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Calculating EOFs and principal component time-series

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This is a note to clarify the most common conventions used in principal component analysis for atmospheric sciences, commonly called Empirical Orthogonal Function (EOF) analysis. It is a full recipe to determine EOFs and their corresponding time-series. I wrote it because regularly students would ask me why their own EOF program produced such strange numbers. Often the confusion is about the normalization that is commonly used. While working through all the relevant equations I will gloss over most of the mathematical background. There are plenty of textbooks on linear algebra and statistics if more clarification is required.

We start with a data matrix X where the data are a function of time and space. An element of X is denoted X_{ij} with i the index for the time dimension with n points and j the index for the space dimension with m points. See the end of this note for a few remarks on some properties of the data matrix.

The covariance matrix S is defined as:

$$\mathsf{S} = \frac{1}{n-1}\mathsf{X}^T\mathsf{X}, \tag{1}$$

so that each entry in the $m \times m$ matrix S contains the temporal covariance between the two corresponding spatial points. Eigenvectors of S satisfy:

$$\mathsf{S}\boldsymbol{\psi}^\alpha = \lambda_\alpha \boldsymbol{\psi}^\alpha, \tag{2}$$

where α is the index of the eigenvector $\boldsymbol{\psi}$ and eigenvalue λ. Because S is selfadjoint ($\mathsf{S}^T = \mathsf{S}$) the eigenvectors satisfy the orthogonality relationship:

$$(\lambda_\alpha - \lambda_\beta)\boldsymbol{\psi}^\alpha \cdot \boldsymbol{\psi}^\beta = 0 \tag{3}$$

We can normalize the eigenvectors $\boldsymbol{\psi}^\alpha$ any way we want. It is common to choose:

$$|\boldsymbol{\psi}^\alpha|^2 = \boldsymbol{\psi}^\alpha \cdot \boldsymbol{\psi}^\alpha = \lambda_\alpha. \tag{4}$$

Because the physical dimension of the eigenvalues is the square of the physical dimension of the data we find that the eigenvectors $\boldsymbol{\psi}^\alpha$ have the same dimension as the data. We call these eigenvectors the *Empirical Orthogonal Functions (EOFs)* or the *Principal Components*. For example, a set of gridded pressure data has pressure fields as EOFs. This normalization has other advantageous properties as well —see below.

We can write any spatial pattern $\boldsymbol{\psi}$ as a linear combination of these eigenvectors/EOFs. So this is also the case for every column in the data matrix. It follows that we can decompose the data matrix as:

$$X_{ij} = \sum_\alpha p_i^\alpha \psi_j^\alpha, \tag{5}$$

with p_i^α the coefficient of EOF number α in the linear combination at time i. The vector of coefficients $\boldsymbol{p}^\alpha$ is often called the *principal component time-series* of the EOF.

From the decomposition of the data matrix and the orthogonality of the EOFs we can see that:

$$\mathsf{X}\boldsymbol{\psi}^\beta = \sum_\alpha \boldsymbol{p}^\alpha \boldsymbol{\psi}^\alpha \cdot \boldsymbol{\psi}^\beta = \boldsymbol{p}^\beta |\boldsymbol{\psi}^\beta|^2. \tag{6}$$

We can next use the normalization of the EOFs Eq. 4 to find an equation for the principal component time-series as:

$$\lambda_\alpha \boldsymbol{p}^\alpha = \mathsf{X}\boldsymbol{\psi}^\alpha. \tag{7}$$

We can multiply this equation with $\mathsf{X}^T/(n-1)$ and use the eigenvector equation Eq. 2 to find:

$$\boldsymbol{\psi}^\alpha = \frac{1}{n-1}\mathsf{X}^T \boldsymbol{p}^\alpha. \tag{8}$$

These two equations are very useful as they relate the EOFs and their principal component time-series through a simple matrix multiplication.

By decomposing S in Eq. 2 in its constituent parts and multiplying the equation with X we find:

$$\frac{1}{n-1}\mathsf{X}\mathsf{X}^T\mathsf{X}\boldsymbol{\psi}^\alpha = \lambda_\alpha \mathsf{X}\boldsymbol{\psi}^\alpha. \tag{9}$$

Now substituting the expression for $\boldsymbol{p}^\alpha$ from Eq. 7 this equation can be rewritten as:

$$\mathsf{T}\boldsymbol{p}^\alpha = \lambda_\alpha \boldsymbol{p}^\alpha, \tag{10}$$

with:

$$\mathsf{T} = \frac{1}{n-1}\mathsf{X}\mathsf{X}^T. \tag{11}$$

So, like the EOFs, the principal component time-series also follow from an eigenvalue problem resulting in the same eigenvalues as those of the EOFs.

