Statistical Learning

Dimension Reduction Techniques

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Introduction

- Well-structured data set: Consider any well-structured data set.
- Data matrix: X, with size $n \times p$.
- Sample size: n.
- Dimension: p.
- Curse of dimensionality: If the ratio n/p is not large enough, some problems might be intractable.
- Particularly: If p is large (even larger than n), data visualization becomes very difficult (if not impossible) and standard classification methods perform poorly.
- Thus: In these scenarios, it is very complicated to find interesting features in the data because of the accumulation of noise.

Introduction

- Noise features: Data sets with many variables use to contain many uninformative features.
- Dimension reduction: The main idea of dimension reduction techniques is to transform the data matrix X into another data matrix with a smaller dimension (same sample size).
- Important: The transformed data set should maintain the important features in X and should not contain the irrelevant features (noise) in X.
- Thus: The resulting transformed data matrix should:
  - Be more simple to analyze and to visualize.
  - Have larger discrimination power than the original data set, if possible.
- Note: A dimension reduction tool is more of a means to an end rather than an end in themselves, because they frequently serve as an intermediate step in another analysis.

Introduction

- Principal component analysis (PCA): The most popular method for dimension reduction.
- Idea: Perform a linear transformation of the original data matrix, X, preserving its important features and reducing the noise.
- Properties of PCA:
  - The transformed variables are uncorrelated, thus they do not share linear information.
  - Powerful method to interpret the relationship between the variables that form the data set.
  - Use to reveal unsuspected relationships and thereby allows interesting interpretations.
  - Clusters and outliers in the original data set are usually clearly shown in the transformed data set.
  - Sometimes increases the discriminatory power of the data set.

Introduction

- As we shall see: PCA depends solely on the sample covariance (or correlation) matrix of X.
- Sparse PCA: Similar to PCA but attempt to simplify the interpretation of the PCs.
- Independent Component Analysis (ICA): Tries to obtain independent variables instead of uncorrelated variables.
- Nevertheless: The mathematical treatment of ICA and other alternatives becomes more difficult and computation becomes more complex.

Introduction

- The rest of this chapter is devoted to:
  - Establish the main ideas of the principal component analysis.
  - Describe how to perform principal component analysis in practice.
  - Introduce sparse principal component analysis and independent component analysis.
  - Illustrate these techniques with real data examples.

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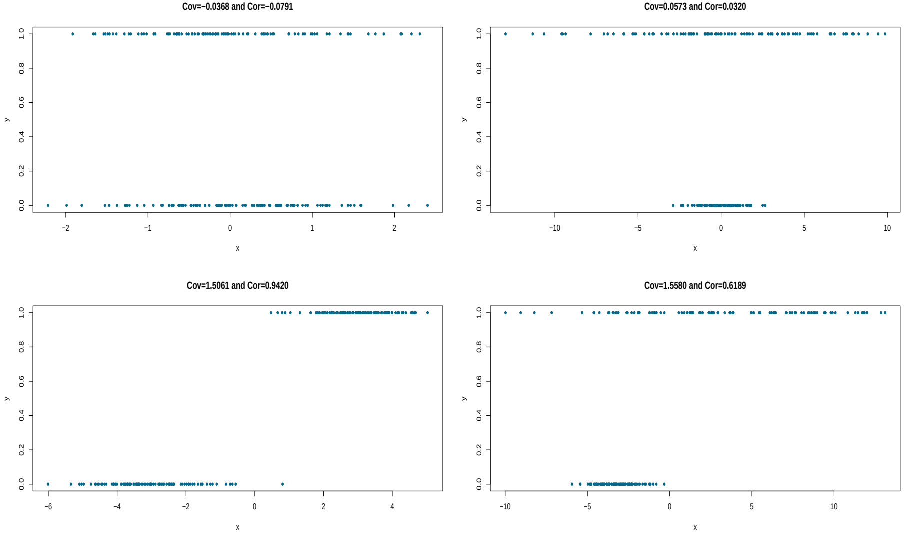
Principal component analysis

- Data matrix: X, with size $n \times p$.
- Quantitative variables: X should only contains quantitative variables.
- Binary variables: There is not a consensus on the inclusion of binary variables in a PCA.
- Sample covariance and sample correlation matrices: PCA are based on the information given by one of these two matrices.
- Interpretation: The interpretation of the sample covariance and correlation coefficients between a quantitative variable and a binary variable differ from those between quantitative variables.

