# 13 Analysis of Climate Variability: EOF/PCA Analysis

*Suggested textbooks*:

a) Statistical Methods in the Atmospheric Sciences. D. S. Wilks, Second Edition, International Geophysics Series, Academic Press, 2006

b) Statistical Analysis in Climate Research. H. von Storch and F. W. Zwiers, Cambridge University Press, 1999

c) Analysis of Climate Variability. H. von Storch, A. Navarra (Eds.), Springer, 1995.

d) Or simply look things up on Wikipedia...............

## 13.1 Motivation

The problem and necessity of the *analysis of climate variability* becomes clear if we consider the series of 500 hPa winter mean anomaly fields shown in Fig. 71. Lacking a precise theory of what we are seeing (apart from the fact that we know that what we see are solutions of the complex Navier-Stokes equations), how can we try to find some order in the *chaos* that we are confronted with? One way to tackle this problem is the *Empirical Orthogonal Function (EOF)* analysis (guess who introduced this in climate analysis?) or *Principle Component Analyisis (PCA)*.

## 13.2 What does the EOF analysis do?

The EOF analysis solves our problem (how, see below) by finding orthogonal functions (EOFs) to represent a time series of horizontal fields in the following way:

$$Z'(x,y,t) = \sum_{l=1}^{L} PC_l(t) EOF_l(x,y) \quad . \qquad (273)$$

$Z'(x,y,t)$ is the original (anomaly) time series as a function of time (t) and (horizontal) space (x,y), for example the fields that are displayed in Fig. 71. $EOF_l(y,x)$ show the spatial structures of the major factors that can account for the temporal variations of $Z'$. $PC_l(t)$ are the principal components that tell you how the amplitude of each EOF varies with time. In practice, time and space dimensions are discretized (as in the Numerical Methods Course!). Therefore, dealing with $Z'(x,y,t)$ and $EOF_l(y,x)$ means to deal with matrices.

## 13.3 Some useful specific definitions and notations

In the following, matrices will be denoted by capital boldface roman letters (**A**,**B**, **Y**, etc.). Vectors will be denoted by a lowercase boldface letters. Let's consider the data matrix:

$$\mathbf{Z} = \begin{bmatrix} z_{11} & z_{12} & \dots & z_{1k} \\ z_{21} & z_{22} & \dots & z_{2k} \\ \vdots & \vdots & & \vdots \\ z_{n1} & z_{n2} & \dots & z_{nk} \end{bmatrix} \tag{274}$$

In the following we assume that time and space are discretized and time is represented by the columns of this matrix, whereas space is represented by the rows (space (x,y) is just discretized a one vector, i.e. order $f(i,j)$ as one long vector $f(i,1), f(i,2), ..., f(i,M), i = 1,\ N,$ with $N \times M\ = k$). EOF analysis is based on anomalies, therefore anomaly data has to be defined. In order to define anomalies, a mean has to be defined. This is done in time, meaning a k-dimensional vector of means can be defined by averaging along the columns of the matrix of Eq. 274 (i.e. the time mean at every grid point). This mean has to be subtracted at every time and gridpoint in order to define the anomaly matrix. The mean subtracted is in general different at different gridpoints, but must be the same at a fixed gridpoint. An elegant way to write this is:

$$\mathbf{Z}' = \mathbf{Z} - \frac{1}{n}\mathbf{1}\ \mathbf{Z} \quad , \tag{275}$$

where $\mathbf{1}$ is a $n \times n$ matrix that contains 1 everywhere which is multiplied with $\mathbf{Z}$ (to confirm, simply try this procedure with a 2x2 matrix!).

