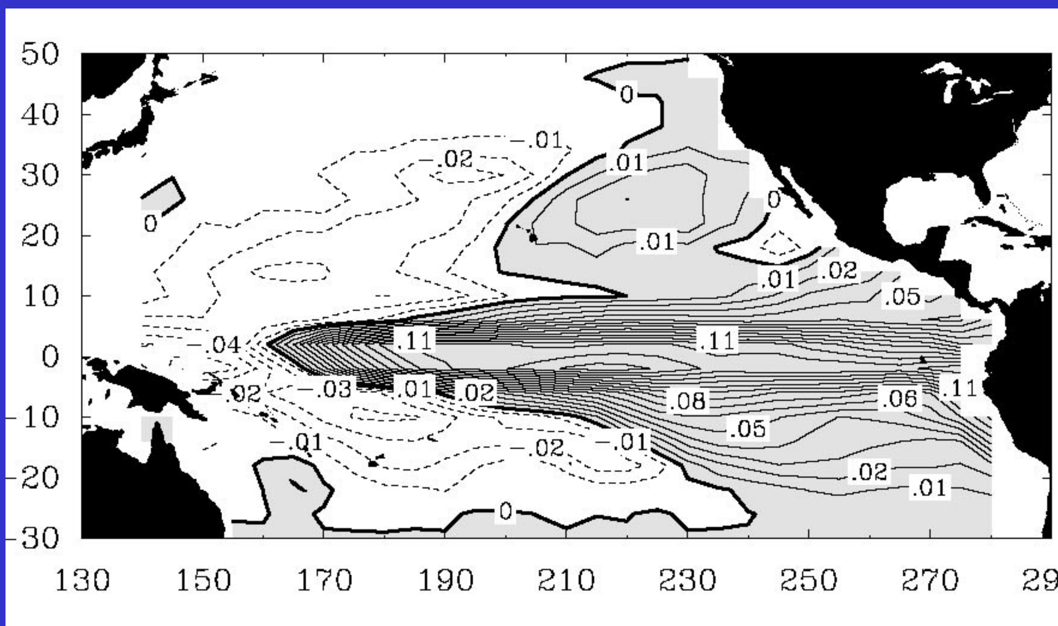
Part 4: Time Series II



- EOF Analysis
- Principal Component
- Rotated EOF
- Singular Value Decomposition (SVD)

Empirical Orthogonal Function Analysis

- Empirical Orthogonal Function (EOF) analysis attempts to find a relatively small number of independent variables (predictors; factors) which convey as much of the original information as possible without redundancy.
- EOF analysis can be used to explore the structure of the variability within a data set in a objective way, and to analyze relationships within a set of variables.
- EOF analysis is also called principal component analysis or factor analysis.

What Does EOF Analysis do?

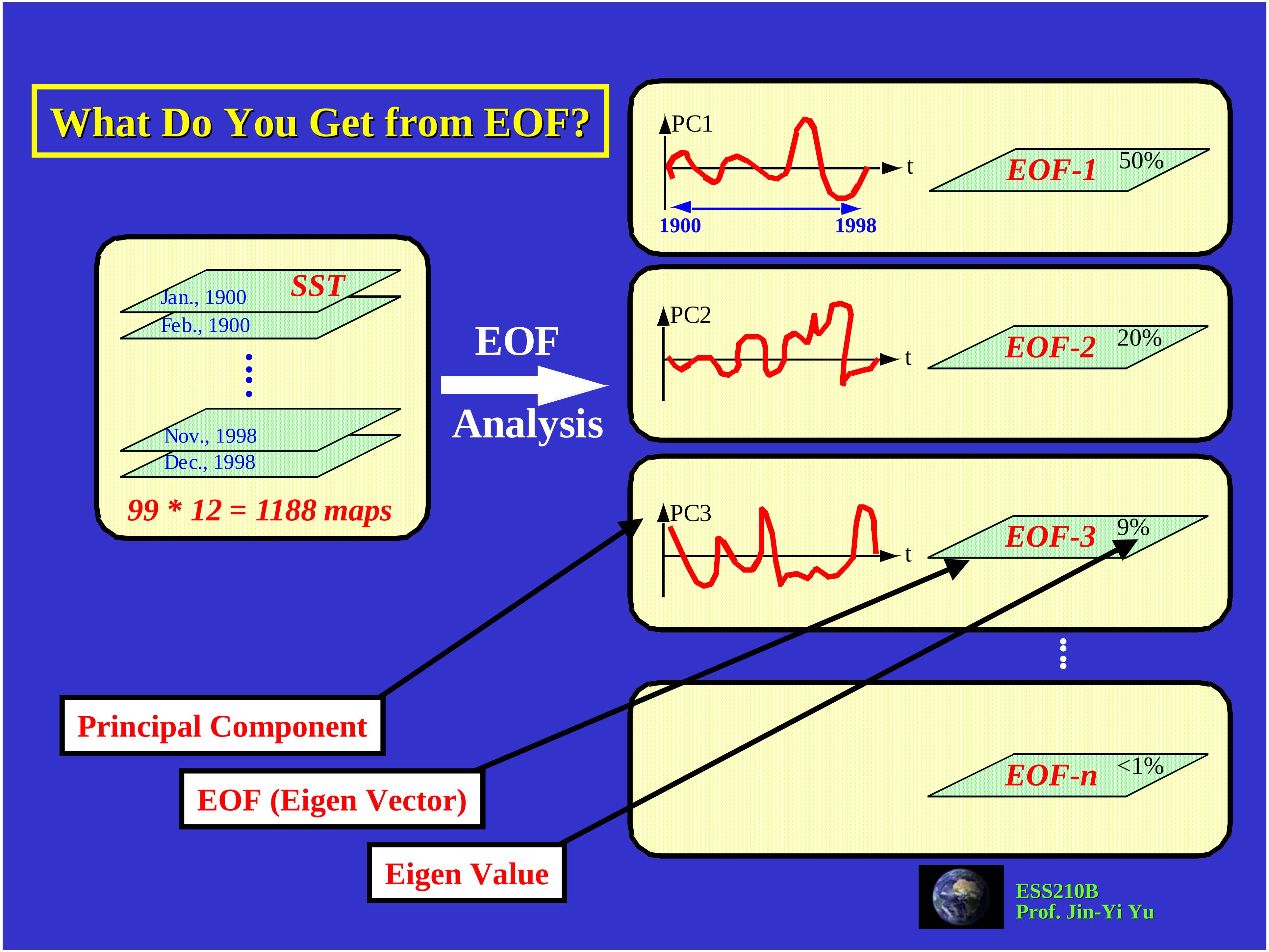
- In brief, EOF analysis uses a set of orthogonal functions (EOFs) to represent a time series in the following way:

$$Z(x, y, t) = \sum_{k=1}^{N} PC(t) \cdot EOF(x, y)$$

- Z(x,y,t) is the original time series as a function of time (t) and space (x, y).

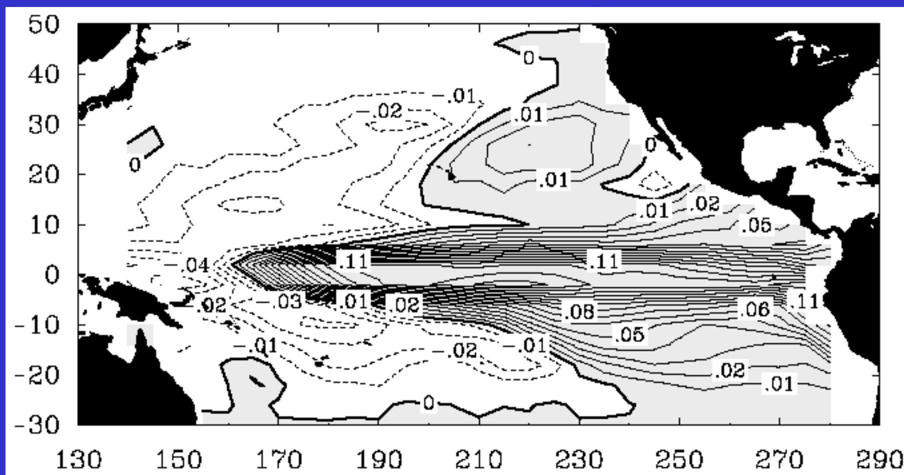
EOF(x, y) show the spatial structures (x, y) of the major factors that can account for the temporal variations of Z.

PC(t) is the principal component that tells you how the amplitude of each EOF varies with time.

