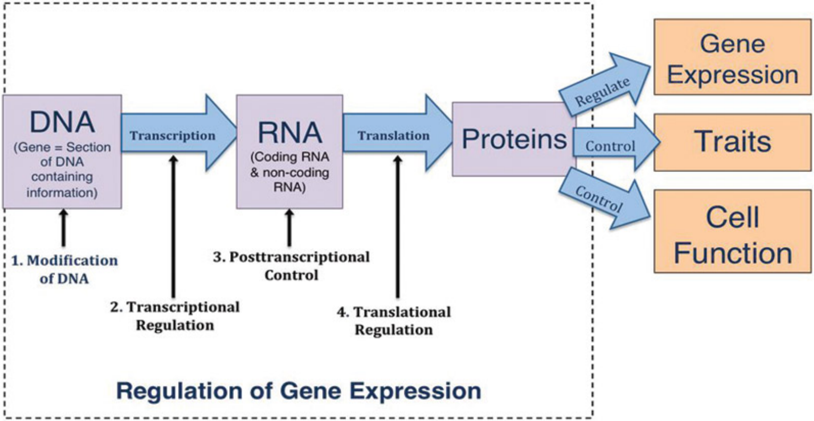
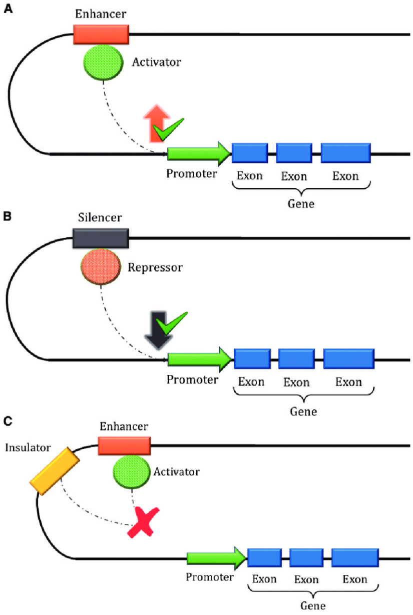
SVD and PCA in HD

December 5, 2023

Motivation - Gene Expression


DNA
(Gene = Section of DNA containing information)
Transcription
RNA
(Coding RNA & non-coding RNA)
Translation
Proteins
Regulate
Control
Control
Gene Expression
Traits
Cell Function
1. Modification of DNA
2. Transcriptional Regulation
3. Posttranscriptional Control
4. Translational Regulation
Regulation of Gene Expression

Transcription factors



PCA - reduction of dimensionality of ”omics” data

$X_{n \times p}$ - data matrix (e.g. gene expressions), $n = k \times 100$, $p \approx 20000$ - number of genes

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Practical goal - data compression, several basis vectors [Principal Components] may contain most of the information and be applied for prediction (of the patient’s response to the therapy)

Principal Components Analysis (2)

Method - Singular Value Decomposition:

$$X = U_{n\times l} D_{l\times l} V^T_{l\times p} \quad ,$$

$U^T U = I_{l\times l}, V^T V = I_{l\times l}, \;\; l = min\{n,p\},$ and D is the diagonal matrix

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$$\hat{M}_k = U_{n\times k} D_{k\times k} V^T_{k\times p} = \underset{M:rank(M)=k}{\arg\min} \sum_{ij} (X_{ij} - M_{ij})^2$$

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Statistical Goal - determining rank k of matrix M

PESEL (PEnalized SEmi-integrated Likelihood)

Sobczyk, Bogdan, Josse, Journal of Computational Graphical Statistics, 2017

Bayesian Information Criterion (BIC) (1)

$A_1 \in A_2 \in A_3 \ldots$ - nested sequence of statistical models

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$l(X, \theta)$ - likelihood function (density of the distribution describing the data)

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In general situation BIC suggests selecting the model maximizing

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Idea - reduction of the number of parameters by integrating them out with respect to some prior distribution

PESEL for large p

Assume that $M = TW^T$, where
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$$w_{j\cdot} \sim N(0, I_k) \quad ,$$

which implies, that $x_{\cdot 1}, \ldots, x_{\cdot p}$ są are iid random vectors from the distribution

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The related criterion is called PESEL (Penalized SEmi-integrated Likelihood).

Consistency of PESEL

Let $\hat{k}_0(p, n)$ be the PESEL estimator of the rank of M.