With these notations Equation 273 may be re-written in (discretized) matrix notation as

$$\mathbf{Z}' = \sum_{l=1}^{k} \mathbf{pc_l}\ \mathbf{e_l}^T \quad , \tag{276}$$

where $\mathbf{pc_l}$ is a $nx1$ vector and $\mathbf{e_l}$ is a $kx1$ vector, therefore the transpose $\mathbf{e_l}^T$ is a $1xk$ vector. Note that the product of an arbitrary $nx1$ vector $\mathbf{a}$ and a $1xk$ vector $\mathbf{b}^T$ is results in

$$\mathbf{ab}^T \equiv \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} \begin{bmatrix} b_1, & b_2, & \dots, & b_k \end{bmatrix} \equiv \begin{bmatrix} a_1b_1 & a_1b_2 & \dots & a_1b_k \\ a_2b_1 & a_2b_2 & \dots & a_2b_k \\ \vdots & \vdots & & \vdots \\ a_nb_1 & a_nb_2 & \dots & a_nb_k \end{bmatrix} \tag{277}$$

If we demand the vectors $\mathbf{e_l}$ to be orthogonal unit vectors, such that $\mathbf{e}_i^T\mathbf{e}_j = 0$ for $j \neq j$, and $\mathbf{e}_l^T\mathbf{e}_l = 1$, then we have

$$\mathbf{Z}'\mathbf{e_m} = \sum_{l=1}^{k} \mathbf{pc_l}\ \mathbf{e_l}^T\mathbf{e_m} = \sum_{l=1}^{k} \mathbf{pc_l}\ \delta_{lm} = \mathbf{pc_m} \quad , \tag{278}$$

where $\delta_{lm} = 1$ if l=m and zero otherwise. We call $\mathbf{Z}'\mathbf{e_m}$ the *projection* (or in climate analysis sometimes called *regression*) of the data matrix onto the subspace defined by the EOF $\mathbf{e_m}$. Thus the principle components corresponding the $m$th EOF can simply be derived by projection of the data matrix $\mathbf{Z}'$ onto the $m$th EOF. The vector $\mathbf{pc}_m$ has therefore n components.

## 13.4 Minimum criterium leading to EOF definition

EOF analysis can be interpreted as a recursive process, we start to determine the first EOF ($\mathbf{e}_1$), then the second, and so on. The criterion to determine the first EOF is the minimization of the residual

$$\epsilon_1 = \parallel \mathbf{Z}' - \mathbf{Z}'\mathbf{e}_1\mathbf{e}_1^T \parallel^2 , \tag{279}$$

with respect to the $k$ dimensional vector $\mathbf{e}_1$ designing the first EOF in our notation. Here, if $\mathbf{Y}$ is any matrix,

$$\parallel \mathbf{Y} \parallel^2 = \frac{1}{(nk)}\mathbf{Y}^T : \mathbf{Y} \equiv \mathrm{tr}\left(\frac{1}{(nk)}\mathbf{Y}^T\mathbf{Y}\right) = \frac{1}{(nk)}\sum_{i=1}^{n}\sum_{j=1}^{k} y_{ij}^2 \quad . \tag{280}$$

This means first the matrix product of $\mathbf{Y}^T$ and $\mathbf{Y}$, then the trace of the resulting matrix by summing up the diagonal elements and this is the total variance of $\mathbf{Y}$. The normalization by $(nk)$ is arbitrary, but represents the *natural* definition of the total variance. In some cases you may find that the normalization is just done by $n$, meaning in time. The final results is however independent of this. The meaning of Eq. 279 is that we are searching for a $k$- dimensional subspace $\mathbf{e}_1$ to represent the data such that the residual (279) is minimal.

Note that $\mathbf{Z}'\mathbf{e}_1$ is a n-dimentional vector to be matrix multiplied by the k-dimentional vector $\mathbf{e}_1^T$ to give a kxn matrix according to Eq. 277. Also note that $\mathbf{Z}'\mathbf{e}_1$ is just the definition of the vector of (discretized) Principle Components corresponding to the first EOF in Eq. 276. Some further manipulation leads to:

$$\epsilon_1 = \parallel \mathbf{Z}' \parallel^2 - \parallel \mathbf{Z}'\mathbf{e}_1 \parallel^2 , \tag{281}$$

which means that minimizing $\epsilon_1$ according to Eq. 279 with respect to $\mathbf{e}_1$ is equivalent to maximizing the principle component projections

$$\epsilon_{proj} = \parallel \mathbf{Z}'\mathbf{e}_1 \parallel^2 \tag{282}$$

with respect to $\mathbf{e}_1$ (see, e.g. Wikipedia). This leads to the often used 2-dimensional example of the *geometrical* interpretation of EOFs shown in Fig. 73, where samples of 2-dimensional data vectors are considered and we search for the unit vector (EOF) that maximizes the variance of the projection of the data on this vector (straight line).