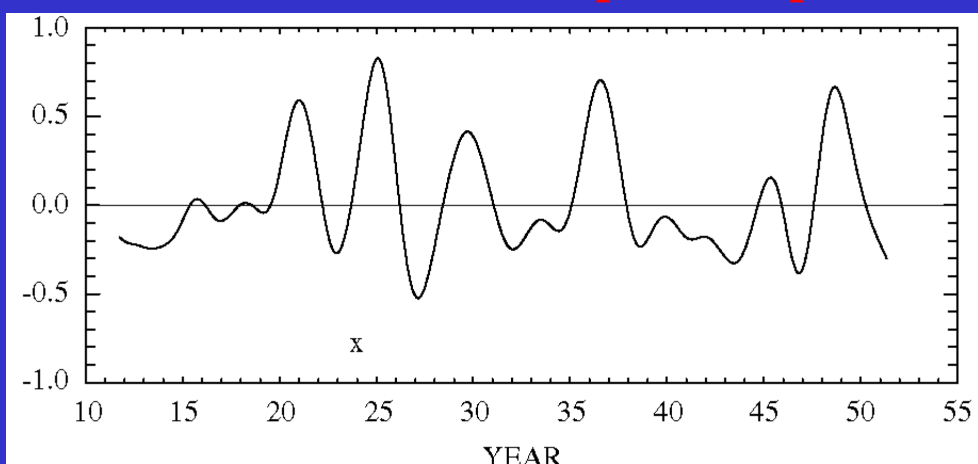

What Do You Get from EOF?
SST
Jan., 1900
Feb., 1900
Nov., 1998
Dec., 1998
99 * 12 = 1188 maps
EOF
Analysis
PC1
t
1900
1998
EOF-1
50%
PC2
t
EOF-2
20%
PC3
t
EOF-3
9%
EOF-n
<1%
Principal Component
EOF (Eigen Vector)
Eigen Value
ESS210B
Prof. Jin-Yi Yu

An Example

Leading EOF Mode

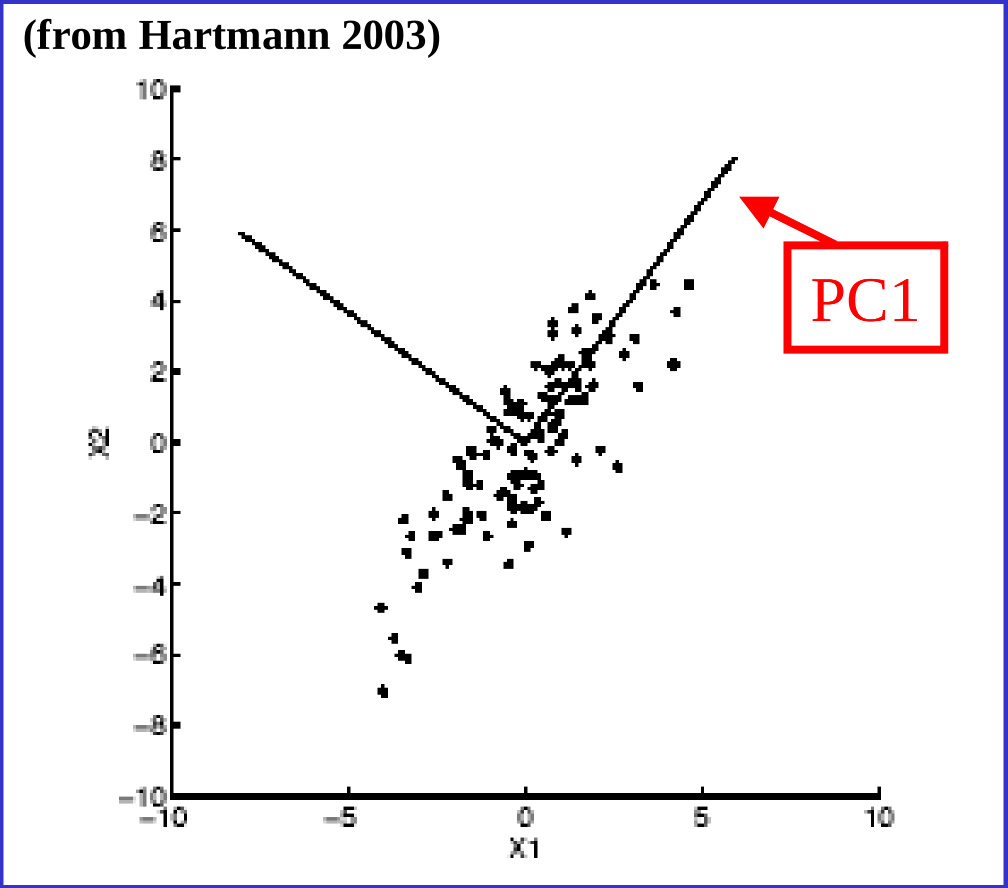


Principal Component



- We apply EOF analysis to a 50-year long time series of Pacific SST variation from a model simulation.
- The leading EOF mode shows a ENSO SST pattern. The EOF analysis tells us that ENSO is the dominant process that produce SST variations in this 50-year long model simulation.
- The principal component tells us which year has a El Nino or La Nina, and how strong they are.

Another View of the Rotation



ESS210B
Prof. Jin-Yi Yu

Rotation of Coordinates

- Suppose the Pacific SSTs are described by values at grid points: x_1, x_2, x_3, ...x_N. We know that the x_i's are probably correlated with each other.

- Now, we want to determine a new set of independent predictors $\boldsymbol{z_i}$ to describe the state of Pacific SST, which are linear combinations of $\boldsymbol{x_i}$:

$$z_1 = e_{11}x_1 + e_{12}x_2 + e_{13}x_3 + \ldots + e_{1M}x_M$$
$$z_2 = e_{21}x_1 + e_{22}x_2 + e_{23}x_3 + \ldots + e_{2M}x_M$$
$$.. \quad = \quad ..... \quad ..... \quad ..... \quad ... \quad .....$$
$$z_M = e_{M1}x_1 + e_{M2}x_2 + eM3x_3 + \ldots + e_{MM}x_M$$

- Mathematically, we are rotating the old set of variable (x) to a new set of variable (z) using a projection matrix (e):

$$Z_i = e_{i,j} \cdot X_j$$

PC

EOF

Determine the Projection Coefficients

- The EOF analysis asks that the projection coefficients are determined in such a way that:

  (1) z_1 explains the maximum possible amount of the variance of the x's;

  (2) z_2 explains the maximum possible amount of the remaining variance of the x's;

  (3) so forth for the remaining z's.

  the orthogonal requirement in time !

- With these requirements, it can be shown mathematically that the projection coefficient functions (e_{ij}) are the eigenvectors of the covariance matrix of x's.

- The fraction of the total variance explained by a particular eigenvector is equal to the ratio of that eigenvalue to the sum of all eigenvalues.

Eigenvectors of a Symmetric Matrix

- Any symmetric matrix **R** can be decomposed in the following way through a diagonalization, or eigenanalysis:

$$\mathbf{R}\mathbf{e}_i = \lambda_i \mathbf{e}_i$$

$$\mathbf{RE} = \mathbf{LE}$$

- Where **E** is the matrix with the eigenvectors e_i as its columns, and **L** is the matrix with the eigenvalues λ_i, along its diagonal and zeros elsewhere.

- The set of eigenvectors, $\boldsymbol{e}_i$, and associated eigenvalues, λ_i, represent a coordinate transformation into a coordinate space where the matrix **R** becomes diagonal.

Covariance Matrix

- The EOF analysis has to start from calculating the covariance matrix.
- For our case, the state of the Pacific SST is described by values at model grid points X_i.
- Let's assume the observational network in the Pacific has 10 grids in latitudinal direction and 20 grids in longitudinal direction, then there are 10x20=200 grid points to describe the state of pacific SST. So we have 200 state variables:

$$X_m(t),\ m = 1, 2, 3, 4, \ldots, 200$$

- In our case, there are monthly observations of SSTs over these 200 grid points from 1900 to 1998. So we have N (12*99=1188) observations at each Xm:

$$X_{mn} = X_m(t_n),\ m=1, 2, 3, 4, \ldots, 200$$
$$n=1, 2, 3, 4, \ldots, 1188$$

Covariance Matrix – cont.

- The covariance between two state variables X_i and X_j is:

$$\overline{X_i X_j} = \frac{1}{N}\sum_{j=1}^{N}(X_i - \overline{X_i})(X_j - \overline{X_j})$$

Here $N = 1188$

- The covariance matrix is as following:

$$\begin{vmatrix} X_{11} & X_{12} & X_{13} & \bullet\bullet\bullet\bullet\bullet & X_{1,M-1} & X_{1M} \\ X_{21} & X_{22} & X_{23} & \bullet\bullet\bullet\bullet\bullet & X_{2,M-1} & X_{2,M} \\ X_{31} & X_{32} & X_{33} & \bullet\bullet\bullet\bullet\bullet & X_{3,M-1} & X_{3,M} \\ & & & & & \\ X_{M-1,1} & X_{M-1,2} & X_{M-1,3} & \bullet\bullet\bullet\bullet\bullet & X_{M-1,M-1} & X_{M-1,M} \\ X_{M,1} & X_{M,2} & X_{M,3} & \bullet\bullet\bullet\bullet\bullet & X_{M,M-1} & X_{M,M} \end{vmatrix}$$

Here $M = 200$

Eigenvectors of a Symmetric Matrix

- Any symmetric matrix **R** can be decomposed in the following way through a diagonalization, or eigenanalysis:

$$\mathbf{R}\mathbf{e}_i = \lambda_i \mathbf{e}_i$$

$$\mathbf{R}\mathbf{E} = \mathbf{L}\mathbf{E}$$

- Where **E** is the matrix with the eigenvectors e_i as its columns, and **L** is the matrix with the eigenvalues λ_i, along its diagonal and zeros elsewhere.

