Section 6: Principal Component and Maximum Covariance Analyses

Maximum Covariance Analysis (MCA)

Purpose

- **Purpose**
  - Find correlated patterns in TWO datasets (i.e. are frequently met simultaneously). E.g. patterns of temperature that go along with patterns of pressure.

- **Applications**
  - Study the coupling between parameters to understand physical mechanisms of climate variations. E.g. how does atmospheric circulation influence the distribution of temperature?
  - Statistical downscaling. (Translate GCM derived climate change scenarios to the local/regional scale.)
  - Reconstruction / Forecasting

Paired Multivariate Datasets

- **Two paired multivariate datasets**

$$\mathbf{x}(i) = \left(x_1(i),\ldots,x_n(i)\right) \qquad \mathbf{y}(i) = \left(y_1(i),\ldots,y_m(i)\right)$$

  - $i=1,\ldots,N$, joint observations of $\mathbf{x}$, $\mathbf{y}$
  - Two data clouds in two phase spaces
  - Centered (means subtracted!), (just for more simple notation!)
  - E.g. $\mathbf{x}$: anomalies of SLP Europe/Atlantic (n gridpoints),
    $\mathbf{y}$: Temperature anomalies in CH (m stations)

- **Data Matrices**

$$\mathbf{X} = \begin{bmatrix} x_1(1) & \cdots & x_n(1) \\ \vdots & \ddots & \vdots \\ x_1(N) & \cdots & x_n(N) \end{bmatrix} \qquad \mathbf{Y} = \ldots$$

Cross-Covariance

Call me
cross-covarofant

- **Cross-covariance matrix**

$$\mathbf{S}_{xy} := \begin{bmatrix} \mathrm{cov}(x_1, y_1) & \mathrm{cov}(x_1, y_j) & \mathrm{cov}(x_1, y_m) \\ \mathrm{cov}(x_i, y_1) & \mathrm{cov}(x_i, y_j) & \vdots \\ \mathrm{cov}(x_n, y_1) & \ldots & \mathrm{cov}(x_n, y_m) \end{bmatrix} = \frac{1}{(N-1)} \mathbf{X}^T \cdot \mathbf{Y}$$

  - Univariate cross-covariances between all pairs of components
  - n x m matrix
  - In general not square and not symmetric
  - diagonal elements do not have special meaning (i.e. different from var. matrix)

Cross-Correlation

- **Cross-Correlation matrix**

$$\mathbf{C}_{xy} := \begin{bmatrix} \operatorname{cor}(x_1, y_1) & \operatorname{cor}(x_1, y_j) & \operatorname{cor}(x_1, y_m) \\ \operatorname{cor}(x_i, y_1) & \operatorname{cor}(x_i, y_j) & \vdots \\ \operatorname{cor}(x_n, y_1) & \dots & \operatorname{cor}(x_n, y_m) \end{bmatrix}$$

  - Analogous to $\mathbf{S}_{xy}$ but divided by standard deviations
  - All matrix elements in {–1,+1}

$$\mathbf{C}_{xy} = \frac{1}{N-1} \mathbf{D}_x^{-\frac{1}{2}} \cdot \mathbf{X}^T \cdot \mathbf{Y} \cdot \mathbf{D}_y^{-\frac{1}{2}} = \mathbf{D}_x^{-\frac{1}{2}} \cdot \mathbf{S}_{xy} \cdot \mathbf{D}_y^{-\frac{1}{2}}$$

$$\mathbf{D}_x^{-\frac{1}{2}} = \left[1/\sigma_{x_k} \right] \qquad \mathbf{D}_y^{-\frac{1}{2}} = \left[1/\sigma_{y_k} \right]$$

MCA Mathematical Procedure

- **Singular Value Decomposition (SVD)**

>> Appendix A

$$\mathbf{S}_{xy} = \mathrm{cov}(\mathbf{X}, \mathbf{Y})$$ the cross-covariance matrix (n x m)

- There are r real numbers $\{\omega_1, \omega_2, ..., \omega_r\}$, $\omega_k>0$, *singular values*, (sorted in decreasing order $\omega_1 \geq \omega_2 \geq \omega_3 \ldots \geq \omega_r$), …
- … and r vectors $\{\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_r\}$, n-dimensional, unit-length, orthogonal, and r vectors $\{\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_r\}$, m-dimensional, unit-length, orthogonal, called *left* ($\mathbf{u}_k$) and *right* ($\mathbf{v}_k$) *singular vectors*, …
- … such that:

$$\mathbf{S}_{xy} = \mathbf{U}^T \cdot \Omega \cdot \mathbf{V}$$

$$\Omega = [\omega_k], \quad \text{diagonal}, r \times r$$

$$\mathbf{U} = [\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_r], \quad \mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_r], \quad \text{vectors in columns}$$

`R: svd`

MCA Interpretation

- **Singular Vectors, Coefficients**
  - Consider singular vectors anchored in center of data clouds, spanning sub-spaces of the phasespaces of each dataset (new variables). They are not necessarily a basis system, because $r \le n, r \le m$
  - Consider projections of data $\mathbf{x}(i)$ onto singular vectors as new data coordinates:

$$a_j(i) = \mathbf{x}(i)^T \cdot \mathbf{u}_j, \quad b_j(i) = \underbrace{\mathbf{y}(i)^T \cdot \mathbf{v}_j}_{\text{projection of data vector on singular vector}}, \quad j = 1,..,r$$

  - New coordinates are linear combinations of original variables.
  - $a_j(i)$: left coefficients, (also left SVD scores)
    $b_j(i)$: right coefficients, (also right SVD scores)

MCA Interpretation

- **Singular values, cross-covariance**
  - $\mathbf{\Omega}$ is the cross-covariance matrix of the new coordinates $\{a_k\}$, $\{b_k\}$:

$$\operatorname{cov}(a_i(.),b_j(.)) = 0 \quad \text{for } i \neq j, \quad \operatorname{cov}(a_i(.),b_i(.)) = \omega_i$$

>> Appendix B

  - Coordinates corresponding to different indices of singular vectors are mutually uncorrelated.
  - The first pair of singular vectors $\{\mathbf{u}_1, \mathbf{v}_1\}$ are the phase-space directions, for which the projections have the largest possible cross-covariance. *First coupled mode*.
  - Subsequent vector pairs $\{\mathbf{u}_k, \mathbf{v}_\mathrm{k}\}$ maximize cross-covariance subject to orthogonality to previous pairs. *k^{th} coupled mode*.

MCA Interpretation

- **Within space variance**
  - Singular vectors do not maximize variance in individual spaces.
  - Singular vectors are not necessarily aligned along directions of large data spread or cloud symmetry.
  - Left and right coefficients are in general not uncorrelated between themselves:

$$\mathrm{var}\left(a_i, a_j\right) \neq 0 \quad \mathrm{var}\left(b_i, b_j\right) \neq 0 \quad \text{for } i \neq j$$

  - *Cumulative Explained Variance Fraction* of first l modes

$$CEVF_x^l = \sum_k^l \mathrm{var}(a_k) \Big/ \mathrm{tr}\left(\mathbf{S}_{xx}\right) \qquad CEVF_y^l = \sum_k^l \mathrm{var}(b_k) \Big/ \mathrm{tr}\left(\mathbf{S}_{yy}\right)$$

