Clustering Methods and Correlated Data: Simulations

Parker Knight

9/29/2021

Overview

1. Review of methods
2. Simulation design
3. Results
4. Directions

Methods of Interest

1. K-means
2. Hierarchical clustering
3. Spectral clustering

K-means

Let $X \in \mathbb{R}^{n \times p}$ be a given data matrix. Our goal is to partition the n data points into k non-overlapping clusters, denoted by the set $S = \{S_1, S_2, ..., S_k\}$.

The k-means algorithms does so by minimizing the Euclidean distance between each point and the centroid of it's assigned cluster:

$$\min_{S} \sum_{i=1}^{k} \sum_{X_j \in S_i} ||X_j - \mu_i||_2^2$$

where μ_i is centroid of the points in S_i.

K-means (cont.)

Key points:

- k must be specified up front
- Computation is NP-hard (objective function is not convex)
- By default, uses Euclidean distances
  - alternate versions exist (K-medoids)
- Assumes separation between clusters is convex

Hierarchical clustering

Let $D = \mathrm{dist}(X)$ be the pairwise distance matrix of the n samples.

In agglomerative HC, we start with every observation in a singleton cluster, join clusters G and H together based on the following criteria:

i. $d_{SL} = \min_{i \in G, j \in H} d_{i,j}$ (single linkage)
ii. $d_{CL} = \max_{i \in G, j \in H} d_{i,j}$ (complete linkage)
iii. $d_{GA} = \frac{1}{N_G N_H} \sum_{i \in G} \sum_{j \in H} d_{i,j}$ (group average)

In divisive HC, we begin with data all in one cluster and split into sub-clusters with K-means.

HC (cont.)

Key points:

- don't need to specify k up front, can 'cut' the tree at any depth
- relies on pairwise distances, sensitive to outliers
- greedy algorithm
- 'big data' issues

Spectral clustering

Refers to a broad class of methods, but the general idea is as follows:

1. Compute spectral composition of X to yield a low-rank approximation
2. Cluster the low-rank data with a standard method (usually k-means)

I'll focus on two approaches: Graph-based spectral clustering (GSC) and 'simple' spectral clustering (SSC).

Graph Spectral Clustering

Described in detail by von Luxburg (2007).

From our data matrix X, compute a similarity matrix $S \in \mathbb{R}^{n \times n}$. Then:

1. Compute a similarity graph from S, and define W to be the 'weighted' adjacency matrix
2. Construct the Laplacian L from W
3. Compute $L = UDU^T$
4. Cluster the first k columns of U using k-means

GSC (cont.)

Key points:

- How do we construct S? How do we construct a graph from S?
- Normalized or unnormalized Laplacian?
- Need to specify k
- Can handle non-convexity between clusters

Simple Spectral Clustering

1. Compute the SVD $X = USV^T$
2. Run k-means on the first k columns of $US^{1/2}$

SSC (cont.)

Key points:

- Simple implementation
- Need to specify k
- Assumes clusters are convex in $\mathbb{R}^k$

Simulation Design

Question: how robust are these methods to correlation structure between the samples in X?

We vary the following parameters:

- n $= 100$
- p $=$ 50,100,200
- $\#$ of clusters $=$ 2, 3, 4
- $\#$ of groups $=$ 2, 10, 50
  - the 'groups' determine the block-diagonal structure of the covariance matrix
- $\rho =$ 0.2,0.5,0.8
  - within-group correlation
- difference in mean between groups: 0.25,1
  - 'signal strength'

Simulation Design (cont.)

Given a set of parameters, repeat R times:

1. Generate block-diagonal Σ with `ngroups` blocks, set within-group correlation ρ

```
Sigma <- Matrix::bdiag(lapply(1:(n/ngroups), function(i){
    I <- (1-rho) * diag(ngroups)
    ones <- rho * rep(1 ,ngroups) %*% t(rep(1, ngroups))
    I + ones
  }))
```

Simulation Design (cont.)

2. Generate vector of cluster assignments $\mathbf{C} = (C_1, C_2, ..., C_n)^T$ where C_i may equal 1, 2, ..., k. Set the mean vector $\mu = (\mu_{C_1}, \mu_{C_2}, ..., \mu_{C_n})^T$ where μ_{C_i} is the mean of cluster C_i.

```
cluster_names <- LETTERS[1:nclust]
cluster_assignment <- sample(cluster_names,
                             size = n,
                             replace = TRUE)
mu <- (0:(nclust - 1)) * mu_step_size
mu_vec <- rep(0, n)
for (cl in 1:length(cluster_names))
    mu_vec <- mu_vec + ifelse(cluster_assignment ==
                                cluster_names[cl],
                              mu[cl],
                              0)
```

Simulation Design (cont.)