- The set of eigenvectors, $\boldsymbol{e}_i$, and associated eigenvalues, λ_i, represent a coordinate transformation into a coordinate space where the matrix **R** becomes diagonal.

Orthogonal Constrains

- There are orthogonal constrains been build in in the EOF analysis:

(1) The principal components (PCs) are orthogonal in time.

There are no simultaneous temporal correlation between any two principal components.

(2) The EOFs are orthogonal in space.

There are no spatial correlation between any two EOFs.

- The second orthogonal constrain is removed in the rotated EOF analysis.

Mathematic Background

- I don’t want to go through the mathematical details of EOF analysis. Only some basic concepts are described in the following few slids.

- Through mathematic derivations, we can show that the empirical orthogonal functions (EOFs) of a time series Z(x, y, t) are the eigenvectors of the covarinace matrix of the time series.

- The eigenvalues of the covariance matrix tells you the fraction of variance explained by each individual EOF.

Some Basic Matrix Operations

- A two-dimensional data matrix ***X***:

$$\mathbf{X} = M\overset{N}{\begin{bmatrix} \quad & \quad \end{bmatrix}} = X_{i,j} \; where \; i = 1, M; \; j = 1, N$$

- The transpose of this matrix is $\boldsymbol{X^T}$:

$$\mathbf{X}^T = N\overset{M}{\begin{bmatrix} \quad \\ \quad \end{bmatrix}} = X_{j,i} \; where \; i = 1, M; \; j = 1, N$$

- The inner product of these two matrices:

$$\mathbf{X}\mathbf{X}^T = M\overset{N}{\begin{bmatrix} \quad & \quad \end{bmatrix}}\overset{M}{\begin{bmatrix} \quad \\ \quad \end{bmatrix}}N = \overset{M}{\begin{bmatrix} \quad \end{bmatrix}}M$$

How to Get Principal Components?

- If we want to get the principal component, we project a single eigenvector onto the data and get an amplitude of this eigenvector at each time, $\boldsymbol{e^T X}$**:**

$$
\begin{bmatrix} e_{11} & e_{21} & e_{31} & \dots & e_{M1} \end{bmatrix}
\begin{bmatrix}
x_{11} & x_{12} & x_{13} & \dots & x_{1N} \\
x_{21} & x_{22} & x_{23} & \dots & x_{2N} \\
x_{31} & x_{32} & x_{33} & \dots & x_{3N} \\
\dots & \dots & \dots & \dots & \dots \\
x_{M1} & x_{M2} & x_{M3} & \dots & x_{MN}
\end{bmatrix}
= \begin{bmatrix} z_{11} & z_{12} & z_{13} & \dots & z_{1N} \end{bmatrix}
$$

- For example, the amplitude of EOF-1 at the first measurement time is calculated as the following:

$$
z_{11} = e_{11}x_{11} + e_{21}x_{21} + e_{31}x_{31} + \dots + e_{M1}x_{M1}
$$

Using SVD to Get EOF&PC

- We can use Singular Value Decomposition (SVD) to get EOFs, eigenvalues, and PC's directly from the data matrix, without the need to calculate the covariance matrix from the data first.

- If the data set is relatively small, this may be easier than computing the covariance matrices and doing the eigenanalysis of them.

- If the sample size is large, it may be computationally more efficient to use the eigenvalue method.

What is SVD?

- Any m by n matrix A can be factored into

$$\mathbf{A} = \mathbf{U}\,\Sigma\,\mathbf{V}^T$$

original time series ($\mathbf{A}$) — **EOFs** ($\mathbf{U}$) — **normalized PCs** ($\mathbf{V}^T$)

- The columns of **U** (m by m) are the EOFs
- The columns of **V** (n by n) are the PCs.
- The diagonal values of Σ are the eigenvalues represent the amplitudes of the EOFs, ***but not the variance explained by the EOF***.
- The square of the eigenvalue from the SVD is equal to the eigenvalue from the eigen analysis of the covariance matrix.

An Example – with SVD method

```
>> clear
>> a=[2 4 -6 8; 1 2 -3 4]
a =
     2     4    -6     8
     1     2    -3     4
```

Do SVD of that data matrix to find its component parts.

```
>> [u, s, v]=svd(a)
```

First U, which contains the spatial singular vectors as columns.

```
u =
    0.8944   -0.4472
    0.4472    0.8944
```

Then the singular value matrix, which only contains one value. This means the data matrix is singular and one structure function and one temporal function can explain all of the data, so only the first column of the spatial eigenvector matrix is significant. The singular value contains all of the amplitude information. The spatial and temporal singular vectors are both of unit length.

```
s =
   12.2474         0         0         0
         0         0         0         0
```

Finally, the temporal structure matrix. Only the first column is meaningful in this context and it gives the normalized temporal variation of the amplitude of first spatial structure function.

```
v =
    0.1826   -0.1195   -0.9759         0
    0.3651   -0.2390    0.0976   -0.8944
   -0.5477   -0.8367    0.0000    0.0000
    0.7303   -0.4781    0.1952    0.4472
```

We can reconstruct the data matrix by first multiplying the singular value matrix times the transpose of the temporal variation matrix.

```
>> sv=s*v'
sv =
    2.2361    4.4721   -6.7082    8.9443
         0         0         0         0
```

Only the first row of this matrix has nonzero values, because the amplitude of the second structure function is zero. The second spatial structure is the left null space of the data matrix. If you multiply it on the left of the data matrix, it returns zero. The first row of sv is the principal component vector, including the dimensional amplitude. Finally we can recover the data matrix by multiplying the spatial eigenvector matrix times the previous product of the singular value and the temporal structure matrices. This is equivalent to multiplying the eigenvector matrix times the PC matrix, and gives us the original data back.

```
>> A=u*sv
A =
    2.0000    4.0000   -6.0000    8.0000
    1.0000    2.0000   -3.0000    4.0000
```

(from Hartmann 2003)

An Example – With Eigenanalysis

First, enter the data matrix a, as before.

```
>> clear
>> a=[2 4 -6 8; 1 2 -3 4]
a =
     2     4    -6     8
     1     2    -3     4
```

Now compute the covariance matrix AA^T. We won't even bother to remove the mean.

```
>> c=a*a'
c=
   120    60
    60    30
```

Next do the eigenanalysis of the square covariance matrix c.

```
>> [v,d]=eig(c)
v =
   -0.8944    0.4472
   -0.4472   -0.8944
d=
   150     0
     0     0
```

(from Hartmann 2003)

v contains the eigenvectors as columns. We get the same normalized eigenvector in the first column as before, except that its sign is reversed. The sign is arbitrary in linear analysis, so let's just leave it reversed. The one eigenvalue (d) is 150, the total variance of the data set. It's all explained by one function.

We can get the PCs by projecting the eigenvectors on the original data. The result will be exactly as we got in the SVD method, except for that pesky change of sign. Take the transpose of the eigenvector matrix and multiply it on the left into the original data.

```
>> p=v'*a
p =
   -2.2361   -4.4721    6.7082   -8.9443
         0         0         0         0
```

Finally recover the original data again by multiplying the eigenvector matrix(v) times the PC matrix(p).

```
>> A=v*p
A =
    2.0000    4.0000   -6.0000    8.0000
    1.0000    2.0000   -3.0000    4.0000
```

Correlation Matrix

- Sometime, we use the correlation matrix, in stead of the covariance matrix, for EOF analysis.
- For the same time series, the EOFs obtained from the covariance matrix will be different from the EOFs obtained from the correlation matrix.
- The decision to choose the covariance matrix or the correlation matrix depends on how we wish the variance at each grid points (X_i) are weighted.
- In the case of the covariance matrix formulation, the elements of the state vector with larger variances will be weighted more heavily.
- With the correlation matrix, all elements receive the same weight and only the structure and not the amplitude will influence the principal components.

Correlation Matrix – cont.

- The correlation matrix should be used for the following two cases:

(1)The state vector is a combination of things with different units.

(2) The variance of the state vector varies from point to point so much that this distorts the patterns in the data.

Presentations of EOF – Variance Map

- There are several ways to present EOFs. The simplest way is to plot the values of EOF itself. This presentation can not tell you how much the real amplitude this EOF represents.
- One way to represent EOF's amplitude is to take the time series of principal components for an EOF, normalize this time series to unit variance, and then regress it against the original data set.
- This map has the shape of the EOF, but the amplitude actually corresponds to the amplitude in the real data with which this structure is associated.
- If we have other variables, we can regress them all on the PC of one EOF and show the structure of several variables with the correct amplitude relationship, for example, SST and surface vector wind fields can both be regressed on PCs of SST.