MCA Interpretation

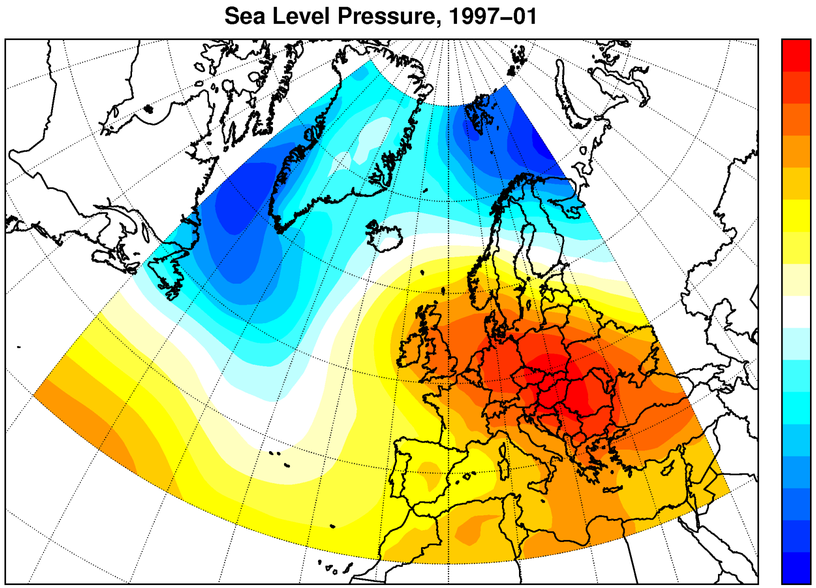
- **Singular vectors describe patterns of anomalies in each dataset that tend to occur simultaneously (are linearly correlated). *Modes of co-variability*, *coupled modes*, *canonical pairs*.**

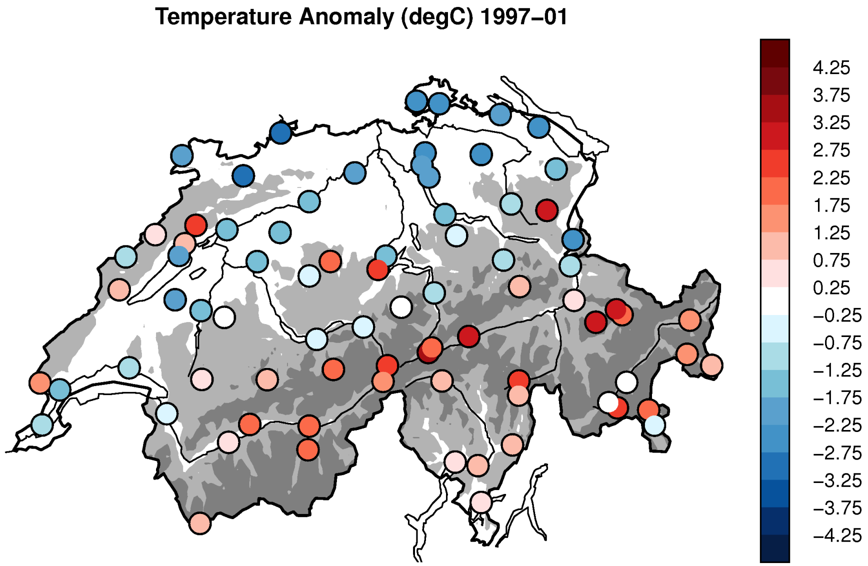
- **Coefficients represent amplitude (emphasis) of the respective patterns in each sample.**

- **The first few coefficient pairs have large cross-covariance and often show high correlations. *Dominant modes*.**

Example: Swiss T <> SLP

How does sea level pressure influence the distribution of winter-time temperature anomalies in Switzerland?



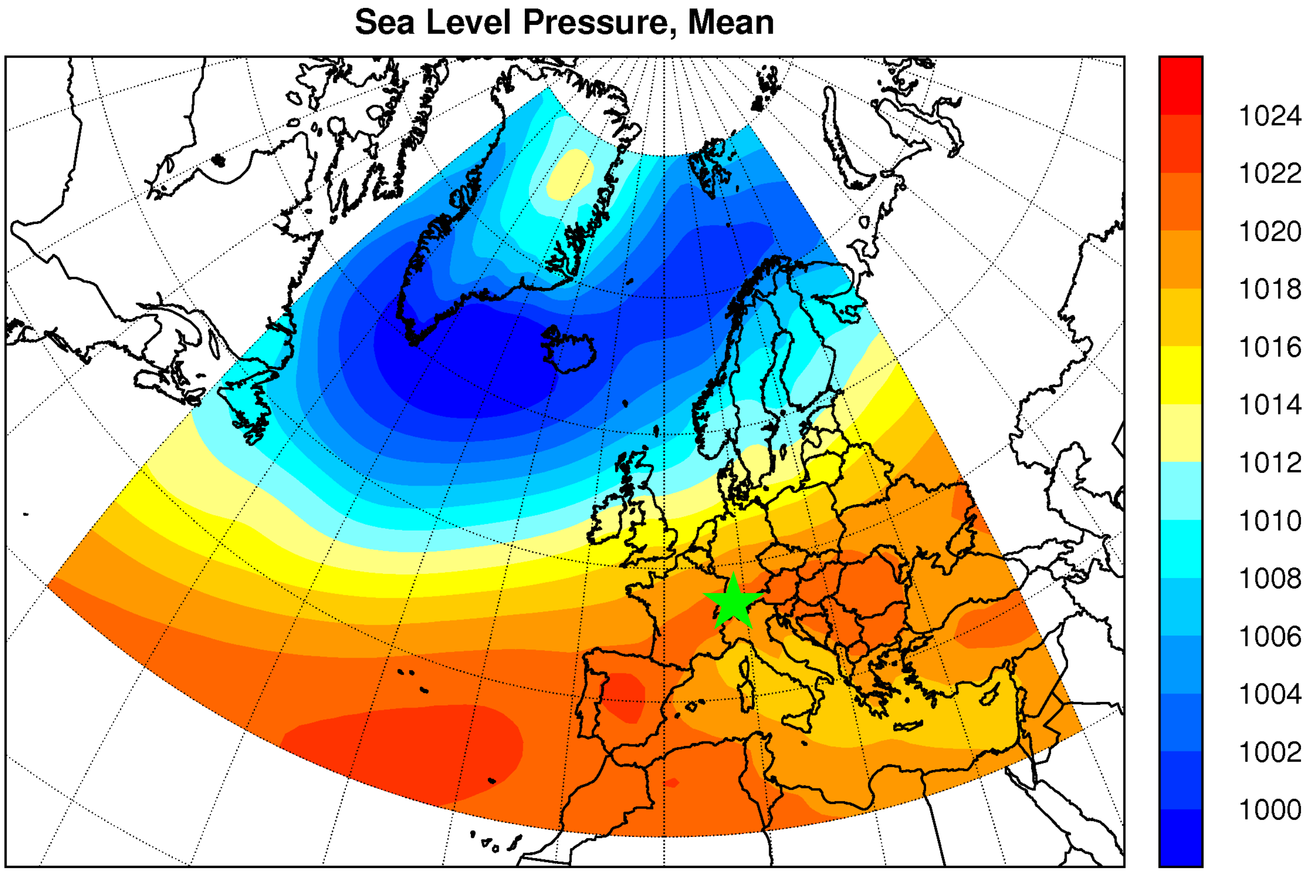


SLP: DJF, 1981 – 2010
(60°W–40°E, 30°N–80°N)
101 x 51 grid points, 1 degrees
ECMWF, ERA-Interim

