Variable Selection for Consistent Clustering

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Classification Society, 2017

Typical Questions in Cluster Analysis

How many clusters?

Which variables should we use?

Which clustering method?

Typical Questions in Cluster Analysis

How many clusters?

- Model-Based Cluster Analysis *(Fraley & Raftery, 1998)*
- Gap Statistic *(Tibshirani et al., 2001)*
- Maximum Clustering Similarity
  (Albatineh & Niewiadomska-Bugaj, 2011)

Which variables should we use?

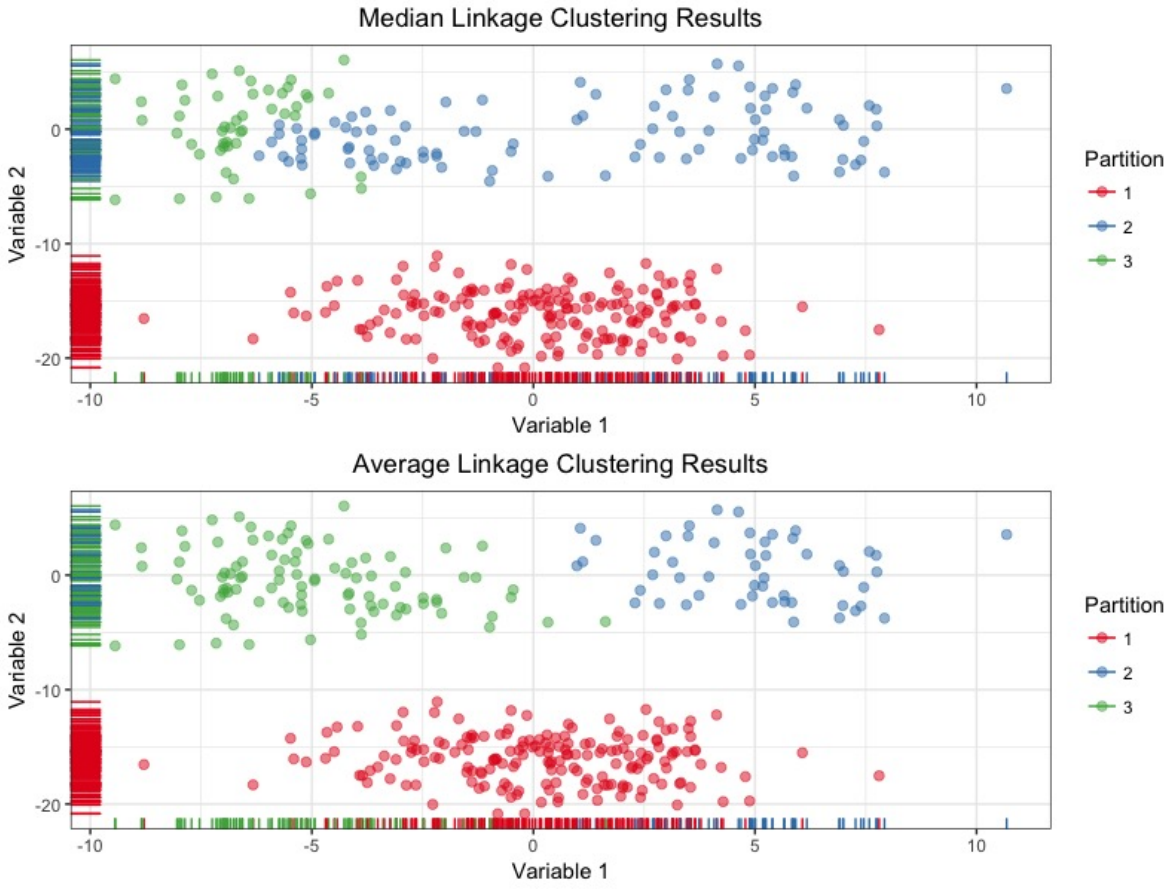
- HINoV Method *(Carmone et al., 1999)*
- Heuristic for K-Means *(Brusco & Cradit, 2001)*
- Model-Based Clustering *(Raftery & Dean, 2006)*

Which clustering method?

- Clustering Validation *(Milligan, 1996)*
- Comparison of Heuristic Procedures *(Brusco & Steinley, 2007)*

Inconsistent Clustering

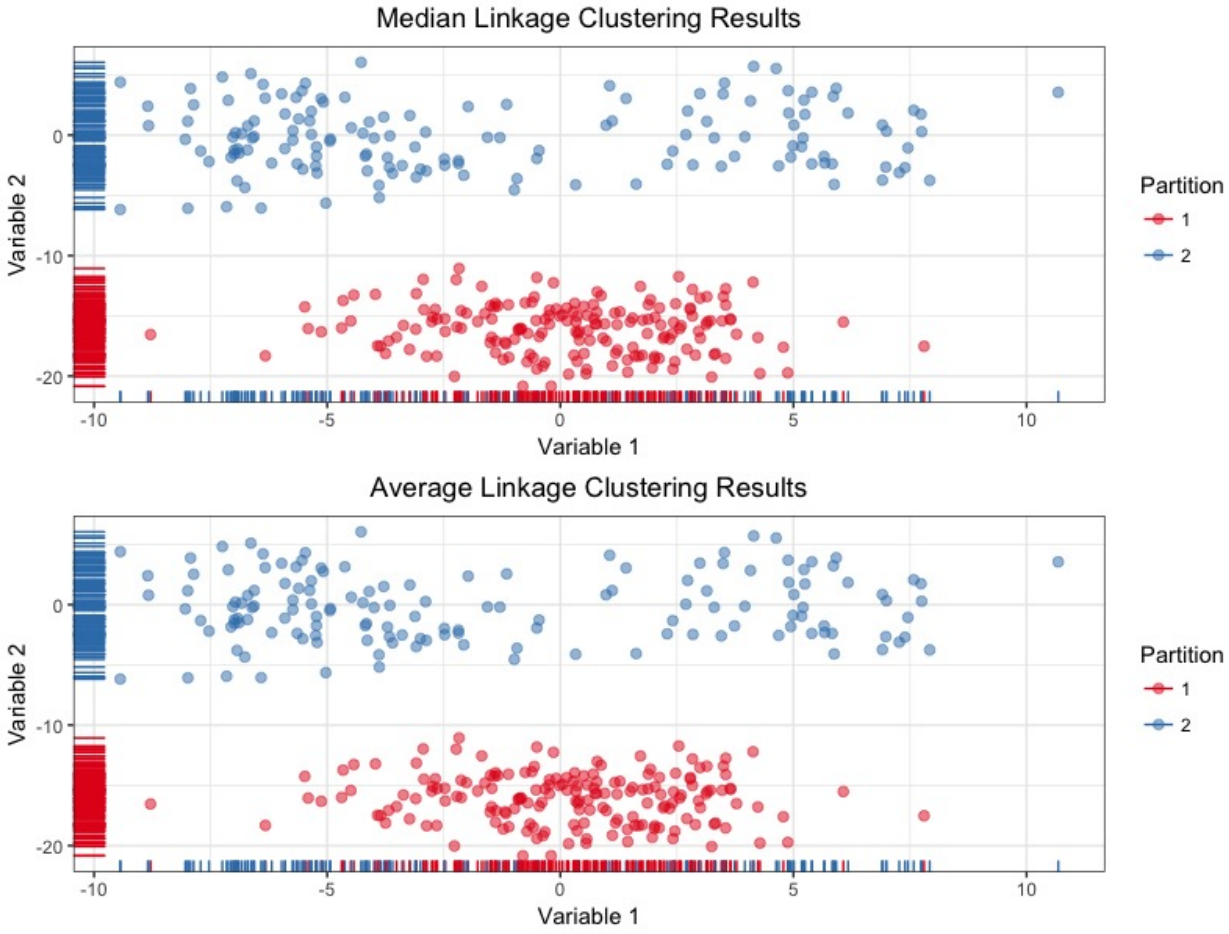
Clustering with both variables and 3 clusters



Disagree on 2 of the 3 clusters,
probably since they're not well separated along Variable 1

Consistent Clustering

Clustering only with Variable 2 and 2 clusters



Perfectly agree on 2 well separated clusters

Variable Selection for Consistent Clustering

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

Variable Selection for Consistent Clustering

Combine variable selection and method agreement

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Variable Selection:

- Greedy search - find best variable for clustering, given that variable find the next best, repeat
- *Variable Selection for Model-Based Clustering (Raftery & Dean, 2006)*

Variable Selection for Consistent Clustering

Combine variable selection and method agreement

Variable Selection:

- Greedy search - find best variable for clustering, given that variable find the next best, repeat
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Method Agreement:

- Measure agreement between methods using similarity indices to compare clustering partitions
- Adjusted Rand Index (ARI) *(Hubert & Arabie, 1985)*, expected value of 0 and closer to 1 the better
- *MCS: A Method for Finding the Number of Clusters (Albatineh & Niewiadomska-Bugaj, 2011)*

Algorithm Notation

- $\mathbf{X} = N \; x \; D$ data matrix, where $d \in \{1, \ldots, D\}$
- $M =$ set of clustering methods considered, where $m \in \{1, \ldots, |M|\}$
- $S =$ set of variables selected for inclusion
- $U =$ set of unselected variables, where $S \cup U = \{1, \ldots, D\}$ and $S \cap U = \{\emptyset\}$

Algorithm Notation

- $p_{m,S}$ = $(1\ x\ N)$-dimensional row vector that defines a partition with method m given set of variables S
- $ARI(p_{m_i,S},\ p_{m_j,S})$ = ARI between partitions of two different methods m_i and m_j
- $\overline{ARI}_S = \frac{1}{\binom{|M|}{2}} \sum_{i \neq j} ARI(p_{m_i,S},\ p_{m_j,S})$ measures the **consistency** for set of variables S

Algorithm

Step 0: Initialize $S = \{\emptyset\}$, $U = \{1, \ldots, D\}$

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

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

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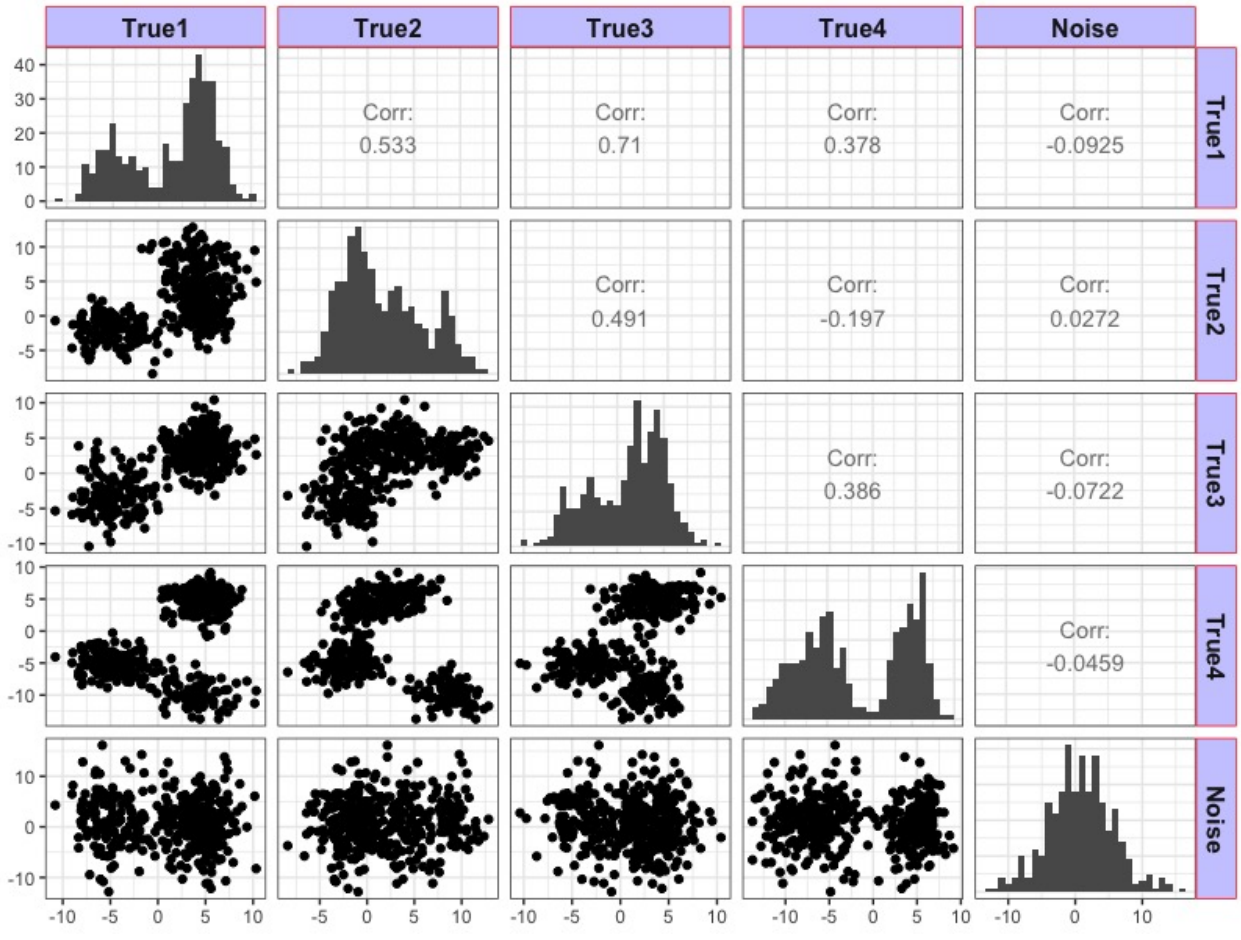
Repeat Steps 1-3 until including d^* meets stopping criteria

Demo Data

402 observations, 5 variables (4 true, 1 noise),
3 known clusters with moderate separation



Generated with `clusterGeneration` *(Qiu & Joe, 2006)*

Algorithm Demo

For now clustering with known number of 3 clusters

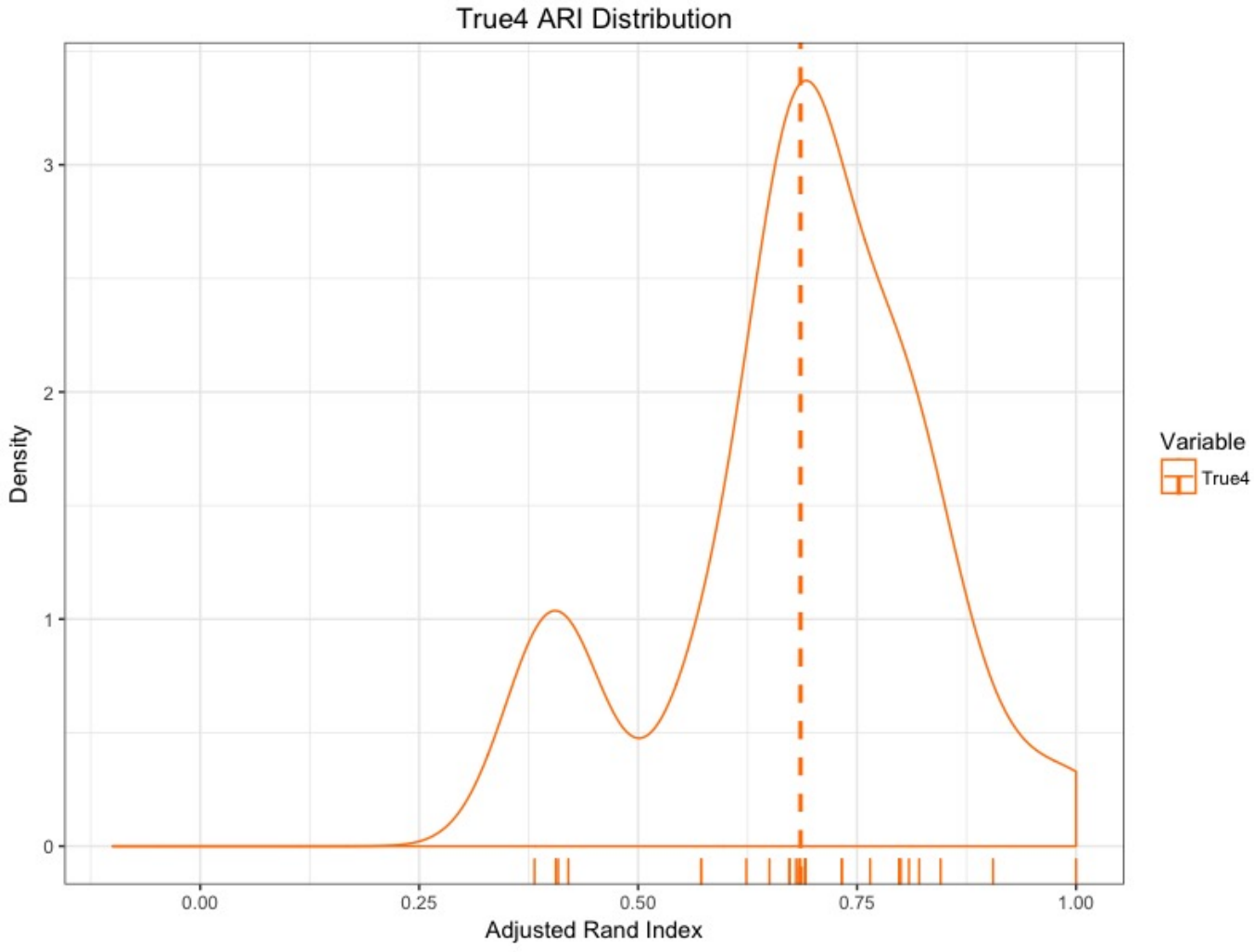
Let $M =$
$\{complete, single, Ward, average, McQuitty, median, centroid, kmeans\}$

For each variable, ARI distribution has $\binom{8}{2} = 28$ values:

Variable	**Method 1**	**Method 2**	**ARI**
True1	Complete	K-Means	0.4583
True2	Complete	K-Means	0.7799
True3	Complete	K-Means	0.3246
True4	Complete	K-Means	0.6803
Noise	Complete	K-Means	0.6400
True1	Complete	Average	0.7195
⋮	⋮	⋮	⋮

