Reordering and selecting continuous variables

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Introduction

- Handling big, unknown data sets with a huge number of numerical variables is challenging
- Overviewing the correlation structure or finding more general two-dimensional anomalies can be quite difficult, **but**
  - two-dimensional structures are a good starting point for discovering interactions
  - interactions between two variables are visualizable and can be easily interpreted in scatterplots

  $\Longrightarrow$ It's useful to be able to handle them

- The talk tries to help with two concepts:
  - Present a convenient graphic to overview the whole correlation structure
  - Select a scatterplot matrix to allow a first deeper insight in the real data

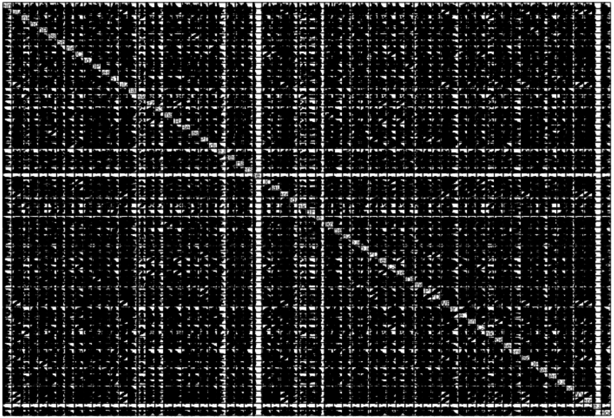
German election

- 299 cases (Germans electoral districts)
- 70 variables
  - vote shares of the parties in 2009 and 2005
  - demographic and economic information about the districts (e.g. unemployment rate, population density, birth rate)

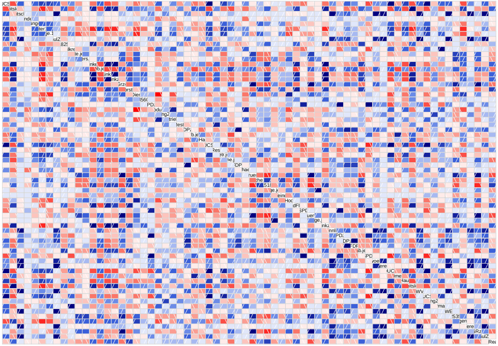
68 numeric variables $\Longrightarrow$ 2278 possible two-dimensional plots

How can we overview the correlation structure visually?

Overview of all bivariate structures: A scatterplot matrix



A *corrgram*[1] with all numerical variables in random order



- Visualizes the correlation matrix
- Direction of correlation is visualized by the color (blue for positive correlation, red for negative)
- Strength is visualized by the color intensity

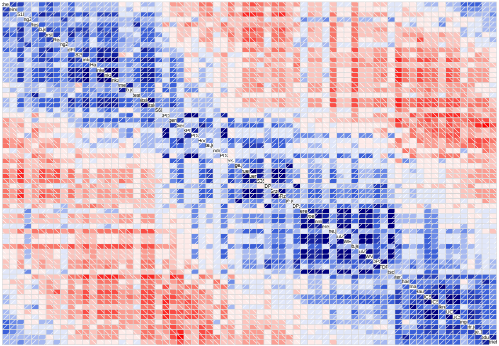
More to see, but still unclear $\Longrightarrow$ we need a new order

[1] Michael Friendly (2002), implemented in the package **corrgram**

Reordering based on angles of principal components

Based on eigenvectors v_1, v_2 of the correlation matrix we consider for each variable the loading on the first two principal components $((v_{i1}, v_{i2})^T)$
The angles to the x-axis of these vectors can be used as a measure of similarity:

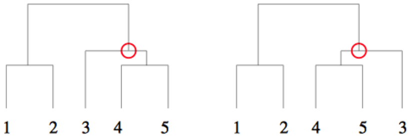
$$\alpha_i = \begin{cases} \arctan\left(\frac{v_{i2}}{v_{i1}}\right) & \text{if } v_{i1} > 0, \\ \arctan\left(\frac{v_{i2}}{v_{i1}}\right) + \pi & \text{else} \end{cases}$$



For a comparison: Optimal leaf ordering (OLO)[2]

Approach:

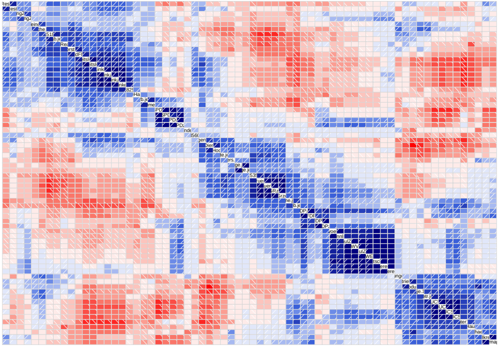
- Hierarchical clustering (average linking) of the variables based on correlation matrix
- Reordering of the leaves to maximize the sum of the correlations of adjacent variables



from: Fast optimal leaf ordering for hierarchical clustering (Ziv Bar-Joseph et al)

[2]practical algorithm from Ziv Bar-Joseph et al (2001), implemented in the package **seriation**

A corrgram with variables in OLO based order



- Seems even more ordered (over the PCA based ordering)
- Can also help to make a choice for the number of clusters (alternative to dendrograms)

Selecting q variables to show in a scatterplot matrix

Goal: Show q variables with maximal correlation in terms of:

$$\max g(i_1, i_2, ..., i_q) = \sum_{j=1}^{q} \sum_{k=j+1}^{q-1} Cor(X_{i_j}, X_{i_k}) \quad (1)$$
$$\text{where } i_1 < i_2 < ... < i_q \text{ and } i_j \in \{1, ..., p\} \forall\, i_j$$

Easiest approach: Checking all possible combinations, which is computationally intensive.

- There are more than 10 million possibilities to select 5 variables from the *German election* dataset and
- more than 500 million to select 8 variables.

How can the reordering help?

Approach to find q variables with maximal correlation

Based on the new order of the variables $X_1, ..., X_p$ both goals are (approximatively) reachable with the following steps:

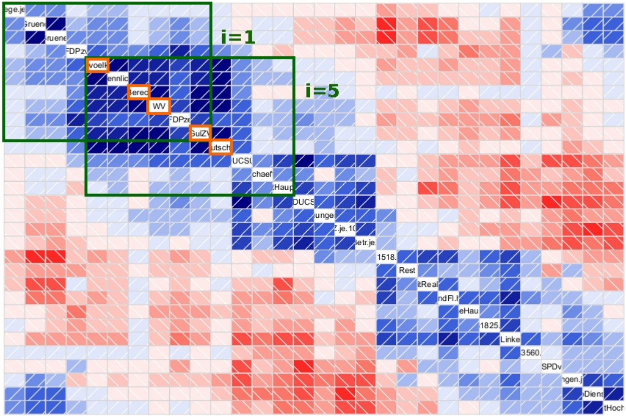
1. Choose $r \geq q$
2. For all $i \in \{1, ..., p\}$ calculate:

$$\begin{aligned} sumCor_i = & \max g(i_1, i_2, ..., i_q) \\ & \text{where } i_1 < i_2 < ... < i_q \\ & \text{and } i_j \in \{i, (i+1) \bmod p, ..., (i+r-1) \bmod p\} \\ & \forall\, i_j \text{ with } (p \bmod p) := p \end{aligned} \tag{2}$$

3. Find $\max_i sumCor_i$

Illustration of the approach

$r = 10, q = 5$



Comparison

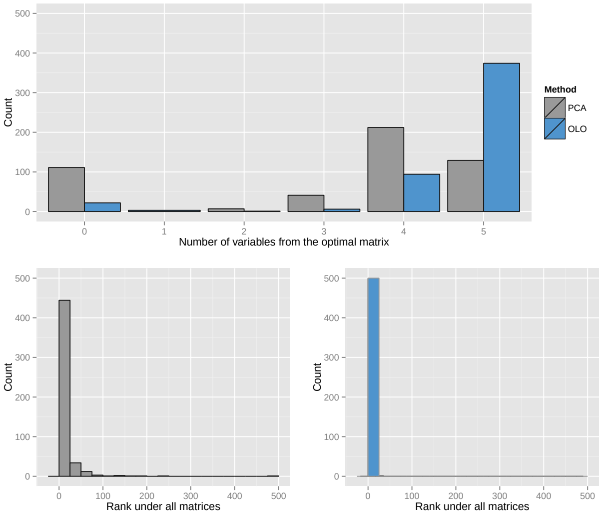
- Consider randomly chosen samples (30 variables) from dataset *German election* (500 times)
- Compare the results from the PCA based and from the optimal leaf reordering with the real optimum
- Vary r

Of interest is for different numbers of r:

- How many variables from real optimal matrix are found?
- Which rank has the approximative matrix under all possible in terms of the maximum correlation?

