Lecture 37

Principal component analysis (PCA)

STAT 8020 Statistical Methods II
November 25, 2019

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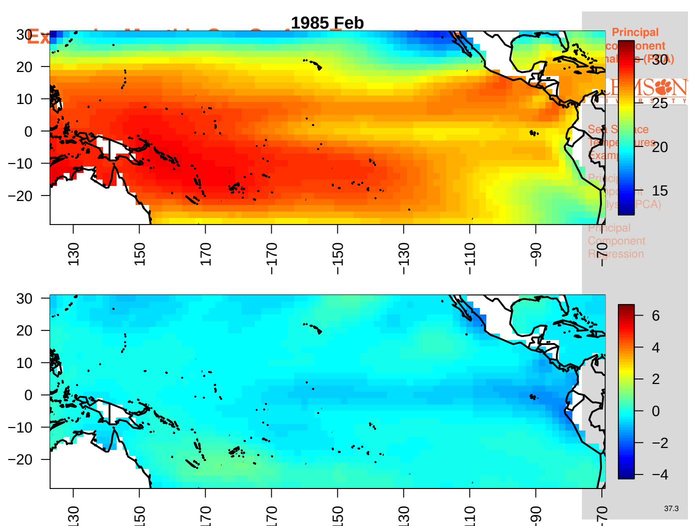
Notes

Agenda

1. Sea Surface Temperatures Example
2. Principal component analysis (PCA)
3. Principal Component Regression

Notes



Notes

Sea Surface Temperatures and Anomalies

- The "data" are gridded at a 2° by 2° resolution from $124^{\circ}E - 70^{\circ}W$ and $30^{\circ}S - 30^{\circ}N$. The dimension of this SST data set is
  2303 (number of grid points in space) ×
  552 (monthly time series from 1970 Jan. to 2015 Dec.)
- Sea-surface temperature anomalies are the temperature differences from the climatology (i.e. long-term monthly mean temperatures)
- We will demonstrate the use of Empirical Orthogonal Function (EOF) analysis to uncover the low-dimensional structure of this spatio-temporal data set

Notes

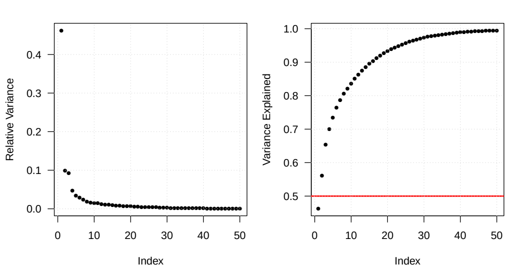
The Emipirical Orthogonal Function (EOF) Decomposition

Two parts:

- Basis functions – spatial fields in the SST example
  - Basis functions determined in an optimal way (in terms of least square) from the same data ⇒ "empirical"
- Coefficients – monthly time series in the SST example
  - Coefficients found by least squares

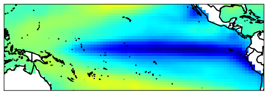
Notes

Screen Plot for EOFs

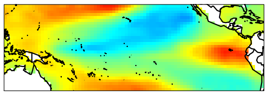


Notes

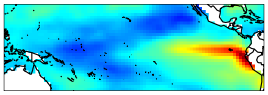
The First 3 EOFs



EOF1: The classic ENSO pattern



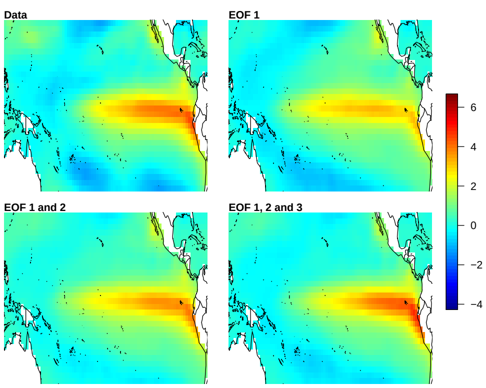
EOF2: A modulation of the center



EOF3: Messing with the coast of SA and the Northern Pacific.

Notes

1998 Jan El Niño Event



Notes

Principal Component Analysis

Given a random sample from a p-dimensional random vector $X_i = \{X_{1,i}, X_{2,i}, \cdots, X_{p,i}\}, \quad i = 1, \cdots, n$

- Dimension reduction technique
  - Large number of variables (p)
  - Number of variables (p) may be greater than number of observations (n)
- Create new, uncorrelated variables for the follow up analysis
  - Principal Component Regression
  - Interpretation of new variables?