Principal component analysis

- Four different situations with a quantitative variable and a qualitative variable:
  - $x \sim N(0,1)$, for $y = 0$, and $x \sim N(0,1)$, for $y = 1$.
  - $x \sim N(0,1)$, for $y = 0$, and $x \sim N(0,5)$, for $y = 1$.
  - $x \sim N(-3,1)$, for $y = 0$, and $x \sim N(3,1)$, for $y = 1$.
  - $x \sim N(-3,1)$, for $y = 0$, and $x \sim N(3,5)$, for $y = 1$.
- Dependency structure: There is no linear dependency between the variables.
- However: The sample covariance and correlation coefficients are quite different.
- High correlations: Appear because the two groups are well separated.
- Conclusion: Better not to include them.

Principal component analysis



Principal component analysis

- Center the data: PCA starts by centering the variables in the data matrix.
- Why?: The linearly transformed data set will be centered as well, thus, we avoid sample mean vectors for the new variables.
- Centered data matrix: $\widetilde{X} = X - 1_n \overline{x}'$, where $\overline{x}$ be the sample mean vector of X and 1_n is the $n \times 1$ vector of ones.
- Goal of PCA: Obtain a linear transformation of $\widetilde{X}$, $Z = \widetilde{X} C$, where C is a matrix of size $p \times r$ such that:
  1. Z has smaller dimension than $\widetilde{X}$, i.e., $r < p$.
  2. Z contains the important features in $\widetilde{X}$.
  3. Z does not contain the irrelevant features in $\widetilde{X}$.

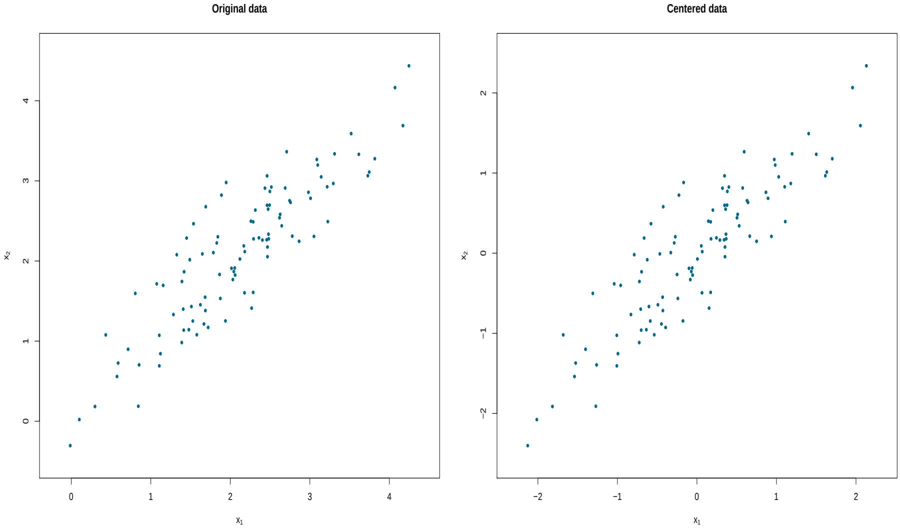
Principal component analysis

- Assume we want $r = 1$: Then, the new data matrix Z has dimension $n \times 1$.
- Then: We want to obtain a linear combination of $\widetilde{X}$ that contains the most important features in the data.
- In other words: Find the vector $c = (c_1, \ldots, c_p)'$ such that:
  - $Z = \widetilde{X}c$.
  - Z represents $\widetilde{X}$ best.
- The question is: What does best mean here?
- Toy example: Simple example with $p = 2$.

Principal component analysis

- Sample size: $n = 100$.
- Dimension: $p = 2$.
- Data matrix: X with size 100×2.
- First thing to do: Center the data, i.e., from X, we obtain the centered data matrix $\widetilde{X} = X - 1_n \overline{x}'$, that also has size 100×2.