Presentations of EOF – Correlation Map

- Another way to present EOF is to correlate the principal component of an EOF with the original time series at each data point.

- This way, present the EOF structure in a correlation map.

- In this way, the correlation map tells you what are the co-varying part of the variable (for example, SST) in the spatial domain.

- In this presentation, the EOF has no unit and is non-dimensional.

How Many EOFs Should We Retain?

- There are no definite ways to decide this. Basically, we look at the eigenvalue spectrum and decide:

(1) The 95% significance errors in the estimation of the eigenvalues is:

$$\Delta\lambda = \lambda\sqrt{2 / N^*}$$

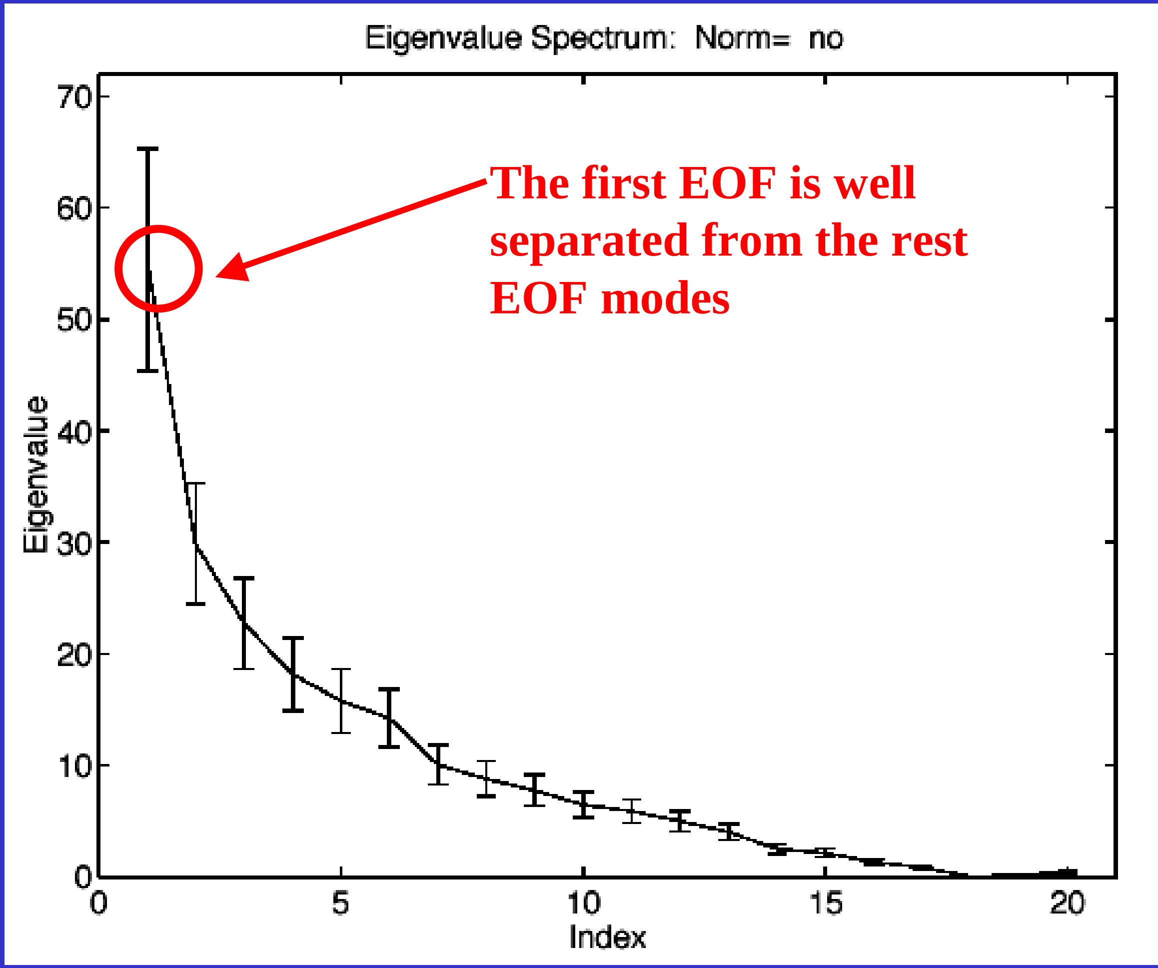
effective numbers of degree of freedom

If the eigenvalues of adjacent EOF's are closer together than this standard error, then it is unlikely that their particular structures are significant.

(2) Or we can just look at the slope of the eigenvalue spectrum.

We would look for a place in the eigenvalue spectrum where it levels off so that successive eigenvalues are indistinguishable. We would not consider any eigenvectors beyond this point as being special.

An Example



(from Hartmann 2003)

Rotated EOF

- The orthogonal constrain on EOFs sometime cause the spatial structures of EOFS to have significant amplitudes all over the spatial domain.
  - ➔ We can not get localized EOF structures.
  - ➔ Therefore, we want to relax the spatial orthogonal constrain on EOFs (but still keep the temporal orthogonal constrain).
  - ➔ We apply the Rotated EOF analysis.

- To perform the rotated EOF analysis, we still have to do the regular EOF first.
  - ➔ We then only keep a few EOF modes for the rotation.
  - ➔ We “rotated” these selected few EOFs to form new EOFs (factors). based on some criteria.
  - ➔ These criteria determine how “simple” the new factors are.

Criteria for the Rotation

- Basically, the criteria of rotating EOFs is to measure the "simplicity" of the EOF structure.

- Basically, simplicity of structure is supposed to occur when most of the elements of the eigenvector are either of order one (absolute value) or zero, but not in between.

- There are two popular rotation criteria:

(1) Quartimax Rotation

(2) Varimax Rotation

Quartimax and Varimax Rotation

- Quartimax Rotation

  It seeks to rotate the original EOF matrix into a new EOF matrix for which the variance of squared elements of the eigenvectors is a maximum.

$$s_{b^2}^2 = \frac{1}{mM} \sum_{j=1}^{M} \sum_{p=1}^{m} \left(b_{jp}^2 - \overline{b^2} \right)^2$$

b_{jp}: the jth loading coefficient of the pth EOF mode

- Varimax Rotation (more popular than the Quartimax rotation)

  It seeks to simplify the individual EOF factors.

$$s_p^2 = \frac{1}{M} \sum_{j=1}^{M} \left\{ b_{jp}^2 \right\}^2 - \frac{1}{M^2} \left\{ \sum_{j=1}^{M} b_{jp}^2 \right\}^2 \quad , p = 1, 2, \ldots, m$$

The criterion of simplicity of the complete factor matrix is defined as the maximization of the sum of the simplicities of the individual factors.

Reference For the Following Examples

- The following few examples are from a recent paper published on Journal of Climate:

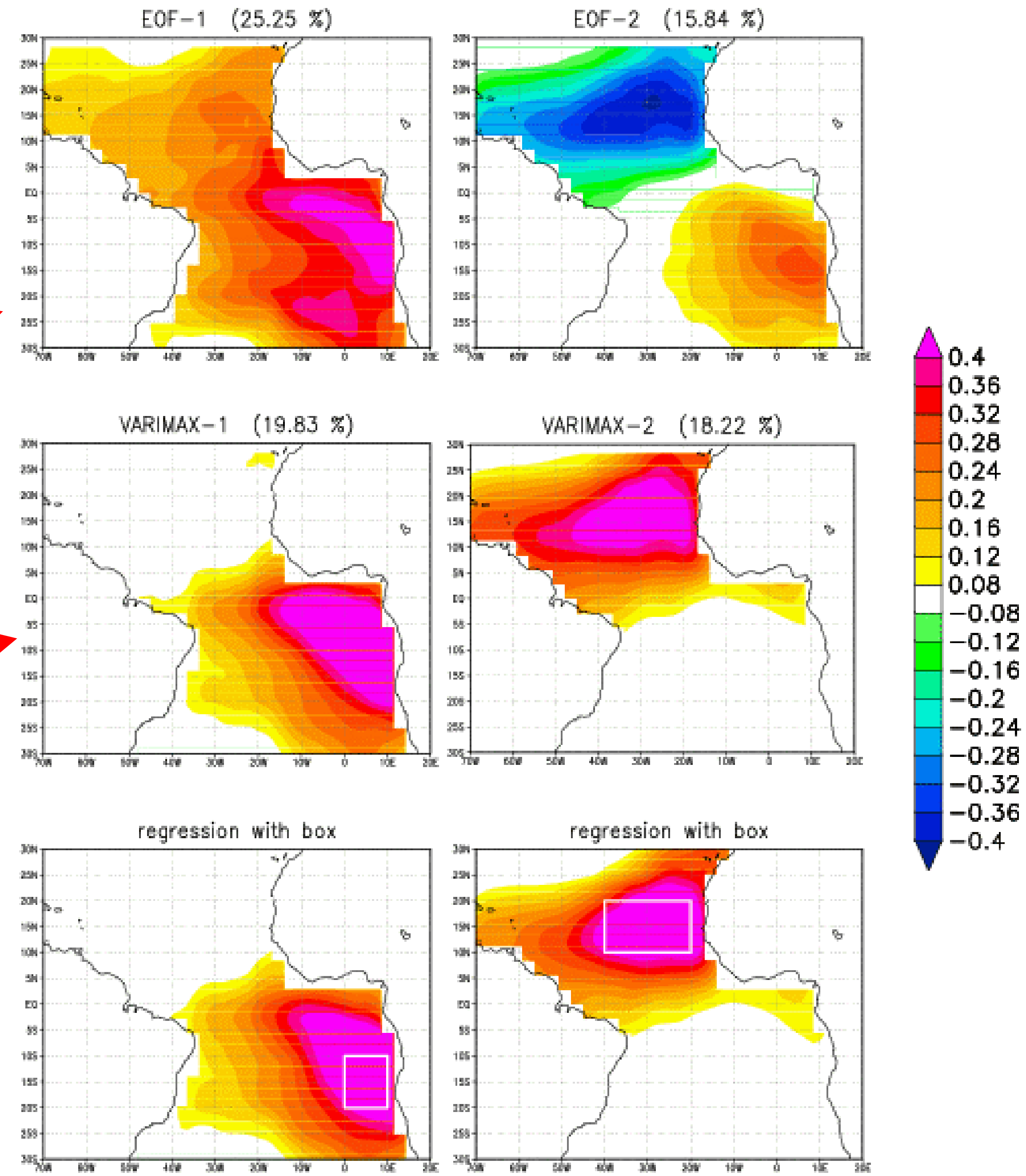
Dommenget, D. and M. Latif (2002): A Cautionary Note on the Interpretation of EOF. *J. Climate*, Vol. 15, No.2, pages 216-225.