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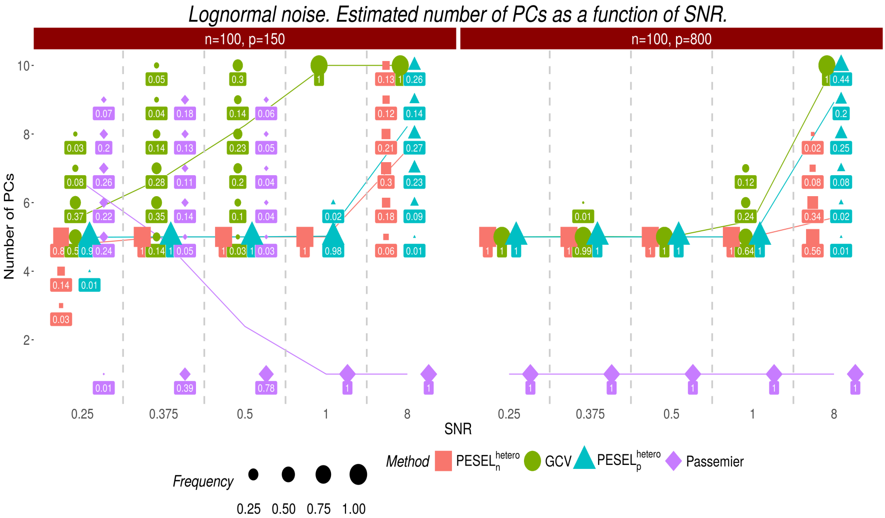
Then, for n fixed and under mild regularity conditions it holds

$$P(\exists p_0 \; \forall p > p_0 \quad \hat{k}_0(p, n) = k_0) = 1.$$

Errors from the log-normal distribution



Varclust

Multiple Latent Component Clustering, Sobczyk, Wilczyński, Bogdan, Graczyk, Josse, Panloup, Seegers, 2020

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Package *varclust* by P. Sobczyk and S. Wilczyński- Algorithm K-centroids around PCs. Estimation of the number of clusters and their dimensions by modifications of BIC.

Methodology

K-centroids algorithm

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Centers - PCs, distance - BIC

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Estimation of clusters dimensions by PESEL

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Repeat for different K and estimate K by mBIC

Overview of the algorithm

Algorithm: Multiple Latent Clustering Components

```
Input: $n$ - number of individuals, $p$ - number of variables,
  $X_{n \times p} = (x_1, \ldots, x_p)$ - data set, $d$ - maximal subspace
  dimension, $N$ - number of runs of the algorithm
  Scale $X$ to have columns with mean 0 and unit variance
  for $i \in \{1, \ldots, N\}$ do
     Find the model using K-means and store its value of mBIC
  end for
  Choose the model with the highest value of mBIC and return
  the model (segmentation, mBIC, factors) as the result. =0
```

K-means step

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   - For every variable x_j and every cluster factors $F_{j'}$ fit a linear regression model without intercept $lm(x_j \sim F_{j'})$ and store BIC value as $BIC_{jj'}$
   - Assign variable x_j to the cluster M_q where

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   - For every cluster M_i use PESEL to estimate its dimensionality k_i with an upper bound of d. Use PCA to compute the first k_i principal components and store them in F_i

Convergence (1)

Both the partition (BIC) and the center's selection (PESEL) steps lead to increase of Laplace approximations to the model posterior probability.

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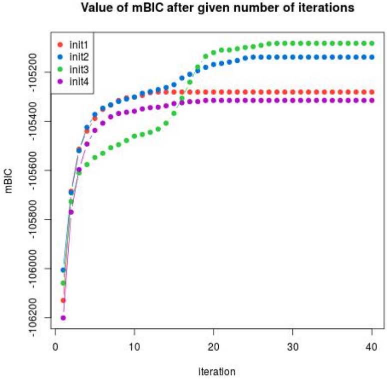
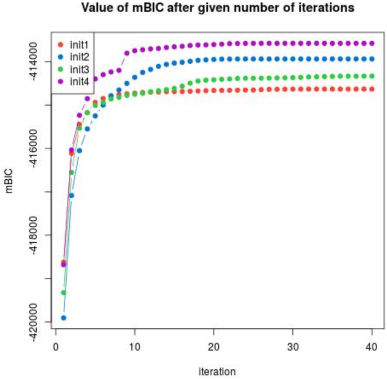
For sufficiently large *n* and *p* each step of the algorithm leads to increase of mBIC.