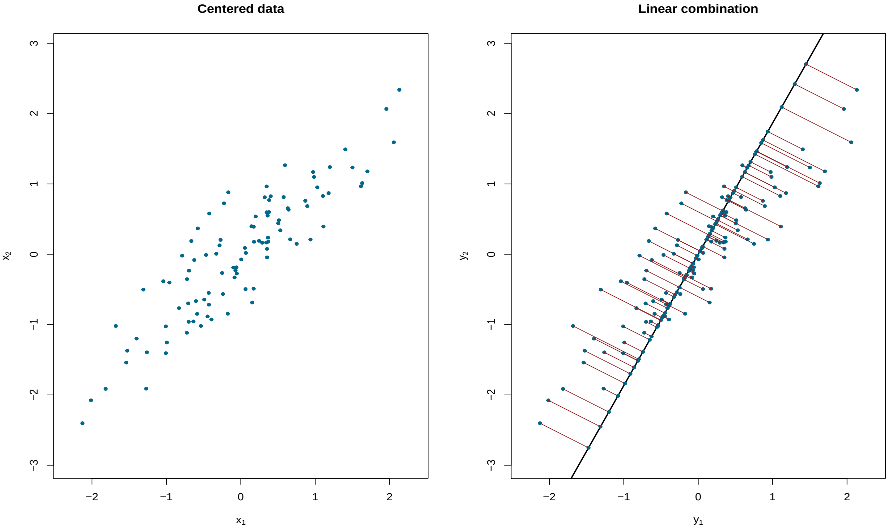
Principal component analysis



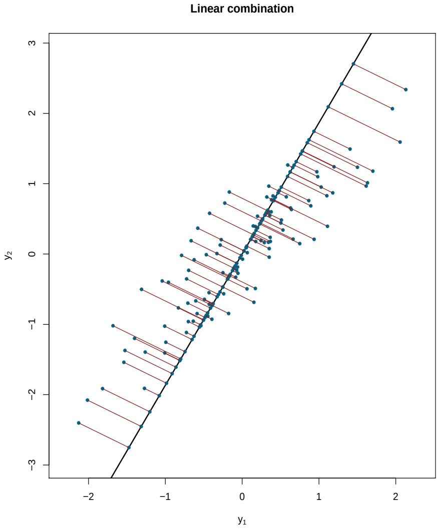
Principal component analysis

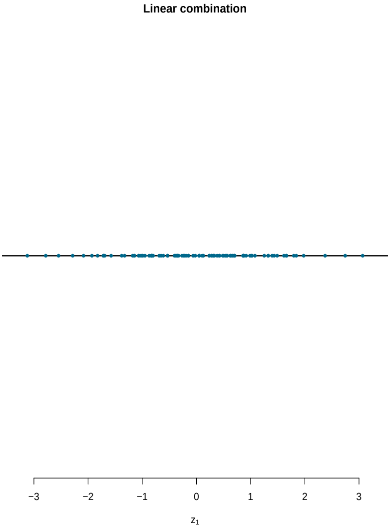
- Linear combination of $\widetilde{X}$: $Z = \widetilde{X}c$, where $c = (c_1, c_2)'$.
- Size of Z: 100×1.
- What is Z from a geometrical point of view?
- Idea: Project orthogonally the points in $\widetilde{X}$ into the straight line with slope given by $\frac{c_2}{c_1}$.
- Then: The points in Z are the points obtained after rotating this line (and thus the projected points) to the horizontal axe.

Principal component analysis



Principal component analysis

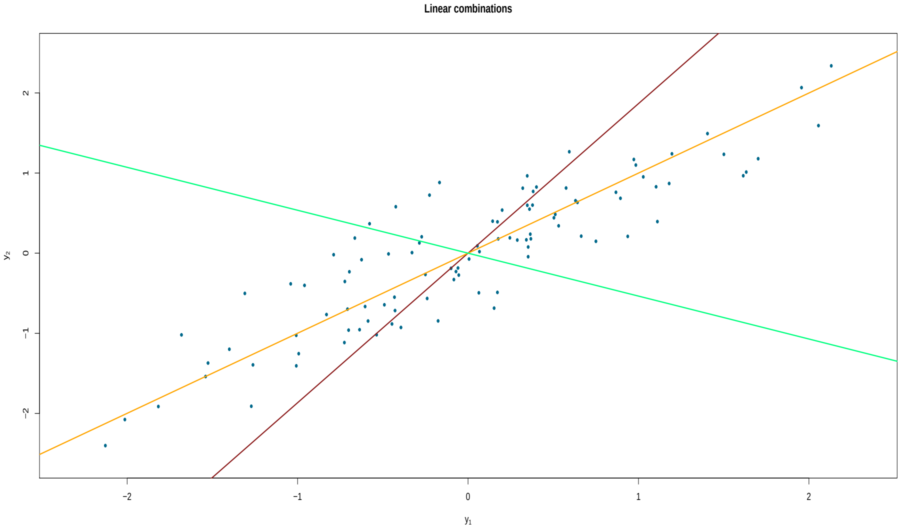




Principal component analysis

- The question is: Which vector $c = (c_1, c_2)'$ represents $\widetilde{X}$ best?
- See several possibilities in the next slide.
- Which one is the best option?