The minimization (a lot of matrix calculus) leads to the eigenvalue problem

$$\mathbf{S}\mathbf{e}_1 = \lambda\mathbf{e}_1 \quad , \tag{283}$$

where $\lambda$ is the largest eigenvalue and $\mathbf{S} = \frac{1}{nk}\mathbf{Z}'^T\mathbf{Z}'$ is the kxk variance-covariance matrix of the anomalies. Therefore the first EOF $\mathbf{e}_1$ becomes the eigenvector of the matrix $\mathbf{S}$ corresponding to the largest eigenvalue. The other EOFs are found by simply iteratively minimizing the reduced residual

$$\epsilon_2 = \parallel \mathbf{Z}' - \mathbf{Z}'\mathbf{e}_1\mathbf{e}_1^T - \mathbf{Z}'\mathbf{e}_2\mathbf{e}_2^T \parallel^2 \; ' \tag{284}$$

and

$$\epsilon_l = \parallel \mathbf{Z'} - \mathbf{Z'}\mathbf{e}_1\mathbf{e}_1^T - \mathbf{Z'}\mathbf{e}_2\mathbf{e}_2^T - ... - \mathbf{e}_l\mathbf{e}_l^T \parallel^2 , \tag{285}$$

and the results is that $\mathbf{e}_2$ is the eigenvector of $\mathbf{S}$ that corresponds to the second largest eigenvalue, and $\mathbf{e}_l$ is the eigenvector of $\mathbf{S}$ that corresponds to the $l$th largest eigenvalue. Since $\mathbf{S}$ has k eigenvectors we can continue this until l=k.

### 13.5 Some further properties

Note that also the principal components are orthogonal, that is $\mathbf{pc}_i \cdot \mathbf{pc}_j^T = 0$ for $j \neq j$. For practice purposes, we hope that a good approximation for the data matrix is given by

$$\mathbf{Z'} \approx \sum_{l=1}^{N} \mathbf{pc_l}\ \mathbf{e_l}^T \quad , \tag{286}$$

with $N \ll k$.

A further property is

$$\sum_{l=1}^{k} \lambda_l = \frac{1}{(nk)} \mathbf{Z'}^T : \mathbf{Z'} = \frac{1}{(nk)} \sum_{i=1}^{n} \sum_{j=1}^{k} z'^2_{ij} \quad , \tag{287}$$

which means that the sum of all eigenvalues gives the trace of the variance-covariance matrix $\mathbf{S}$ which is the total variance of $\mathbf{Z'}$ . To evaluate the importance of EOFs it is useful to consider the portion of variance explained by it:

$$\text{expl var of } \lambda_i = \frac{\lambda_i}{\sum_{l=1}^{k} \lambda_l} \tag{288}$$

