Empirical Orthogonal Functions (Principal Components):

Introductory Review

This is an effective multivariate analysis of dominant patterns of variability (Hotelling, 1935, Lorenz, 1956, van den Dool, class notes and forthcoming book, based on his classes in this course!!!). In meteorology, EOFs refer to the spatial patterns of variability, and "principal components" refer to their time varying amplitudes.

Suppose that we have a long series of gridded maps, where *s* represents the spatial index (in two dimensions, the grid points would be ordered into a single long vector of length *K*), and t represents the time index:

$$X(t,s) = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1K} \\ x_{21} & x_{22} & \cdots & x_{2K} \\ \cdots & \cdots & \cdots & \cdots \\ x_{N1} & x_{N2} & \cdots & x_{NK} \end{bmatrix}$$ gridded maps anomalies, with

$$s = 1,\dots,K, \quad t = 1,\dots,N$$

$$X(t,s) = X_{total}(t,s) - \overline{X(t,s)}^{t}$$ anomalies

The goal is to express the anomalies in terms of a small number of EOFs $e_m(s)$, which represent the spatial variability, with amplitudes (PCs) $u_m(t)$:

$$X(t,s) = \sum_{m=1}^{M} u_m(t) e_m(s)$$

To do this we compute the covariance matrix of *X*. The normal way to compute the covariance matrix is to do it in space:

$$S = \begin{pmatrix} s_{11} & s_{12} & \cdots & s_{1K} \\ s_{21} & s_{22} & \cdots & s_{2K} \\ \cdots & \cdots & s_{ij} & \cdots \\ s_{K1} & s_{K2} & \cdots & s_{KK} \end{pmatrix} = X(t,s)^T X(t,s)$$

S is the normal (space) covariance

where each element is computed as the product of the anomalies at two different space grid points, and we average in time:

$$s_{ij} = \frac{1}{N}\sum_{t=1}^{N} X(t,s_i)X(t,s_j)$$

S is a symmetric matrix, and therefore it has orthogonal eigenvectors $e_m(s)$ and has real, positive eigenvalues λ_m :

$$Se_m = \lambda_m e_m .$$

The eigenvectors (EOFs) are orthogonal, which means:

$$\sum_{s=1}^{K} e_m(s)e_n(s) = 0 \text{ if } m \neq n$$

and the principal components (time amplitudes) can be obtained by projecting the original field on each EOF:

$$u_m(t) = \sum_{s=1}^{K} X(t,s)e_m(s) .$$

The principal components $u_m(t)$ can also be obtained as eigenvectors of the alternative covariance in time (vanden Dool, 2007).

The alternative covariance $S^a(t_i,t_j) = X(t,s)X^T(t,s)$ is a covariance in time, and the average is done in space:

$$s^a_{i,j} = \frac{1}{K}\sum_{s=1}^{K} X(t_i,s)X(t_j,s)$$

Since $S^a(t_i,t_j)$ is also symmetric, the $u_m(t)$ are also orthogonal in time:

$\sum_{t=1}^{N} u_m(t)u_n(t) = 0$ if $m \neq n$. The fact that the PCs are orthogonal in time is a very important property of the *empirical* functions. If the space functions used as basis are orthogonal but defined analytically rather than empirically from the covariance matrix (for example, if we use spherical harmonics as basis), then their amplitudes are not orthogonal in time.

If the number of grid points is much smaller than the number of time levels (K<<N), it is better to use the regular covariance. If N<<K, it is less expensive to use the alternative covariance. In either case, one obtains M eigenvectors, where M is the smaller of N, K.

The total (space and time) variance of the data is given by

$$STV = \sum_{s=1}^{K}\sum_{t=1}^{N}\frac{X(t,s)^2}{KN}.$$

Replacing $X(t,s) = \sum_{m=1}^{M} u_m(t)e_m(s)$ into *STV* we obtain

$$STV = \sum_{m=1}^{M}\sum_{t=1}^{N}\frac{u_m^2(t)}{KN}$$

This shows that the space time variance corresponding to the mode *m*, is

$STV_m = \sum_{t=1}^{N} \frac{u_m^2(t)}{KN}$, and the "explained variance" corresponding to the mode *m*

is $\frac{STV_m}{STV}$, and is given by the ratio of the *m* space (or time) eigenvalue divided by the trace of the space (or time) covariance.

Minimalist example: two grid points, 3 time observations

$$X = \begin{matrix} t_1 \\ t_2 \\ t_3 \end{matrix} \begin{pmatrix} 1 & 1 \\ 0 & -1 \\ -1 & 0 \end{pmatrix}$$
$$\qquad\qquad s_1 \quad s_2$$