3. Draw $X \sim MVN(\mu, \Sigma)$.

```
X <- t(MASS::mvrnorm(n = p, mu = mu_vec, n/nclust,
        Sigma = Sigma))
```

4. Cluster the rows of X with each method to get an estimated cluster assignment $\hat{\mathbf{C}} = (\hat{C}_1, ..., \hat{C}_n)^T$ and compare results...

Simulation Design (cont.)

How do we evaluate the performance of each clustering method?
Rand index:

$$RI = \frac{1}{\binom{n}{2}} \sum_{i=1}^{n} \sum_{j \neq i} I\left[(C_i = C_j \wedge \hat{C}_i = \hat{C}_j) \vee (C_i \neq C_j \wedge \hat{C}_i \neq \hat{C}_j) \right]$$

Simulation Design (cont.)

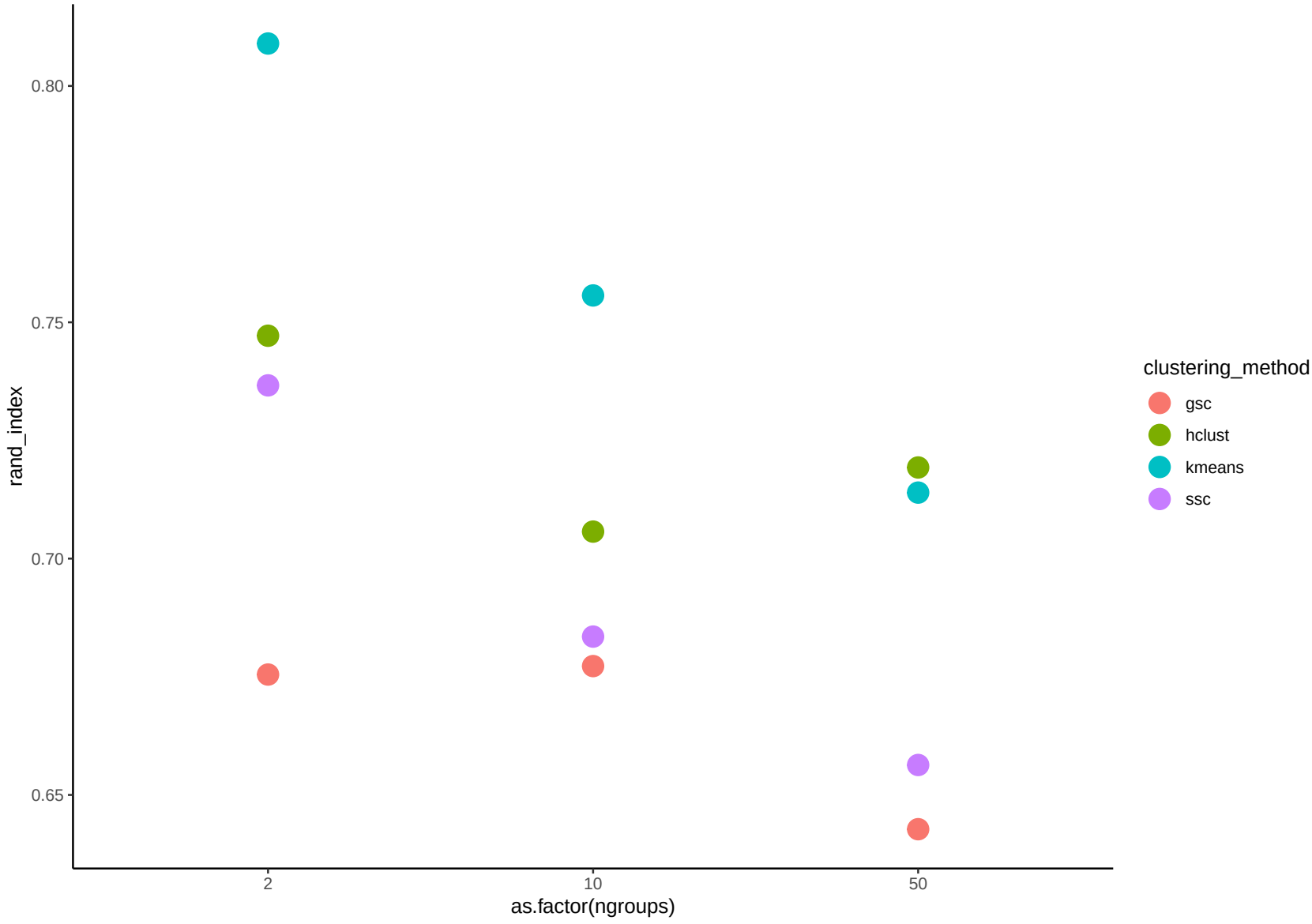
Some immediate concerns:

1. We set k to be the true number of clusters
2. We assume that cluster means are equally spaced apart (signals are equally strong).
3. Many options for graph spectral clustering... our method (after some trial-and-error) is:
   - Construct S with a Gaussian similarity kernel with $\sigma^2 = 25$
   - Build an unweighted K-nearest neighbors graph with $K = 25$ (relatively dense)
   - Use a normalized Laplacian $L = I - D^{-1/2}AD^{-1/2}$

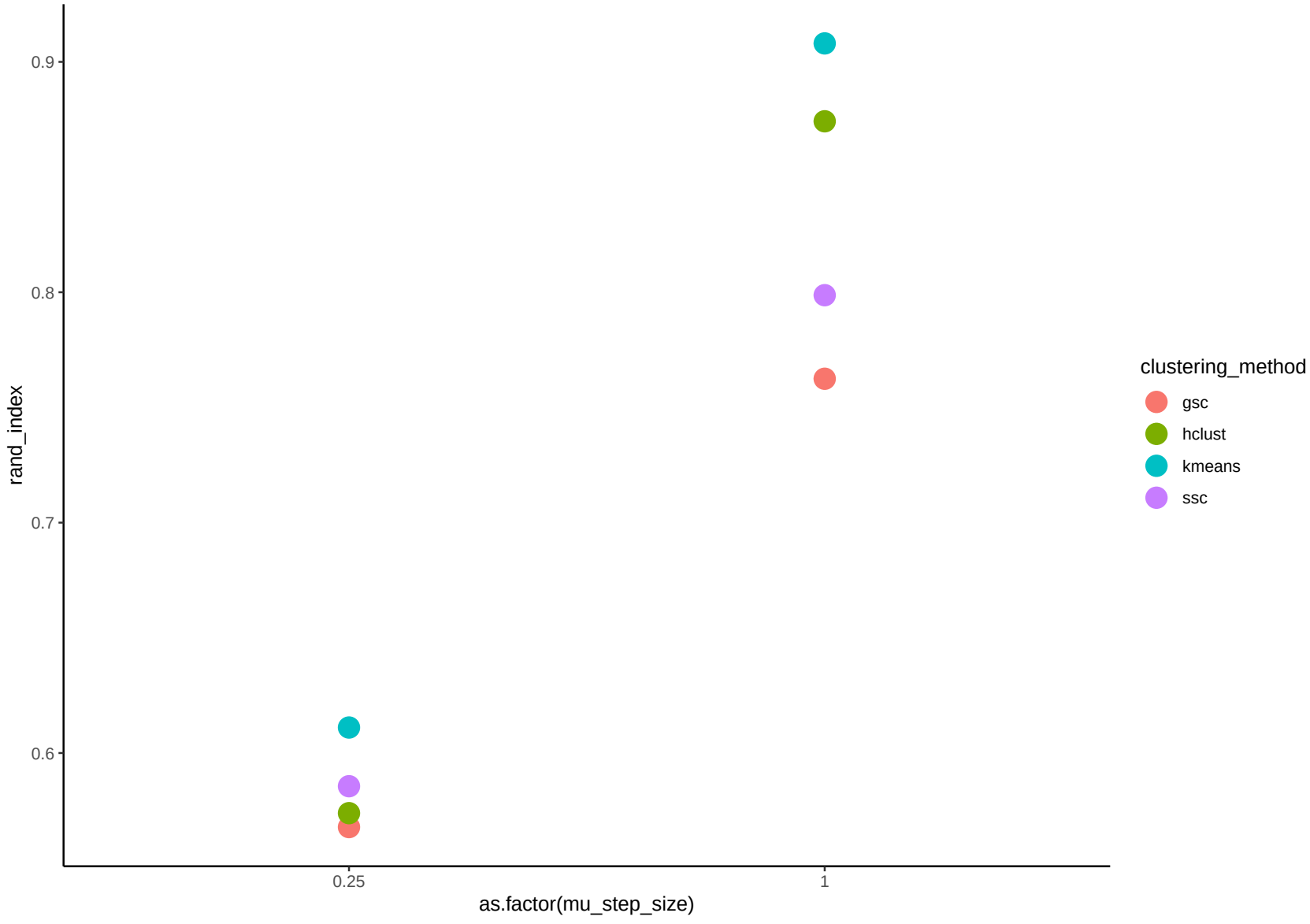
Results

clustering_method	average_ri
gsc	0.6651614
hclust	0.7240498
kmeans	0.7595413
ssc	0.6921627