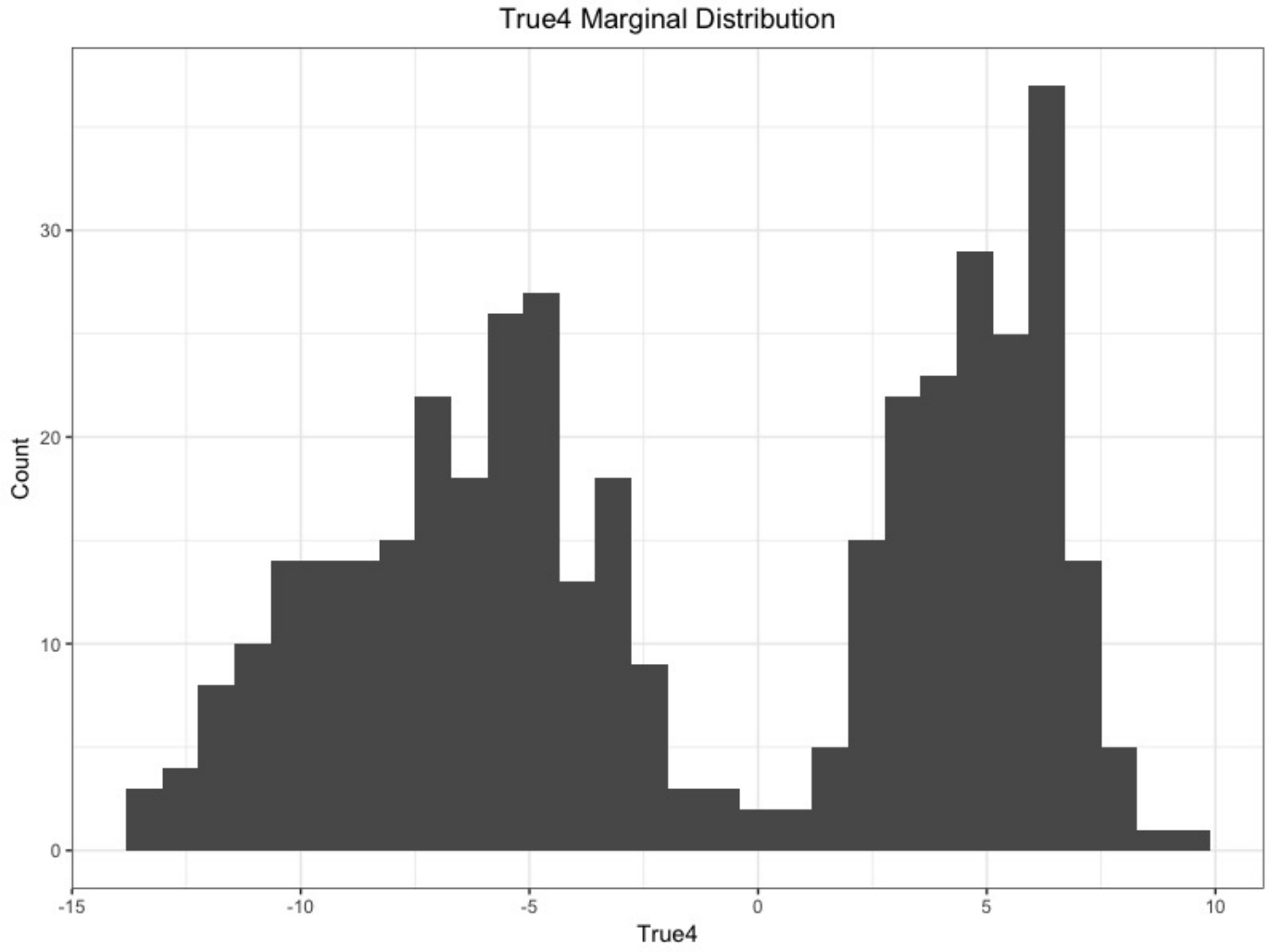
Most Consistent Variable: True4

True4's ARI distribution and dashed line at $\overline{ARI}_{\{True4\}} = 0.6854$



Revisit True4 Marginal Distribution

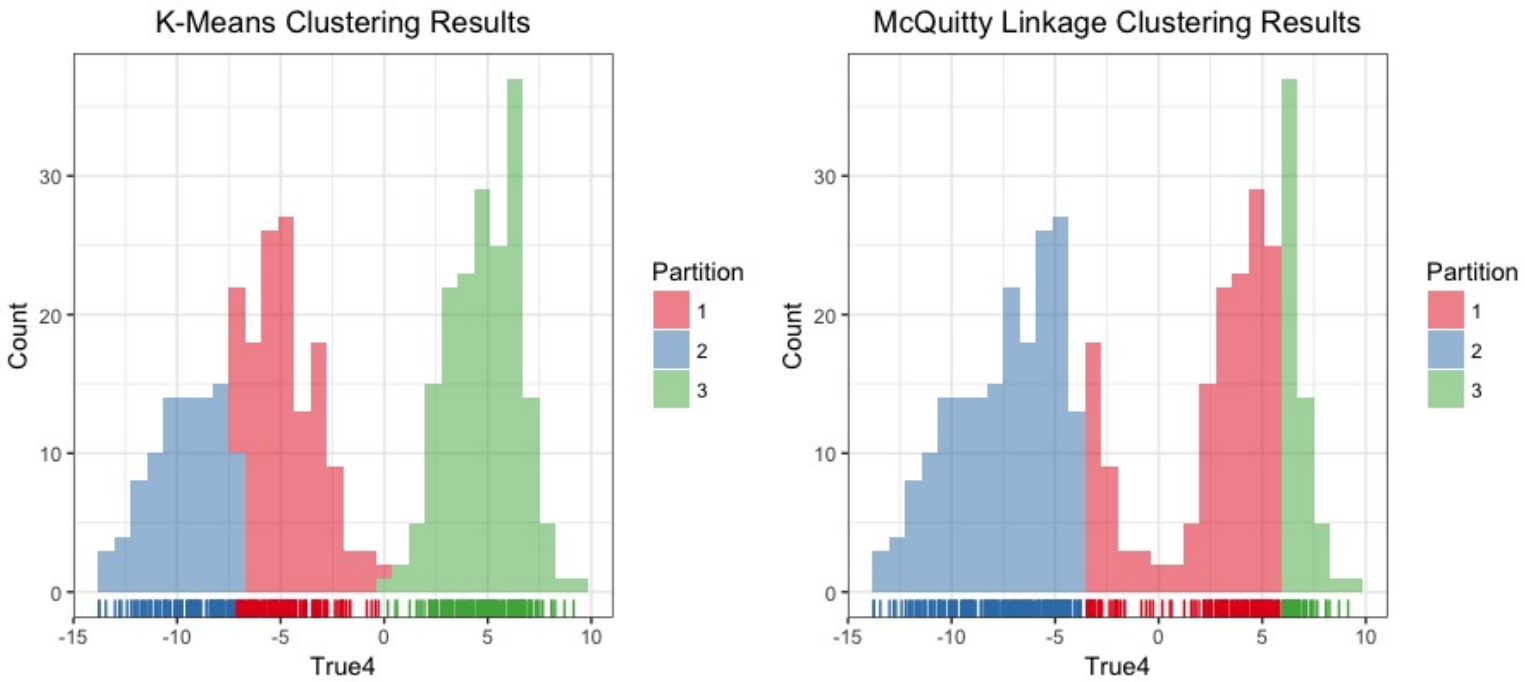
Clear bimodal distribution, but asking for 3 clusters



Clustering Disagreement Example

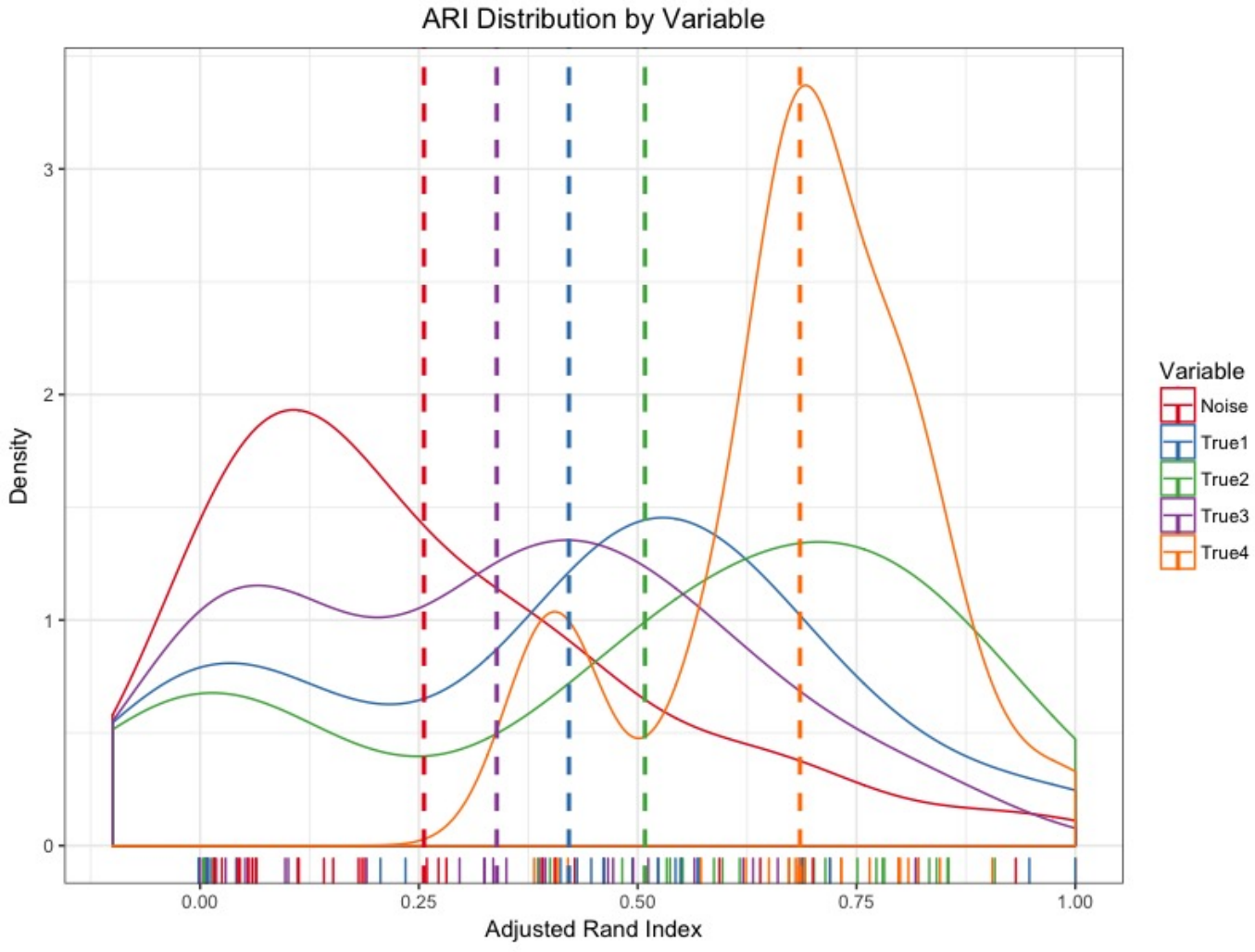
$ARI(p_{kmeans,\{True4\}},\ p_{McQuitty,\{True4\}}) = 0.3816$

Lower mode of ARI values for True4 all involved McQuitty



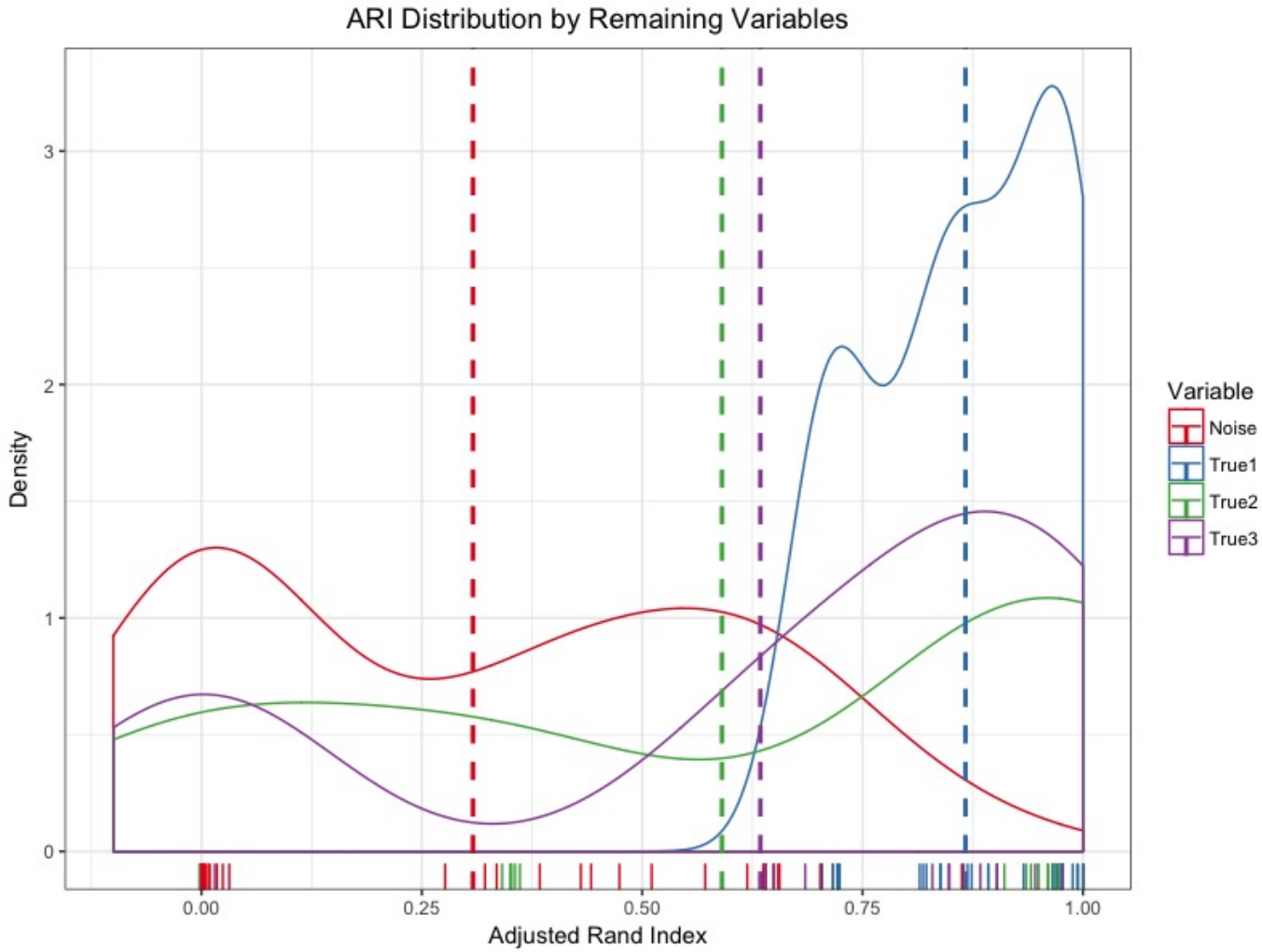
Comparison of ARI Distributions

Can easily view how other variables compare to True4



Given {True4}, Most Consistent: True1

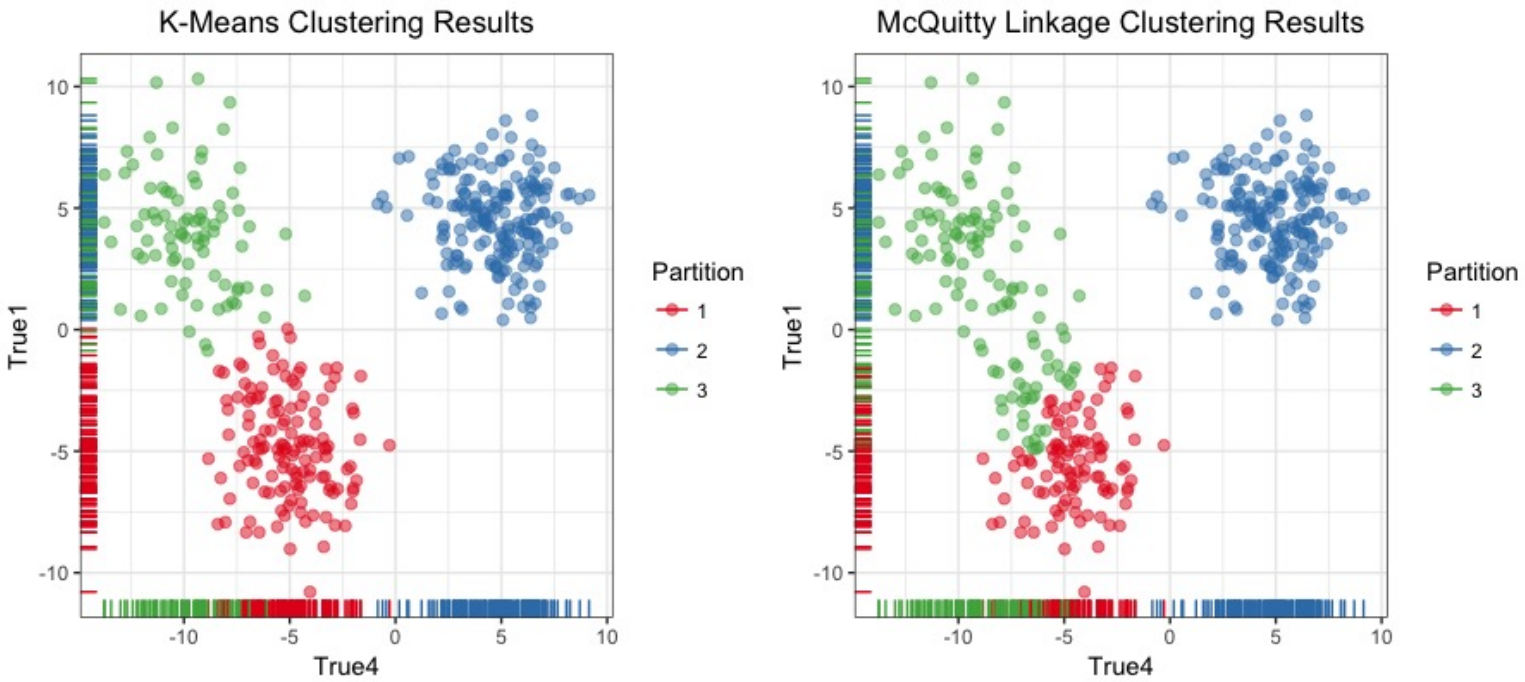
More consistent results, $\overline{ARI}_{\{True4, True1\}} = 0.8668$



Change In Clustering Disagreement

$$ARI(p_{kmeans,\{True4,True1\}},\ p_{McQuitty,\{True4,True1\}}) = 0.8224$$

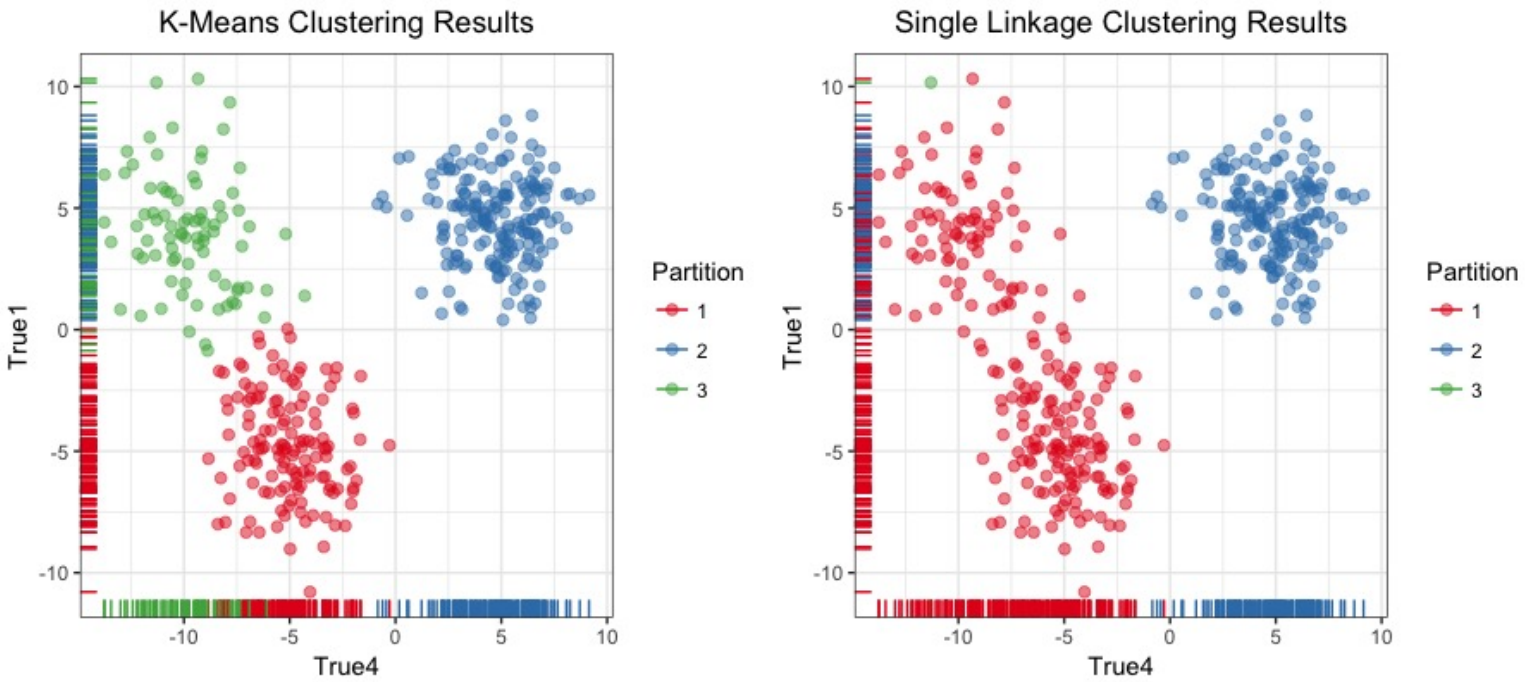
McQuitty is no longer the lower mode of ARI values...