T: DJF, 1981 – 2010
79 stations, MeteoSwiss
Anomaly from Mean

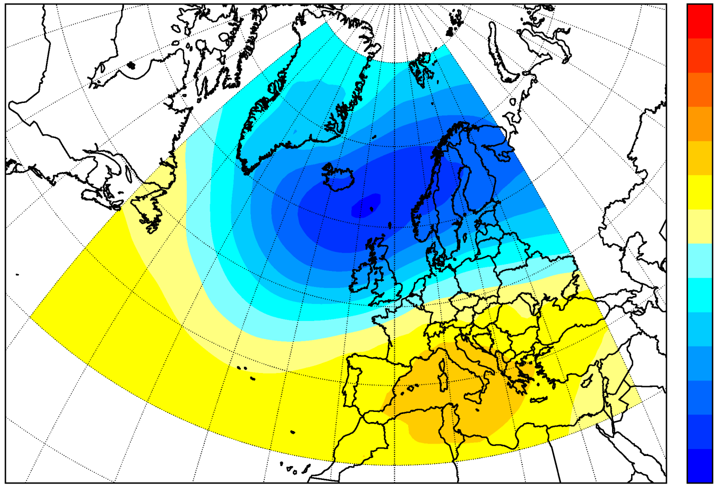
Begert et al. 2005, Dee et al. 2011

Example: Mean winter SLP

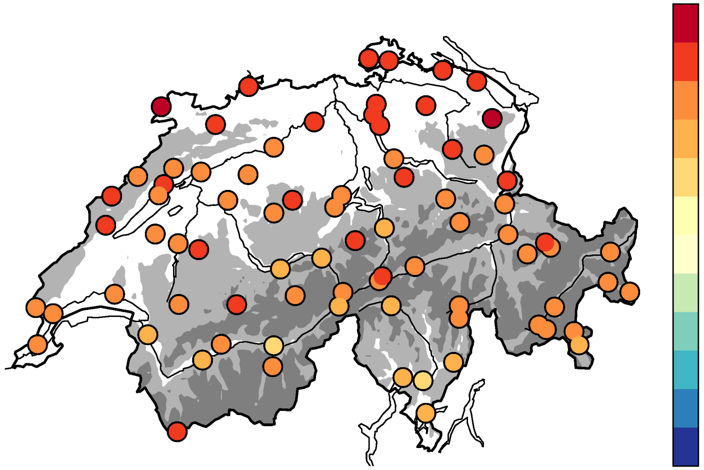


Example: Singular Vector Pair 1

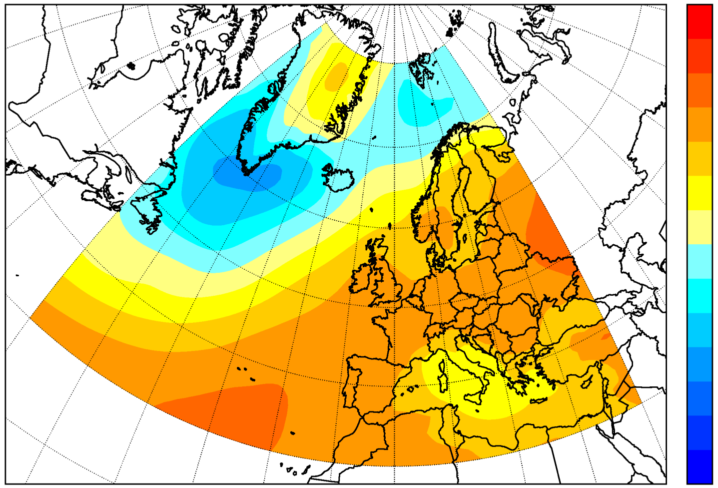
SLP Anomaly, Left Singular Vector 1



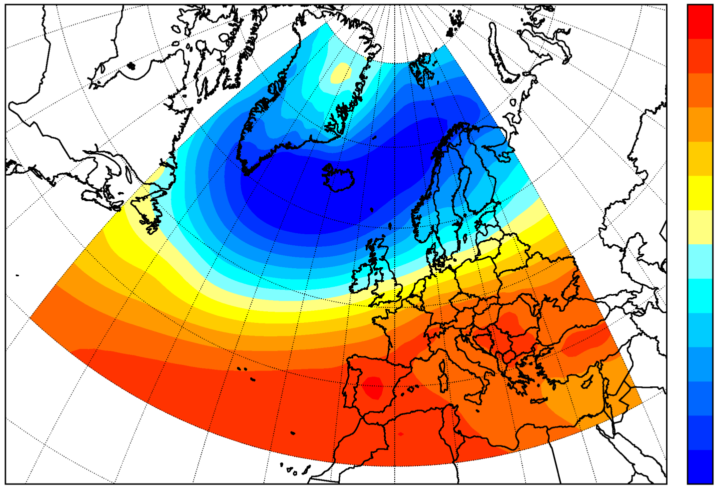
Temperature Anomaly, Right Singular Vector 1