Example 1: Atlantic SST Variability

EOF

Rotated EOF

Linear Regression



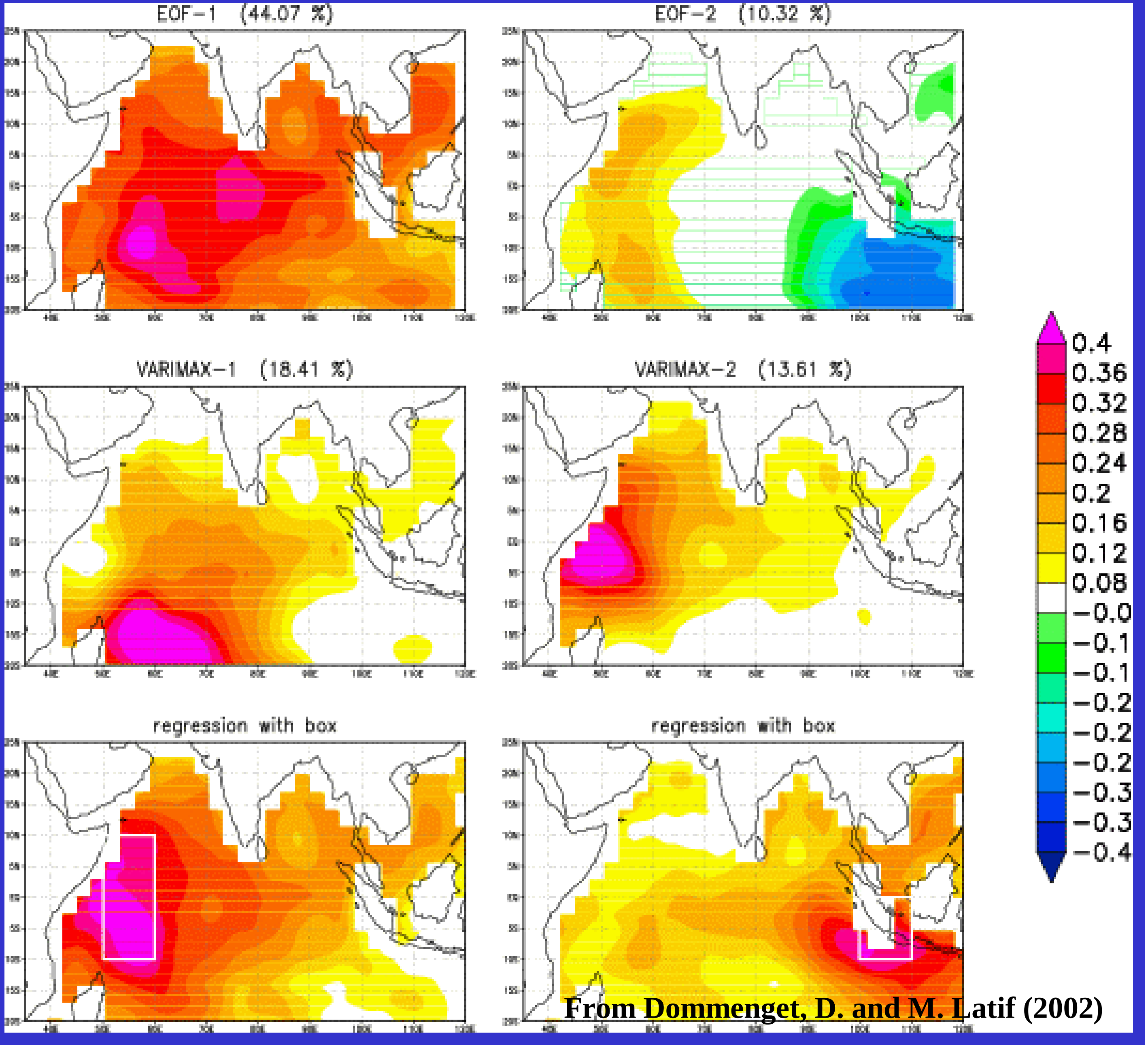
From Dommenget, D. and M. Latif (2002)

Example 2: Indian Ocean SST Variability

EOF

Rotated EOF

Linear Regression



From Dommenget, D. and M. Latif (2002)

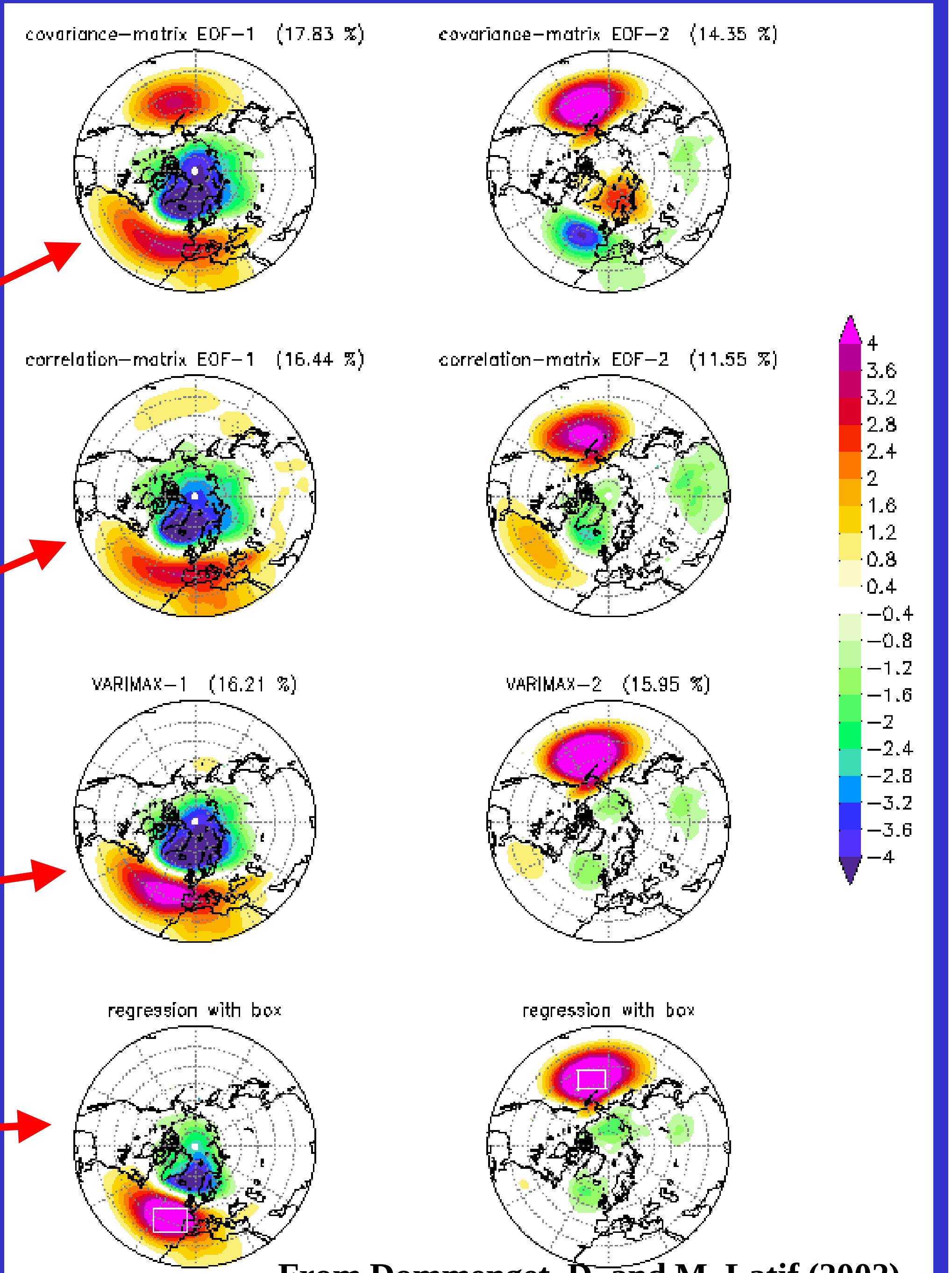
Example 3: SLP Variability (Arctic Oscillation)

