) the temporal orthogonality is relaxed and the time series are no longer constrained to be uncorrelated. In fact, as shown in Table V of Mestas-Nuñez and Enfield (1999), the cross-correlation between the North and South Atlantic REOFs is 0.02, and between the North and central equatorial Pacific REOFs is -0.4. This led Mestas-Nuñez and Enfield (1999) to conclude that the North and South Atlantic modes of non-ENSO variability may, indeed, be independent (see also Enfield *et al.*, 1999), but the North Pacific and central tropical Pacific modes may not.

7. SUMMARY AND DISCUSSION

An apparent confusion found in the literature regarding the orthogonality properties of orthogonally rotated empirical modes is clarified. It is shown that the confusion arises from using two (equivalent) formulations of the modal decomposition defined by the analysis (Equation (2)) and synthesis (Equation (3)) equations. These two formulations lead to respective normalized forms of the analysis (Equation (4)) and synthesis (Equation (5)) equations. The normalized form of the analysis formulation (Equation (4)) consists of multiplying both the space patterns and time series by the normalization matrix K. The normalized form of the synthesis formulation (Equation (5)) consists of multiplying the space patterns by K, and the time series by K^{-1}. The synthesis formulation is preferred because it allows us to recover the data matrix by direct multiplication of the unrotated or rotated modes. Along with the two normalized forms of the modal decomposition, three possible choices of the normalization matrix K were considered. These choices of K include two commonly used cases in oceanography and meteorology ($K=S$ which defines the PCA model and $K=I$ which defines the EOF model) and one more unusual case considered by Jolliffe (1995) ($K=S^{-1}$).

Using the normalized form of the analysis formulation given by (Equation (4)) and the three choices of K, the spatial orthogonality and temporal uncorrelatedness properties of the rotated modes presented by Jolliffe (1995) were reproduced. Briefly, $K=S$ (PCA model, the default case in some computer packages) preserves neither property, $K=I$ (EOF model) preserves only spatial orthogonality, and $K=S^{-1}$ preserves only temporal uncorrelatedness. In contrast, using the normalized form of the synthesis formulation given by (Equation (5)) leads to different properties—except of course for $K=I$. Briefly, $K=S$ (PCA model) preserves only temporal uncorrelatedness and $K=S^{-1}$ preserves neither property.

As noted above, when an orthogonal rotation is applied to the synthesis formulation (Equation (5)) of the PCA model ($K=S$), the orthogonality is preserved in time, but relaxed in space. This choice is useful to avoid getting predictable space patterns for the second and higher modes when the leading space pattern is known. For example, when the leading space pattern has the same sign over all the domain—as is the case of ENSO in the tropics—one generally expects that the second space pattern will have a zero crossing near the maximum of the leading mode. Applications that used this approach to avoid getting predictable higher order patterns include Houghton and Tourre (1992) and Kawamura (1994). Other applications of this approach can be found in the study of atmospheric circulation patterns. These are based on the apparent property of atmospheric modes to be approximately uncorrelated in time, and not necessarily orthogonal in space (Horel, 1981; Barnston and Livezey, 1987).

When an orthogonal rotation is applied to the EOF or unit eigenvector model ($K=I$), independently of using the analysis or synthesis formulations, the spatial orthogonality is preserved but the temporal uncorrelatedness is not. This is useful when using the rotated modes to define regional temporal indexes because they are not constrained to be uncorrelated in time. This approach has the effect of not prejudicing conclusions regarding the possibility of temporal couplings between the rotated modes, especially those representing subregions of the same ocean basin. An application of the rotated EOF approach (Mestas-Nuñez and Enfield, 1999; see also Enfield *et al.*, 1999), and how it compares to a rotated PCA approach, was illustrated with an example using a global SST anomaly dataset (Section 6).

ACKNOWLEDGEMENTS

I am thankful to D. Enfield, C. Thacker, I. Jolliffe and an anonymous reviewer for helpful comments. This research has been carried out under the auspices of the Cooperative Institute for Marine and Atmospheric Studies (CIMAS), a joint institute of the University of Miami and the National Oceanic and Atmospheric Administration (NOAA), cooperative agreement #NA67RJO-149. This work has also been supported by a grant from the NOAA Pan-American Climate Studies program.

APPENDIX A. DERIVATION OF THE ORTHOGONALITY PROPERTIES

The orthogonality properties of the normalized modes given by Equations (4) and (5) are

$$\hat{A}^T\hat{A} = KA^TAK = K^2,$$

$$\hat{Z}^T\hat{Z} = KSU^TUSK = KS^2K$$

and

$$\tilde{A}^T\tilde{A} = \hat{A}^T\hat{A} = K^2,$$

$$\tilde{Z}^T\tilde{Z} = K^{-1}SU^TUSK^{-1} = K^{-1}S^2K^{-1},$$

respectively.

Similarly, the orthogonality properties of the rotated modes given by Equations (6) and (7) are

$$\hat{A}^{*T}\hat{A}^* = T^T\hat{A}^T\hat{A}T = T^TK^2T,$$

$$\hat{Z}^{*T}\hat{Z}^* = T^T\hat{Z}^T\hat{Z}T = T^TKS^2KT$$

and

$$\tilde{A}^{*T}\tilde{A}^* = T^T\tilde{A}^T\tilde{A}T = T^TK^2T,$$

$$\tilde{Z}^{*T}\tilde{Z}^* = T^T\tilde{Z}^T\tilde{Z}T = T^TK^{-1}S^2K^{-1}T,$$

respectively.

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