SLP, Mean − Singular Vector 1

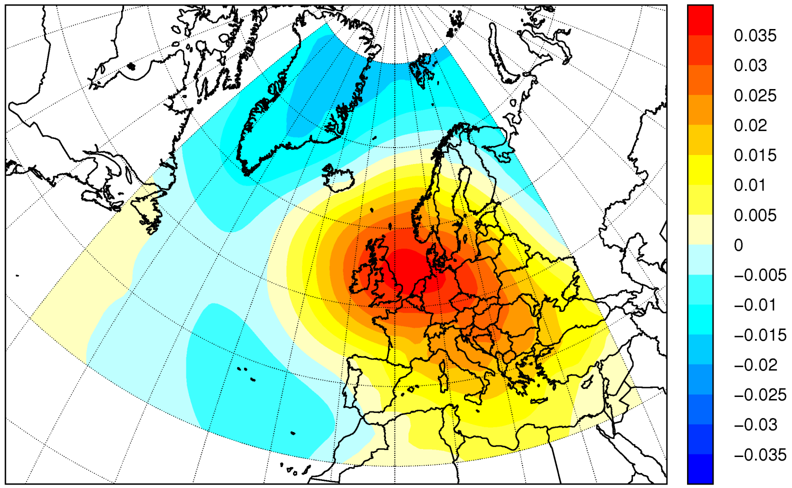


SLP, Mean + Singular Vector 1

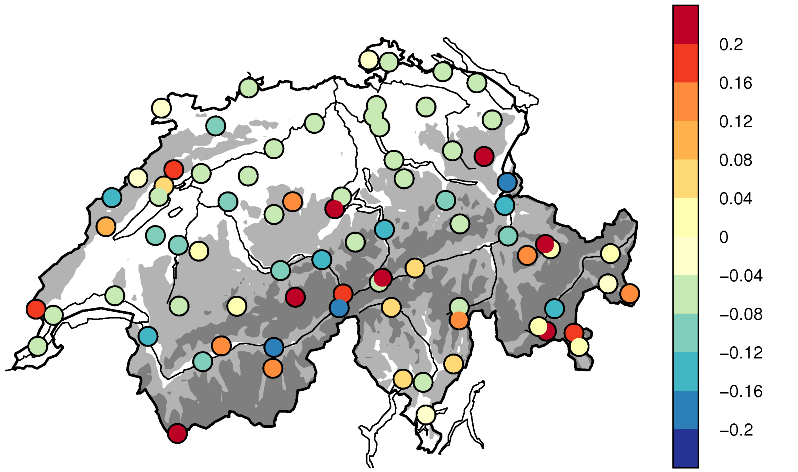


Example: Singular Vector Pair 2

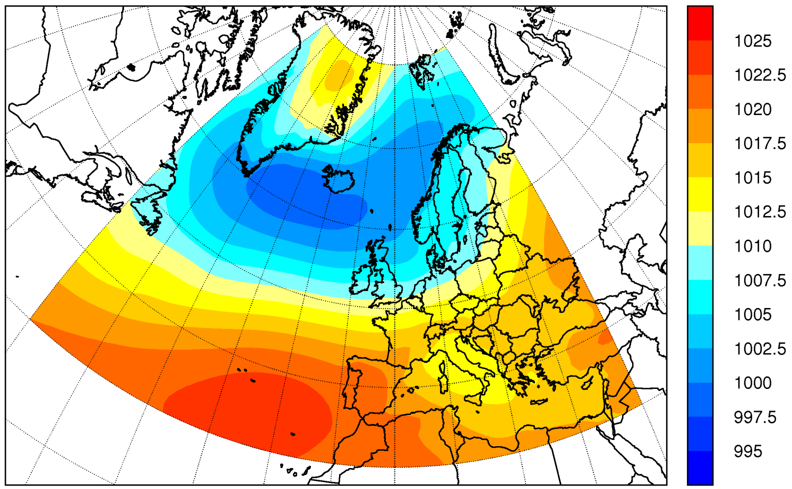
SLP Anomaly, Left Singular Vector 2



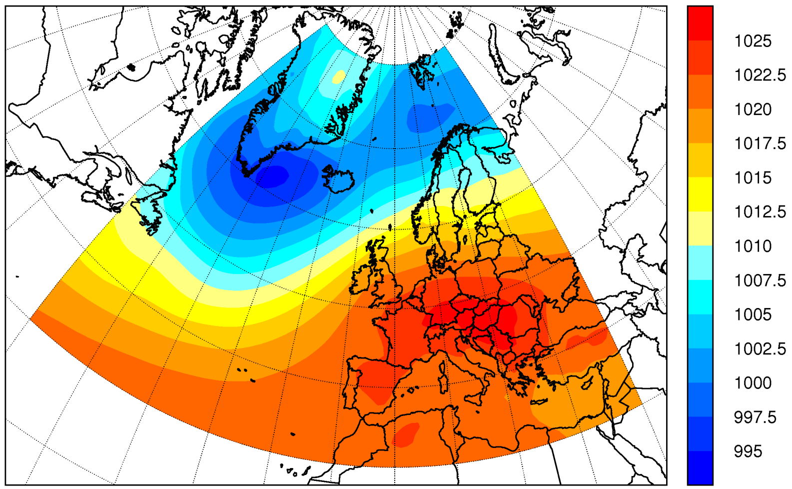
Temperature Anomaly, Right Singular Vector 2



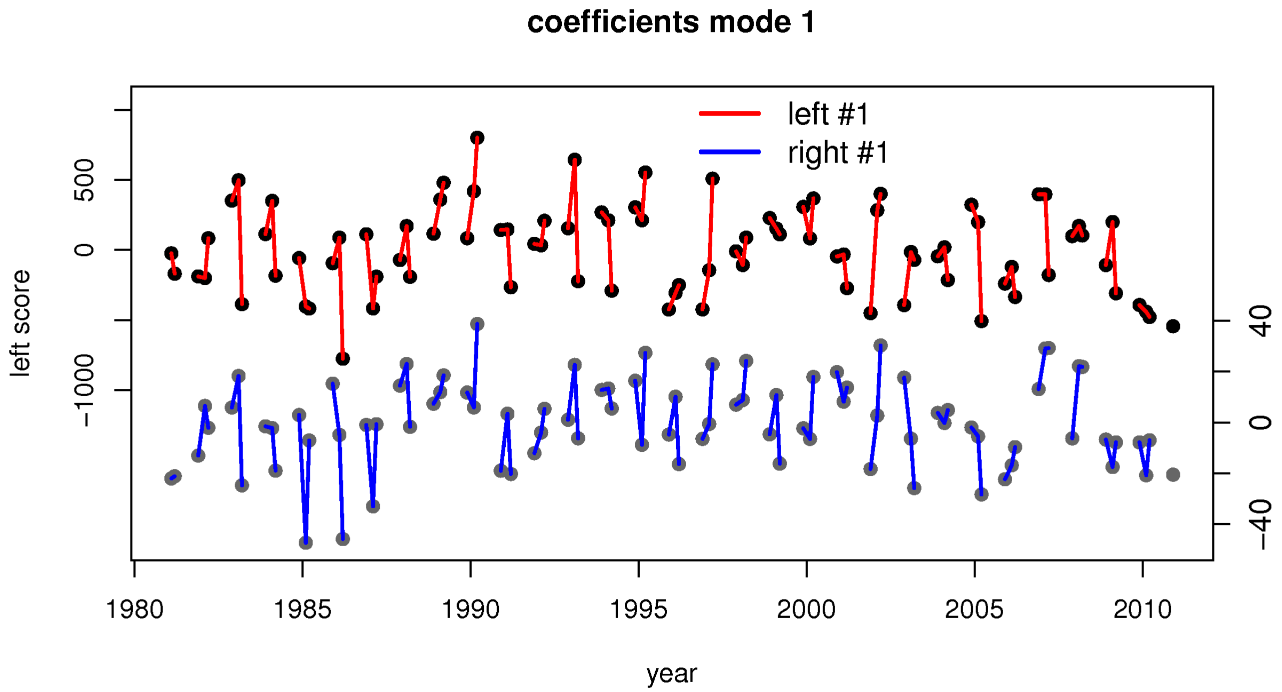
SLP, Mean – Singular Vector 2



SLP, Mean + Singular Vector 2

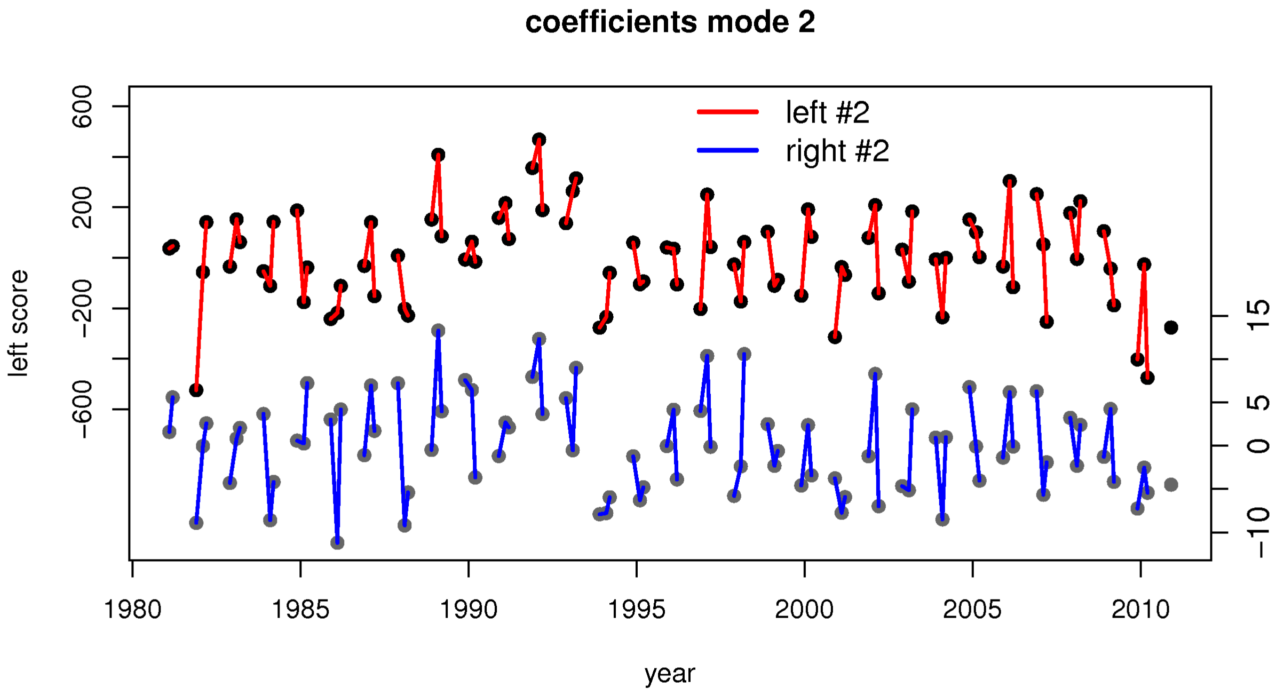


Example: Coefficients



Mode	Correlation
1	0.63 ☆
2	0.68
3	0.56
4	0.43
5	0.39
6	0.37
7	0.42
8	0.31

Example: Coefficients



Mode	Correlation
1	0.63
2	0.68 ☆
3	0.56
4	0.43
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7	0.42
8	0.31

Measuring Cross-Covariance

- **Total squared cross-covariance:**

$$\left\| S_{xy} \right\|_F := \sum_i^n \sum_j^m s_{ij}^2 = \sum_i^r \omega_i^2$$

Frobenius Norm

  - Note all matrix elements (different from PCA!)