Change In Clustering Disagreement

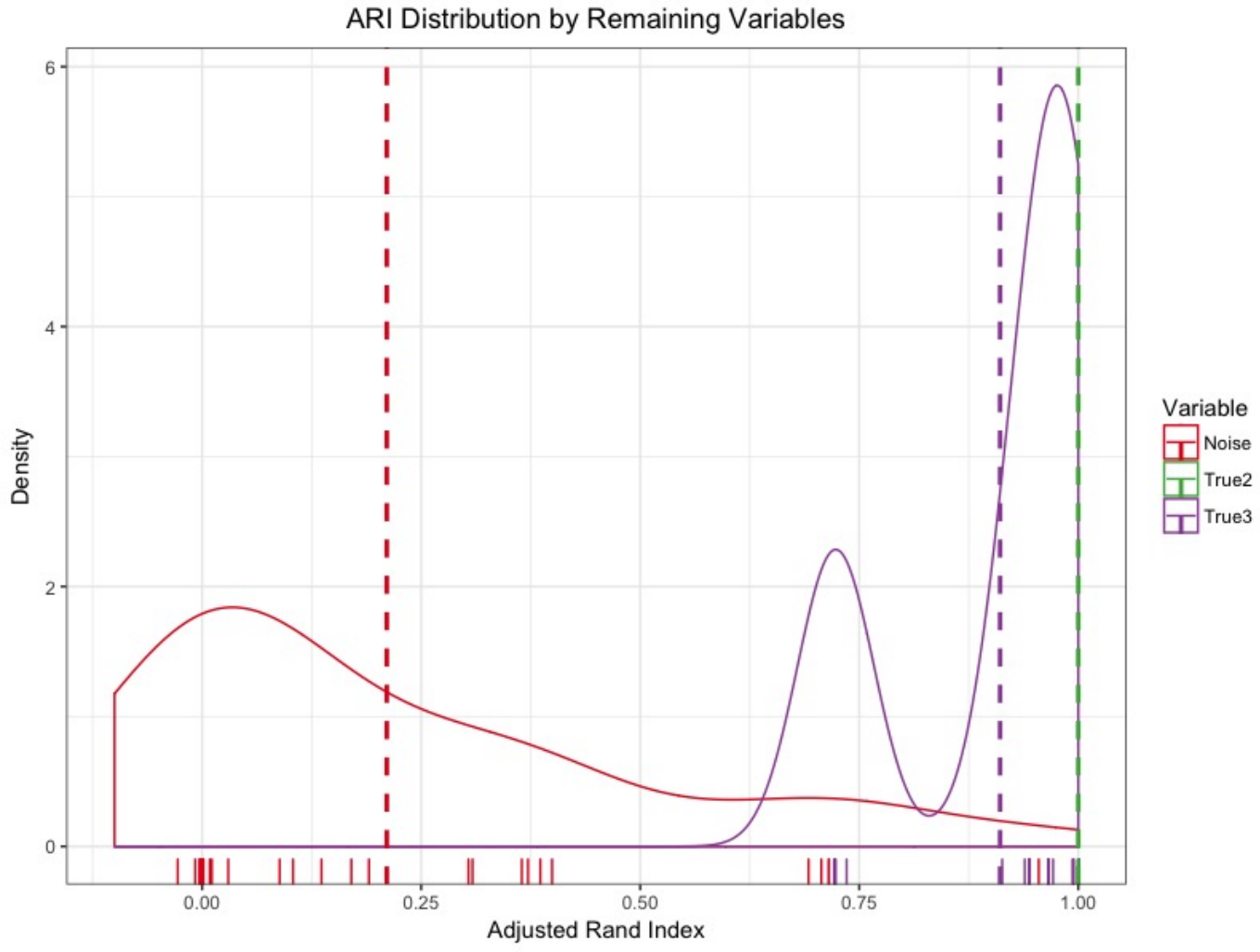
$$ARI(p_{kmeans,\{True4,True1\}},\ p_{single,\{True4,True1\}}) = 0.7213$$

Single linkage makes up the lower mode



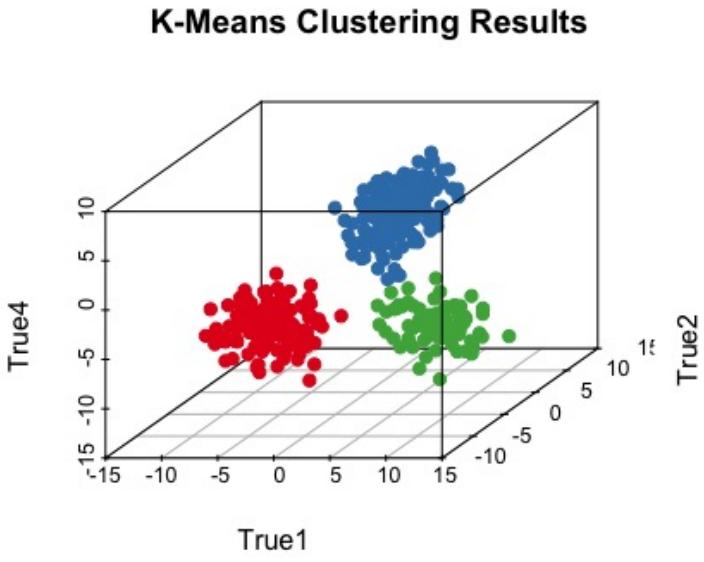
Given {True4, True1}, Most Consistent: True2

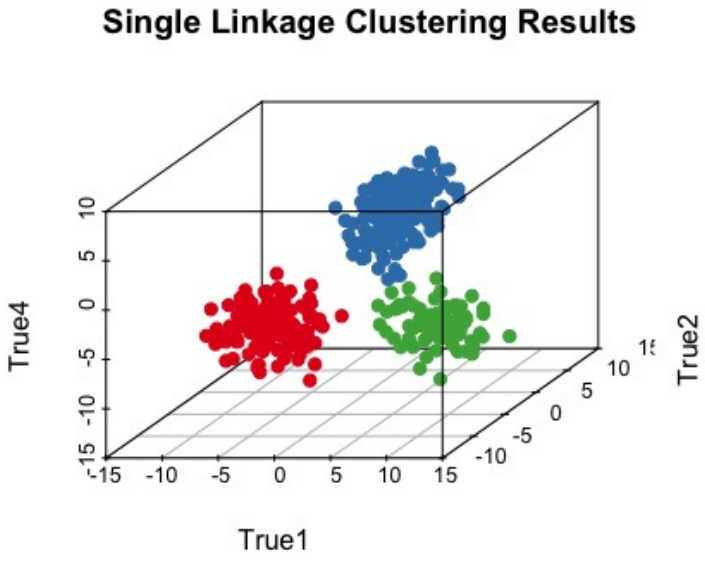
Perfect agreement, $\overline{ARI}_{\{True4, True1, True2\}} = 1$



Consistent Clustering Agreement

$ARI(p_{m_1,\{True4,True1,True2\}},\ p_{m_2,\{True4,True1,True2\}}) = 1,$
across all 28 pairs of methods

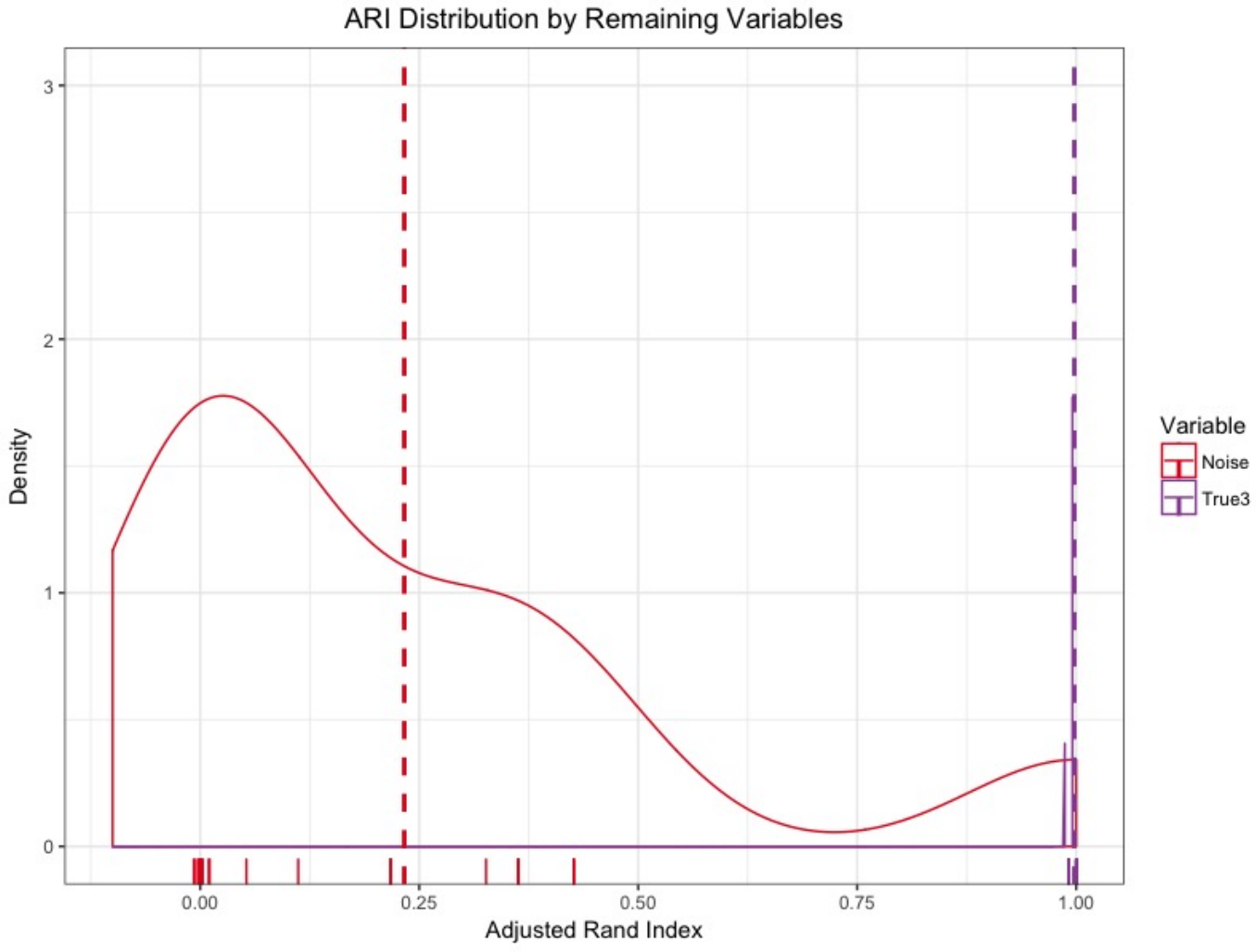




Identified 3 well separated clusters

Given {True4,True1,True2} Most Consistent: True3

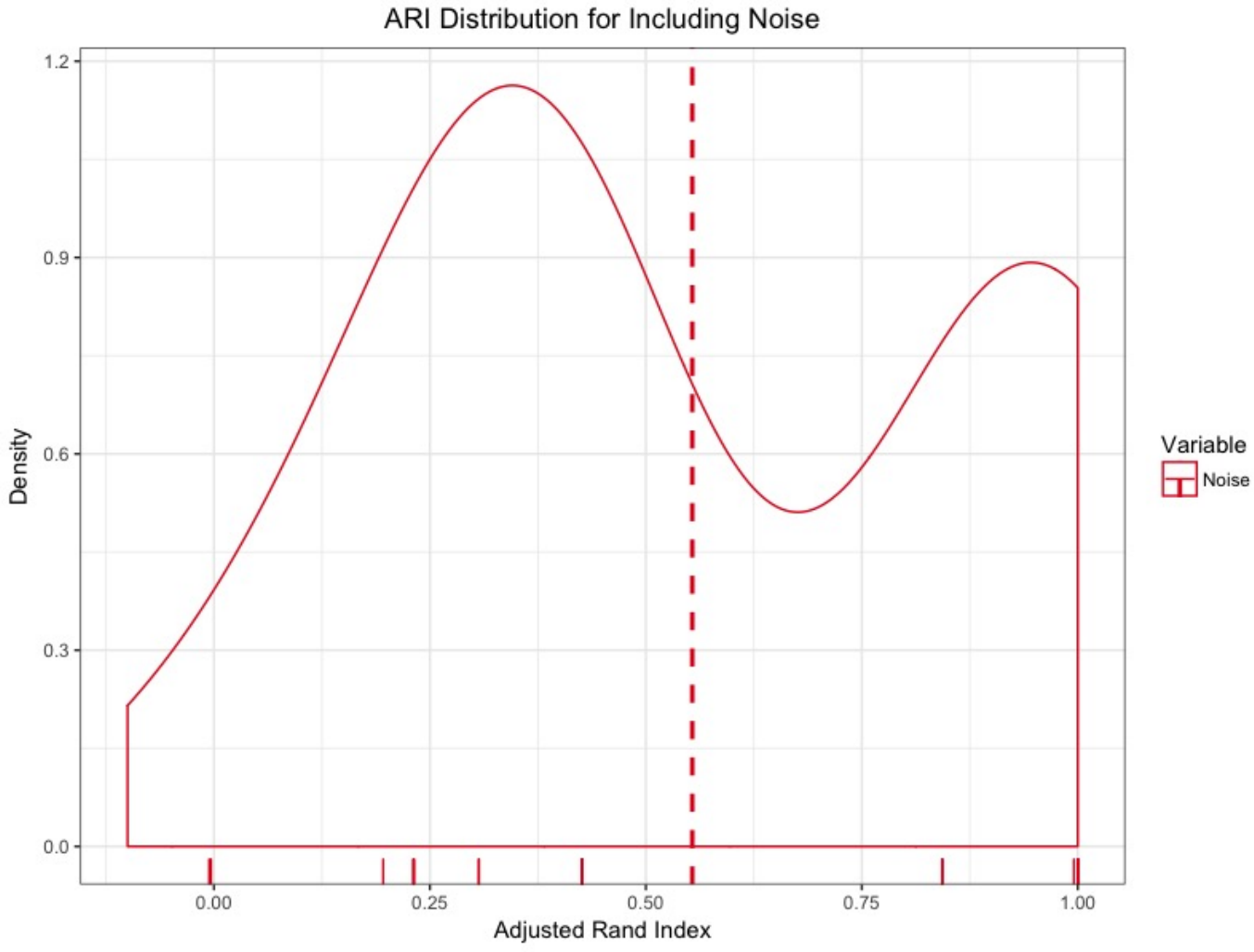
Still consistent results, $\overline{ARI}_{\{True4, True1, True2, True3\}} = 0.9979$



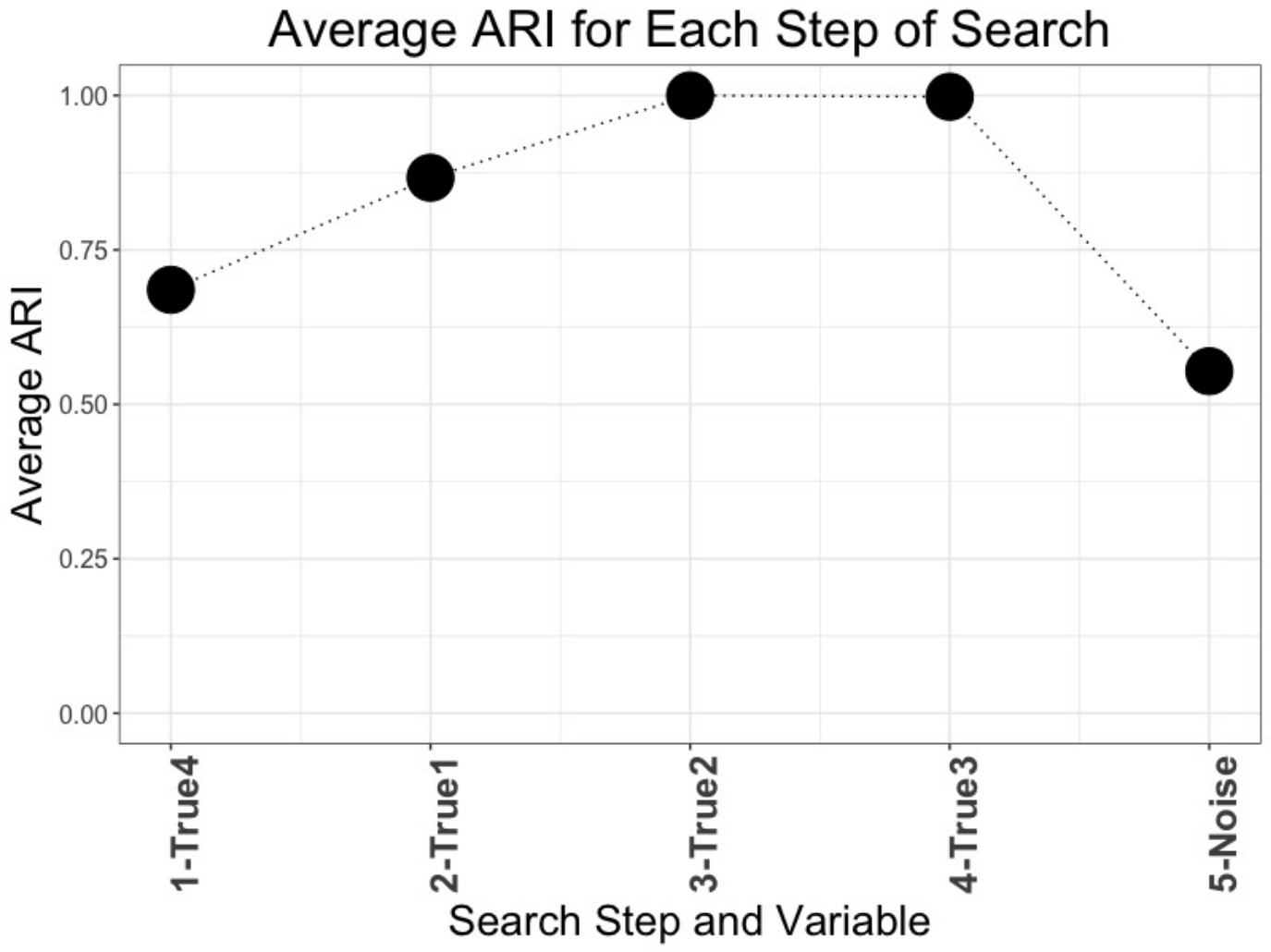
What About Including Noise?