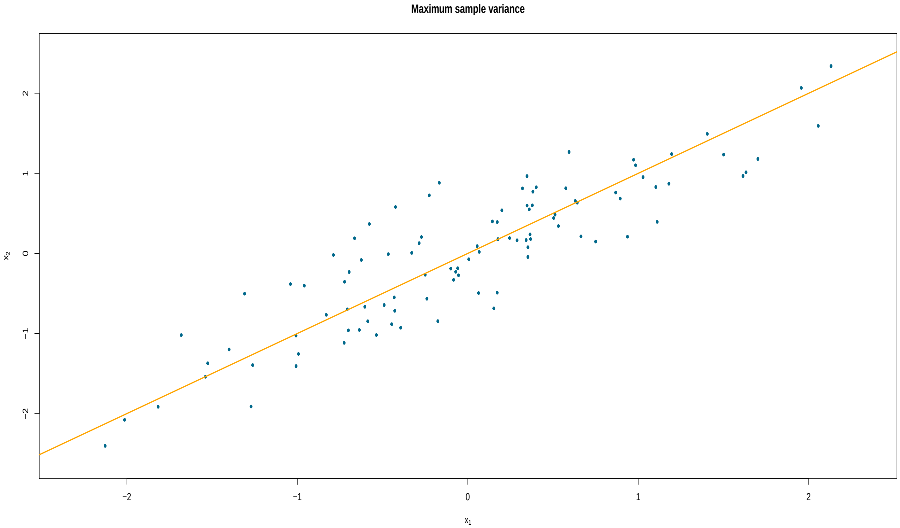
Principal component analysis



Principal component analysis

- PCA: The linear combination that represents $\widetilde{X}$ best is the one that maximizes the sample variance of the projected data.
- Problem: How to get such linear combination in practice?

Principal component analysis



Principal component analysis

- First principal component: $Z = z_1 = \widetilde{X} c_1$ such that z_1 has maximum sample variance.
- Sample variance of z_1: $s_{z_1}^2 = c_1' S_x c_1$, where S_x is the sample covariance matrix of X.
- However: $c_1' S_x c_1$ can be increased by multiplying c_1 with any constant larger than 1.
- Eliminate this indeterminacy: Restrict attention to coefficient vector of unit length, i.e., assume that $c_1' c_1 = 1$.
- Then: First PC corresponds to the linear combination, c_1, that solves:

$$\underset{s.t.\ c_1' c_1 = 1}{\arg\max}\ c_1' S_x c_1$$

Principal component analysis

- Remember: S_x is a positive semi-definite matrix.
- Thus: S_x has p positive eigenvalues, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \geq 0$ with associated eigenvectors $v_1, \ldots, v_p$, such that, $S_x v_j = \lambda_j v_j$, for $j = 1, \ldots, p$.
- Solution to the optimization problem: c_1 is the eigenvector of S_x, v_1, associated with the largest eigenvalue, λ_1.
- First PC: $z_1 = \widetilde{X} v_1$.
- Sample variance of z_1:

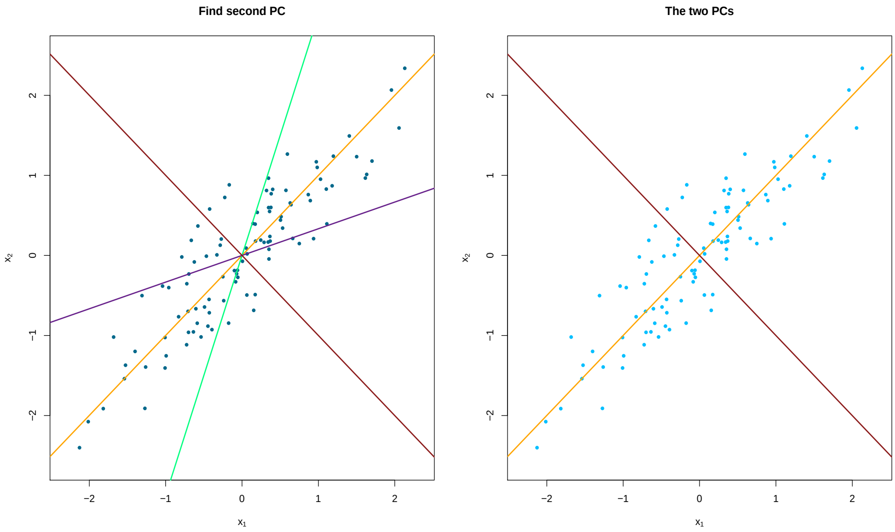
$$s_{z_1}^2 = v_1' S_x v_1 = \lambda_1 v_1' v_1 = \lambda_1$$

- In other words: The sample variance of the first PC is the largest eigenvalue of S_x, λ_1.