Notes

Finding Principal Components

Principal Components (PC) are uncorrelated **linear combinations** $\tilde{X}_1, \tilde{X}_2, \cdots, \tilde{X}_p$ determined sequentially, as follows:

1. The first PC is the linear combination $\tilde{X}_1 = c_1^T X = \sum_{i=1}^p c_{1i} X_i$ that maximize $\mathrm{Var}(\tilde{X}_1)$ subject to $c^T c = 1$
2. The second PC is the linear combination $\tilde{X}_2 = c_2^T X = \sum_{i=1}^p c_{2i} X_i$ that maximize $\mathrm{Var}(\tilde{X}_2)$ subject to $c_1^T c_1 = 1$ and $c_2^T c_1 = 0$

$$\vdots$$

3. The j_{th} PC is the linear combination $\tilde{X}_j = c_j^T X = \sum_{i=1}^p c_{ji} X_i$ that maximize $\mathrm{Var}(\tilde{X}_j)$ subject to $c_j^T c_j = 1$ and $c_j^T c_k = 0 \forall k < j$

Notes

Principal Components

- Let Σ have eigenvalue-eigenvector pairs $(\lambda_i, e_i)_{i=1}^p$ with with $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \geq 0$ Then, the i_{th} principal component is given by

$$\tilde{X}_i = e_i^T X = e_{i1} X_1 + e_{i2} X_2 + \cdots e_{ip} X_p$$

- Then,

$$\mathrm{Var}(\tilde{X}_i) = \lambda_i, \quad i = 1, \cdots, p$$

$$\mathrm{Cov}(\tilde{X}_j, \tilde{X}_k) = 0, \quad \forall j \neq k$$

Notes

PCA and Proportion of Variance Explained

- It can be shown that

$$\sum_{i=1}^p \mathrm{Var}(\tilde{X}_i) = \lambda_1 + \lambda_2 + \cdots + \lambda_p = \sum_{i=1}^p \mathrm{Var}(X_i)$$

- The proportion of the total variance associated with the k_{th} principal component is given by

$$\frac{\lambda_k}{\lambda_1 + \lambda_2 + \cdots + \lambda_p}$$

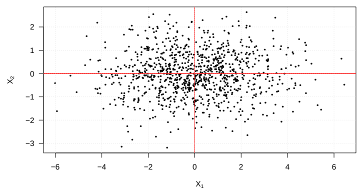
- If a large proportion of the total population variance (say 80% or 90%) is explained by the first k PCs, then we can restrict attention to the first k PCs without much loss of information

Notes

Toy Example 1

Suppose we have $X = (X_1, X_2)^T$ where $X_1 \sim \mathrm{N}(0, 4)$, $X_2 \sim \mathrm{N}(0, 1)$ are independent

- Total variation $= \mathrm{Var}(X_1) + \mathrm{Var}(X_2) = 5$
- X_1 axis explains 80% of total variation
- X_2 axis explains the remaining 20% of total variation

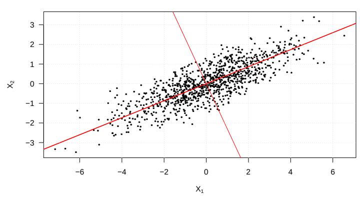


Notes

Toy Example 2

Suppose we have $X = (X_1, X_2)^T$ where $X_1 \sim \mathrm{N}(0, 4)$, $X_2 \sim \mathrm{N}(0, 1)$ and $\mathrm{Cor}(X_1, X_2) = 0.8$

- Total variation $= \mathrm{Var}(X_1) + \mathrm{Var}(X_2) = \mathrm{Var}(\tilde{X}_1) + \mathrm{Var}(\tilde{X}_2) = 5$
- $\tilde{X}_1 = .9175X_1 + .3975X_2$ explains 93.9% of total variation
- $\tilde{X}_2 = .3975X_1 - .9176X_2$ explains the remaining 6.1% of total variation



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Longley's Economic Regression Data

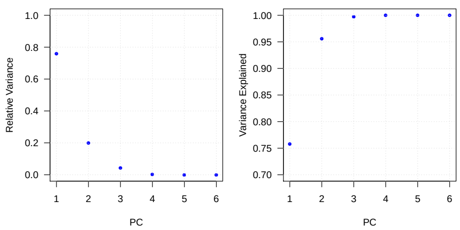
We are going to use Longley's data set, which provides a well-known example of multicollinearity, to illustrate Principal Component Regression

	GNP	Unemployed	Armed.Forces	Population	Year	Employed
GNP	1.00	0.60	0.45	0.99	1.00	0.98
Unemployed	0.60	1.00	-0.18	0.69	0.67	0.50
Armed.Forces	0.45	-0.18	1.00	0.36	0.42	0.46
Population	0.99	0.69	0.36	1.00	0.99	0.96
Year	1.00	0.67	0.42	0.99	1.00	0.97
Employed	0.98	0.50	0.46	0.96	0.97	1.00

```
       GNP   Unemployed Armed.Forces   Population         Year
14350.70398    601.69137     98.18754    558.11084  22897.44840
   Employed
 1064.78369
```


Notes

How Many PCs to Use?



Notes

Principal Component Regression in R

```
# Fit model
pcrFit<-pcr(Employed ~ ., data = longley, valdiation = "cv")

# Summarize the fit
summary(pcrFit)
```

```
Data:   X dimension: 16 6
    Y dimension: 16 1
Fit method: svdpc
Number of components considered: 6
TRAINING: % variance explained
         1 comps  2 comps  3 comps  4 comps  5 comps  6 comps
X          64.96    94.90    99.99   100.00   100.00   100.00
Employed   78.42    89.73    98.51    98.56    98.83    99.55
```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