Severe drop in consistency,

$\overline{ARI}_{\{True4, True1, True2, True3, Noise\}} = 0.5537$



Summary of Demo Search



Clearly see the drop from including Noise

What About The Number Of Clusters?

Only considered the true number of clusters, but...

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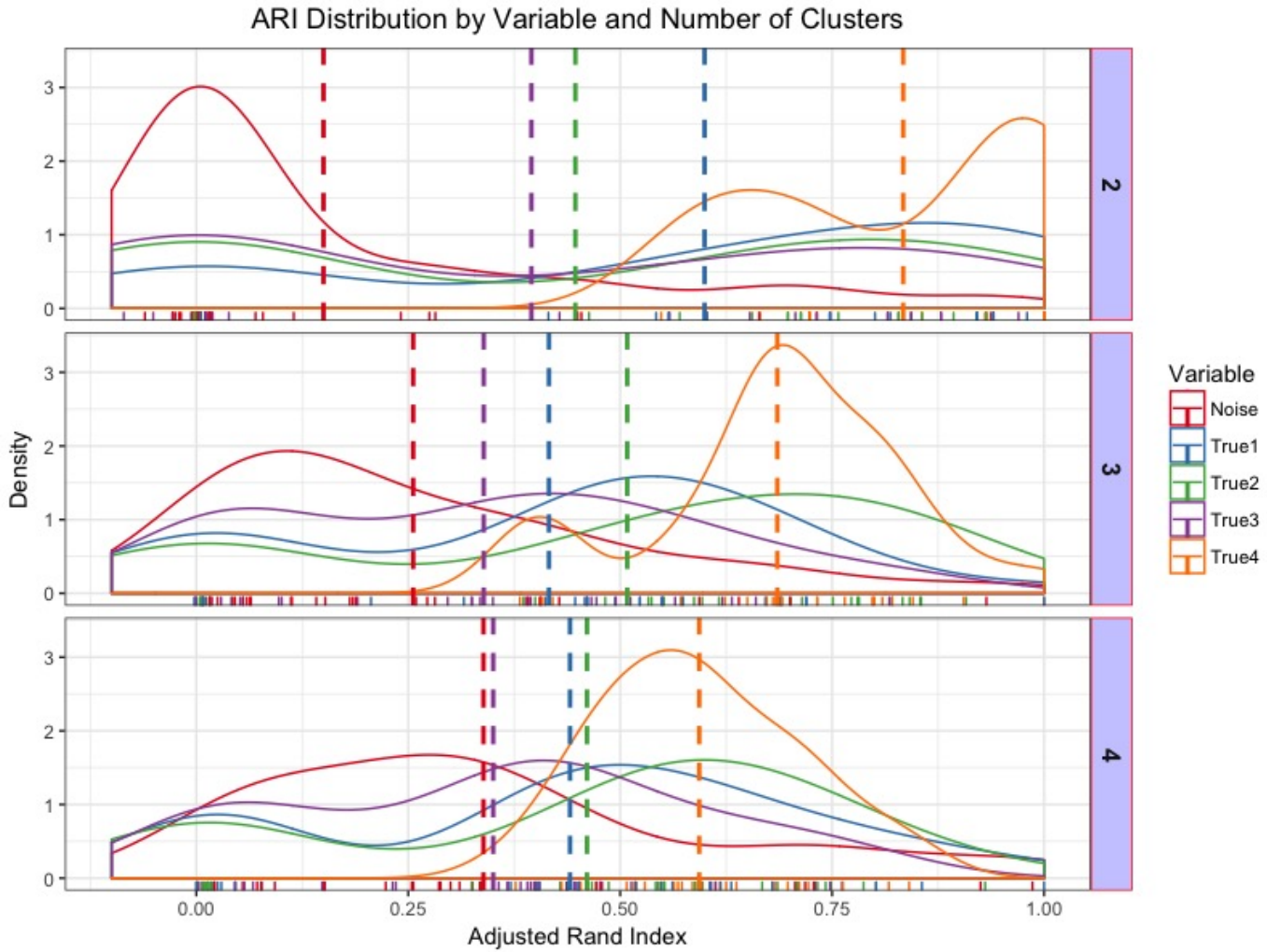
- $k = 1, 2, \ldots, K$ number of clusters
- $p_{m,k,S}$ defines a partition with method m and k clusters, given set of variables S
- $\overline{ARI}_{k,S} = \frac{1}{\binom{|M|}{2}} \sum_{i \neq j} ARI(p_{m_i,k,S},\ p_{m_j,k,S})$ measures the consistency for set of variables S with k clusters

Search over number of clusters and variables to identify the combination consistently agreeing on cluster structure

Most Consistent Combo: k=2, True4

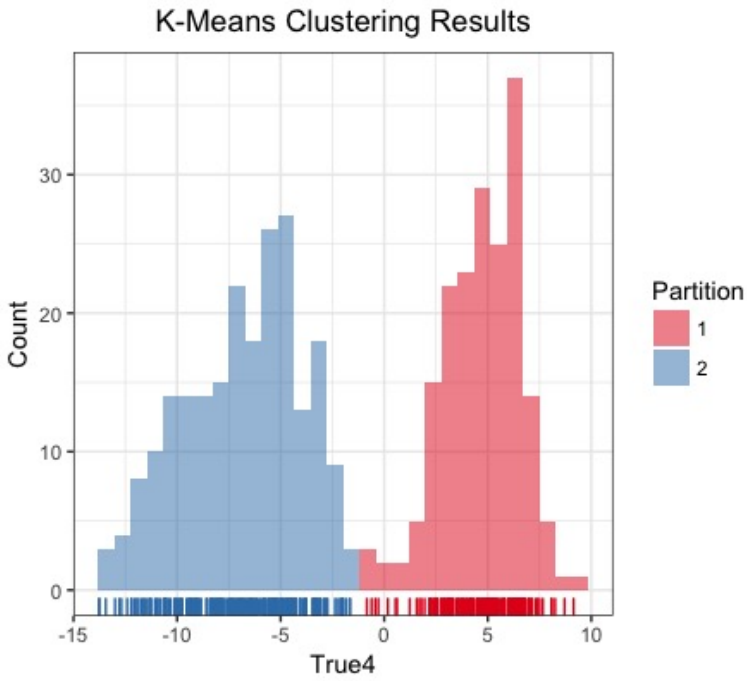
Still True4, but more consistent with 2 clusters

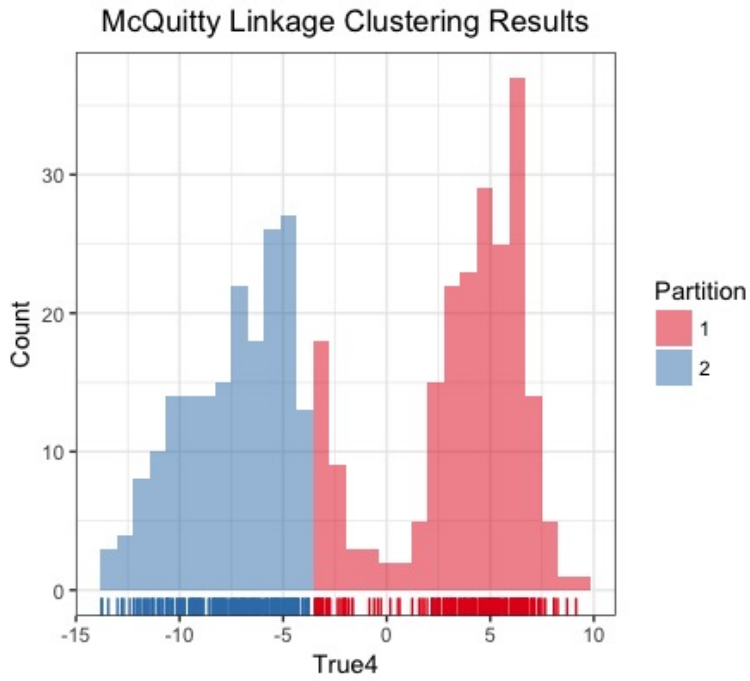
$\overline{ARI}_{2,\{True4\}} = 0.8338$



Consistent Clustering With 2 Clusters

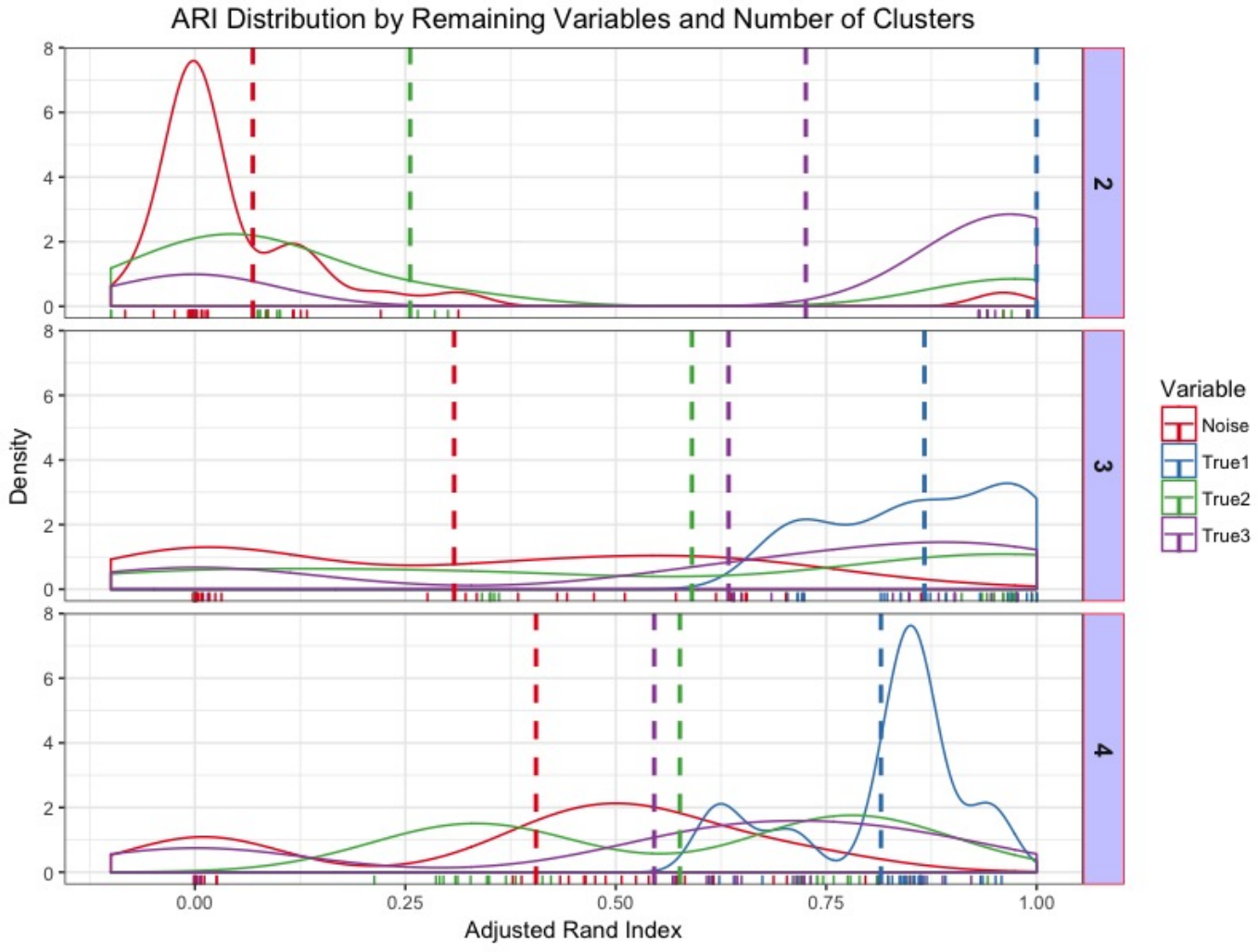
More consistent due to bimodal nature of True4





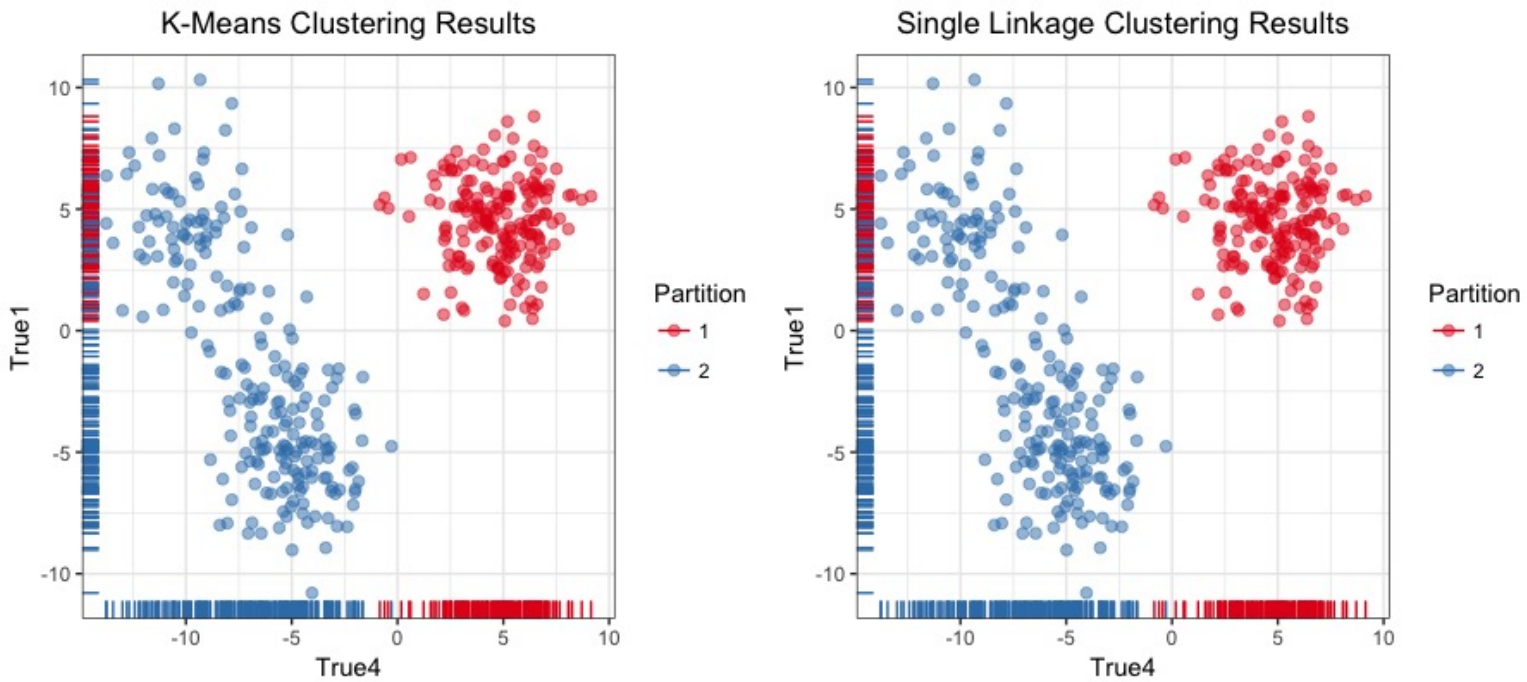
Given {True4}: k=2, True1

Perfect agreement, $\overline{ARI}_{2,\{True4,True1\}} = 1$



Consistent Clustering With 2 Clusters

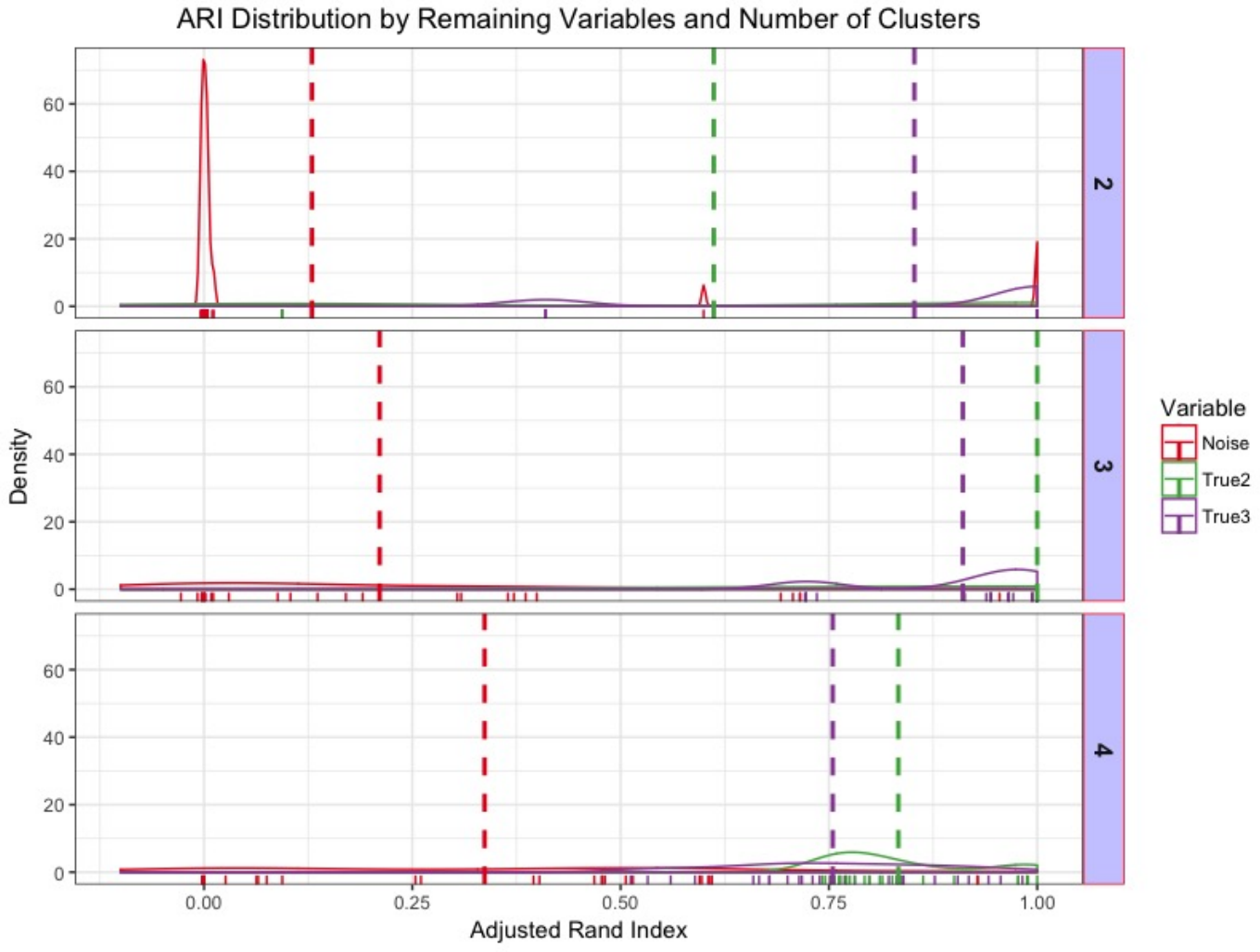
$ARI(p_{m_1,2,\{True4,True1\}},\ p_{m_2,2,\{True4,True1\}}) = 1,$
across all 28 pairs of methods