A further property of eigenvalues of a matrix is of importance for the practical implementation of the EOF analysis, and is indeed used in the fortran program that you will use in the exercises of this section: If $\lambda$ is an eigenvalue of the variance-covariance matrix kxk $\mathbf{Z'}^T\mathbf{Z'}$ (we drop the scaling $1/(nk)$ for here because it is just a factor), then it is also an eigenvalue of the nxn matrix $\mathbf{Z'}\mathbf{Z'}^T$. In this case the variance-covariance matrix is defined as by the spatial variances and covariances. Thus if $n \ll k$, then we may prefer to find the eigenvalues of $\mathbf{Z'}\mathbf{Z'}^T$. If there are m independent eigenvectors $(\mathbf{e}_1, \mathbf{e}_2, ..., \mathbf{e}_s)$ of $\mathbf{Z'}^T\mathbf{Z'}$ the eigenvectors of $\mathbf{Z'}\mathbf{Z'}^T$ are $\mathbf{Z'}\mathbf{e}_1, \mathbf{Z'}\mathbf{e}_2, ..., \mathbf{Z'}\mathbf{e}_s$, which are the projections of the data matrix on the EOFs $\mathbf{e}_s$ which are therefore the (normalized) principal components of the original problem. This means that EOFs and principal components are exchangable. Instead of calculating the eigenvectors of $\mathbf{Z'}^T\mathbf{Z'}$, we may calculate the eigenvectors of $\mathbf{Z'}\mathbf{Z'}^T$, interpret the eigenvectors as the principal components and calculate the EOFs as projections of the transpose data matrix $\mathbf{Z'}^T$ onto the eigenvectors: $\mathbf{e_l} = \mathbf{Z'}^T\mathbf{pc_l}$. In this case the principal components are normalized (that is standard deviation = 1), whereas the EOFs are not. In the approximation 286 it does not matter if the principle component or the EOF is normalized, because they are multiplied with each other.

As stated above EOFs are found by determining the eigenvalues and eigenvectors of the variance-covariance matrix. Do you remember how to find these? You have to demand that the *determinant* of the variance-covariance matrix vanishes, this leads to an equation, the *characteristic equation* that contains kth-order polynomials and has at most k roots. There are standard techniques to find eigenvalues and eigenvectors, you may have learned some in your Numerical Methods course?

### 13.6 Geometric interpretation of PCs and EOFs

The geometric interpretation of the principle components mentioned before is as follows: The eigenvectors empirical orthogonal function (EOF) define a new coordinate system in which to view the data. This coordinate system is oriented such that each new axis is aligned along the direction of the maximum joint variability of the data, consistent with that axis being orthogonal to the preceding one.

The goal is to account for the variation in a sample in as few variables as possible. In the example here, the data is essentially 1-dimensional in the new coordinate system defined by the EOFs.

### 13.7 Interpretation of EOFs

As we have learned by now, EOFs may be useful to compress the information contained in complex data sets and to structure the data (according to the largest variances). As for the physical interpretation of EOFs, it is tempting to try to give physical explanations to the first few EOFs of a complex data set. Indeed, we expect that if the variability of our fields are governed by a strong low-dimensional physical mechanism (e.g. ENSO in the Pacific region), then one of the first EOFs will reflect this mechanism (indeed in case of EOFs of the interannual variability in the tropical Pacific, we find that the first EOF reflects the canonical ENSO pattern). Unfortunately, the opposite is not true: Not every first (or second or third, ...) is related to a simple and unique physical mechanism! Furthermore it is often even misleading to try to provide a physical mechanism for higher EOFs (e.g. EOF4, EOF5, etc.), because of the orthogonality of the EOFs. This constraint may make higher EOFs less 'physical' than the first or second EOF! The EOF analysis applied to the fields in Fig. 71 gives as first 2 EOFs the maps displayed in Fig. 74. Do you have ideas about possible 'physical' explanations of these EOFs? They are at least well know patterns, do you know their names?

### 13.8 Related Methods of Climate Analysis

The EOF analysis is probably the most basic of all analysis methods of climatic fields. For example a different question could arise considering 500 hPa geopotential height fields and sea surface temperature fields together. We may ask the question are the 500 hPa fields and the sea surface temperature (SST) fields we see related? This could be due to the fact that one is *forcing* the other. We may get some idea performing an EOF analysis on both fields separately and then try to connect the emerging EOFs by a physical interpretation (e.g. similar to what we will do in the exercise in this section). We could go one step further and compare (e.g. correlate) the principle components (pcs) of the first EOFs, etc. If we are lucky and the pcs are highly correlated, then there is likely some physical connection between the two first EOFs. However, it could also be that the first pc in geopotential height is a little correlated with the first pc in SSTs and also a little with the second, and so on. This means our interpretation of the connections between 500 hPa geopotential height and SST fields are not much easier after the EOF analysis. There are methods to address this question systematically. For example, the Canonical Correlation Analysis (CCA) or Maximum Covariance Analysis (MCA) provide tools to address the question stated above in a systematic way.