This allows us to gain efficiency in calculating EOFs. Matrix T has size $n \times n$ and matrix S has size $m \times m$. It then makes sense to solve the smallest eigenvalue problem Eq. 2 or 10, and then use Eq. 7 or 8, respectively, to find the corresponding principal component time-series or EOFs, respectively. I did quite a lot of data analysis on series of about 60 fields which contained about 6000 spatial points. With eigenvector routines approximately scaling as the third power of the size of the matrix, this little trick saved me a bit of time.

The temporal variance v of each principal component time-series can be determined starting from Eq. 7:

$$v^\alpha \equiv \frac{1}{n-1}|\boldsymbol{p}^\alpha|^2 = \frac{1}{n-1}\frac{1}{\lambda_\alpha^2}|\mathsf{X}\boldsymbol{\psi}^\alpha|^2 = \frac{1}{\lambda_\alpha^2}\boldsymbol{\psi}^\alpha \cdot \mathsf{S}\boldsymbol{\psi}^\alpha = 1. \tag{12}$$

So by setting the normalization Eq. 4 for the EOFs we find that the corresponding time-series has unit variance. In other words, the field amplitude in the EOFs (sometimes called *loading*) indicates the importance of that EOF to the total field.

In summary, there are two recipes to get the EOFs and corresponding principal component time-series.[1] The first recipe is through Eqns. 1, 2, 4, and 7 respecively. The second recipe is through Eqns. 11, 10, 12, and 8 respectively. Both recipes lead to the same results. The first recipe is most effective when there are more time than space points ($n > m$), the second recipe when there are more space than time points ($m > n$).

Example: suppose there are more space than time points. First use Eq. 11 to determine matrix T. Then calculate the eigenvactors $\boldsymbol{p}^\alpha$ and eigenvalues λ_α of this matrix, Eq. 10. Then multiply each eigenvector with a normalization factor to ensure that each eigenvector $\boldsymbol{p}^\alpha$ has unit variance, Eq. 12. These are then the principal component time-series. The EOFs can subsequently be determined by performing the matrix multiplication in Eq. 8 with the principal component time-series. Done. Note that the normalization Eq. 4 is implied by normalization Eq. 12, and vice-versa.

Finally I need to add some remarks on the data matrix X. Temporal covariances are found as a simple matrix multiplication, Eq. 1. This implies that for each spatial point the temporal average of the data is assumed to be zero. If this is not the case the

[1] There is in fact yet another way of doing the analysis. A singular value decomposition of the data matrix X will give the EOFs, principal comonent time series and the eigenvalues in one operation —albeit a rather complicated operation.

presented EOF analysis has not much meaning. So do ensure that this is the case for your data matrix.

When analyzing equal lat–lon fields on a sphere, as is often the case in meteorology, the data matrix needs to be scaled first with the factor $\sqrt{\cos\phi}$, with ϕ the latitude of the datapoint, so that areas contribute proportionally to the total variance in the field. The whole analysis is then performed on this scaled data matrix. The eigenvectors found from either Eqns. 2 or 8 (depending on which of the two recipes was chosen) then need to be scaled back with the inverse of this factor to find the EOFs.

There is some confusion in the literature on the use of this factor and its inverse and on the corresponding nomenclature. Some people insist that the scaled back version is not an EOF anymore —I do not know where this misunderstanding originated. Suffice to say that there is no relevance in looking at an analysis that does not include this scaling before and inverse scaling after the eigenvalue analysis. The paper by North et al. in Monthly Weather Review (1982, vol. 110, pp. 699–706) nicely clarifies this issue by demonstrating how the matrix algebra in this note is in fact a discrete version of an analysis of fields continuous in space and time where area weighting naturally arises as part of two-dimensional spatial integrals.

To clarify this point: where there is a spatial inner or matrix product in this note the equivalent continuous field version has a spatial integral over the sphere. In polar coordinates such an integral over the sphere will contain a $\cos\phi$ factor (from $\cos\phi\, d\lambda\, d\phi$). An easy way to implement this in the discrete analysis presented here is by rescaling all datapoints with $\sqrt{\cos\phi}$ so that wherever products of such fields occur a $\cos\phi$ is included. This rescaling is just a trick to make the algebra look a bit cleaner. We could as well have decided to omit this rescaling and make sure that wherever in the algebra above a spatial inner or matrix product occurs an integration factor is included; on the sphere this integration factor equals $\cos\phi$.