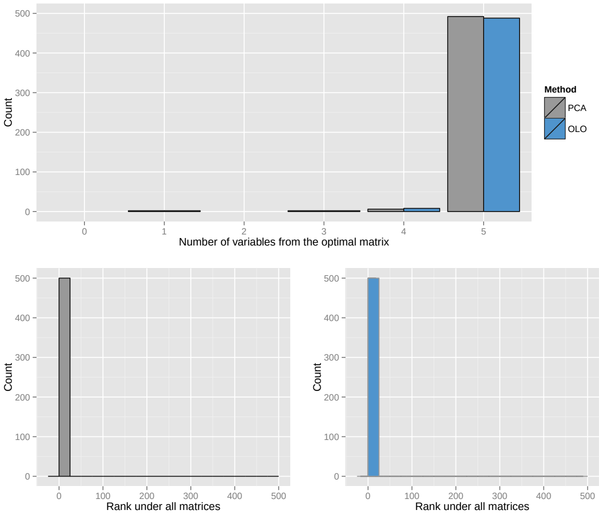
$r = 5$ (check only adjacent variables)

Checking 30 combinations instead of all $\binom{30}{5} = 142506$



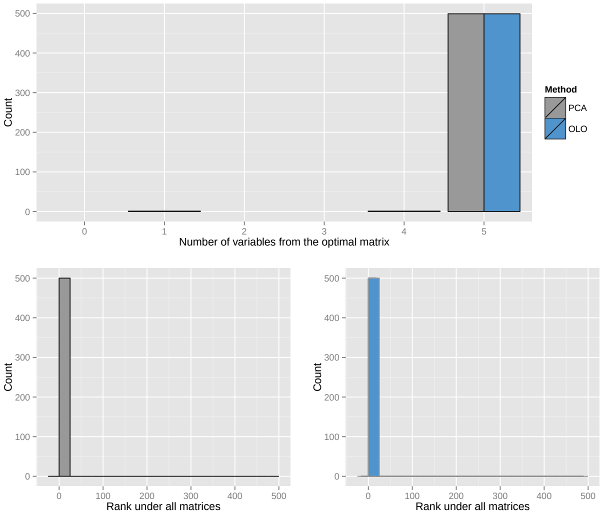
$r = 10$

Checking $30\binom{10}{5} = 7560$ combinations instead of $\binom{30}{5} = 142506$

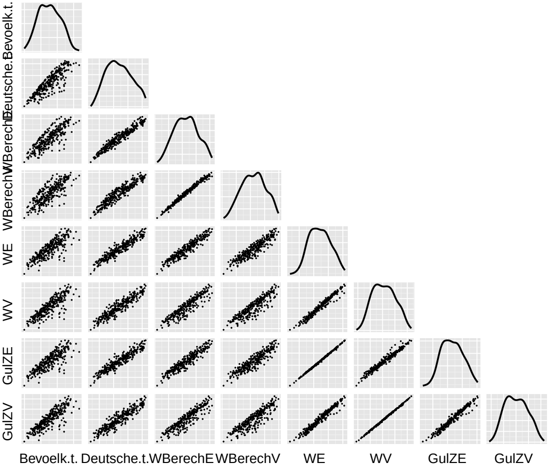


$r = 15$

Checking $30\binom{15}{5} = 90090$ combinations instead of $\binom{30}{5} = 142506$



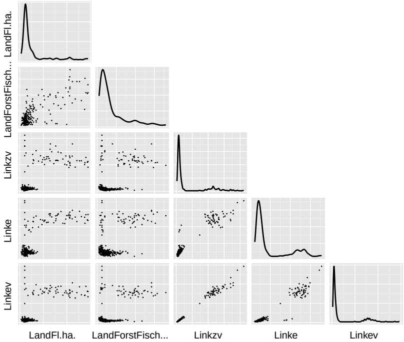
What's the result with the whole dataset?



- $r = 10$: PCA based reordering finds 7 from the 8 variables of the optimal matrix, OLO already delivers the optimal matrix
- $r = 15$: Both methods find the optimal matrix

Possible extensions to select scatterplot matrices

1. Ignore really high correlations (in a second step)
2. Substitute the correlation with a more general dependency measure
3. Based on the *scagnostics* idea, that scatterplots are describable through a few measures, a more complex approach is conceivable:
   - Define a *relevance measure* based on scagnostics measures[3]
   - Use the same approach to find the matrix with "highest relevance"



[3]Some of the measures from package **scagnostics** are used for the example

Conclusions

- Reordering in connection with corrgrams satisfies the goal to offer a good first overview of the correlation structure
- The idea of studying subgroups can bring good insights in the data
- Especially the *scagnostics* approach can offer a general and interesting extension of that idea

References

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