Identified 2 well separated clusters

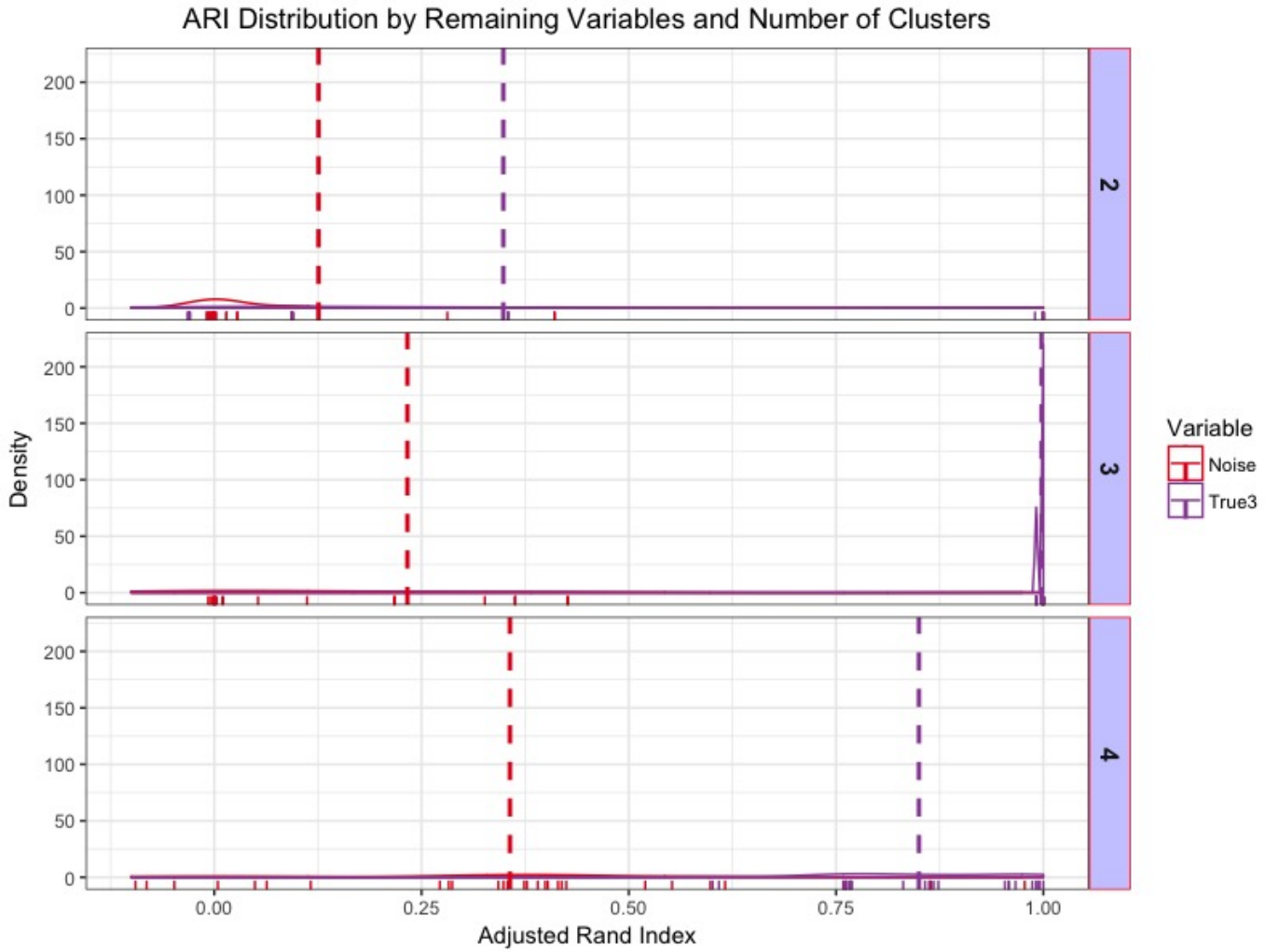
Given {True4, True1}: k=3, True2

Returns to previous result, $\overline{ARI}_{3,\{True4, True1, True2\}} = 1$



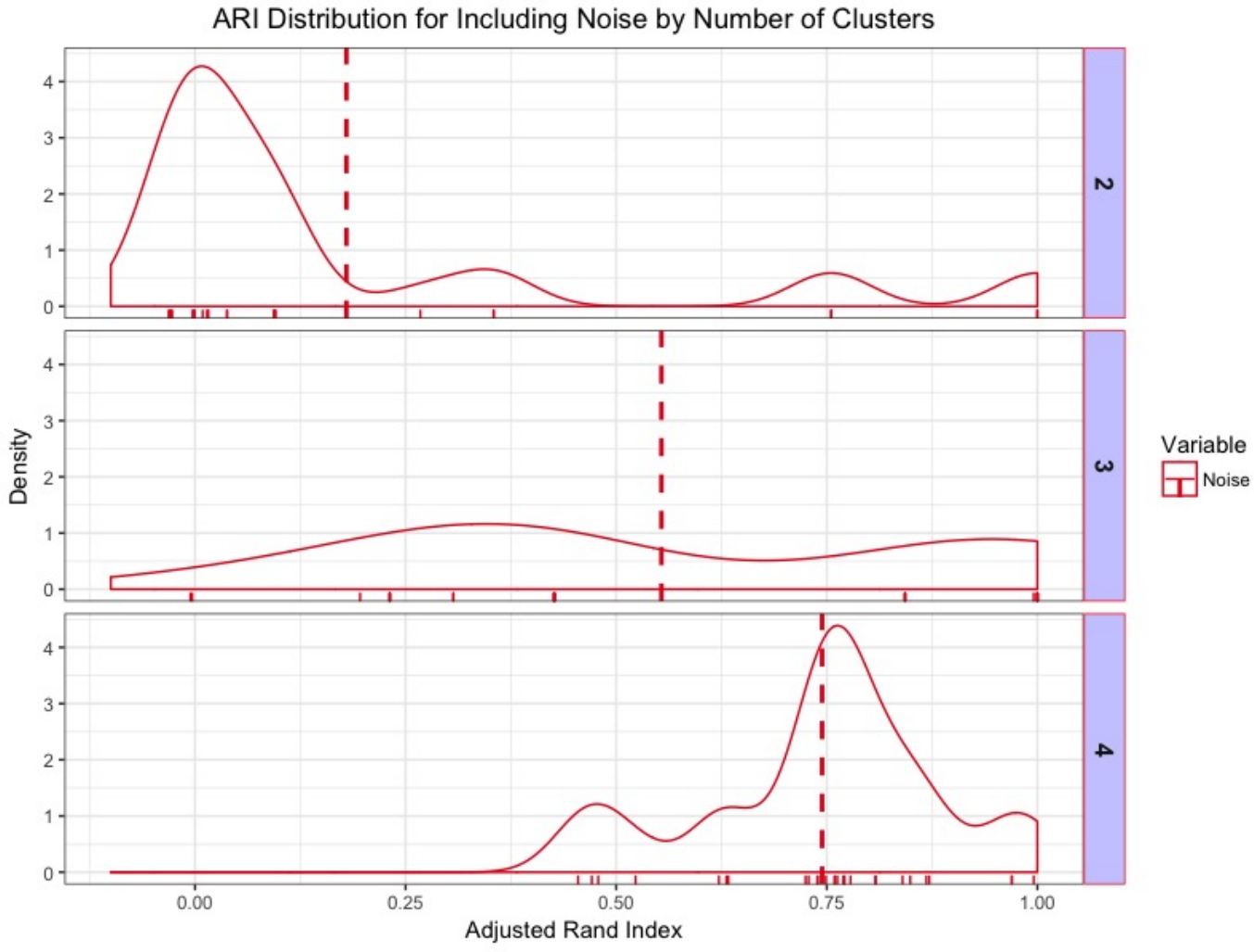
Given {True4, True1, True2}: k=3, True3

Again the same result, $\overline{ARI}_{3,\{True4, True1, True2, True3\}} = 0.9979$

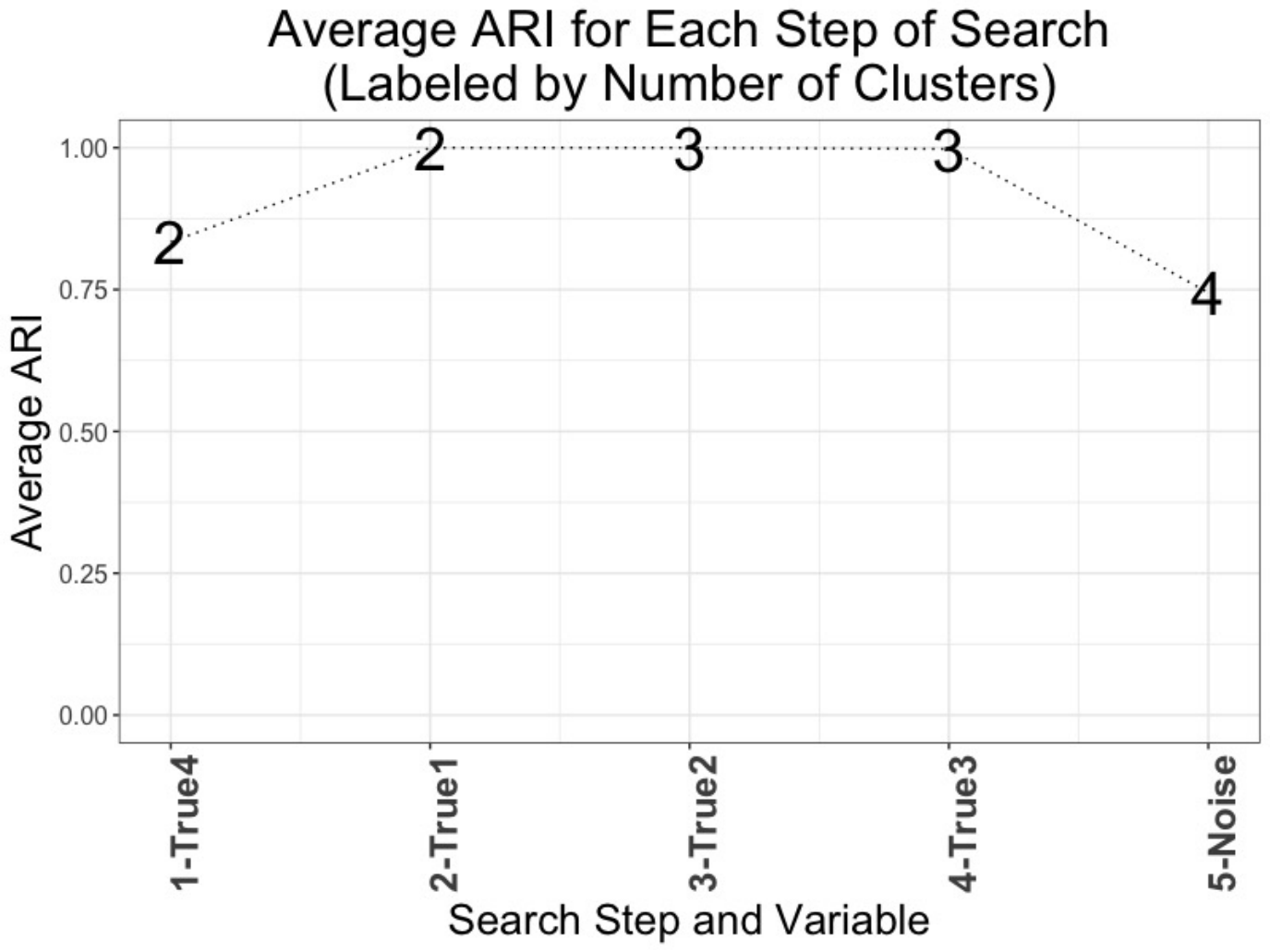


What About Including Noise?

Drop in consistency, $\overline{ARI}_{4,\{True4, True1, True2, True3, Noise\}} = 0.7444$

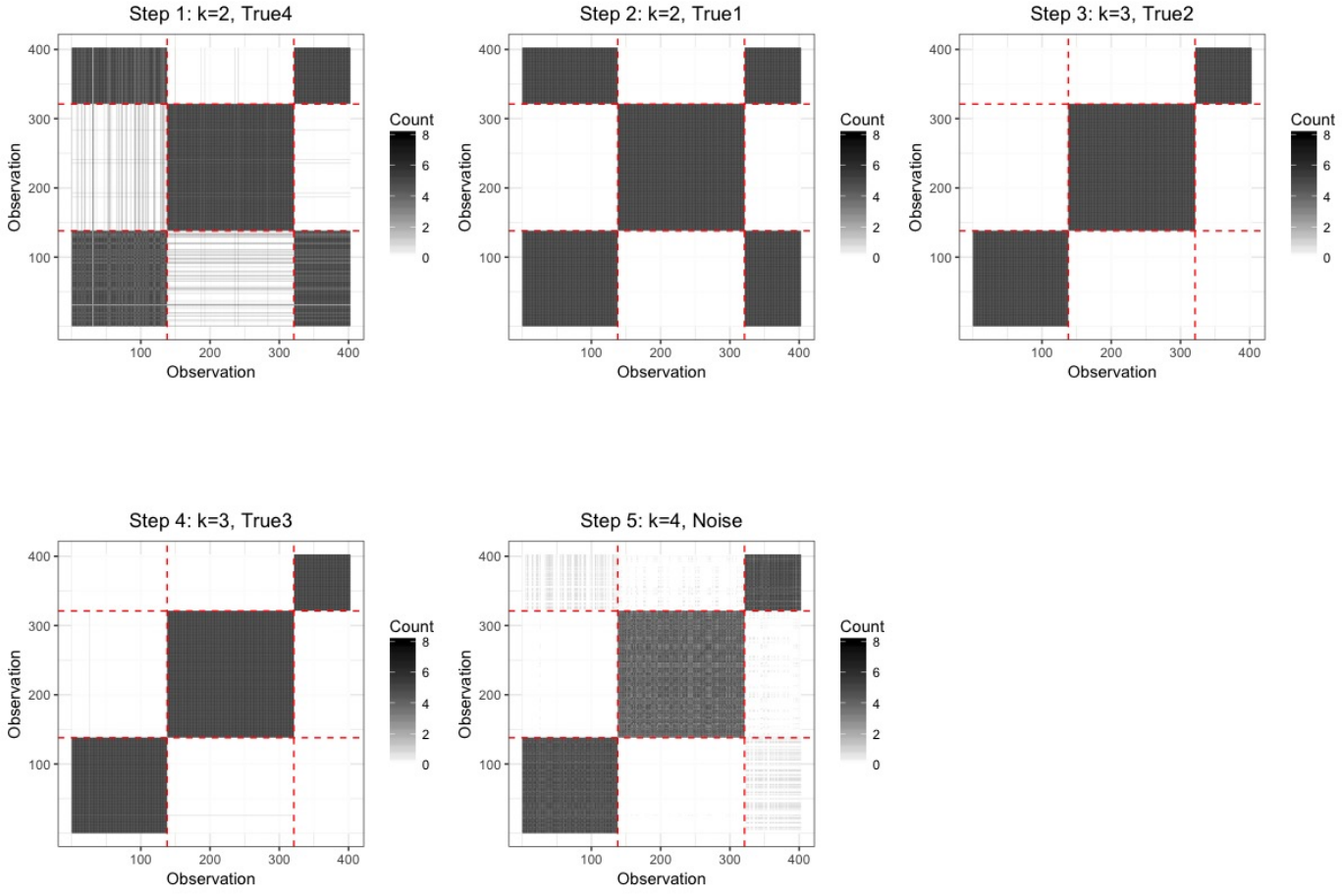


Summary of Demo Search



Clearly see the drop from including Noise

Summary of Demo Search



Stopping Criteria?

Perfect Agreement:

- $\overline{ARI}_{k,S\cup\{d^*\}} = 1$

Minimum Threshold:

- Only include d^* if $\overline{ARI}_{k,S\cup\{d^*\}} > ARI_{min}$

Percentage Drop:

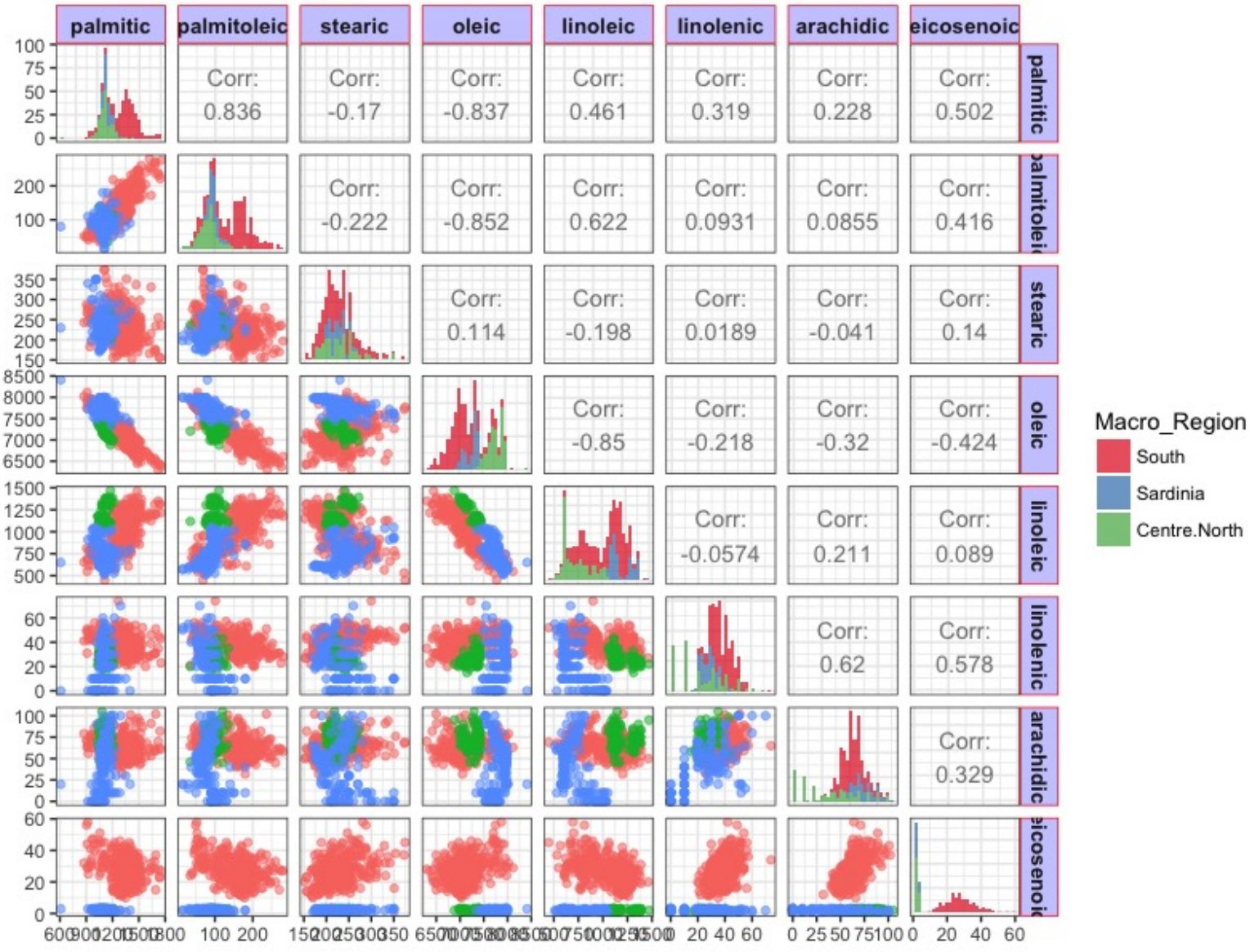
- Only include d^* if $\overline{ARI}_{k,S\cup\{d^*\}} > C * \overline{ARI}_{k,S}$, where C is a percentage

