Variable Selection for Consistent Clustering

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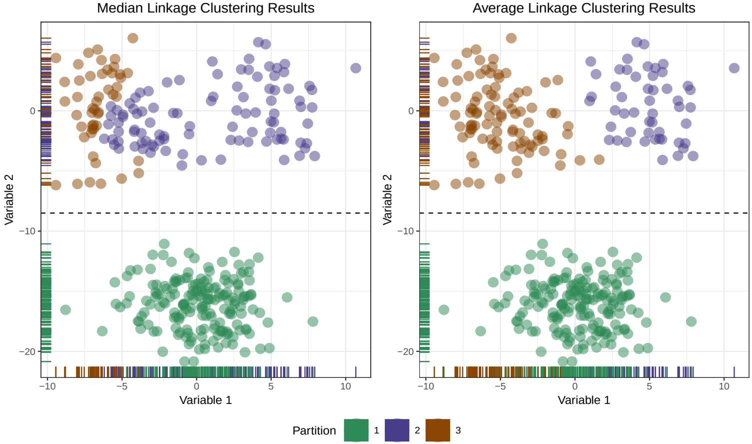
Symposium on Data Science and Statistics 2018

Variable choice ! inconsistent clusters



Methods disagree using both variables,
but **agree** on two consistent clusters with Variable 2

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GOAL:

Search for the variables yielding consistent clusters based on the level of agreement between methods

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We are NOT optimizing for recovery of "true cluster labels"

We ARE optimizing for agreement of obvious group structure

Measuring clustering agreement with ARI

$ARI(p_1; p_2) =$ **Adjusted Rand Index (ARI)**[1], similarity index between two partitions p_1 and p_2

Corrected for chance agreement,

$$\mathbb{E}[ARI(p_1; p_2)] = 0$$

$ARI(p_1; p_2) < 0 \ \rightarrow$ worse than random

$ARI(p_1; p_2) = 1 \ \rightarrow$ identical partitions

[1] [Hubert and Arabie, 1985]

Maximum Clustering Similarity (MCS)[2]

An approach to determine K, number of clusters

Let $M =$ set of clustering methods

Choose K with most frequent max similarity,

$$e.g.\ ARI(p_{1,K}, p_{2,K}) \text{ from } \binom{|M|}{2} \text{ partition pairs}$$

[2] [Albatineh and Niewiadomska-Bugaj, 2011]

Greedy search algorithm for variable selection

Idea: **Greedily search for the most consistent subset of variables across clustering methods and number of clusters** K

Notation:

- $\mathbf{X} = N \times D$ data matrix, $d\ 2\ f1;:::;Dg$
- $S =$ set of selected variables
- $U =$ set of unselected variables, where $S\ [\ U = f1;:::;Dg$ and $S\ \backslash\ U = f;g$
- $M =$ $f$complete, single, Ward, average, McQuitty, median, centroid, kmeans$g$ (*just for illustrative purposes*)

Step 0: Initialize $S = f;g$, $U = f1;:::;Dg$

Greedy search algorithm for variable selection

Step 1: For each variable $d \in U$ and K:

- Create partitions $p_{m_1, K, S \cup \{d\}}, \ldots, p_{m_{|M|}, K, S \cup \{d\}}$
- Compute $ARI(p_{m_i, K, S \cup \{d\}}, p_{m_j, K, S \cup \{d\}})$ for each of the $\binom{|M|}{2}$ pairs of partitions

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Step 2: Select most consistent result:

$$d , K := \arg\max_{d \in U, K} \overline{ARI}_{K, S \cup \{d\}}$$

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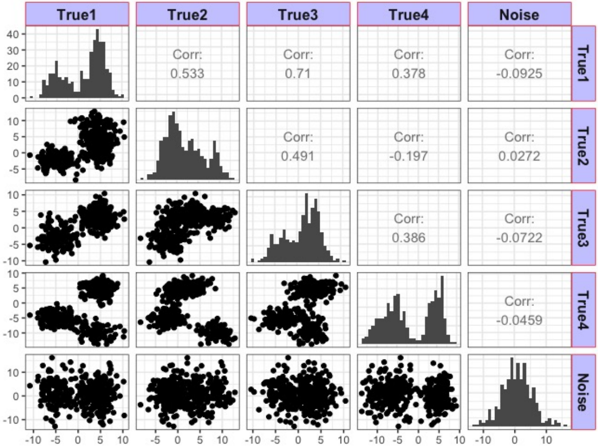
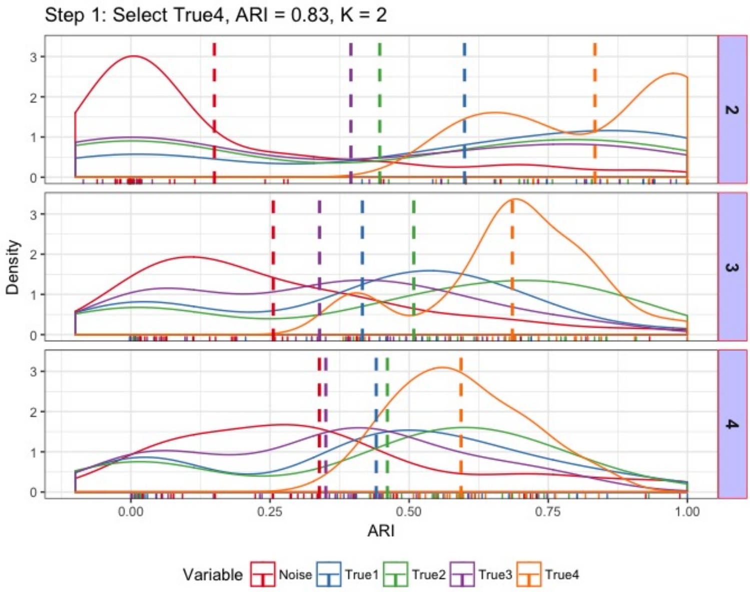
Repeat 1-3 until $U = \{\emptyset\}$ or met stopping criteria

Demo data

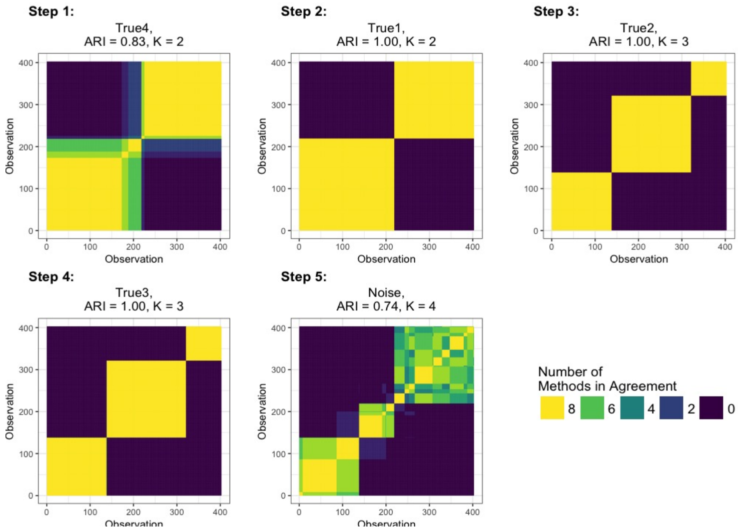
4 true variables, 1 noise variable, and $K = 3$



Step 1 of demo search



Consensus matrices for full search



Bootstrap consistency distributions to address limitations

We want to provide a measure of **con dence** in our decision:

- $f_{K;S}$ = bootstrap distribution for $\overline{ARI}_{K;S}$
- $f_{K;S[fdg}$ = bootstrap distribution for $\overline{ARI}_{K;S[fdg}$
- $overlap(f_{K;S}; f_{K;S[fdg})$ = area of overlap between the two

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Include variable d based on distribution **overlap**

IF $9\ d\ 2\ U$ such that $\overline{ARI}_{K;S\,[\,fdg} > \overline{ARI}_{K;S}$ (more consistent)

$$d\ ;K\ := \arg\min_{d2U;K} overlap(f_{K;S}; f_{K;S\,[\,fdg})\ \text{(minimize overlap)}$$