- **Squared cross-covariance fraction:**
  - of singular vector pair k:

$$SCF_k = \omega_k^2 \Big/ \sum_i^r \omega_i^2$$

  - Note squared quantities (different from PCA!)

Truncation

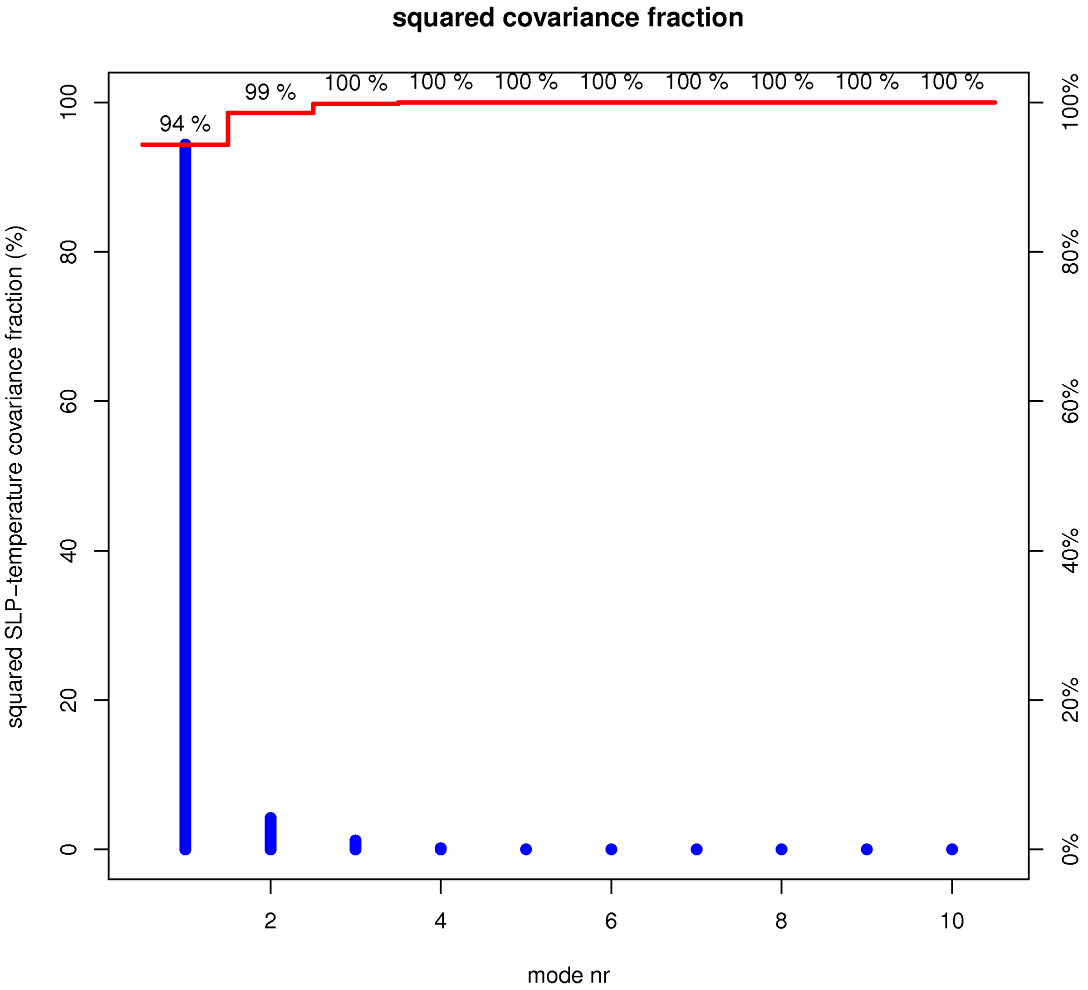
- **Retain only first l coupled modes**
- **Projection onto first l modes**
  - yields an approximation of the original data

$$\tilde{\mathbf{x}}(i) = \sum_{k}^{l} a_k(i) \cdot \mathbf{u}_k \quad \tilde{\mathbf{y}}(i) = \sum_{k}^{l} b_k(i) \cdot \mathbf{v}_k \quad l \le r$$

- **Cumulative squared cross-covariance fraction:**

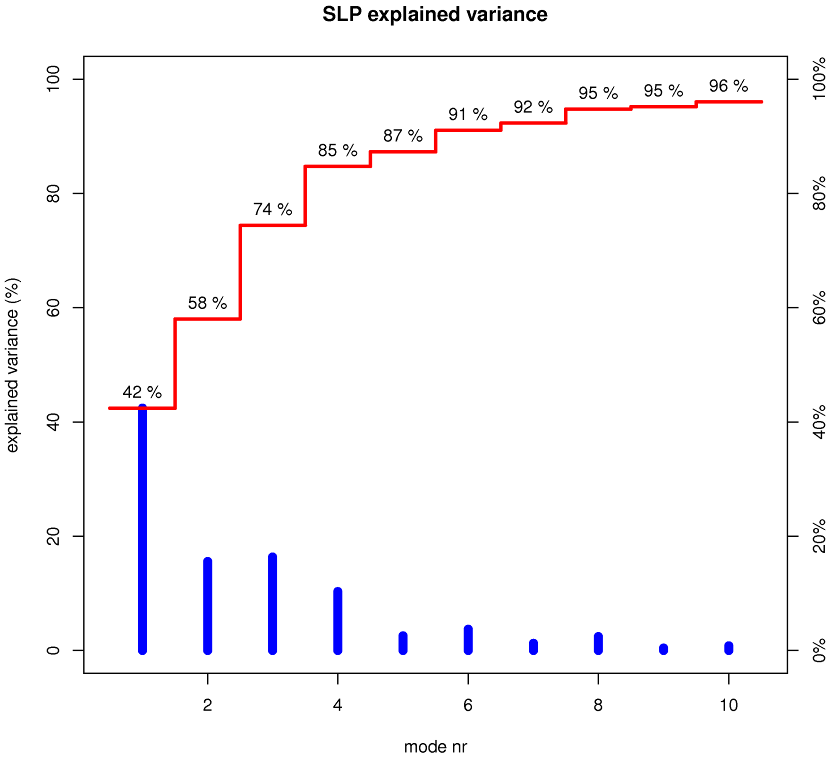
$$CSCF_l = 1 - \frac{\overbrace{\left\| \mathbf{S}_{xy} - \tilde{\mathbf{S}}_{xy} \right\|_F}^{\text{Residual cross-covariance, I.e. not reproduced by approximation}}}{\left\| \mathbf{S}_{xy} \right\|_F} = \sum_{k}^{l} \omega_k^2 \Big/ \sum_{k}^{r} \omega_k^2 = \sum_{k}^{l} SCF_k$$