User can input desired level of consistency

Olive Oil Data

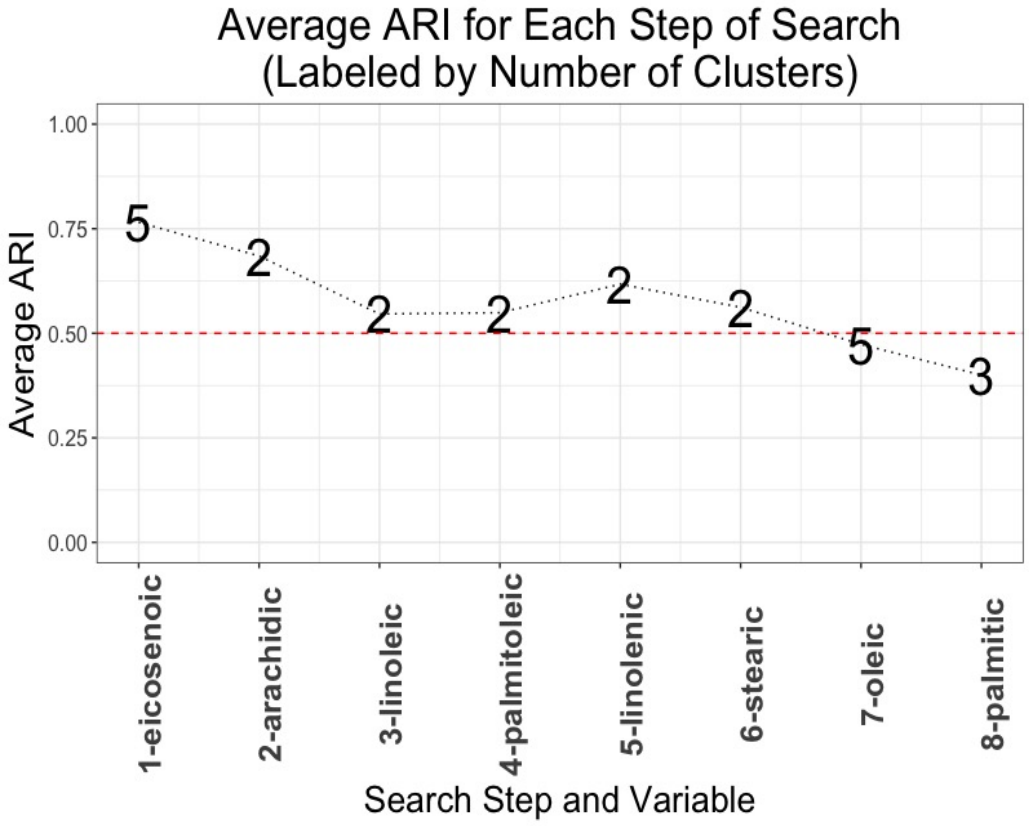
- 572 observations, each a different type of olive oil
- 8 variables for chemical measurements of acids
- 2 known labels:
  - Macro-Regions: 3 groups
  - Sub-Regions: 9 groups

Oils by Macro-Region



Macro-Region Consistency Search

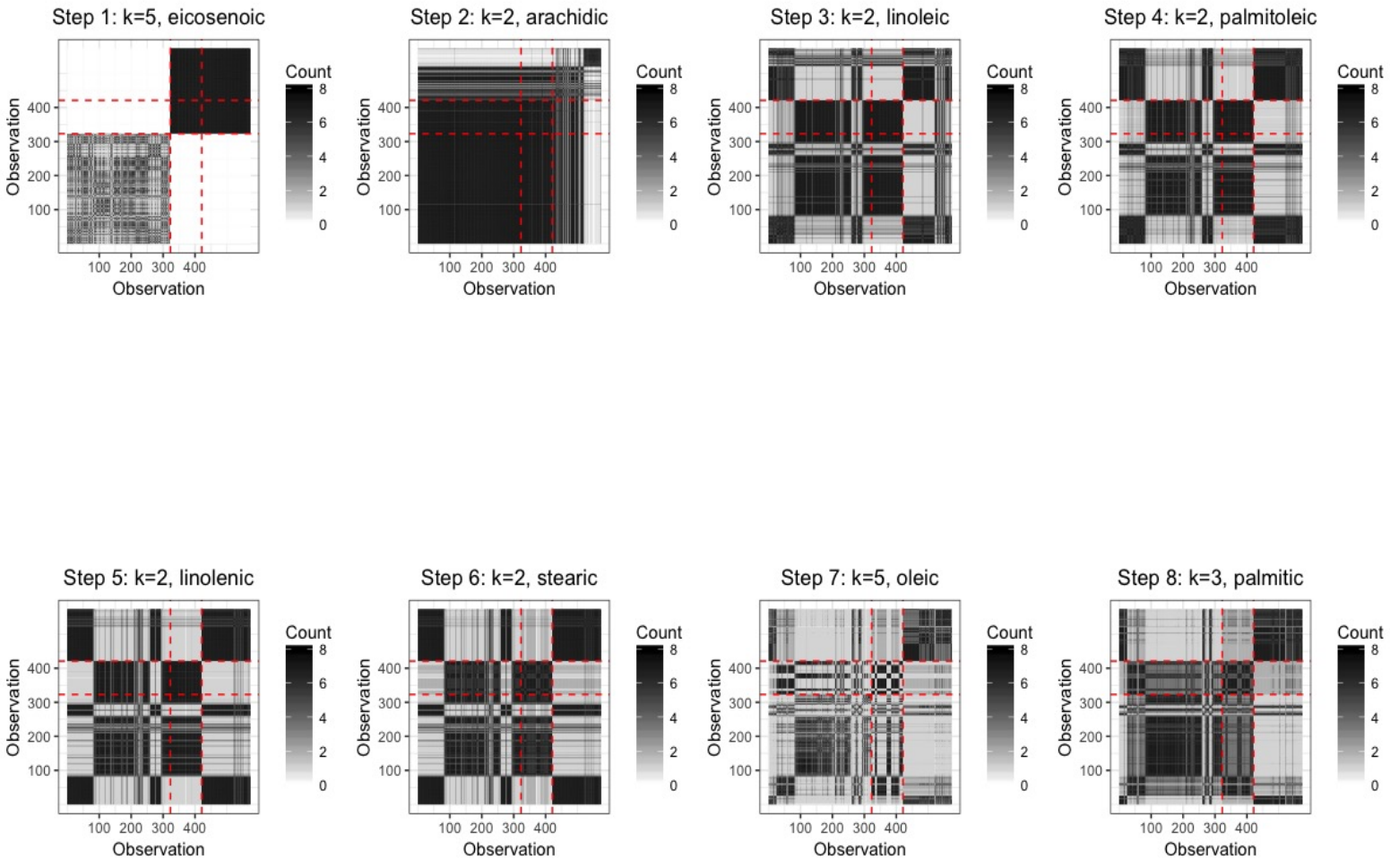
Search over $k = 2, \ldots, 5$: stop after Step 5, $\overline{ARI}_{2,S} = 0.6174$



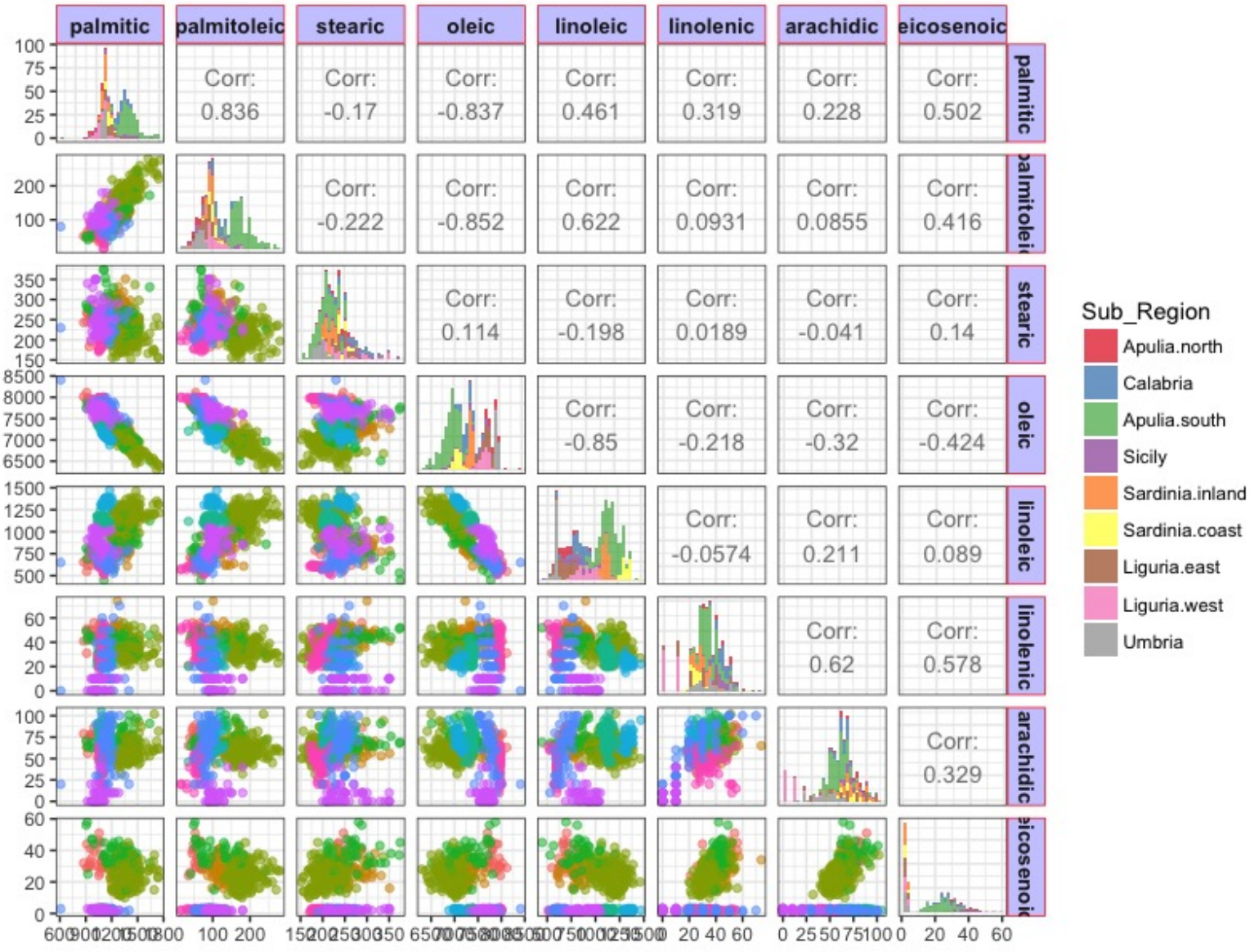
Model-based clustering, with `clustvarsel` *(Raftery & Dean, 2006)*:

Chose all 8 variables, with $k = 5$ (while $\overline{ARI}_{5,S \cup U} = 0.3955$)

Macro-Region Consistency Search

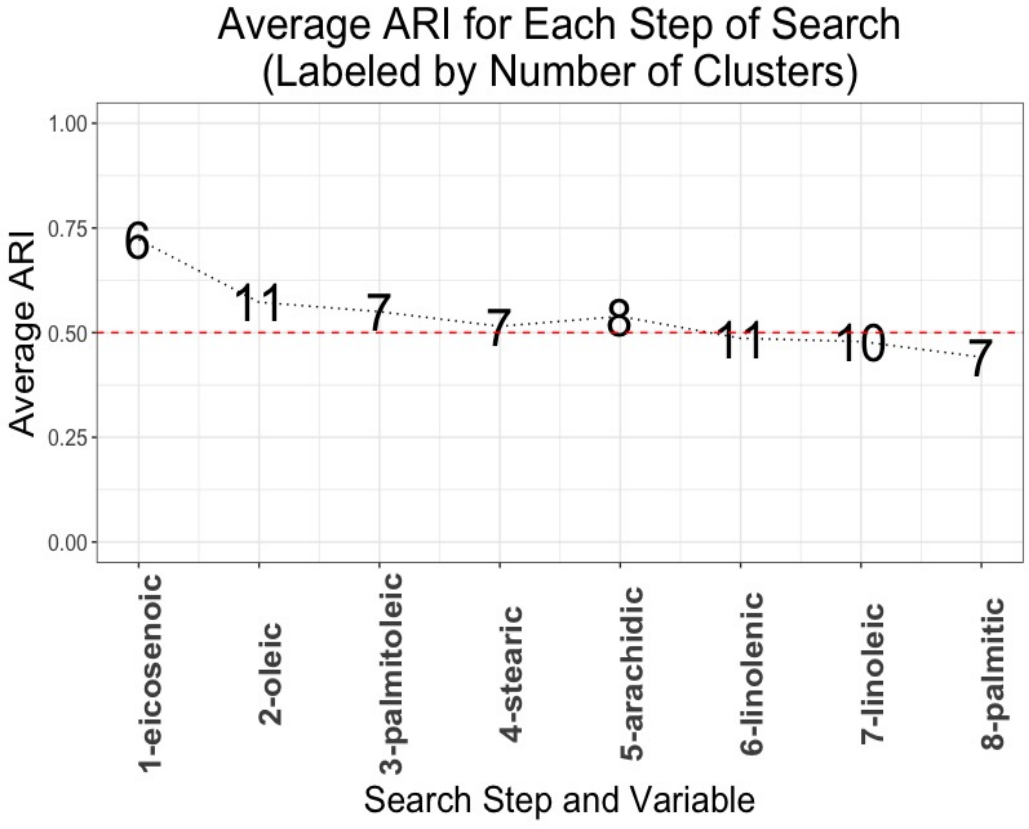


Oils by Sub-Region



Sub-Region Consistency Search

Search over $k = 6, \ldots, 12$: stop after Step 5, $\overline{ARI}_{8,S} = 0.5457$



Model-based clustering:

Chose 7 variables with $k = 9$, didn't select oleic

Future Work

- Include a removal step in the search
- Only considered average ARI, but distributions are multimodal and assymetrical
- Weighting of comparisons,
  e.g. less weight on single vs complete partitions
- Sensitive to methods considered, expand with concept

- Interpretation of changing clusters with different methods
- Mode hunting for specific clustering methods
- Rather than stopping search, consider full sequence path

References I

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[Carmone et al., 1999].
[Albatineh and Niewiadomska-Bugaj, 2011].
[Fraley and Raftery, 1998]. [Raftery and Dean, 2006].
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Maximum clustering similarity

MCS: A Method for Finding the Number of Clusters
(Albatineh & Niewiadomska-Bugaj, 2011)
Use corrected similarity indices to compare clustering methods

- Based on the number of pairs of data points that are (not) placed into the same cluster
- R (Rand, 1971), FM (Fowlkes and Mallows, 1983), K (Kulczynski, 1927)
- Adjusted Rand index (ARI) (Hubert and Arabie, 1985):

$$ARI = \frac{R - E(R)}{1 - E(R)}$$

- ARI close to 0 due to chance, max value of 1

Choose the number of clusters that is most frequently the maximum similarity value across all method comparisons

Variable selection with ARI

HINoV method (Carmone, Kara, & Maxwell, 1999)

- Begin with K-means partition, p_j, using only variable j for each of the $j \in \{1, \ldots, D\}$ variables
- Compute ARI_{jk} between each of the $\binom{D}{2}$ pairs of partitions, $k \in \{1, \ldots, D\}$ and $k \neq j$
- Rank variables by $TOPRI_j = \sum_{k=1}^{D} ARI_{jk}$

Variable selection with ARI

A Variable-Selection Heuristic for K-means Clustering
(Brusco & Cradit, 2001)

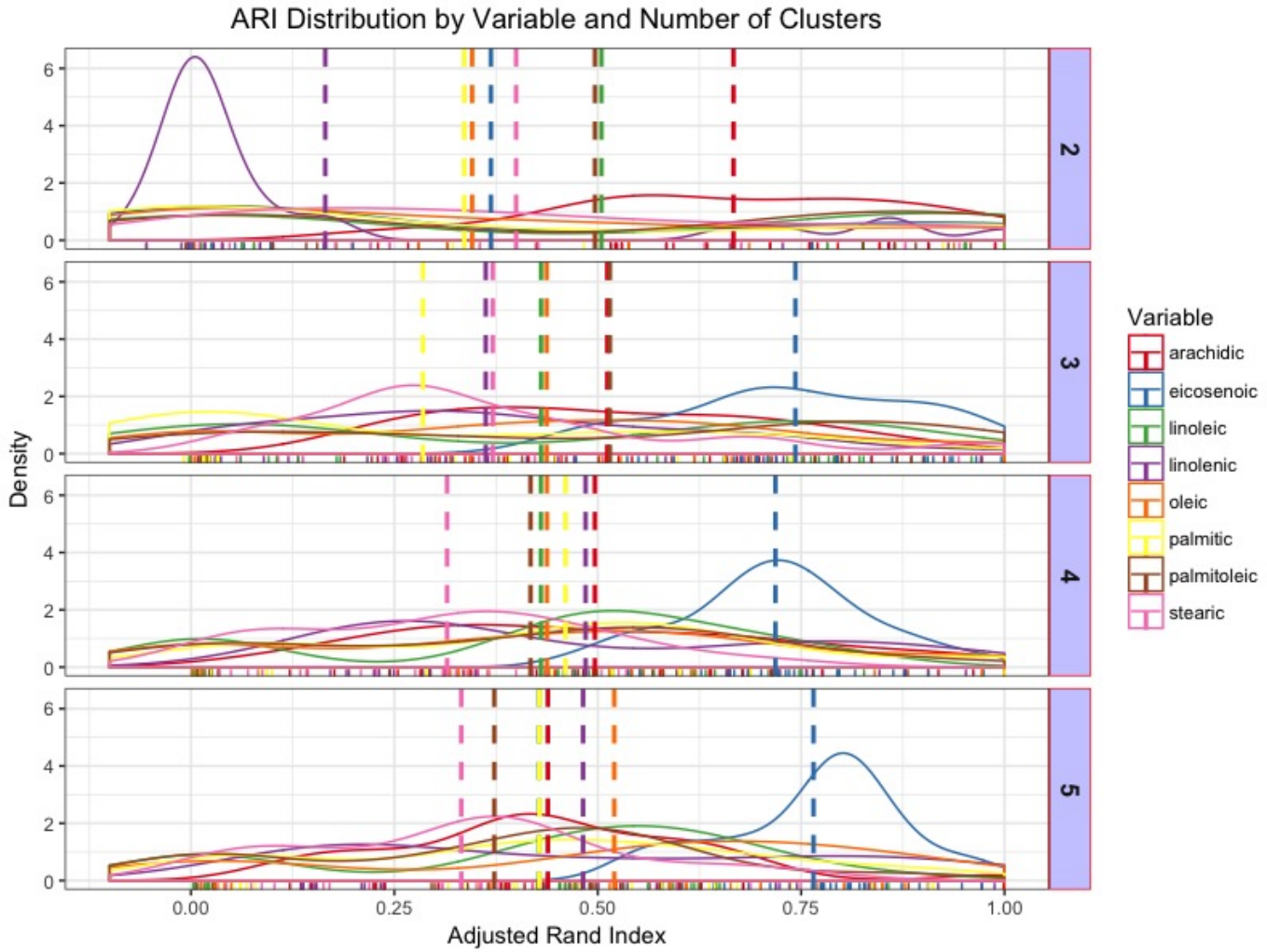
- Begin with K-means partition, p_j, using only variable j for each of the $j \in \{1, \ldots, D\}$ variables
- Compute ARI_{jk} between each of the $\binom{D}{2}$ pairs of partitions, $k \in \{1, \ldots, D\}$ and $k \neq j$
- Create partition w_{jk} with variables j and k, compute ratio of the between cluster sum-of-squares to the total sum-of-squares for partition
- Select variables with highest ratio given ARI_{jk} is above a threshold
- Calculate ARI between w_{jk} and $p_{j'}$ for each of the remaining variables $j' \in \{1, \ldots, D\}$ and $j' \neq j, k$
- Select variable with highest ARI above threshold, repeat until ARI drops below this threshold