Covariance-Based EOF

Correlation-Based EOF

Rotated EOF

Linear Regression



From Dommenget, D. and M. Latif (2002)

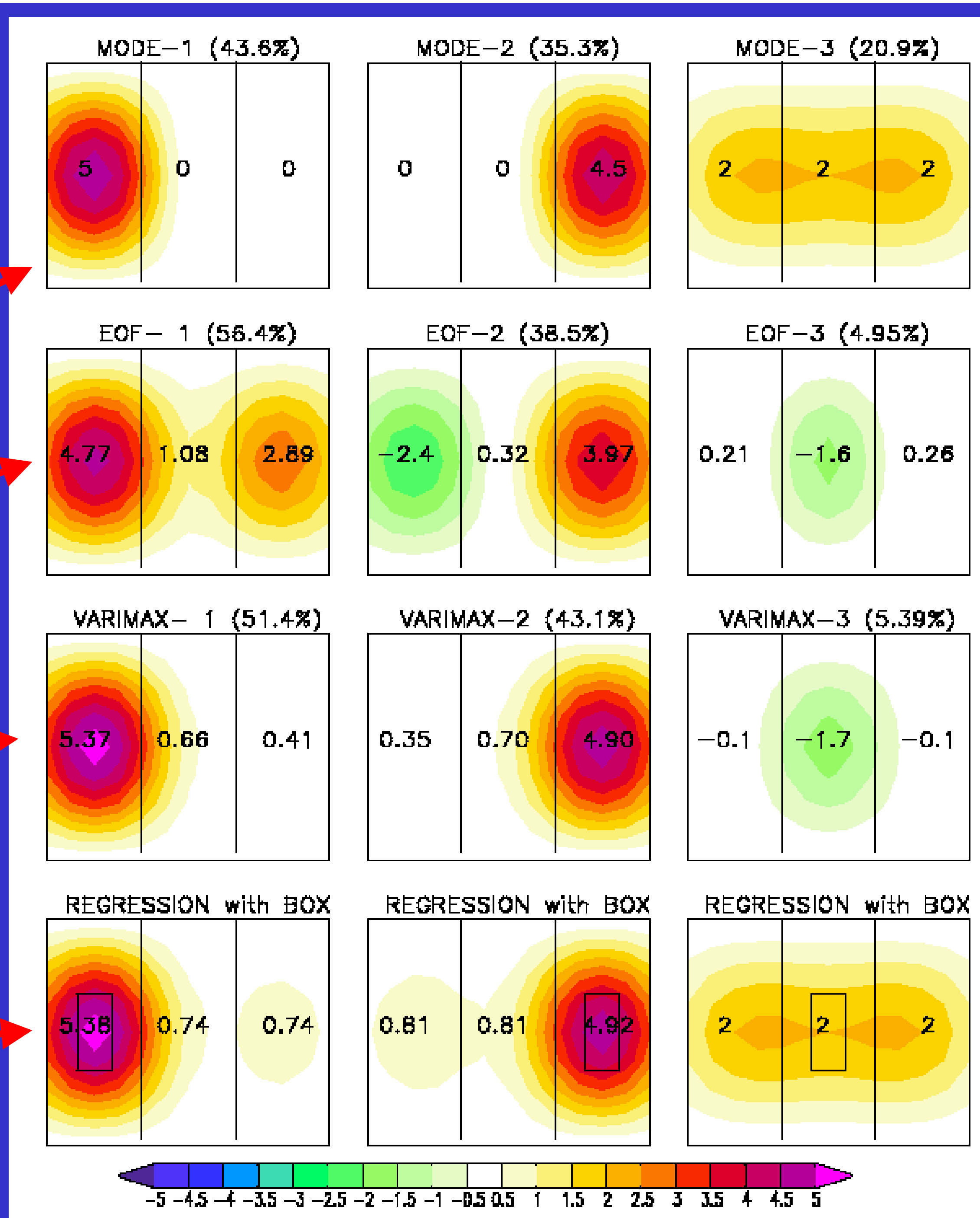
Example 4: Low-Dimensional Variability (Variance Based)

Physical Modes

EOF

Rotated EOF

Linear Regression



From Dommenget, D. and M. Latif (2002)

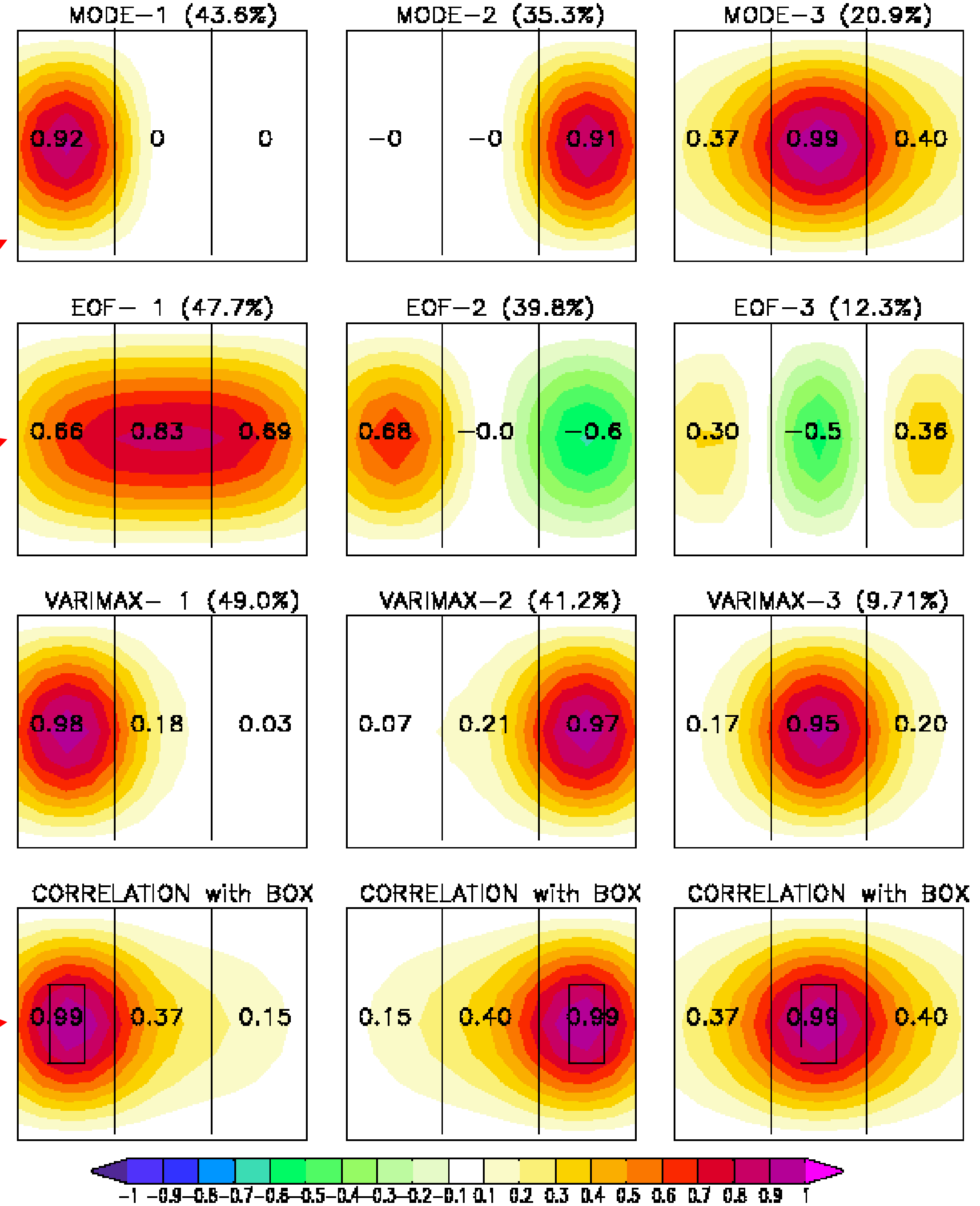
Example 5: Low-Dimensional Variability (Correlation Based)