### Exercises

1. Using the fortran programme provided, calculate the (winter-mean: DJF) EOFs of a) surface temperature and b) 200 hPa geopotential height in the tropical Pacific. Display the covariance of the resulting principal components related to the first EOF with the global surface temperature and 200 hPa geopotential height fields and interpret the results. How much variance does the first EOF explain in each case? Are the first EOFs of surface temperature and 200 hPa geopotential height related? If yes, what could be the physical mechanism?

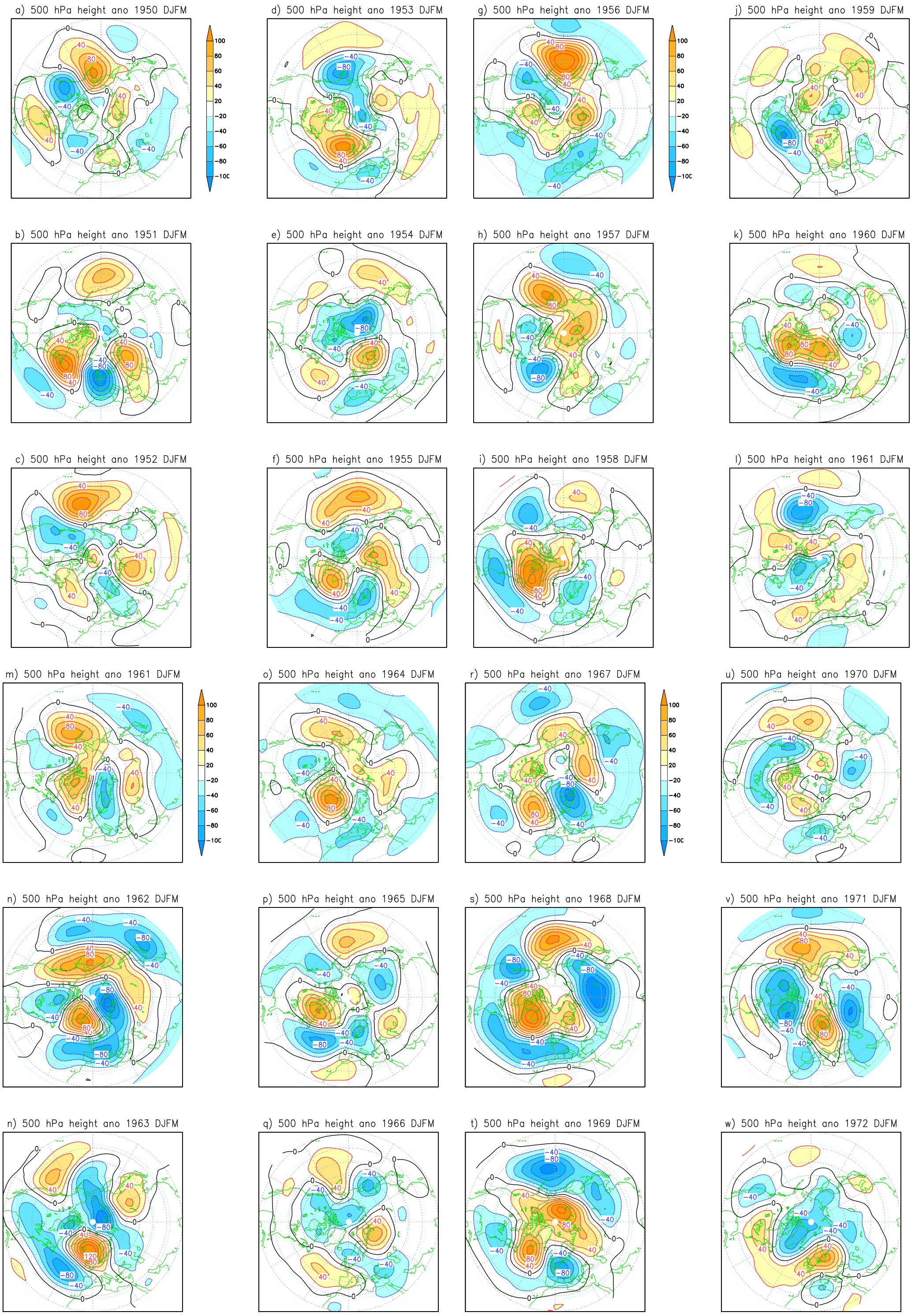


Figure 71: Anomalies of winter 500 hPa height fields for several years. Units are m.

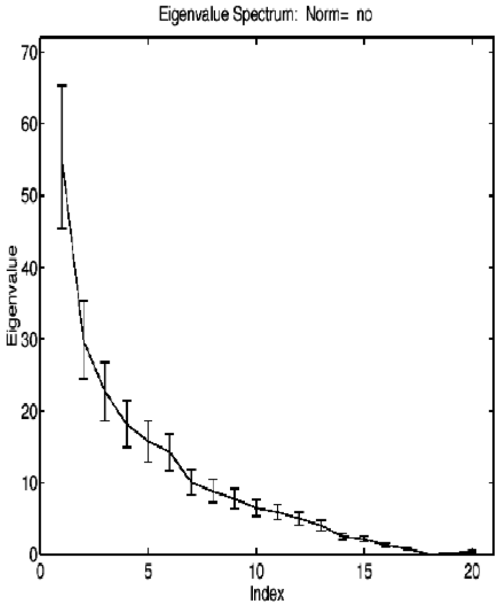


Figure 72: A typical example of the distribution of eigenvalues.

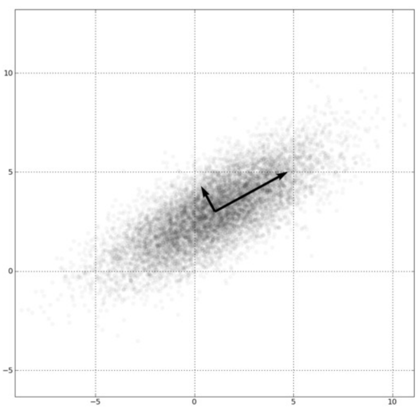

Figure 73: A sample of n observations in the 2-D space $x = (x_1, x_2)$.

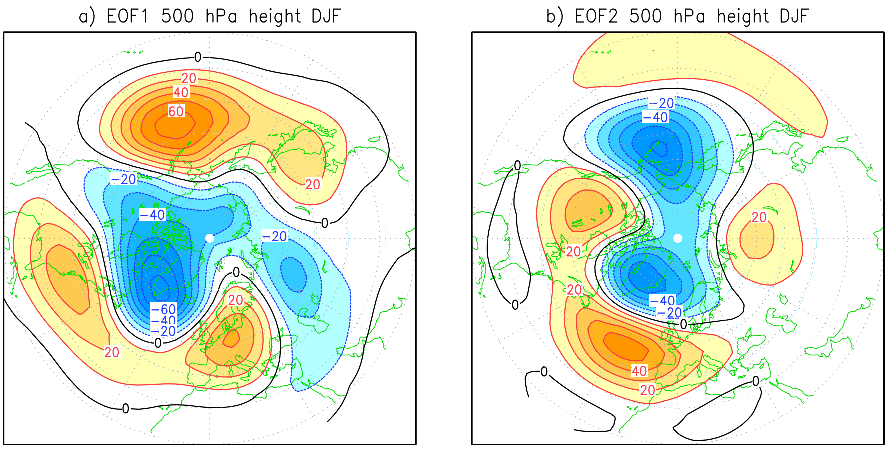


Figure 74: EOFs of the 500 hPa fields presented in Fig . 71