Olive Oil Demo

Search for smaller number of clusters similar to Macro

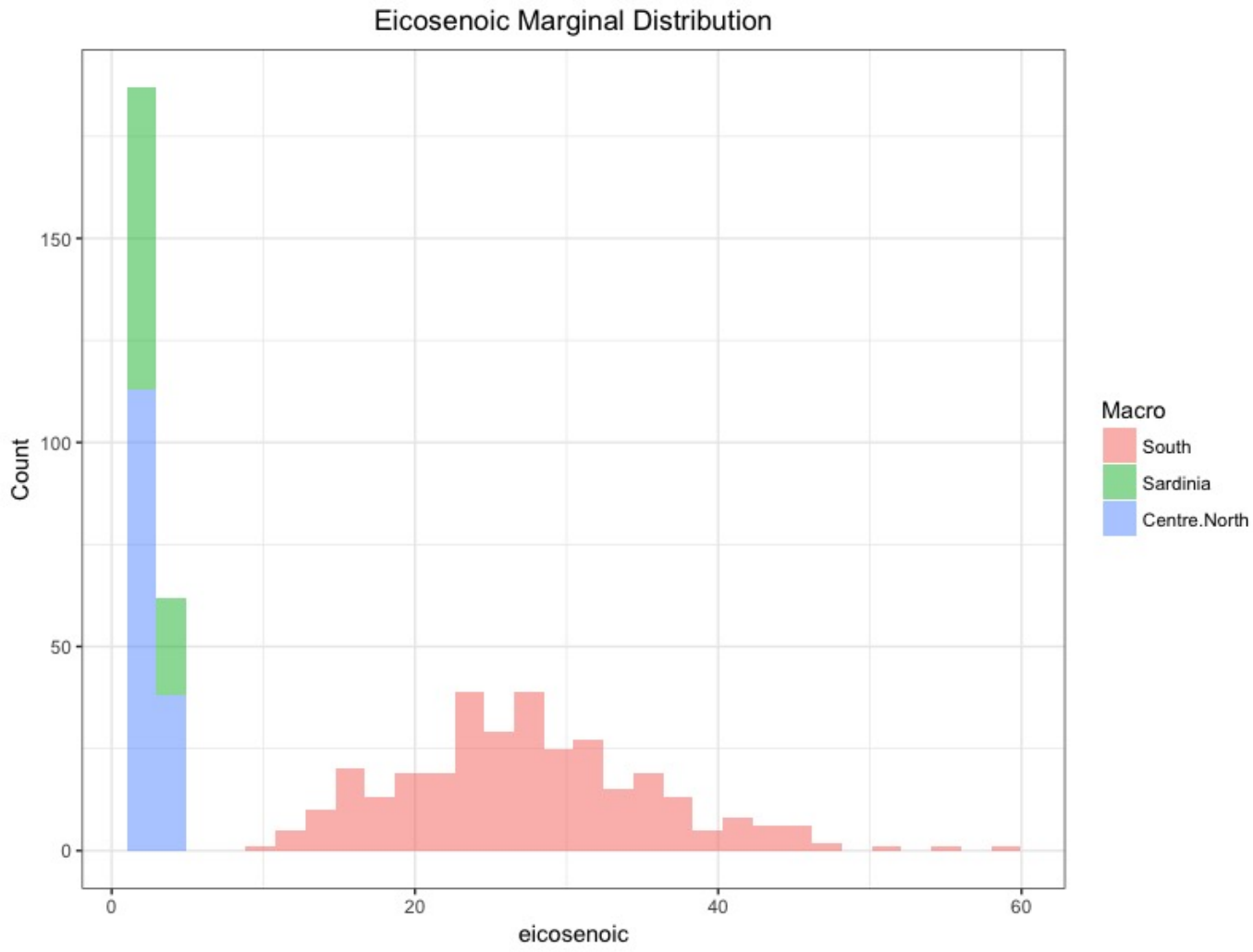
Most Consistent Combo: k=5, eicosenoic

Searching over 2-5 clusters, $\overline{ARI}_{\{eicosenoic\}} = 0.7652$



Why 5 Clusters?

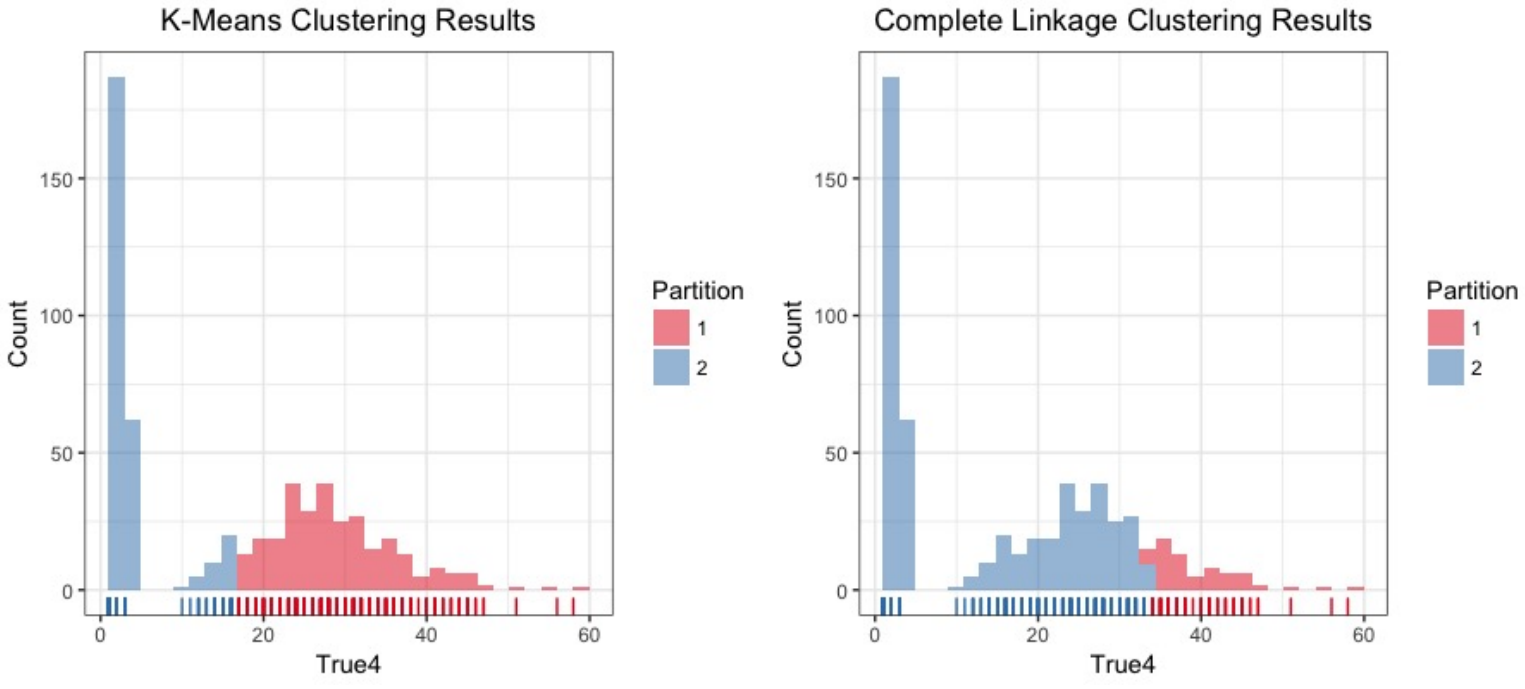
South appears to be separated from the other macro areas



Why 5 Clusters?

Not enough separation for 2 clusters,

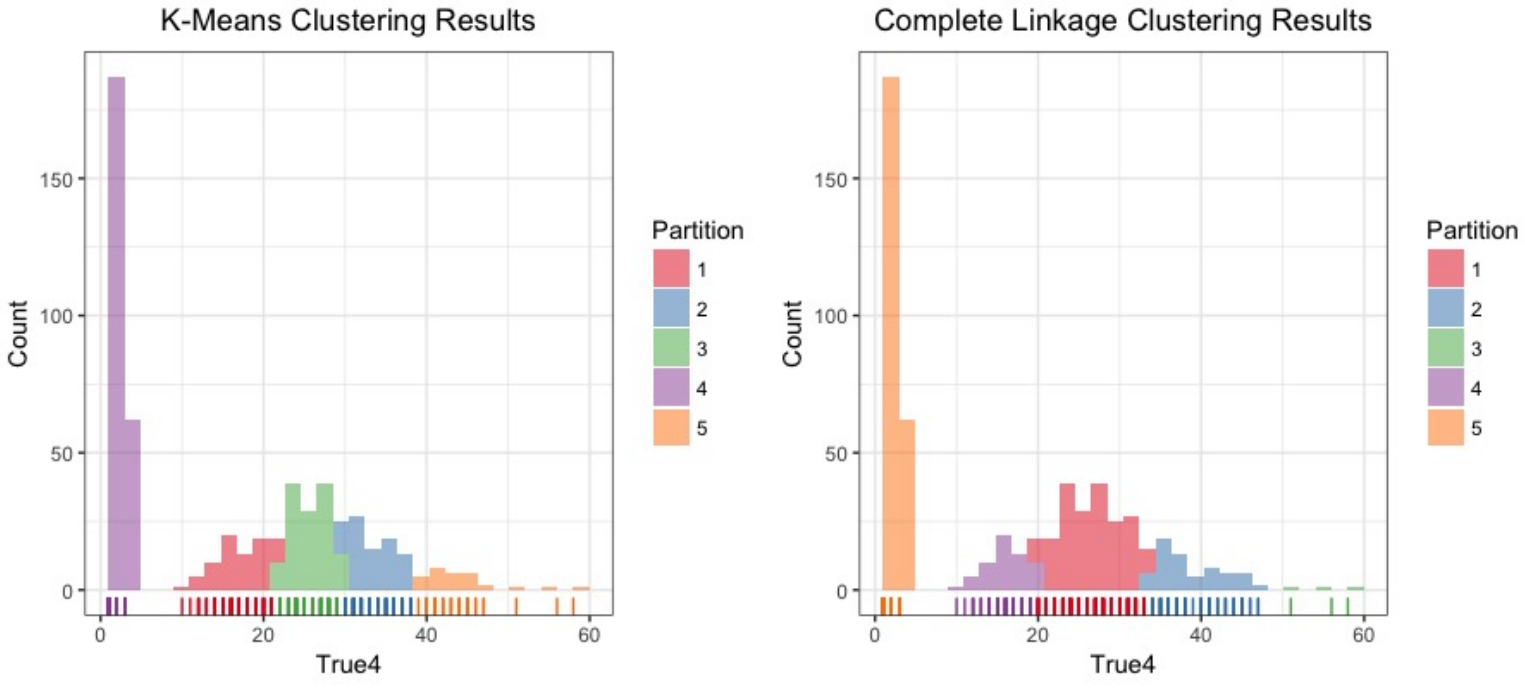
$ARI(p_{kmeans,2,\{eicosenoic\}}, p_{complete,2,\{eicosenoic\}}) = 0.0542$



Why 5 Clusters?

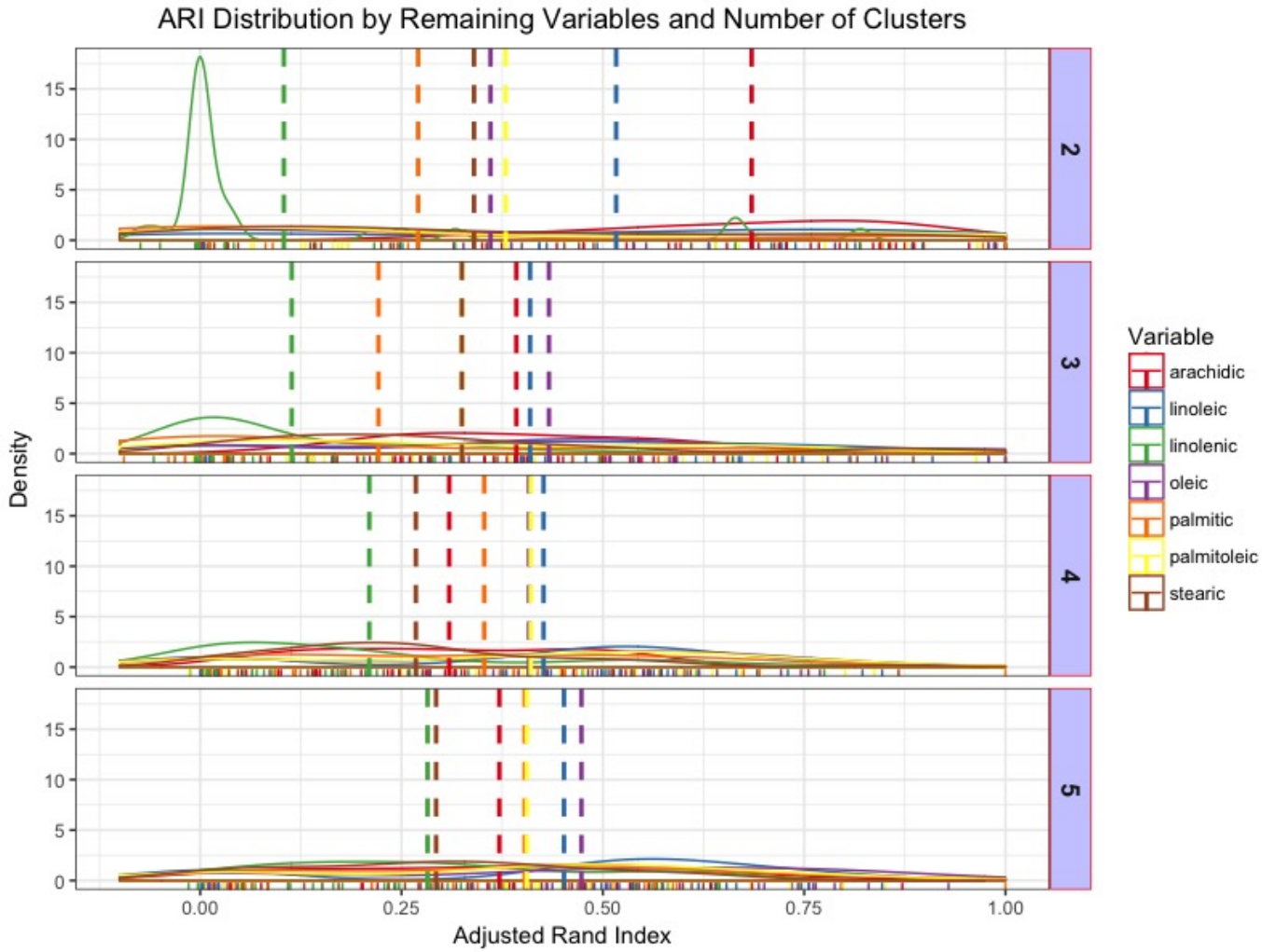
Consistent results with 5 clusters,

$ARI(p_{kmeans,5,\{eicosenoic\}}, p_{complete,5,\{eicosenoic\}}) = 0.8069$



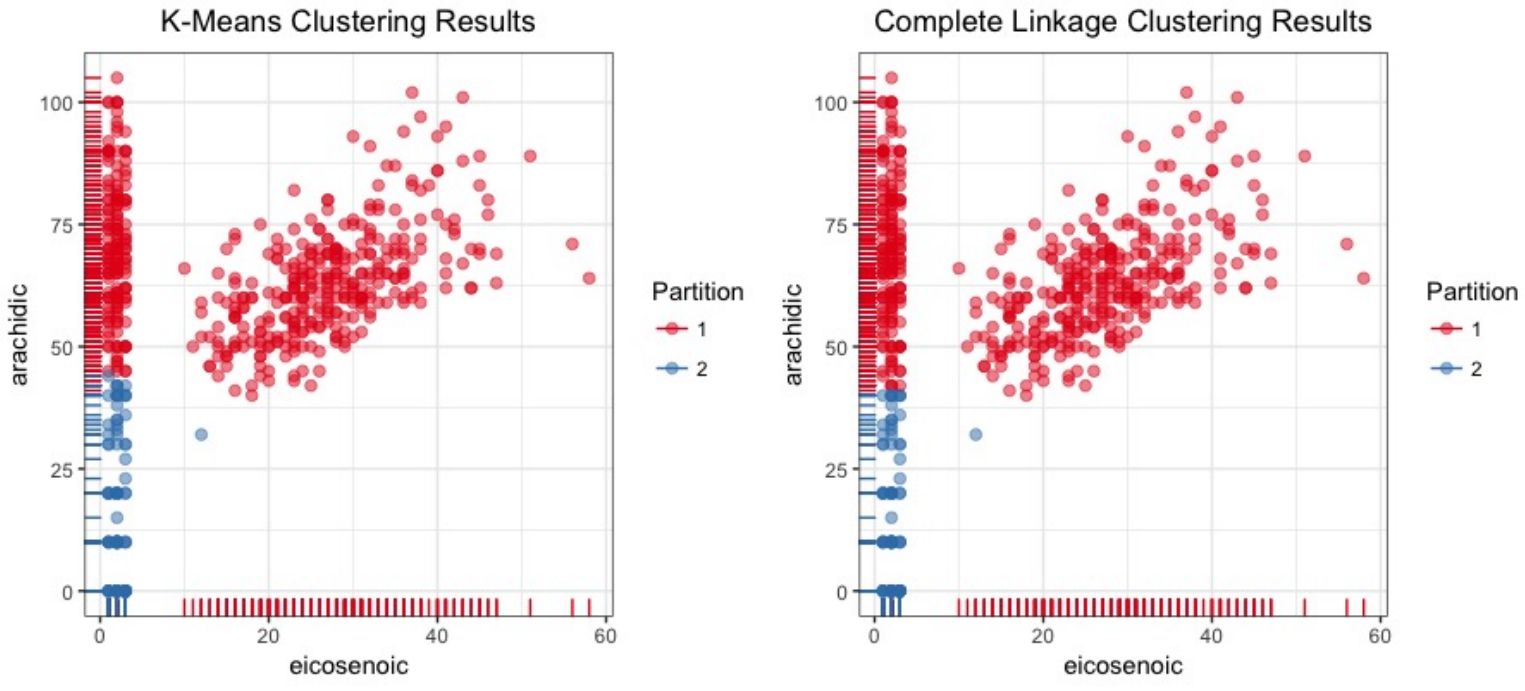
Given {eicosenoic}: k=2, arachidic

Switches to 2 clusters, $\overline{ARI}_{2,\{eicosenoic,arachidic\}} = 0.6848$



Why 2 Clusters?