Convergence (2)

$p = 750 p = 3000$





Informative prior distribution and mBIC

- The problem with BIC (non-informative prior)
- Prior distribution taking into account the number of clusters and maximal dimension of the subspace

$$P(M) = \frac{1}{K^p}\frac{1}{d^K}$$

$$mBIC = \sum_{i=1}^{K} \ln\left(\widehat{P}(X_i|M_i)\right) - p\ln(K) - K\ln(d)$$

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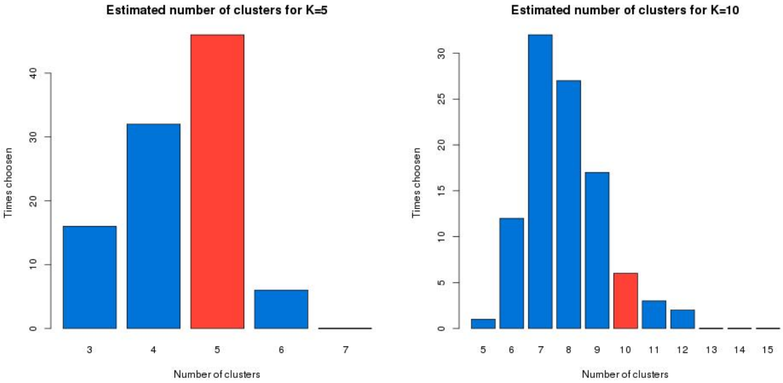
Application

mBIC can be used to compare different models and to choose the number of clusters in the data.

mBIC

Figure: Estimation of the number of clusters. Simulation parameters: $n = 100,\ p = 600,\ d = 3,\ SNR = 1\ mode : not\ shared$.

$K \qquad = \qquad 5K \qquad = \qquad 10$



Compared methods

1. **Sparse Subspace Clustering** (SSC)
2. Low Rank Subspace Clustering (LRSC)
3. **MLCC with random initialization** (MLCC)
4. **MLCC with initialization by the result of SSC** (MLCC_{aSSC})
5. MLCC with initialization by sparse PCA (MLCC_{sPCA})
6. ClustOfVar (COV)

Data generation - shared factors

```
**Input:** $n$, $SNR$, $K$, $p$, $d$
  Number of factors $m \leftarrow K\frac{d}{2}$
  Factors $F = (f_1, \ldots, f_m)$, $f_i \sim N(0, I_n)$
  Draw subspaces' dimension $d_1, \ldots d_K$ uniformly from $\{1, \ldots, d\}$
  **for** $i = 1, \ldots, K$ **do**
    $F_i \leftarrow$ sample of size $d_i$ from columns of $F$
    Draw matrix of coefficients $C_i$ from $U(0.1, 1) \cdot sgn(U(-1, 1))$
    Variables in the $i$-th subspace are $X_i \leftarrow F_i C_i$
  **end for**
  Scale matrix $X = (X_1, \ldots, X_K)$ (columns with unit variance)
  return $X + Z$ where $Z \sim N(0, \frac{1}{SNR} I_n)$ =0
```

Data generation - independent subspaces

Remark

To generate data without shared factors we draw independently i-th subspaces basis F_i as sample of size d_i from standard multivariate normal distribution

Measures of effectiveness

Compare two partitions $A = (A_1, \ldots A_n),\ B = (B_1, \ldots, B_m)$

- Adjusted Rand Index (ARI)
- Integration
- Acontamination
- ARI $\in [-1, 1]$, Integration, Acontamination $\in [0, 1]$.

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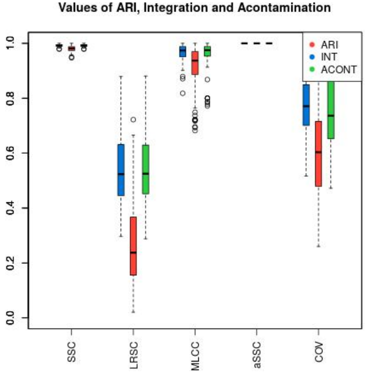
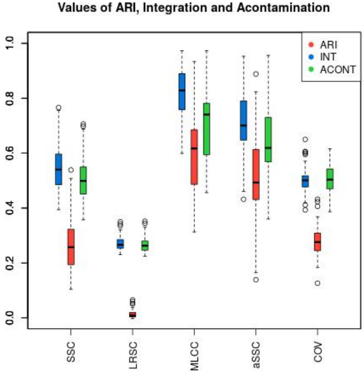
Remark

The bigger the indices, the better the clustering.

Mode

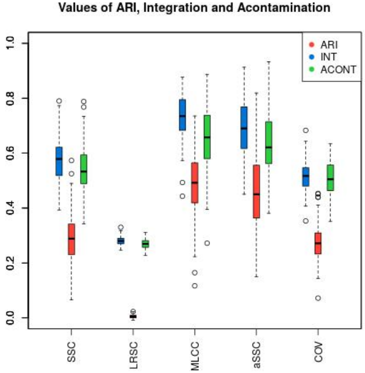


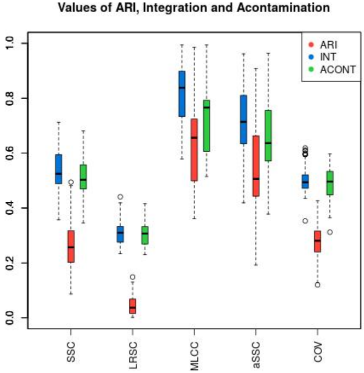
Values of ARI, Integration and Acontamination