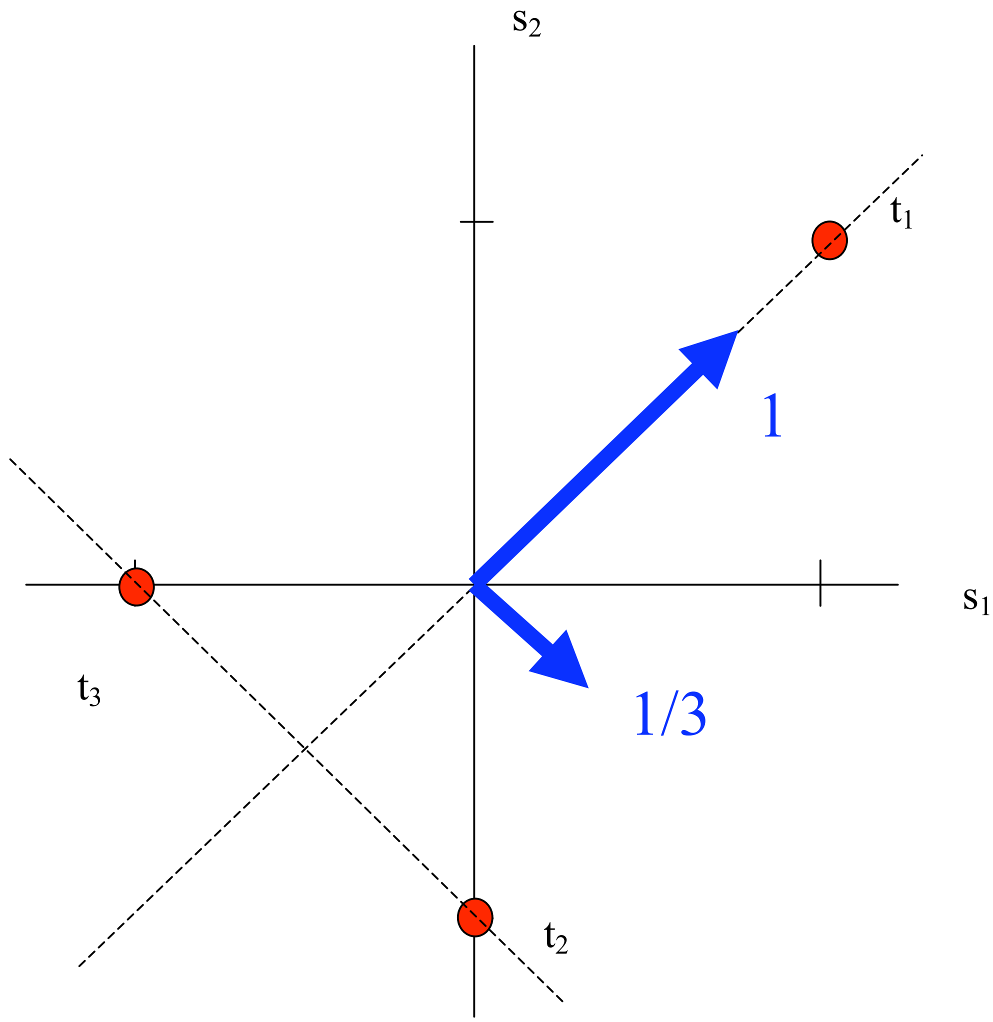
The three "maps" at t_1, t_2 and t_3 are represented by circles in the graph below.

The normal space covariance is $S = \frac{1}{N} X^T X = \begin{pmatrix} 2/3 & 1/3 \\ 1/3 & 2/3 \end{pmatrix}$.

The eigenvalues of *S* are $\lambda_1 = 1, \lambda_2 = 1/3$ with eigenvectors (EOFs)
$e_1 = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}, e_2 = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}$.

The total space variance is the trace of *S*, 4/3. Of this, the first eigenvalue is 3/3, or 75% of the variance, and the second (1/3) is 25% of the variance.

We can see how the eigenvectors represent the variability of the system on the plot (suggested by S. Greybush):



The dashed lines are the directions of covariability of the “maps” (in red) and the blue arrows the EOFs (with their size multiplied by the eigenvalue).

We can compute the PCs (time amplitudes) by projecting X on the EOFs:

$$u_m(t) = \sum_{s=1}^{K} X(t,s) e_m(s)$$

$$\begin{pmatrix} 1 & 1 \\ 0 & -1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \begin{matrix} s_1 \\ s_2 \end{matrix} = \begin{pmatrix} \sqrt{2} & 0 \\ -1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \begin{matrix} t_1 \\ t_2 \\ t_3 \end{matrix} \quad \text{or } XE = U$$

$$\begin{matrix} s_1 & s_2 & & m_1 & m_2 & & m_1 & m_2 \end{matrix}$$

With just the first (leading) mode we can represent most (75% of the variance) of X:

$$u_1(t)e_1^T = \begin{pmatrix} \sqrt{2} \\ -1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ -1/2 & -1/2 \\ -1/2 & -1/2 \end{pmatrix}$$

The second mode represents the rest (25% of the variance) of X:

$$u_2(t)e_2^T = \begin{pmatrix} 0 \\ 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1/2 & -1/2 \\ -1/2 & +1/2 \end{pmatrix}$$

If we compute the alternate (time) covariance we can obtain the $u_m(t)$ directly as its eigenvectors:

$$S^a(t_i, t_j) = XX^T = \begin{pmatrix} 1 & -1/2 & -1/2 \\ -1/2 & 1/2 & 0 \\ -1/2 & 0 & 1/2 \end{pmatrix}$$

