# Clustering Methods and Correlated Data: Simulations

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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 $\mu_i$ 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

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

# Spectral (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

# 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
- # 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 $\Sigma$ with `ngroups` blocks, set within-group correlation $\rho$

```
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 $\mu_{C_i}$ 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.)

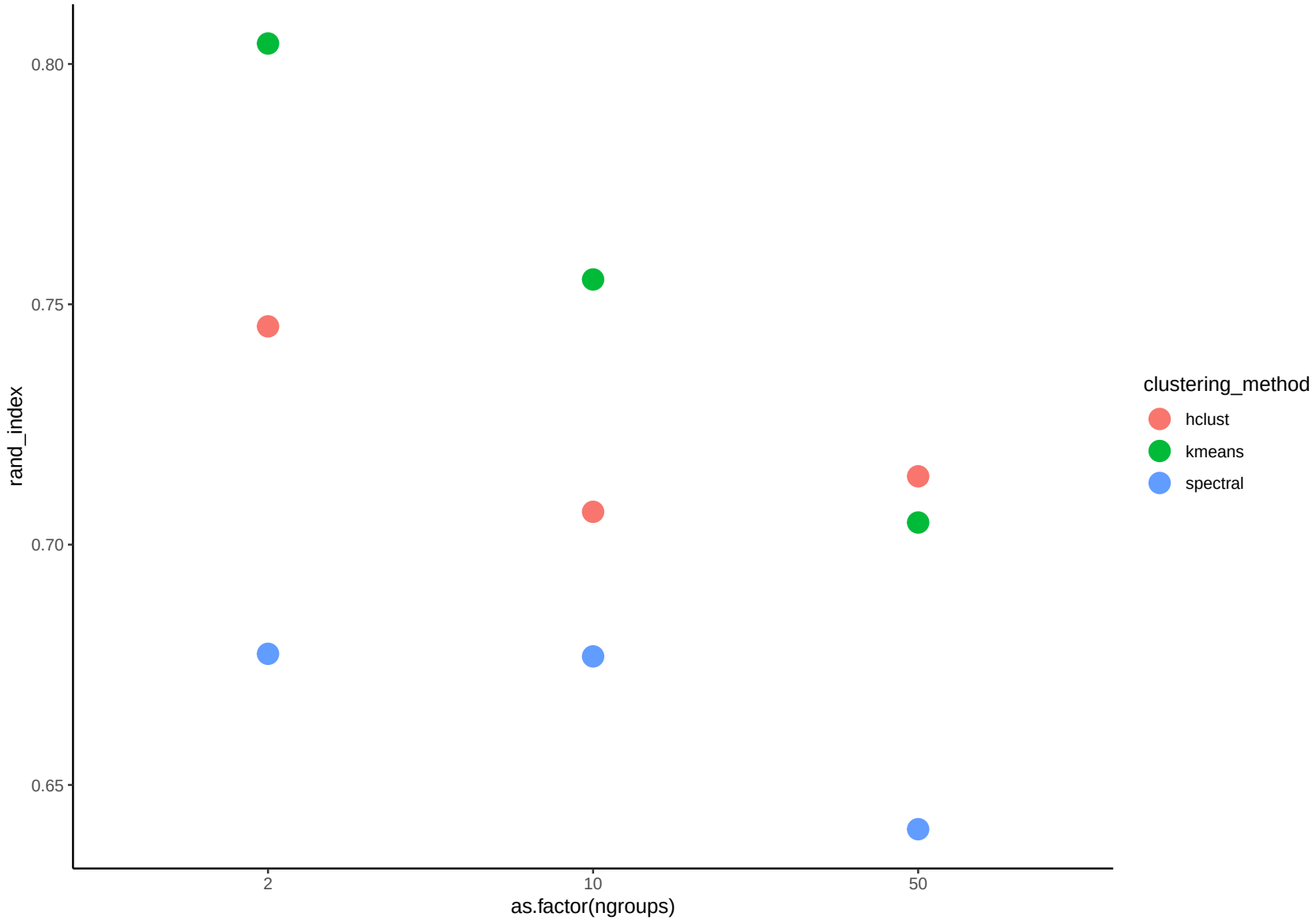
Some immediate concerns:

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 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 $L = I - D^{-1/2}AD^{-1/2}$

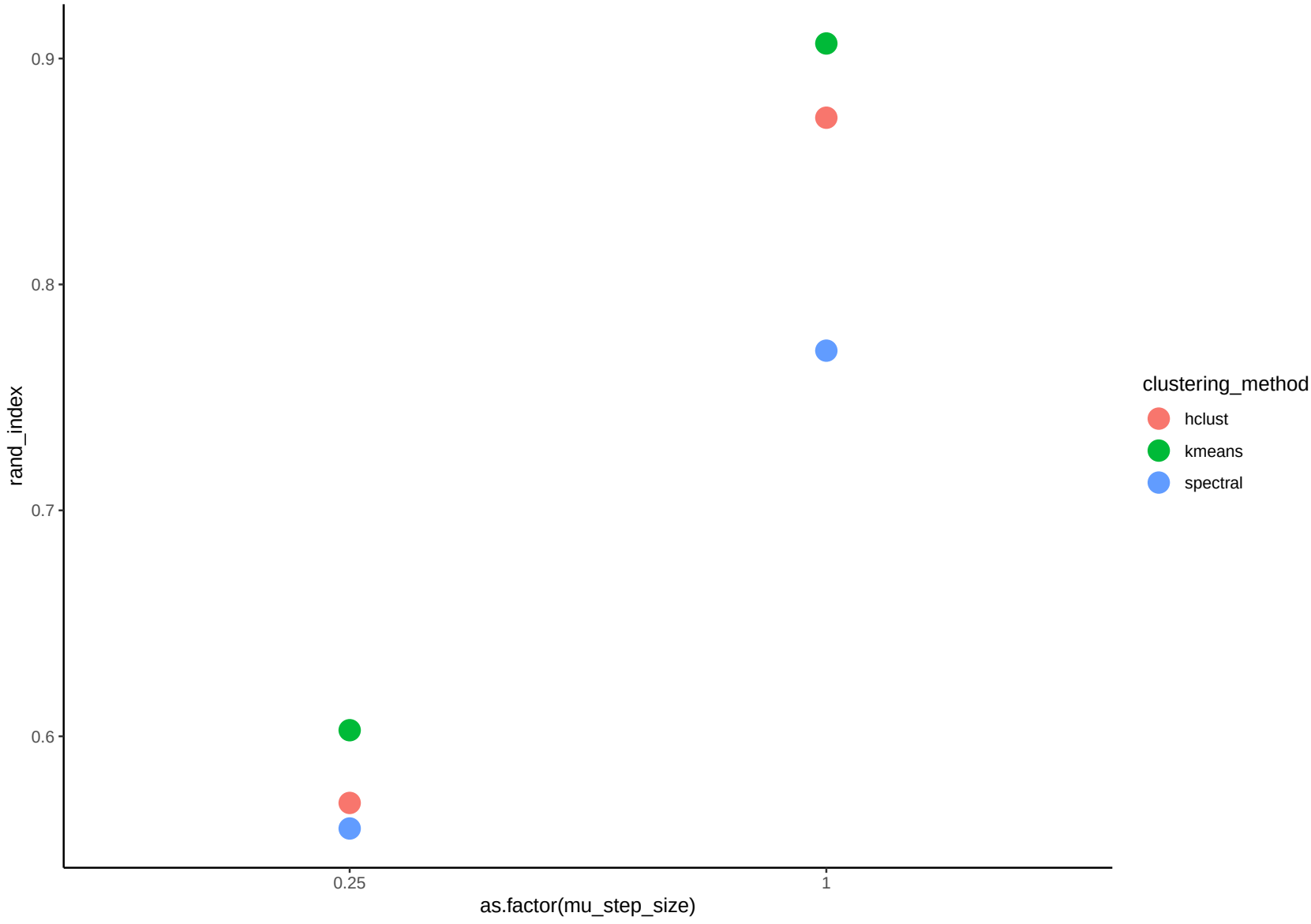
# Results

| clustering_method | average_ri |
|---|---|
| hclust | 0.7221509 |
| kmeans | 0.7546772 |
| spectral | 0.6649400 |

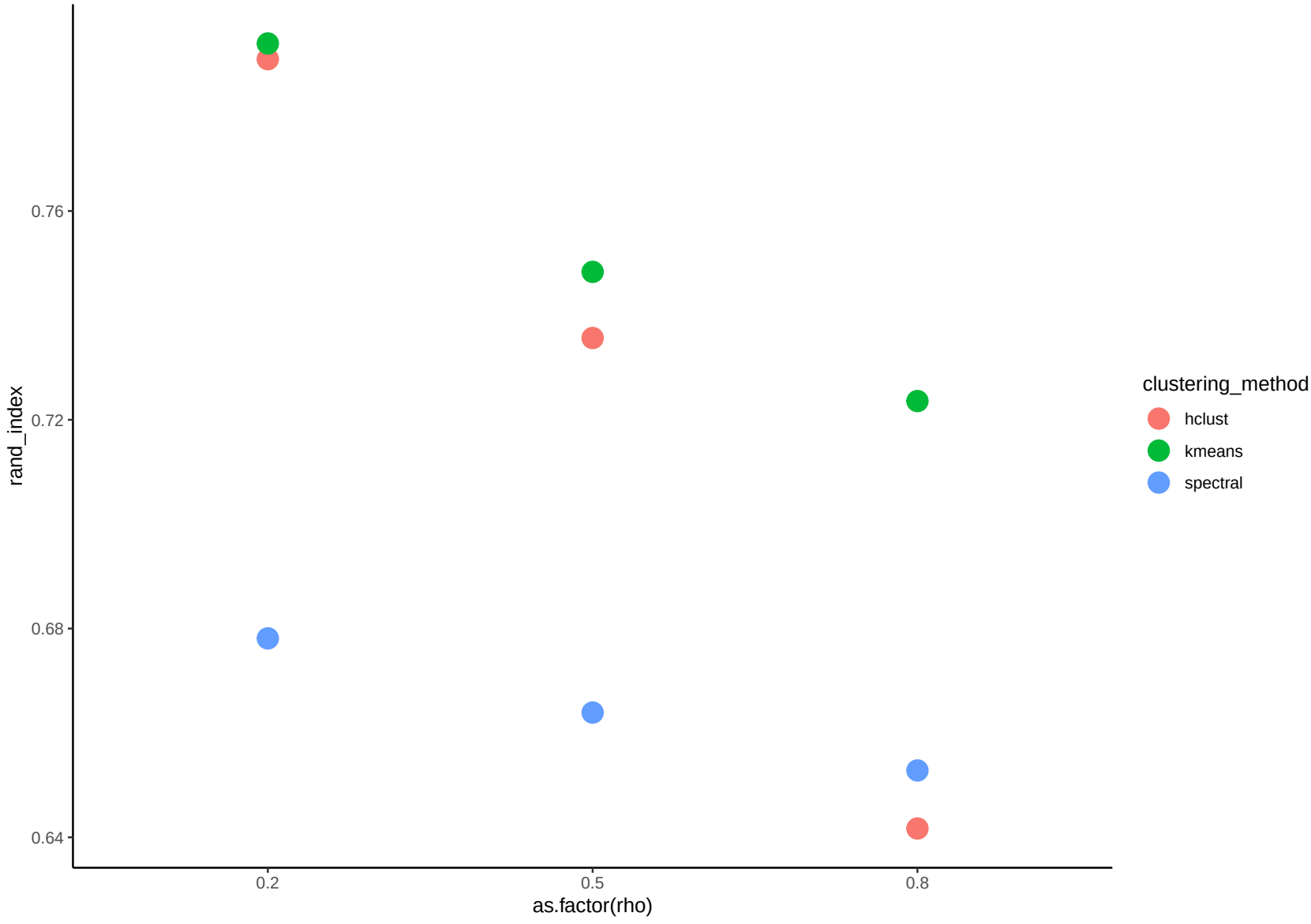
# Results (cont.)



# Results (cont.)



# Results (cont.)



# Directions

1. Improve simulations
   - Bigger $n$ and $p$
   - Move beyond Gaussian data
   - More complex correlation structures
2. Explore variations of spectral clustering
3. More clustering methods
   - Convex clustering?

# Directions (cont.)

Interesting Literature:

1. Kleindessner et al 2019; "Guarantees for Spectral Clustering with Fairness Constraints"
2. Fang and Wang 2011; "Penalized cluster analysis with applications to family data"
3. Donnat and Holmes 2019; "Convex Hierarchical Clustering for Graph-Structured Data"
4. Gittens et al 2014; "Approximate Spectral Clustering via Randomized Sketching"