Example: Squared Covariance Fraction

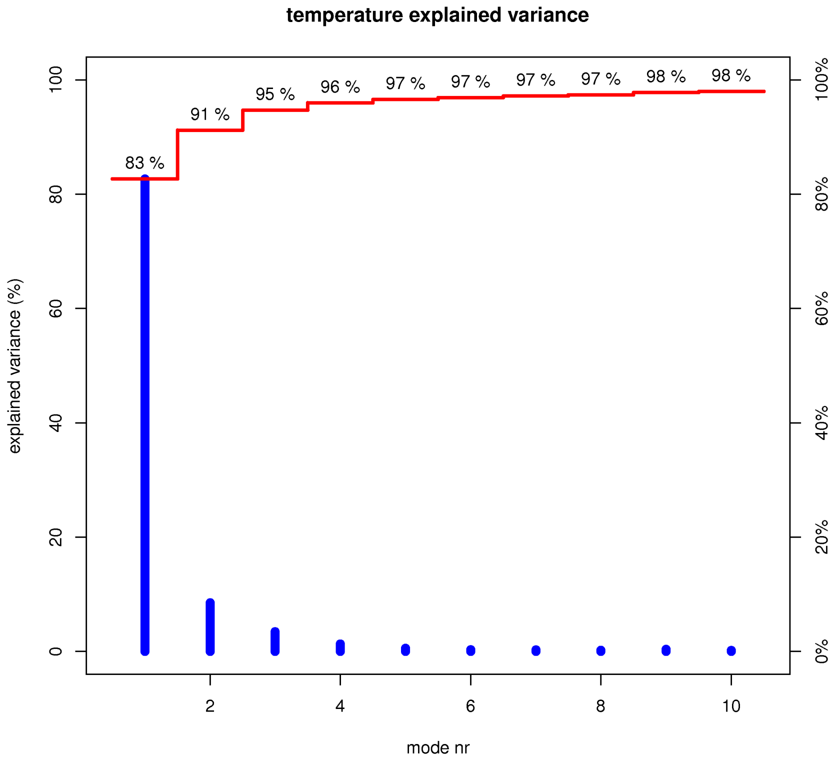


Example: Explained Variance

Sea Level Pressure



Temperature



Reconstruction / Prediction

- **Purpose**
  - Exploit cross-covariance to reconstruct/predict a right data vector from a left data vector (or vice versa).

- **Linear model between left and right coefficients**

right coefficients　　left coefficients (predictors)

$$b_k(i) = \beta_{k0} + \sum_{l}^{r} \beta_{kl} \cdot a_l(i) + \varepsilon_k(i)$$

noise

regression coefficients

  - Simplifies to:

$$b_k(i) = \beta_{kk} \cdot a_k(i), \quad \beta_{kk} = \frac{\omega_k}{\mathrm{var}(a_k)}$$

$$a_k, b_l \quad centered \Rightarrow \beta_{k0} = 0$$

$$\mathrm{var}(a_k, b_l) = 0 \Rightarrow \beta_{kl} = 0, \ k \neq l$$

Reconstruction / Prediction

$$\mathbf{x}$$

a "predictor" data vector
in the left phase space
(centered)

$$\mathbf{a} = \mathbf{U}^T \cdot \mathbf{x}$$

$$\mathbf{b} = \mathbf{G} \cdot \mathbf{a} \qquad \mathbf{G} = \left[\omega_k / \mathrm{var}(a_k)\right]$$

$$\mathbf{y} = \mathbf{V} \cdot \mathbf{b}$$

Operations using singular vectors
and singular values from a prior MCA

the "predictand" data vector
in the right phase space
(centered)

$$\mathbf{y}$$

- **MCA reconstruction equation:**

$$\mathbf{y} = \mathbf{V} \cdot \mathbf{G} \cdot \mathbf{U}^{\mathrm{T}} \cdot \mathbf{x}$$

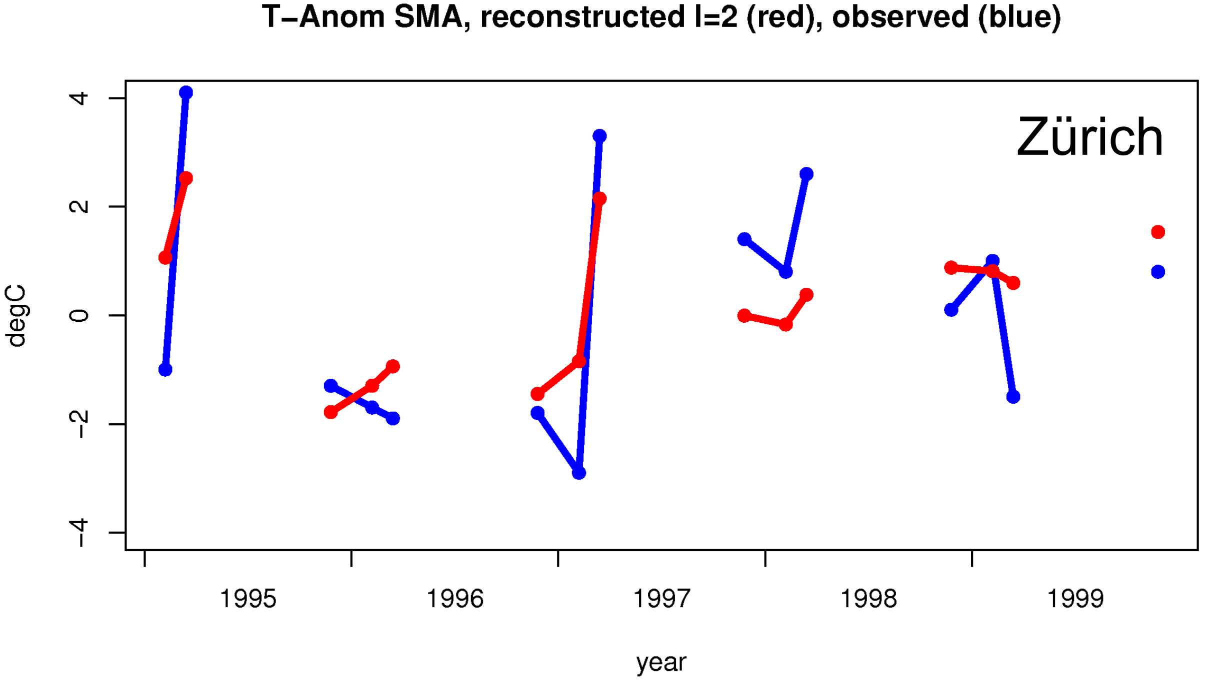
  - Possibly only using a few leading coupled modes. I.e. all matrices truncated to the number of desired modes.

Reconstruction / Prediction

- **Accuracy of reconstruction depends on**
  - The degree of covariance between the two fields.
  - The cumulative squared cross-covariance fraction explained by the modes that are retained (truncation). The more modes the better the reconstruction.
  - The variance explained by the right singular vectors in the right phase space. I.e. the component of the right space that is related to the left space.