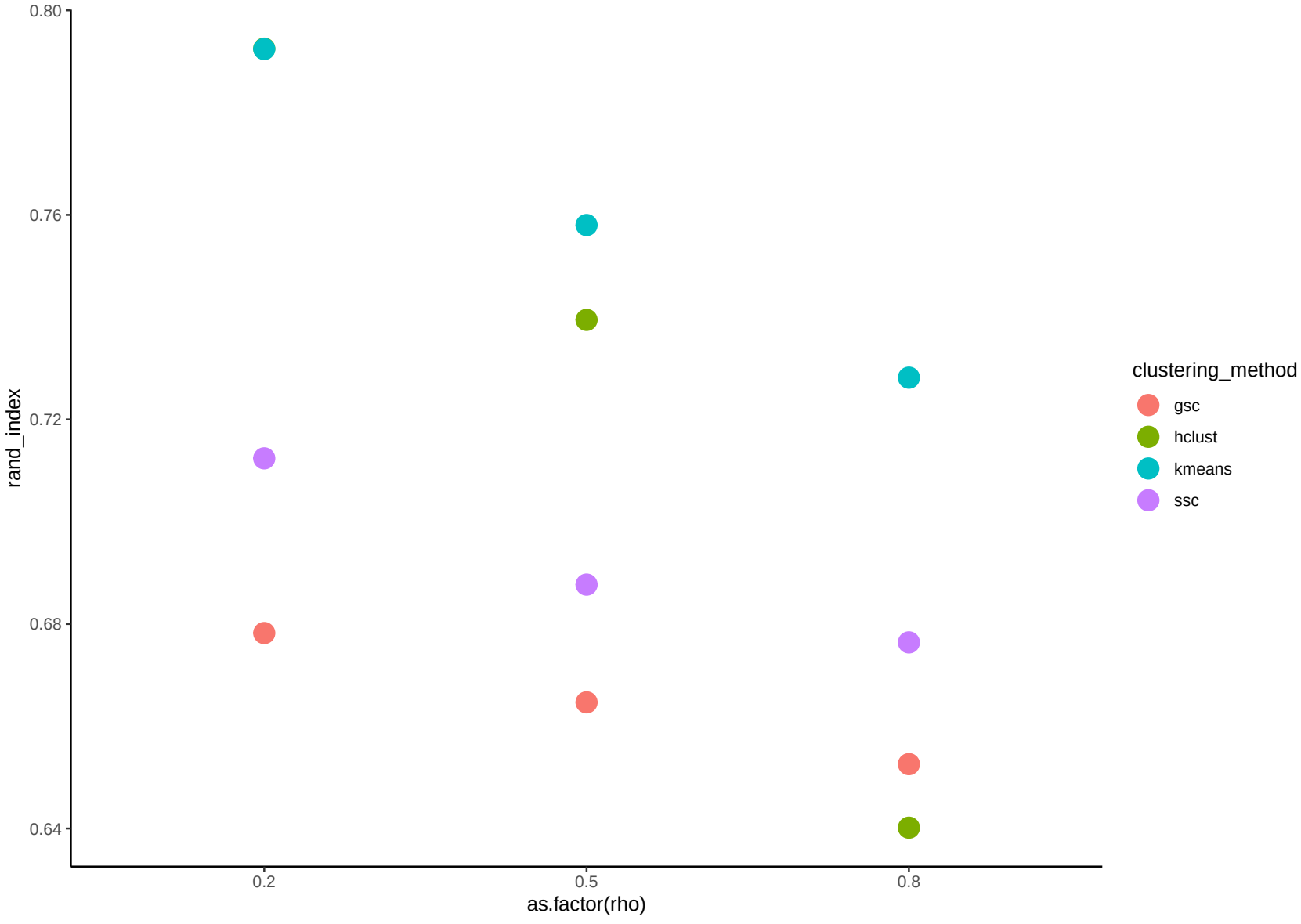
Results (cont.)