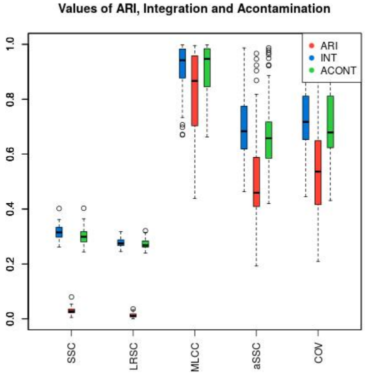
Values of ARI, Integration and Acontamination

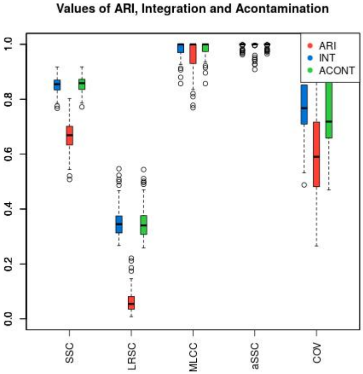
Number of variables





Signal to noise ratio

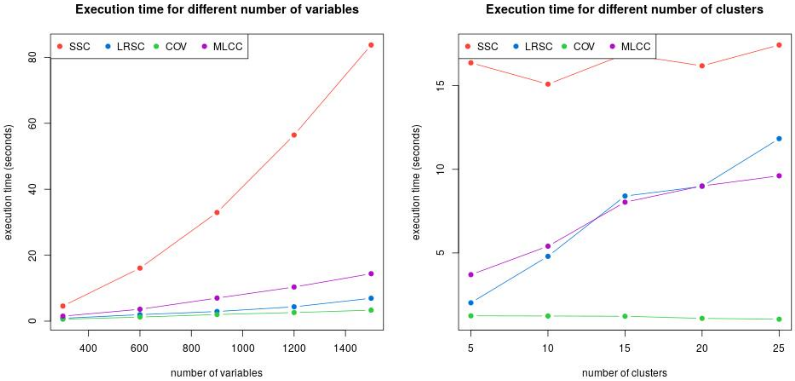




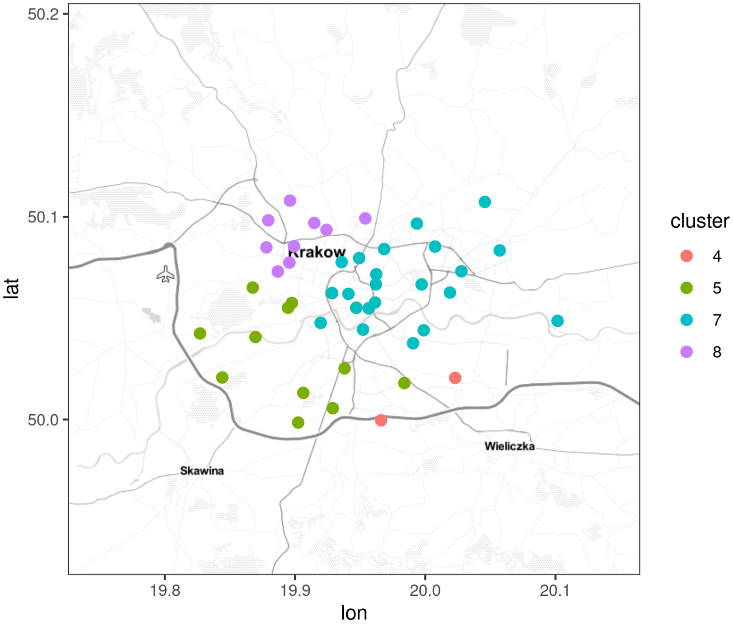
Execution time

Figure: Comparison of the execution time of the methods with respect to p and K. Simulation parameters:$n = 100,\ d = 3,\ SNR = 1\ mode : shared$.

With respect to theWith respect to the
number of variablesnumber of clusters



Particle matter measurements clustered using varclust



Sparse PCA (1)

$$\text{maximize} \;\; a'\Sigma a, \;\text{subject to} \;\; ||a|| = 1 \;\; \text{and}$$

1. $||a||_0 \leq k$
2. $||a||_1 \leq t$ (ScoTLASS)

Sparse PCA in R (*sparsepca*)

$$argmin_B \;\; \frac{1}{2}||X - XBA'|| + \phi(B) \;\; ,$$

where $AA' = I$ and $\phi(B)$ is the sparsity inducing penalty (LASSO or elastic net)