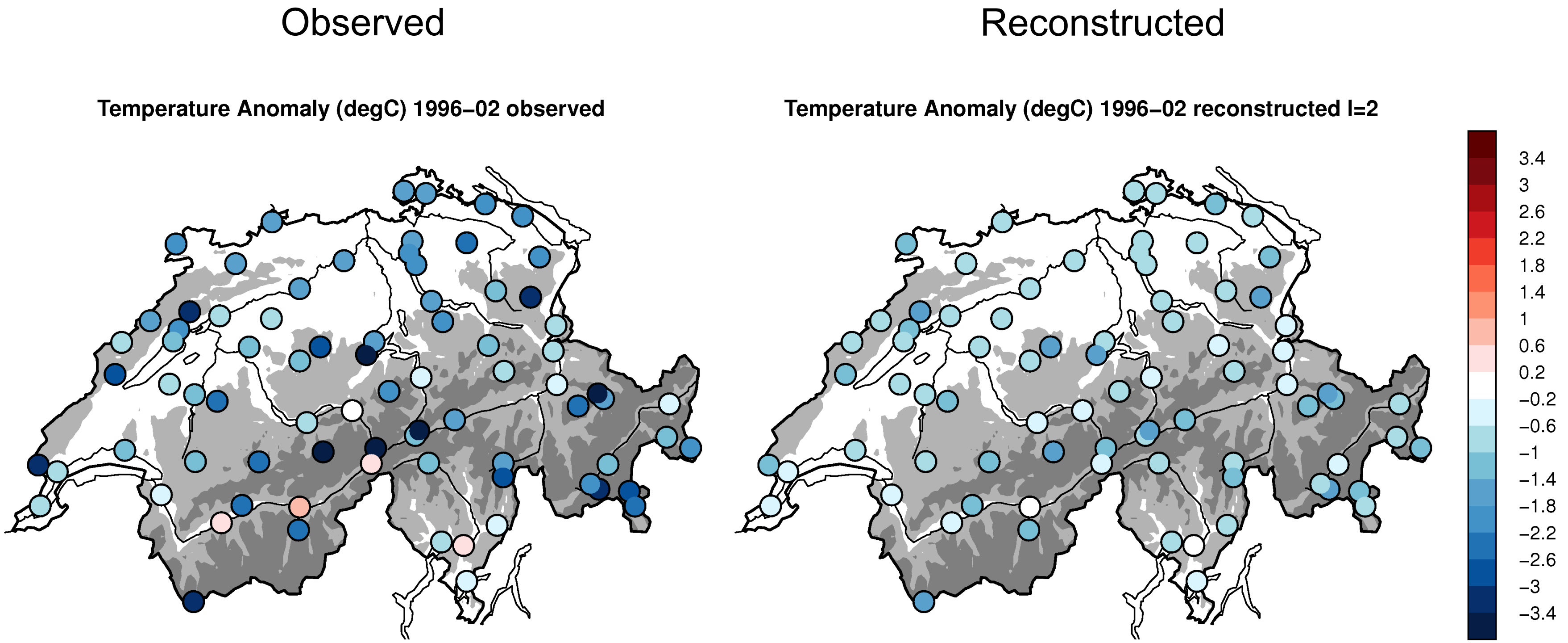
Example: Reconstruction

- **Reconstruction for 1995-1999 (winter months) using**
  - MCA calibrated for 1981-1994 & 2000-2010, i.e. without test period
  - SLP (left field) as predictor
  - 2 leading coupled modes



Example: Reconstruction

February 1996

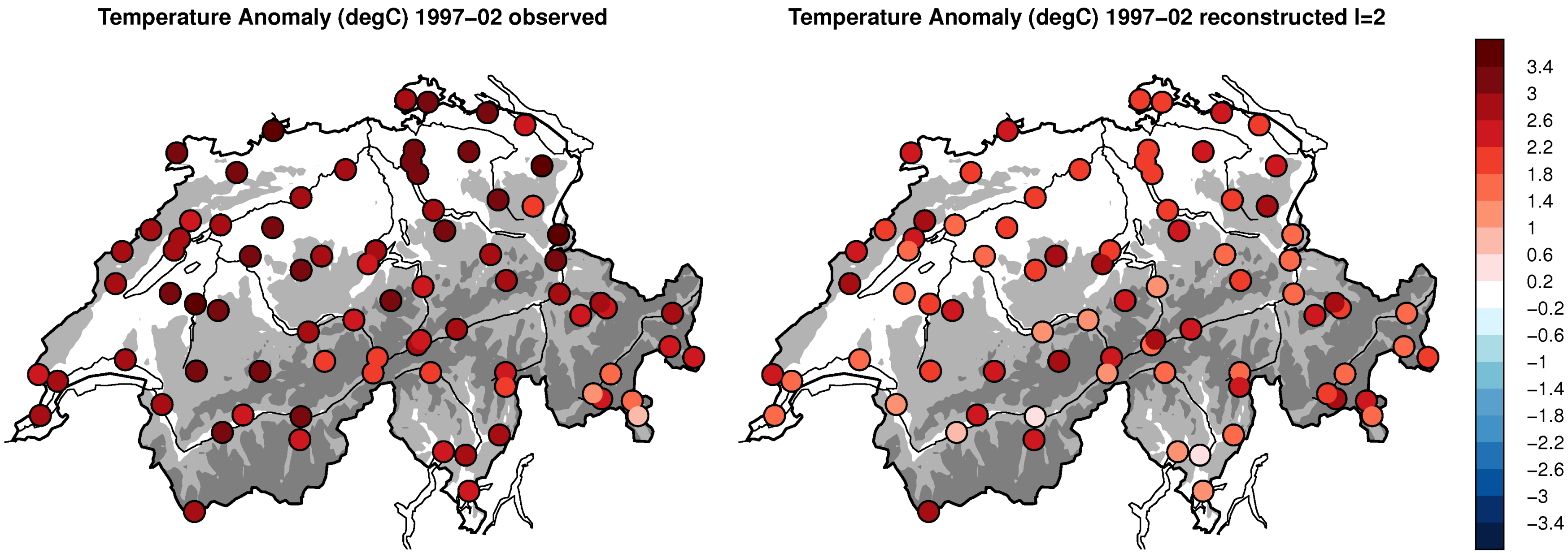


Example: Reconstruction

February 1997

Observed

Reconstructed

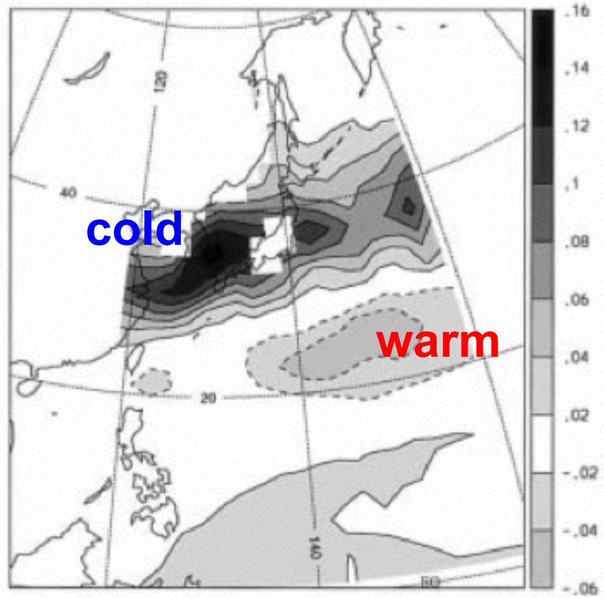


Example

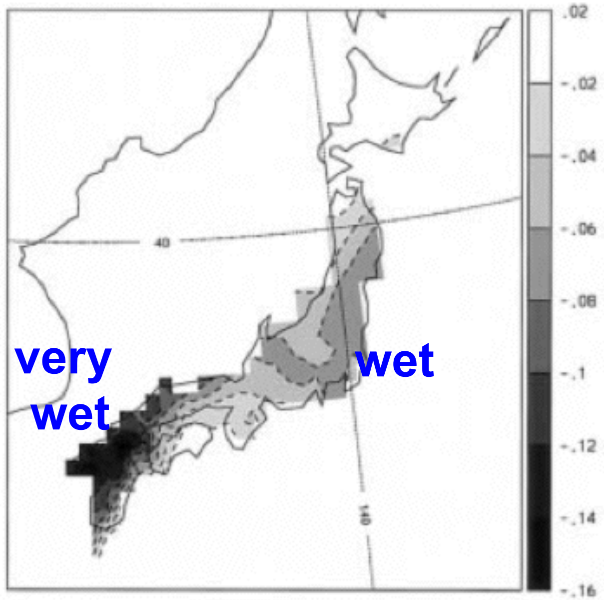
- **Baiu (JJA) Precipitation in Japan coupling to SST**

1st MCA mode

SST anomaly



Precipitation anomaly



What is cause, what is effect?