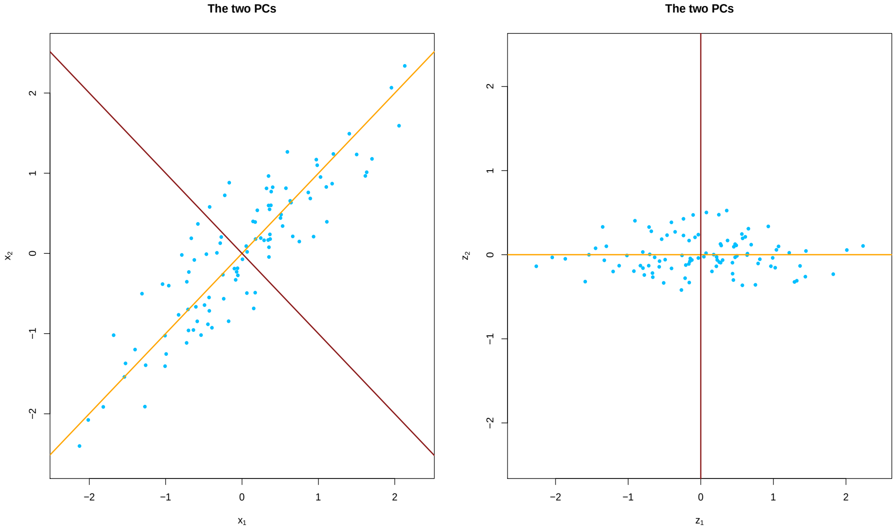
Principal component analysis

- Assume we want $r = 2$: $Z = \widetilde{X}C$, where C is a $p \times 2$ matrix.
- First PC: First column of Z is $z_1 = \widetilde{X}v_1$.
- Second PC: Second column of Z is $z_2 = \widetilde{X}c_2$.
- How to define c_2?
- See several possibilities in the next slide.
- Which one is the best option?

Principal component analysis



Principal component analysis



Principal component analysis

- Thus: The second PC is obtained with a similar argument adding the property that it is uncorrelated with the first PC.
- Why?: The new variables do not share common information.
- Second principal component: $z_2 = \widetilde{X} c_2$ such that z_2 has maximum sample variance and it is uncorrelated to z_2.
- Sample variance of z_2: $s_{z_2}^2 = c_2' S_x c_2$.
- Then: Second PC corresponds to the linear combination, c_2, that solves:

$$\underset{s.t.\ c_2' c_2 = 1,\ c_1' S_x c_2 = 0}{\arg\max} \quad c_2' S_x c_2$$

Principal component analysis

- Solution to the optimization problem: c_2 is the eigenvector of S_x, v_2, associated with the second largest eigenvalue, λ_2.
- Second PC: $z_2 = \widetilde{X} v_2$.
- Sample variance of z_2:

$$s_{z_2}^2 = v_2' S_x v_2 = \lambda_2 v_2' v_2 = \lambda_2$$

- In other words: The sample variance of the second PC is the second largest eigenvalue of S_x, λ_2.

Principal component analysis

- More PCs: This argument can be extended for successive principal components.
- Assume we want r PCs: Define $V_r = [v_1|\dots|v_r]$ with columns the eigenvectors of S_x linked to the r largest eigenvalues $\lambda_1, \dots, \lambda_r$.
- Then: The r PCs are given by the $n \times r$ matrix:

$$Z = \widetilde{X} V_r$$

- Characteristics of Z:
  1. Sample mean vector of Z: $\overline{z} = 0_r$.
  2. Sample covariance matrix of Z: S_z, is the diagonal matrix with elements $\lambda_1, \dots, \lambda_r$.
- PC scores: The observations in Z are usually called PC scores.