Physical Modes

EOF

Rotated EOF

Linear Regression



From Dommenget, D. and M. Latif (2002)

Correlated Structures between Two Variables

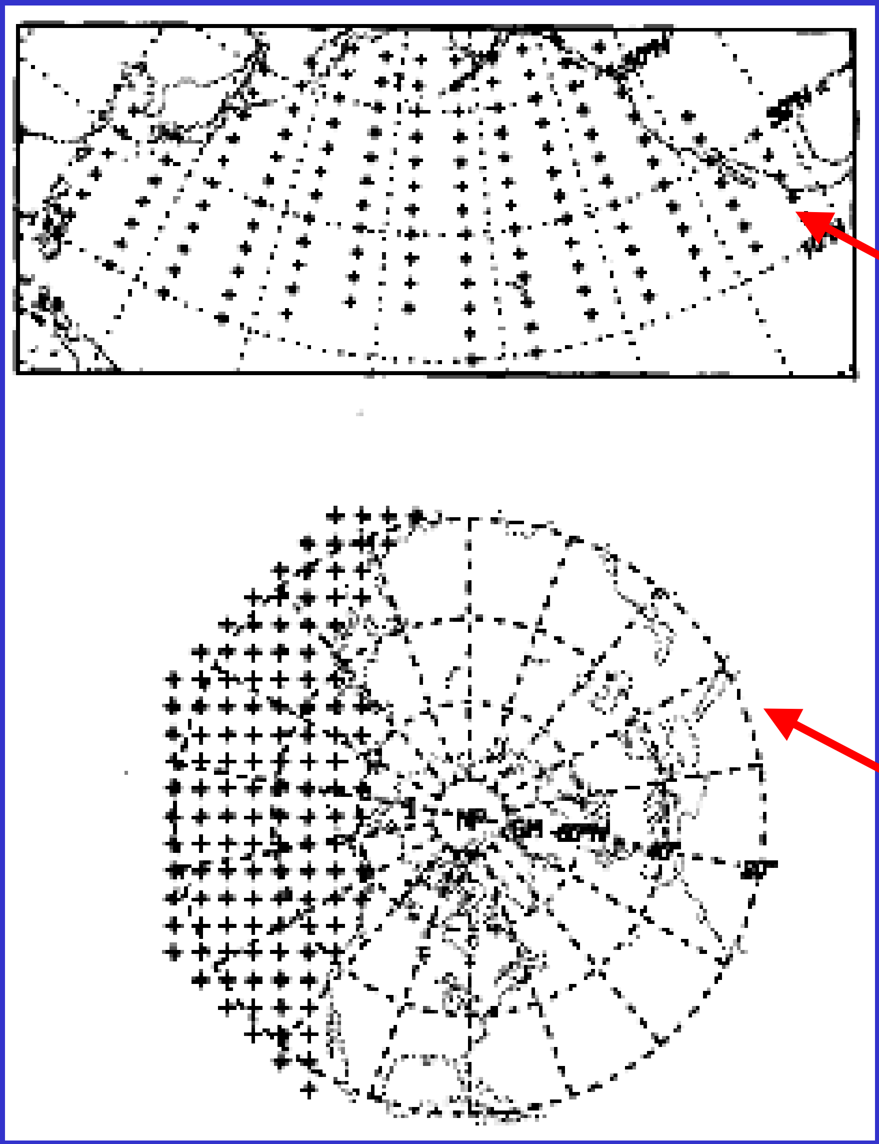
- SVD analysis is also used to reveal the correlated spatial structures between two different variables or fields, such as the interaction structures between the atmosphere and oceans.
- We begin by constructing the covariance matrix between data matrices **X** and **Y** of size ***MxN*** and ***LxN***, where ***M*** and ***L*** are the structure dimensions and N is the shared sampling dimension.
- Their covariance matrix is:

$$\frac{1}{N}\mathbf{X}\mathbf{Y}^T = \mathbf{C}_{XY}$$

or in matrix form:

$$\underset{M \times N}{M\begin{bmatrix} & X & \end{bmatrix}} \underset{N \times L}{\begin{bmatrix} Y^T \end{bmatrix}} N = \underset{M \times L}{\begin{bmatrix} C_{XY} & \end{bmatrix}} M$$

An Example – SVD (SST, SLP)



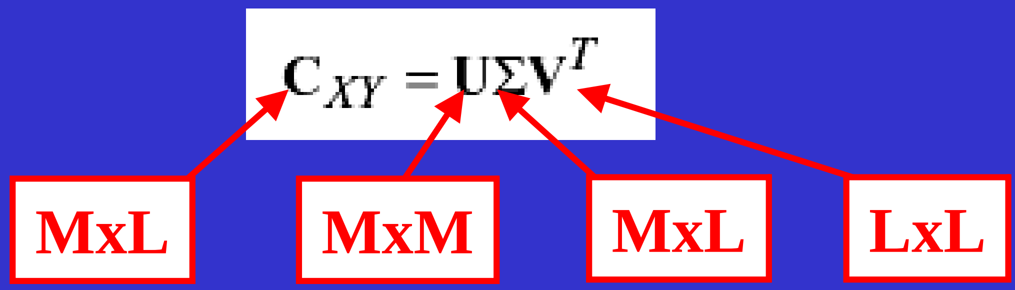
Sea Surface Temperature (SST)

Sea Level Pressure (SLP)

SVD Analysis of Covariance Matrix

- We then apply the SVD analysis to the covariance matrix and obtain:

$$C_{XY} = U\Sigma V^T$$



- ***U:*** The columns of **U** (MxM) are the column space of $\mathbf{C}_{XY}$ and represent the structures in the covariance field of **X**.

  V: The columns of **V** are the row space of $\mathbf{C}_{XY}$ and are those structures in the **Y** space that explain the covariance matrix.

  Σ: The singular values are down the diagonal of the matrix Σ. The sum of the squares of the singular values is equal to the sum of the squared covariances between the original elements of **X** and **Y**.

What Do *U* and *V* mean?

- The column space (in U) will be structures in the dimension M that are orthogonal and have a partner in the row space of dimension L (in V).

- Together these pairs of vectors efficiently and orthogonally represent the structure of the covariance matrix.

- The hypothesis is that these pairs of functions represent scientifically meaningful structures that explain the covariance between the two data sets.

- The 1st EOF in U and the 1st EOF in V together explain the most of the covariance (correlation) between two variables X and Y.

Principal Components

- The principal components corresponding to the EOFs in ***U*** and ***V*** can be obtained by projecting the EOFs (singular vectors) onto the original data:

$$\mathbf{X}^* = \mathbf{U}^T\mathbf{X} \quad ; \quad \mathbf{Y}^* = \mathbf{V}^T\mathbf{Y}$$

- The covariance between each pair (kth) of the principal component should be equal to their corresponding singular value.

$$\sigma_k = \overline{x_k^* y_k^*}$$

Presentation of SVD Vectors

- Similar to the EOS analysis, the singular vectors are normalized and non-dimensional, whereas the expansion coefficients have the dimensions of the original data.

- To include amplitude information in the singular vectors, we can regress (ore correlate) the principal components of U or V with the original data for this purpose.

- (1) For example, normalize the principal component of U.

  (2) Regress this normalized principal component with the original data set Y to produce a "heterogeneous regression map". This map shows the amplitude of covariance between X and Y.

  (3) Regress this normalized principal component with the original data set X to produce a "homogeneous map". This map tells us the spatial structure of X that is most correlated with Y.