S^a It has eigenvalues $\lambda_1^a = 3/2, \quad \lambda_1^a = 1/2, \quad \lambda_3^a = 0$. The total time variance is equal to the trace of the time covariance, 2, and the leading EOF represents 75%, as before. The number of eigenvalues different from zero is the minimum between K=2 and N=3. The eigenvectors of S^a are the PCs

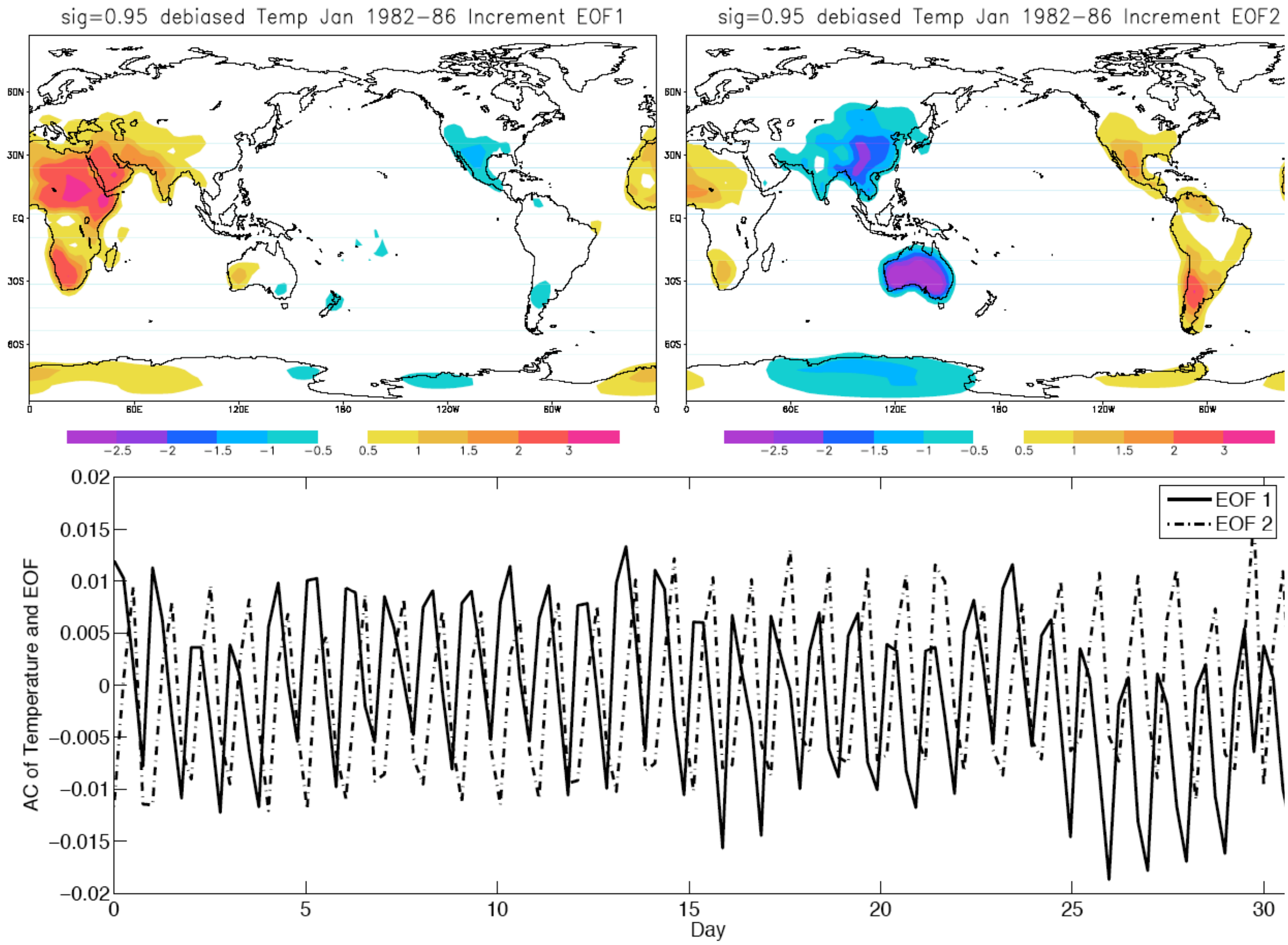
$u_m(t)$, and the EOFs $e_m(s)$ can be obtained by projecting $XU^T=E^T$. We choose the smaller of K and N to create the EOFs/PCs.

If the field is composed by more than one variable in space, such as sea level pressure and SST, it is customary to convert the covariance into a correlation matrix, by dividing by the products of the standard deviation, which gets rid of the units. The nondimensional correlation matrix can then be used to create EOFs and PCs.

Example from Danforth et al (2007)

Estimated the average SPEEDY model error (bias) by averaging over several years the 6 hour forecast (started from reanalysis) minus the reanalysis.

Then they computed the EOFs of the anomaly in the model error, and found two dominant EOFs representing the model error in representing the diurnal cycle:



The PC's are 6 hours apart (like cosines and sines with a period of 24hrs).