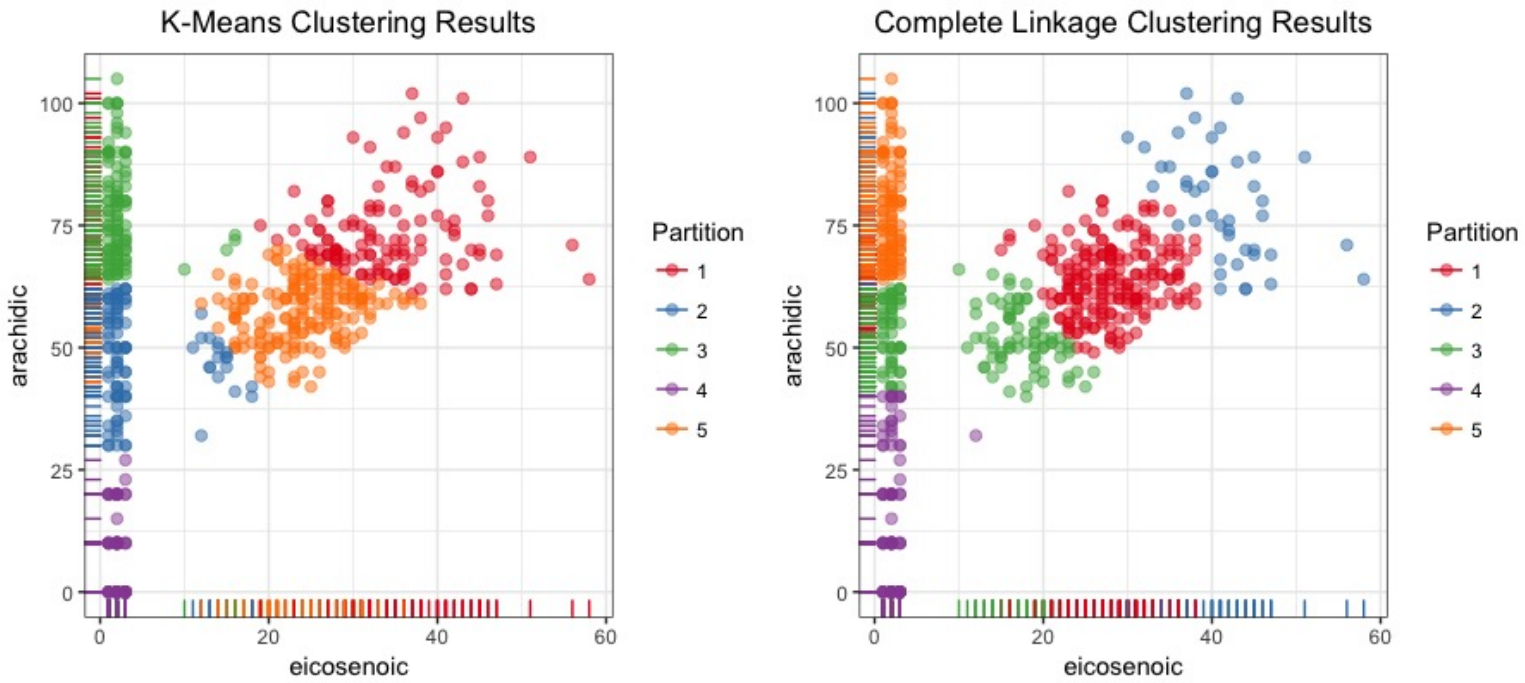
$ARI(p_{kmeans,2,\{eicosenoic,arachidic\}}, p_{complete,2,\{eicosenoic,arachidic\}}) = 0.9548$



Consistent with 2, but not well separated clusters

Why 2 Clusters?

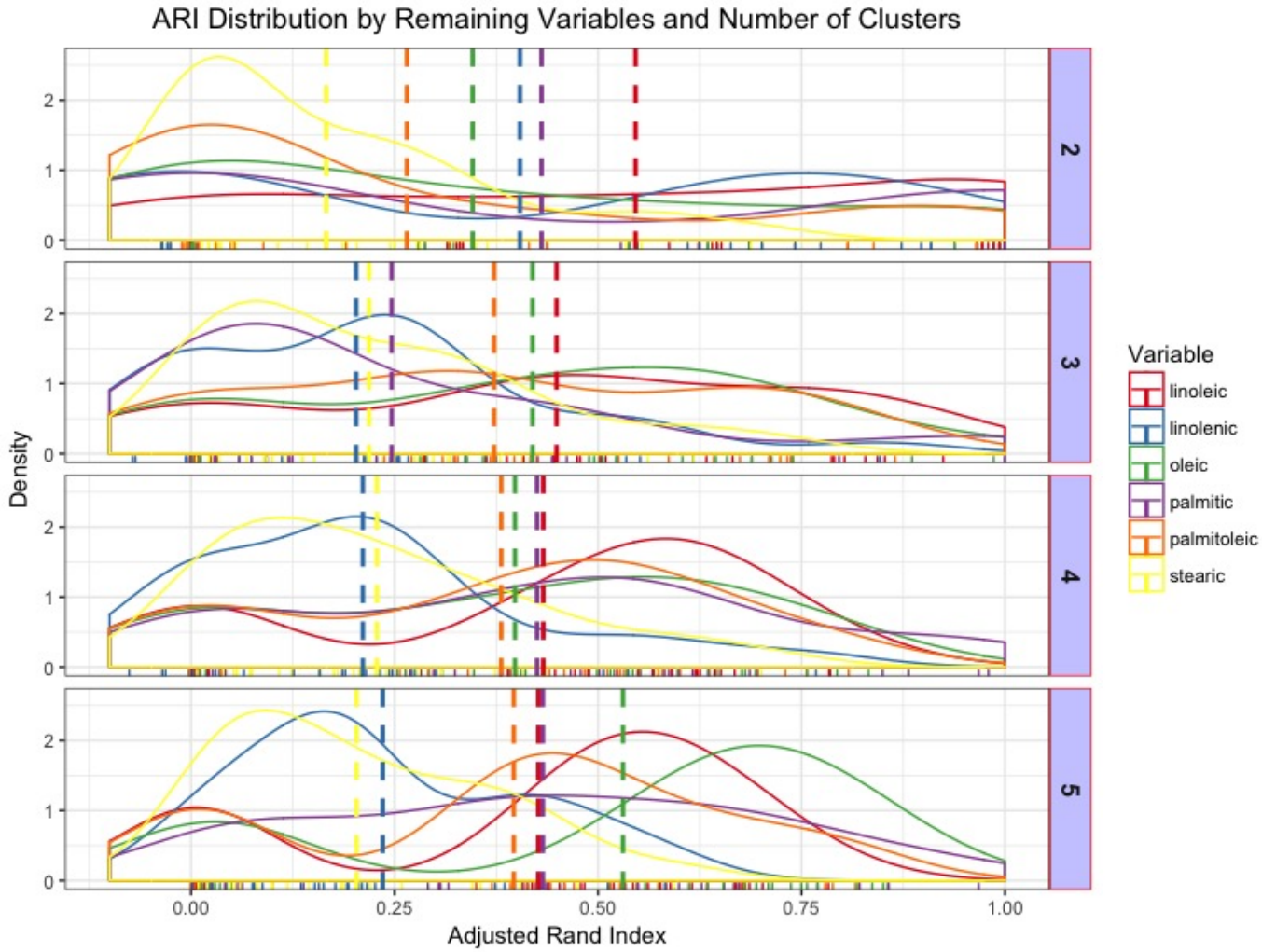
$ARI(p_{kmeans,5,\{eicosenoic,arachidic\}}, p_{complete,5,\{eicosenoic,arachidic\}}) = 0.5134$



Inconsistent with 5 clusters

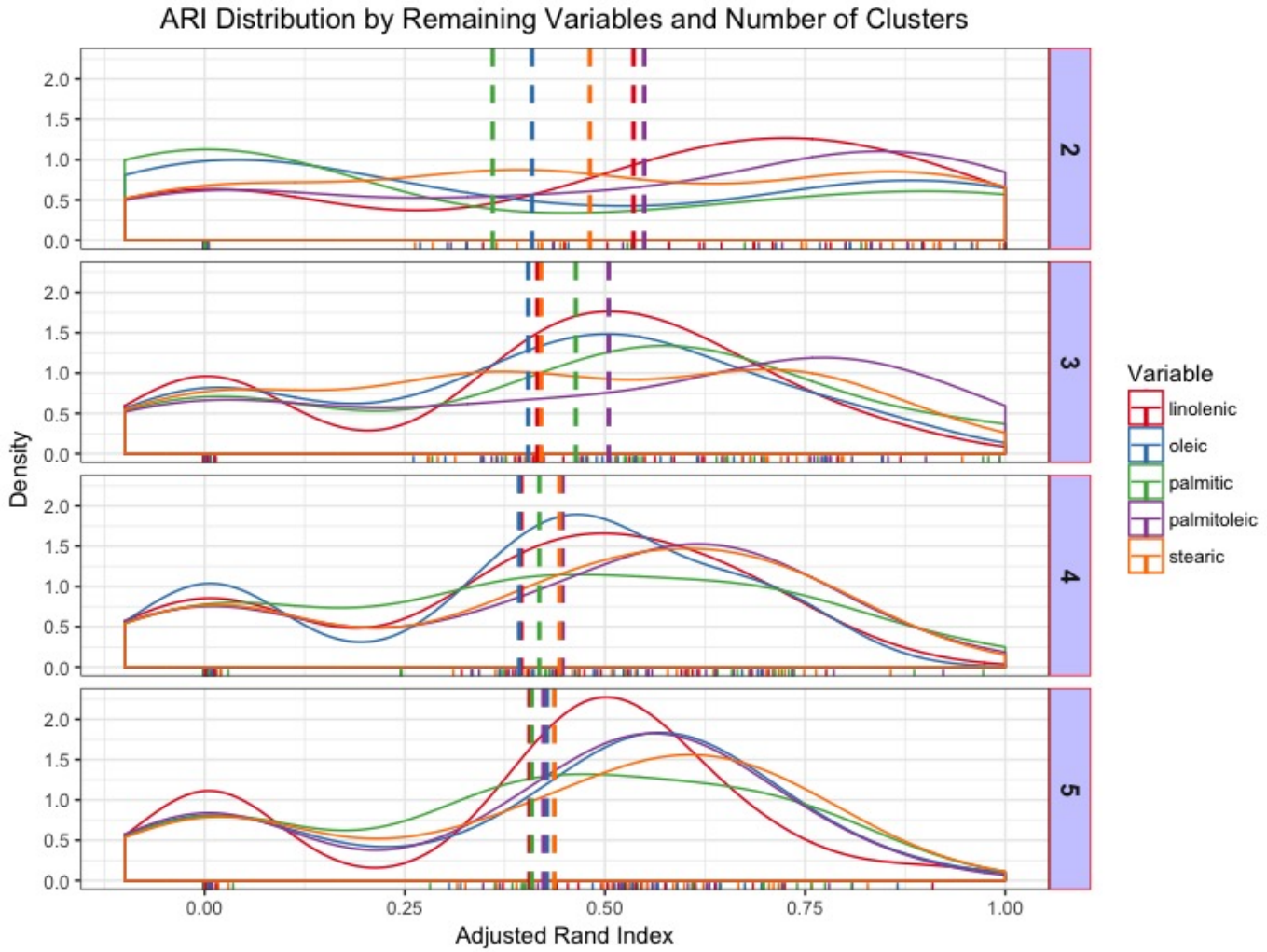
Given {eicosenoic,arachidic}: k=2, linoleic

Stay with 2 clusters, $\overline{ARI}_{2,\{eicosenoic,arachidic,linoleic\}} = 0.5461$



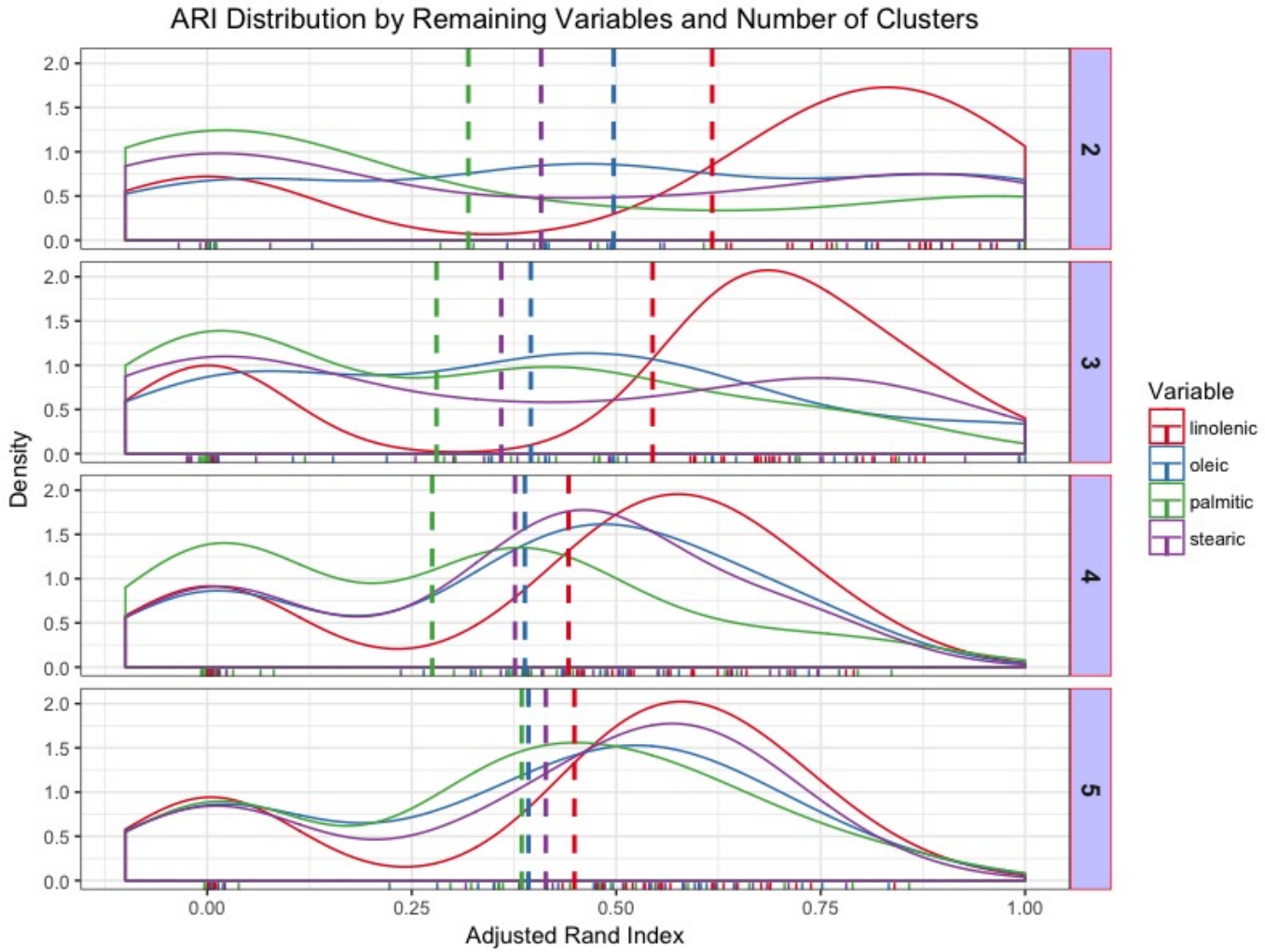
Given {eicosenoic,arachidic,linoleic}: k=2, palmitoleic

Similar results, $\overline{ARI}_{2,\{eicosenoic,arachidic,linoleic,palmitoleic\}} = 0.5491$



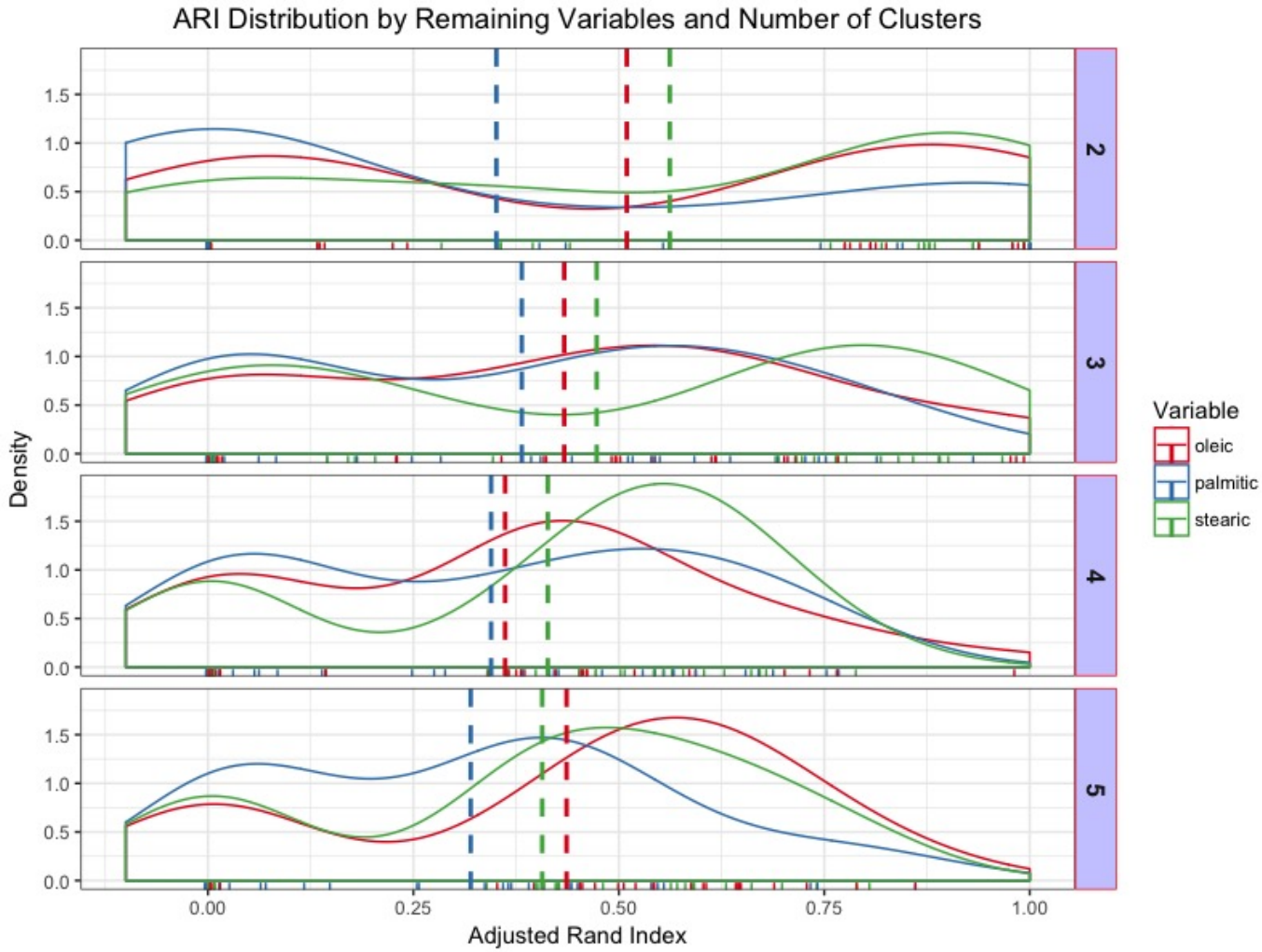
Next: k=2, linolenic

$$\overline{ARI}_{2,\{eicosenoic,arachidic,linoleic,palmitoleic,linolenic\}} = 0.6174$$



Next: k=2, stearic

$$\overline{ARI}_{2,\{eicosenoic,arachidic,linoleic,palmitoleic,linolenic,stearic\}} = 0.5620$$



Stop There

Best option is below 0.5,

$$\overline{ARI}_{5,\{eicosenoic,arachidic,linoleic,palmitoleic,linolenic,stearic,oleic\}} = 0.4733$$