Heterogeneous and Homogeneous Maps

- Heterogeneous regression maps: regress (or correlate) the expansion coefficient time series of the left field with the input data for the right field, or do the same with the expansion coefficient time series for the right field and the input data for the left field.

$$\mathbf{u}_k = \frac{1}{N\sigma_k}\mathbf{X}\mathbf{y}_k^{*T} \quad or \quad u_{jk} = \frac{1}{N\sigma_k}\sum_{i=1}^{N} x_{ji} y_{ik}^{*} = \frac{1}{\sigma_k}\overline{x_j y_k^{*}}$$

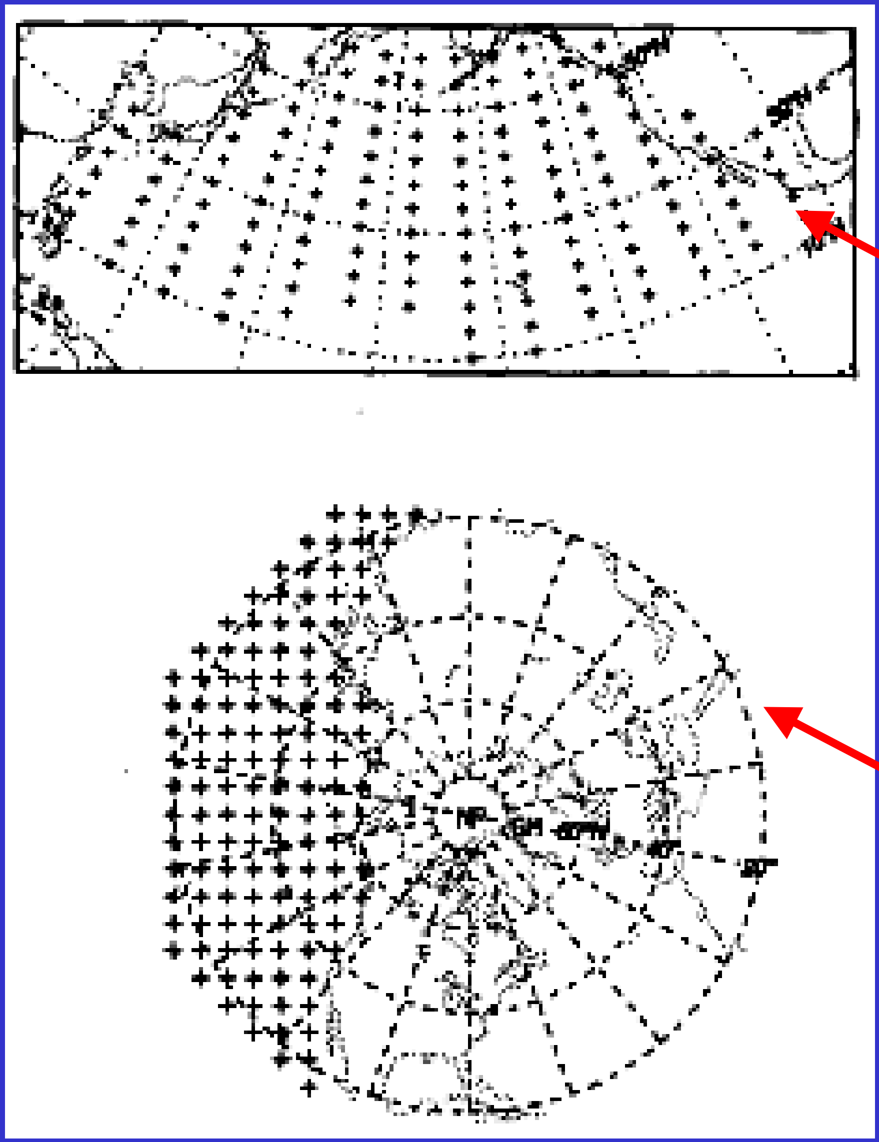
$$\mathbf{v}_k = \frac{1}{N\sigma_k}\mathbf{Y}\mathbf{x}_k^{*T} \quad or \quad v_{jk} = \frac{1}{N\sigma_k}\sum_{i=1}^{N} y_{ji} x_{ik}^{*} = \frac{1}{\sigma_k}\overline{y_j x_k^{*}}$$

- Homogeneous regression maps: regress (or correlate) the expansion coefficient time series of the left field with the input data for the left field, or do the same with the right field and its expansion coefficients.

$$\mathbf{u}_k = \frac{1}{N\sigma_k}\mathbf{X}\mathbf{x}_k^{*T} \quad or \quad u_{jk} = \frac{1}{N\sigma_k}\sum_{i=1}^{N} x_{ji} x_{ik}^{*} = \frac{1}{\sigma_k}\overline{x_j x_k^{*}}$$

$$\mathbf{v}_k = \frac{1}{N\sigma_k}\mathbf{Y}\mathbf{y}_k^{*T} \quad or \quad v_{jk} = \frac{1}{N\sigma_k}\sum_{i=1}^{N} y_{ji} y_{ik}^{*} = \frac{1}{\sigma_k}\overline{y_j y_k^{*}}$$

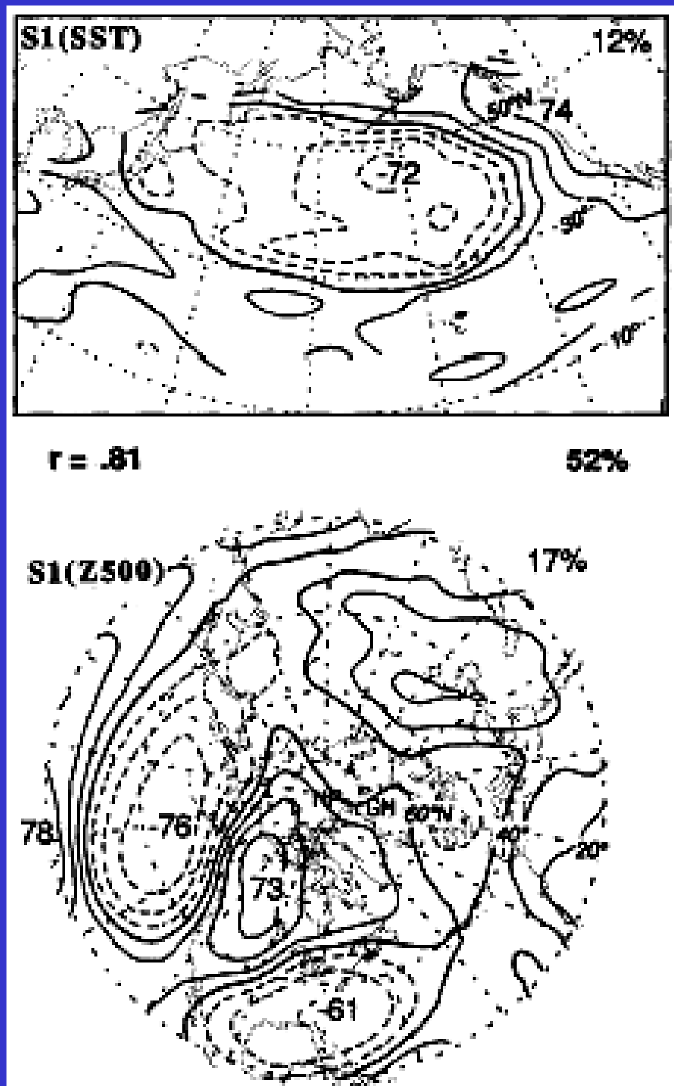
An Example – SVD (SST, SLP)



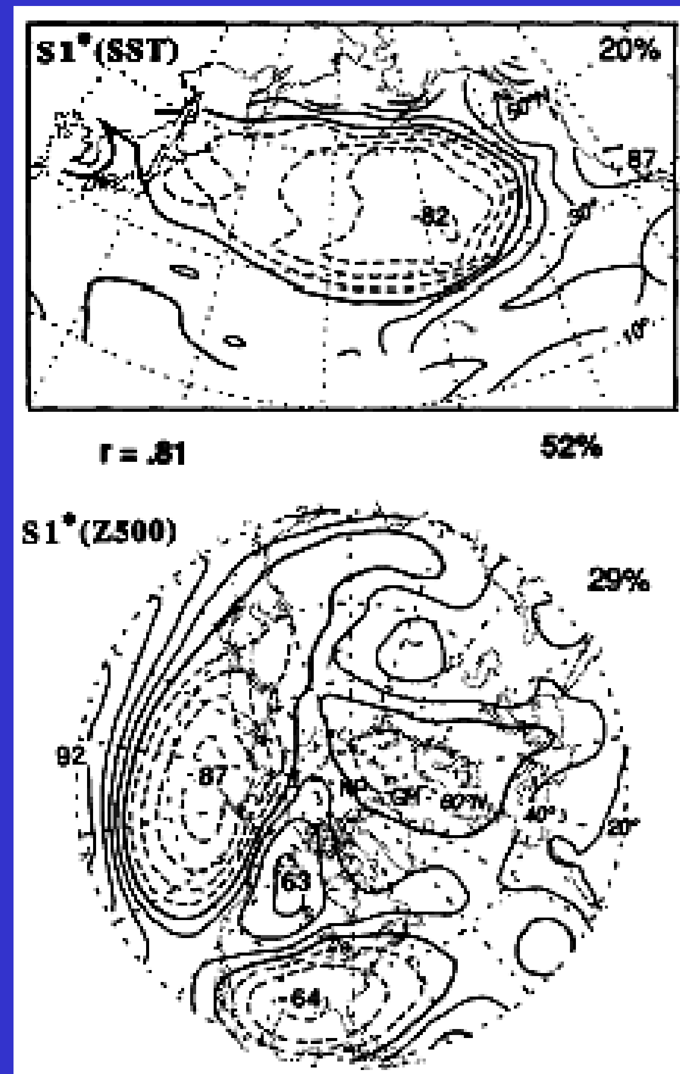
Sea Surface Temperature (SST)

Sea Level Pressure (SLP)

SVD Maps



Heterogeneous Correlation



Homogeneous Correlation

How to Use Matlab to do SVD?

- See pages 27-28 of the paper “A manual for EOF and SVD analysis of climate data” by Bjornsson and Venegas.