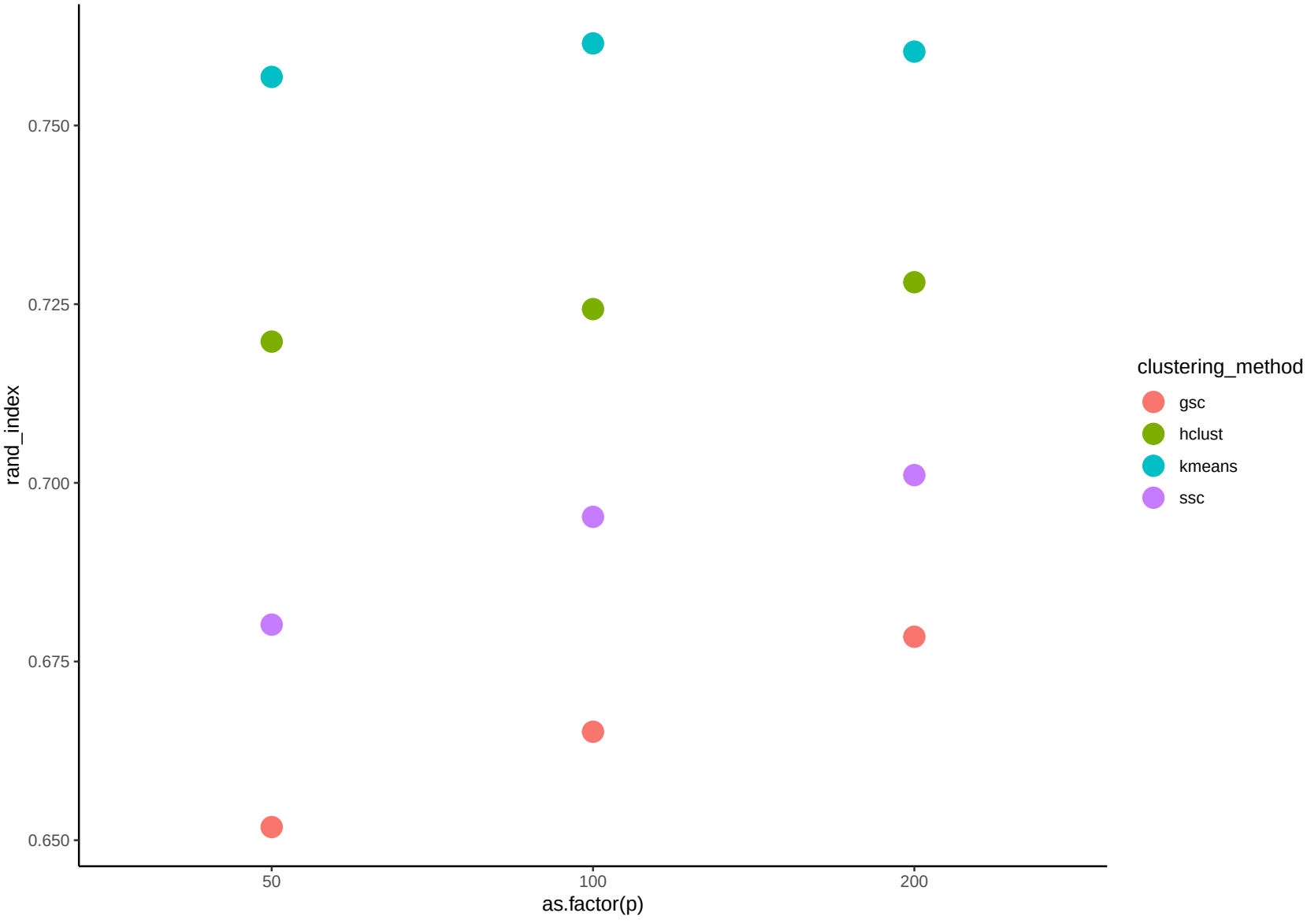
Results (cont.)



Results (cont.)



Results (cont.)



Directions

1. Improve simulations
   - Bigger n and p
   - Move beyond Gaussian data
   - More complex correlation structures
2. More clustering methods
   - Model-based methods
   - Convex clustering

Directions (cont.)

Interesting Literature:

- Kleindessner et al 2019; "Guarantees for Spectral Clustering with Fairness Constraints"
- Fang and Wang 2011; "Penalized cluster analysis with applications to family data"
- Gittens et al 2014; "Approximate Spectral Clustering via Randomized Sketching"
- Joseph and Yu 2016; "Impact of Regularization on Spectral Clustering"
- Loffler et al 2020; "Optimality of spectral clustering in the Gaussian Mixture Model"
- Abbe et al 2021; "An ℓ_p theory of PCA and spectral clustering"