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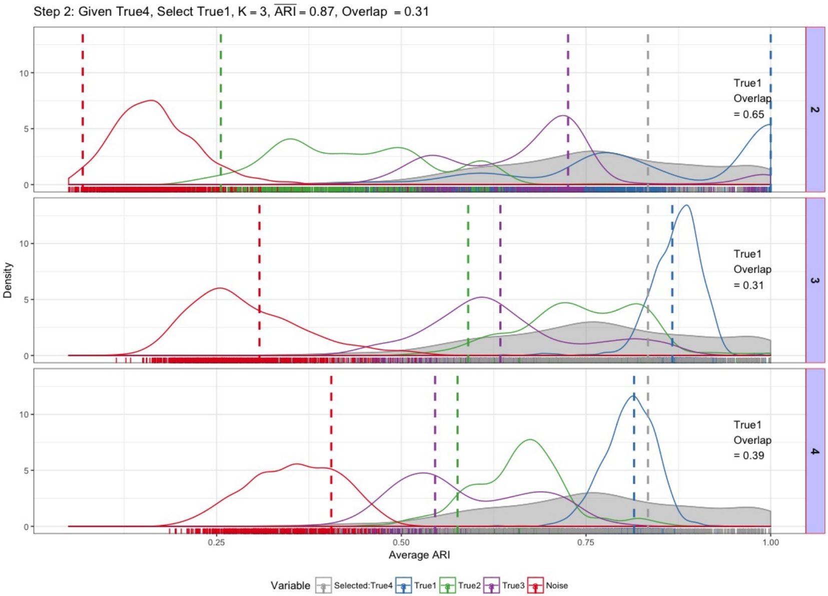
ELSE (less consistent)

$$d\ ;K\ := \underset{d2U;K}{\arg\max}\ overlap(f_{K;S}; f_{K;S\,[\,fdg})\ \text{(maximize overlap)}$$

Bootstrap distributions for step 2 of demo search



Noise has minimal overlap and is not selected

Step	Variable	$\overline{ARI}$	K	Overlap
1	True4	0.8339	2	-
2	True1	0.8668	3	0.3067
3	True2	1.000	3	0.1338
4	True3	0.9979	3	0.3277
5	Noise	0.7444	4	0.0969

By measuring the overlap, we are confident that including Noise leads to inconsistent clustering results

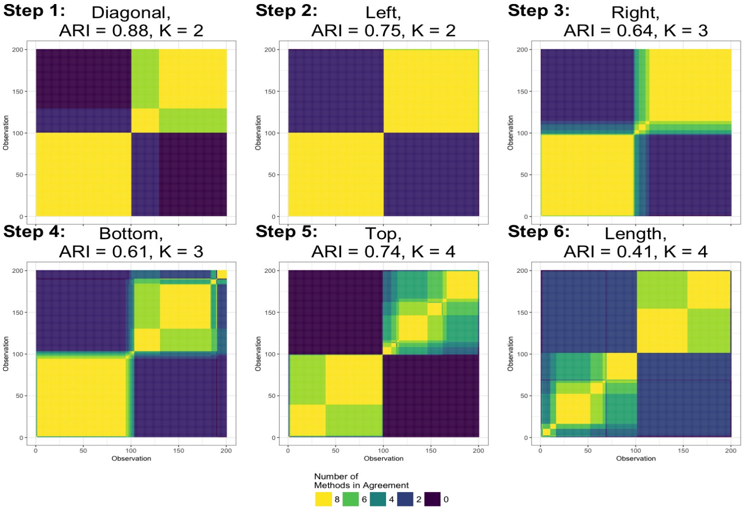
Swiss bank notes example

200 bills that are either counterfeit or real with 6 measurements

Summary of search reveals decrease in consistency:

Step	Variable	$\overline{ARI}$	K	Overlap
1	Diagonal	0.8755	2	-
2	Left	0.7500	2	0.8969
3	Right	0.6418	2	0.8789
4	Bottom	0.6112	3	0.6401
5	Top	0.7438	4	0.7262
6	Length	0.4113	4	0.7916

Swiss bank notes consensus matrices



Future Work

Simulation study, examine properties of ARI values

Explore different notions of stopping criteria

- Only considered average, but distributions are multimodal and assymetrical (e.g. mass above threshold?)

Inclusion of removal step

Consider sensitivity to different types of clustering methods

- What about soft partitions?[3]

[3] [Flynt et al.,]

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