Sparse Principal Component Analysis
for Frequency Data

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Dimensionality Reduction

- **Problems** in high dimensions:
  - Time and storage space
  - Multi-collinearity
  - Visualizing data set
  - Curse of dimensionality
- **Idea:** Reduce the number of variables while preserving structure in the data
- **Approach:** Feature selection methods
- **Approach:** Feature extraction methods

Central Idea

- Reduce dimensionality while retaining as much information as possible
- Linearly project the data to a space of fewer dimensions
- Represent data set regarding newly identified principal components
- Natural order on principal components

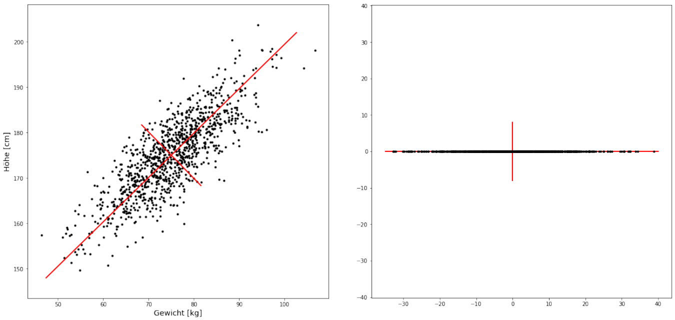


Figure: Some description of the plots

Mathematical Formulation

Let $\mathbf{X} \in \mathbb{R}^{n \times p}$ be a centered data matrix with n samples and p variables. We find the first principal axis by

$$v_1 = \underset{\|v\|_2=1}{\arg\max} \operatorname{Var}[\mathbf{X}v] = \underset{\|v\|_2=1}{\arg\max}\, v^T \mathbf{\Sigma} v$$

where $\mathbf{\Sigma} = \mathbf{X}^T\mathbf{X}$ is the sample covariance matrix. Then we can find the following principal axis successively

$$v_{k+1} = \underset{\|v\|=1}{\arg\max}\, v^T \mathbf{\Sigma} v$$

$$\text{subject to } v_{k+1}^T v_l = 0 \quad \forall 1 \leq l \leq k$$

The new, transformed variables are defined by $Z_i = \mathbf{X}v_i$

The principal axis can also be computed via the eigendecomposition of $\boldsymbol{\Sigma}$.

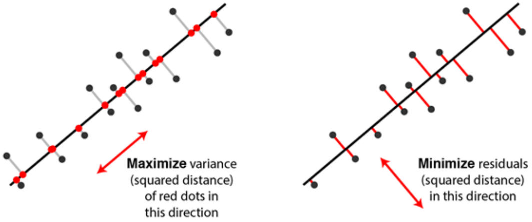
$$\boldsymbol{\Sigma} = \mathbf{V}\mathbf{L}\mathbf{V}^T$$

where $\mathbf{L}$ is a diagonal matrix with eigenvalues λ_i and $\mathbf{V}$ is the matrix of eigenvectors. Closely related is the Singular Value Decomposition (SVD)

$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^T$$

where $\mathbf{D}$ is a diagonal matrix with singular values $d_1, \dots, d_p$, $\mathbf{U}$ a $n \times p$ and $\mathbf{V}$ a $p \times p$ orthogonal matrix.

PCA as a regression problem



Suppose we want to extract the first k principal axis.

$$\hat{\mathbf{V}}_k = \arg\min_{\mathbf{V}_k} \sum_{i=1}^{n} \left\| x_i - \mathbf{V}_k \mathbf{V}_k^T x_i \right\|^2 + \lambda \sum_{j=1}^{k} \|\beta_j\|^2$$

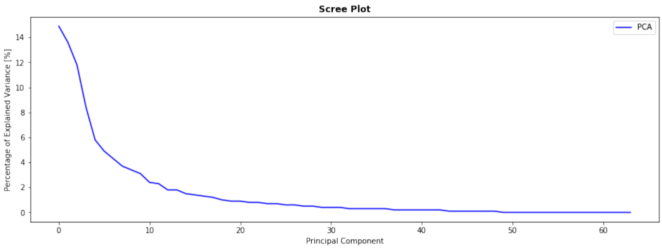
$$\text{subject to } \mathbf{V}_k^T \mathbf{V}_k = I_{k \times k}$$

Succes of PCA is due to the following two important optimal properties

1. Principal Components sequentially capture the maximum variability (among the columns of X, thus guaranteeing minimal information loss)
2. Principal Components are uncorrelated, (so we can talk about one principal component without referring to others)

- Linear Relationship between variables
- Correlation of variables
- Completeness of data set
- Outliers
- Number of variables p ¿¿ Number of Samples n (Inconsistency Theorem)
- Interpreation of principal axis

Application to handwritten digits



Algorithm 1 General SPCA Algorithm

procedure $\mathrm{SPCA}(A, B)$
    $\mathbf{A} \leftarrow \mathbf{V}[, 1\colon k]$, the loadings of the first k ordinary principal components
    while not converged **do**   ▷ Definiere Abbruchkriterium
        Given a fixed $\mathbf{A} = [\alpha_1, \ldots, \alpha_k]$, solve the elastic net problem

$$\beta_j = \arg\min_{\beta} \left\| \mathbf{X}\alpha_j - \mathbf{X}\beta \right\|^2 + \lambda \left\| \beta \right\|^2 + \lambda_{1,j} \left\| \beta \right\|_1$$

        For a fixed $\mathbf{B} = [\beta_1, \ldots, \beta_k]$, compute the SVD of

$$\mathbf{X}^T \mathbf{X} \mathbf{B} = \mathbf{U} \mathbf{D} \mathbf{V}^T$$

        $\mathbf{A} \leftarrow \mathbf{U}\mathbf{V}^T$
    end while
    $\hat{V}_j = \frac{\beta_j}{\|\beta_j\|}$ for $j = 1, \ldots, k$
end procedure

References

- *Beamer Paket*
  http://latex-beamer.sourceforge.net/
- *User's Guide to the Beamer*
- *DANTE e.V.* http://www.dante.de