1st mode explains 70% of total squared covariance fraction.
SST and Precip. Coefficients are correlated by r=0.47 (r^2=0.22).

Fukutome et al. 2003

Canonical Correlation Analysis (CCA)

- **Similar to MCA but searching for maximum correlation**
- **Procedure**
  - Conduct SVD with cross-correlation matrix
- **Interpretation (like for MCA)**
  - Canonical pairs describe coupled modes, emphasis on correlation
- **CCA or MCA?**
  - MCA focuses on covariance: Modes tend to be large where the variance is large. Danger that physical modes are confounded by large variance.
  - CCA focuses on correlation: Coupling is identified also if associated variance is low. Danger that physical modes are confounded by small (insignificant) variations (sampling problems).

see Wilks 2005, Chap 12 for details

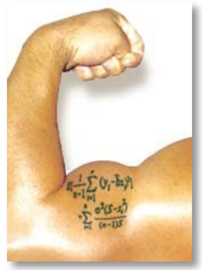
Summary

- **PCA & MCA are interesting techniques for characterising the (co-)variability in spatial datasets.**
- **Results require careful interpretation, corroboration in sensitivity experiments.**
- **Well established instruments in climate science:**
  - Technique of data reduction
  - Parsimonous reconstruction models (e.g. in historical climatology, paleo-climatology).
  - Evaluation of physical mechanisms in climate models.
  - Statistical (empirical) forecasting, climate change downscaling.
  - Source of hypothesis building for later modelling exercises.

Section 6: Principal Component and Maximum Covariance Analyses

Appendix MCA

Appendix A



- **Singular Value Decomposition (SVD)**
  - If $\mathbf{Q}$ is a real-valued n x m matrix (e.g. a cross-covariance matrix) with rank $r \leq \min(n, m)$
  - Then there exist real-valued matrices $\mathbf{U}$, $\mathbf{V}$, Ω such that:

$$\mathbf{Q} = \mathbf{U} \cdot \Omega \cdot \mathbf{V}^T$$

  - Ω: a diagonal r x r matrix with diagonal elements:

    $\omega_1 \geq \omega_2 \geq .. \geq \omega_r > 0$ the singular values

  - $\mathbf{U}$: a n x r matrix $\mathbf{U} = [\mathbf{u}_1, \mathbf{u}_2, .., \mathbf{u}_r]$, with orthonormal vectors: $\mathbf{U}^T \cdot \mathbf{U} = \mathbf{1}$

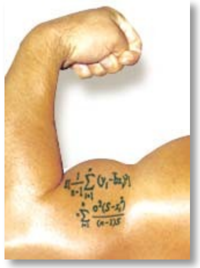
    $\mathbf{u}_k$ $k=1$ .. r the *left singular vectors*

  - $\mathbf{V}$: a m x r matrix $\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, .., \mathbf{v}_r]$, with orthonormal vectors: $\mathbf{V}^T \cdot \mathbf{V} = \mathbf{1}$

    $\mathbf{v}_k$ $k=1$ .. r the *right singular vectors*

See Wilks 2005, Sec. 9.3.5

Appendix A



- The singular vectors $\{\mathbf{u}_k\}$ and $\{\mathbf{v}_k\}$ (k=1,..., r) constitute orthonormal coordinate systems for r-dim subspaces of the n-dim (left) and m-dim (right) phase-spaces.

- I.e. the coordinate systems are not necessarily a basis system for the full phasespaces.

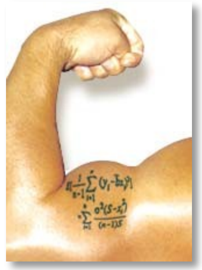
- The sum of squared singular values

$$\|Q\|_F^2 := \sum_i^n \sum_j^m q_{ij}^2 = \sum_i^r \omega_i^2$$

the *Frobenius Norm* = sum of squared matrix elements
= sum of squared singular values

see e.g. Bretherton et al. 1992

Appendix A



- **Calculation of SVD**
  - Singular vectors $\{\mathbf{u}_k\}$ are eigenvectors of $\mathbf{QQ}^{\mathrm{T}}$ (symmetric, n x n) and $\{\mathbf{v}_k\}$ of $\mathbf{Q}^{\mathrm{T}}\mathbf{Q}$ (symmetric, m x m)

$$\left(\mathbf{Q}\cdot\mathbf{Q}^T\right)\cdot\mathbf{U} = \mathbf{U}\Omega\mathbf{V}^T\cdot\mathbf{V}\Omega^T\mathbf{U}^T\cdot\mathbf{U} = \mathbf{U}\cdot\Omega^2, \qquad \text{dito for } \mathbf{V}$$

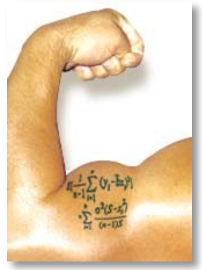
  - Singular left vectors can be obtained directly from singular right vectors (and vice versa):

$$\mathbf{QV} = \mathbf{U}\Omega, \quad \mathbf{Q}^T\mathbf{U} = \mathbf{V}\Omega^T$$

$$\mathbf{Qv}_k = \omega_k\mathbf{u}_k, \quad \mathbf{Q}^T\mathbf{u}_k = \omega_k\mathbf{v}_k, \quad k = 1,..,r$$

  - In practice there is dedicated software to calculate SVD

Appendix B



- **Transformation of Cross-Covariance Matrix**
  - If $\mathbf{X}$, $\mathbf{Y}$ are centered data matrices, the cross-covariance matrix is:

$$\mathbf{S}_{xy} = \frac{1}{N-1}\mathbf{X}^T \cdot \mathbf{Y}$$

  - Let $\mathbf{U}$, $\mathbf{V}$ be transformation matrices (with projection vectors in columns), then the data matrices in transformed coordinates are:

$$\mathbf{A} = \mathbf{X} \cdot \mathbf{U}, \qquad \mathbf{B} = \mathbf{Y} \cdot \mathbf{V}$$

  - The cross-covariance matrix of the transformed variables is:

$$\mathbf{S}_{ab} = \frac{1}{N-1}\mathbf{A}^T \cdot \mathbf{B} = \frac{1}{N-1}\mathbf{U}^T\mathbf{X}^T \cdot \mathbf{Y}\mathbf{V} = \mathbf{U}^T\mathbf{S}_{xy}\mathbf{V}$$

  - I.e. when $\mathbf{U}$, $\mathbf{V}$ are chosen the singular vector systems of $\mathbf{S}_{xy}$ then:

$$\begin{array}{c} \mathbf{S}_{xy} = \mathbf{U}\Omega\mathbf{V}^T \\ \mathbf{U}^T \cdot \mathbf{U} = \mathbf{1},\ \mathbf{V}^T \cdot \mathbf{V} = \mathbf{1} \end{array} \quad \Rightarrow \quad \mathbf{S}_{ab} = \mathbf{U}^T\mathbf{S}_{xy}\mathbf{V} = \mathbf{U}^T\mathbf{U}\Omega\mathbf{V}^T\mathbf{V} = \Omega$$