Principal component analysis

- Indeed: It is possible to take $r = p$, as in the two dimensional data set of the example.
- Total variability of X:

$$Tr\left(S_x\right) = \sum_{j=1}^{p} s_{x_j}^2$$

- Total variability of $Z = \widetilde{X} V_p$:

$$Tr\left(S_z\right) = \sum_{j=1}^{p} \lambda_j$$

- Total variability of X is preserved after a PCA transformation:

$$Tr\left(S_x\right) = Tr\left(S_z\right)$$

Principal component analysis

- Different units of measurement: X should be standardized first.
- Why?: Variables with large sample variances (due to the effect of the units of measurement) will tend to dominate the early components.
- Consequence: First, obtain $Y = \widetilde{X} D_x^{-1/2}$, where D_x is the diagonal matrix that contains the sample variances of the variables in X, and then, obtain PCs.
- Sample covariance of Y is the sample correlation of X:

$$S_y = D_x^{-1/2} S_x D_x^{-1/2} = R_x$$

- Therefore: The PCs are constructed with the eigenvectors of R_x.

Principal component analysis

- How many PCs to select?
- Proportion of variability explained by r-th PC:

$$PV_r = \frac{\lambda_r}{\lambda_1 + \cdots + \lambda_p} \qquad r = 1, \ldots, p$$

where $\lambda_1, \ldots, \lambda_p$ are the eigenvalues of either S_x, or R_x.

- Accumulated proportion of variability explained by the first r PCs:

$$APV_r = \frac{\lambda_1 + \cdots + \lambda_r}{\lambda_1 + \cdots + \lambda_p} \qquad r = 1, \ldots, p$$

- Select r: APV_r larger than a certain quantity, such as 0.7, 0.8 or 0.9.
- Take into account: Trade off between APV_r and the number of PCs selected.

Principal component analysis

- Chapter 2.R script:
  - PCA: NCI60 data set.
  - PCA: College data set.
  - Detect outliers after a PCA: College data set.

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Sparse principal component analysis

- Non-zero weights: As can be seen in the College data set, the PCAs are usually constructed with weights that are non-zero.
- All the variables contribute to all the PCs: This can be problematic when the number of variables is large.
- Two main reasons:
  1. Interpretation can be difficult.
  2. Estimation of eigenvectors can underweight important variables.

Sparse principal component analysis

- Sparse principal components: PCs with many weights forced to be 0.
- Idea: Maximize the variance of linear combinations subject to a norm restriction on the weights and shrinking some of the weights to 0.
- First PC: Solve the following optimization problem:

$$\underset{s.t.\ c_1'c_1=1,\ \|c_1\|_1\leq k}{\arg\max}\quad c_1'S_xc_1$$

  where $\|c_1\|_1 = \sum_{j=1}^{p} |c_{1j}| \leq k$, and k is an integer number.
- The number k: Controls the number of weights that are different than 0.

Sparse principal component analysis

- First sparse principal component: Say w_1.
- Second sparse principal component: Solve the following optimization problem:

$$\underset{s.t.\ c_2'c_2=1,\ w_1'S_x c_2=0,\ \|c_2\|_1\leq k}{\arg\max} \quad c_2' S_x c_2$$

  where $\|c_2\|_1 = \sum_{j=1}^{p} |c_{2j}| \leq k$, and k is an integer number (the same used before).
- Others: Follow the same arguments to get the p sparse principal components, say $w_1, w_2, \ldots, w_p$.

Sparse principal component analysis

- Complex optimization procedures: Resolution of the optimization problems is quite hard.
- Non-orthogonal scores: Usually, the solution obtained in general does not provide with orthogonal scores.
- Nevertheless: Sample correlations between sparse PCs are usually small.

Sparse principal component analysis

- Chapter 2.R script:
  - SPCA: College data set.

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Independent component analysis

- PCA: Given X obtain $Z = \widetilde{X}C$, such that Z of size $n \times r$ with $r < p$, contains uncorrelated variables.
- ICA: Given X obtain $Z = \widetilde{X}C$, such that Z of size $n \times r$ with $r < p$, contains independent variables.
- Mathematical complexity: ICA is much more mathematically challenging than PCA, which is only based on eigenvectors and eigenvalues.
- Idea: Maximize the statistical independence of the independent component scores in Z by maximizing the non Gaussianity of the components of Z.

Independent component analysis

- Standardization: If the variables in X have different units of measurement, it is better to standardize the data first.
- Fix r: It is necessary to fix r in advance.
- Role of r: Different values of r give different ICs.
- New variables: Z have sample mean vector 0_r and sample covariance matrix I_r (at least, it is expected).

Independent component analysis

- Chapter 2.R script:
    - ICA: College data set.

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