Association-Based Spectral Clustering for Mixed Data

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outline

independence-based (IB) vs association-based (AB) dissimilarities

association-based for mixed data

taking into account continuous/categorical interactions

AB spectral clustering

example and future work

(adveRtising)

independence-based (IB) vs association-based (AB) dissimilarities

learning from dissimilarities

some unsupervised learning methods take as input a dissimilarity matrix

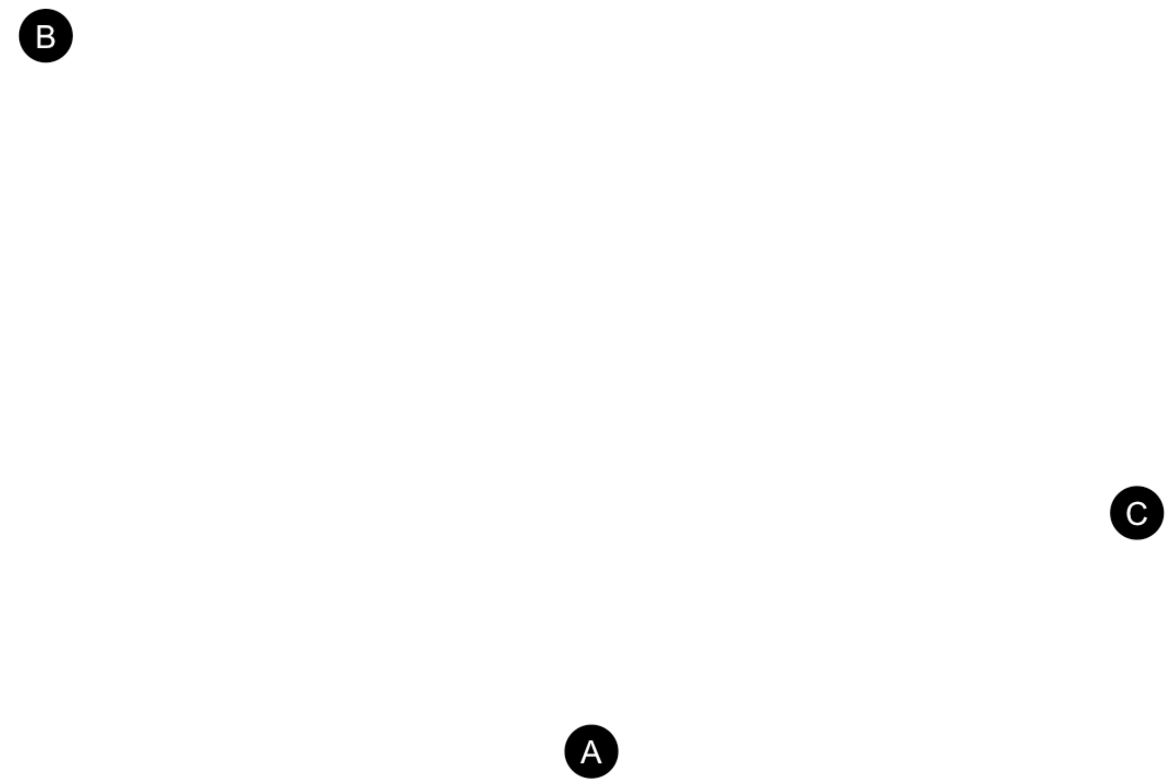
dimension reduction: multidimensional scaling (MDS)[1]

clustering methods: hierarchical (HC) and partitioning around medoids (PAM)[2]

the dissimilarity measure of choice is key, obviously

intuition

2 continuous variables: add up by-variable (absolute value or squared) differences



intuition

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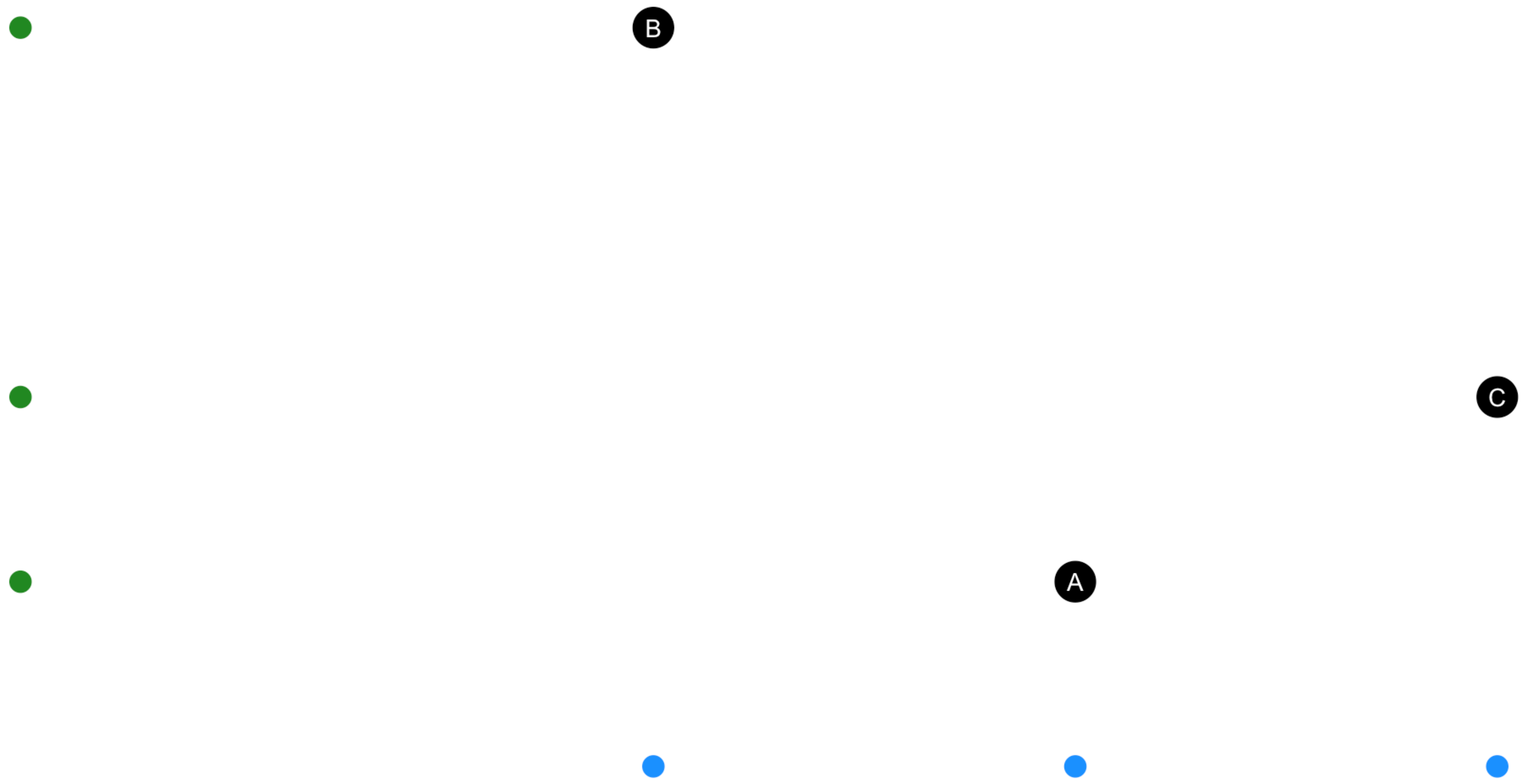

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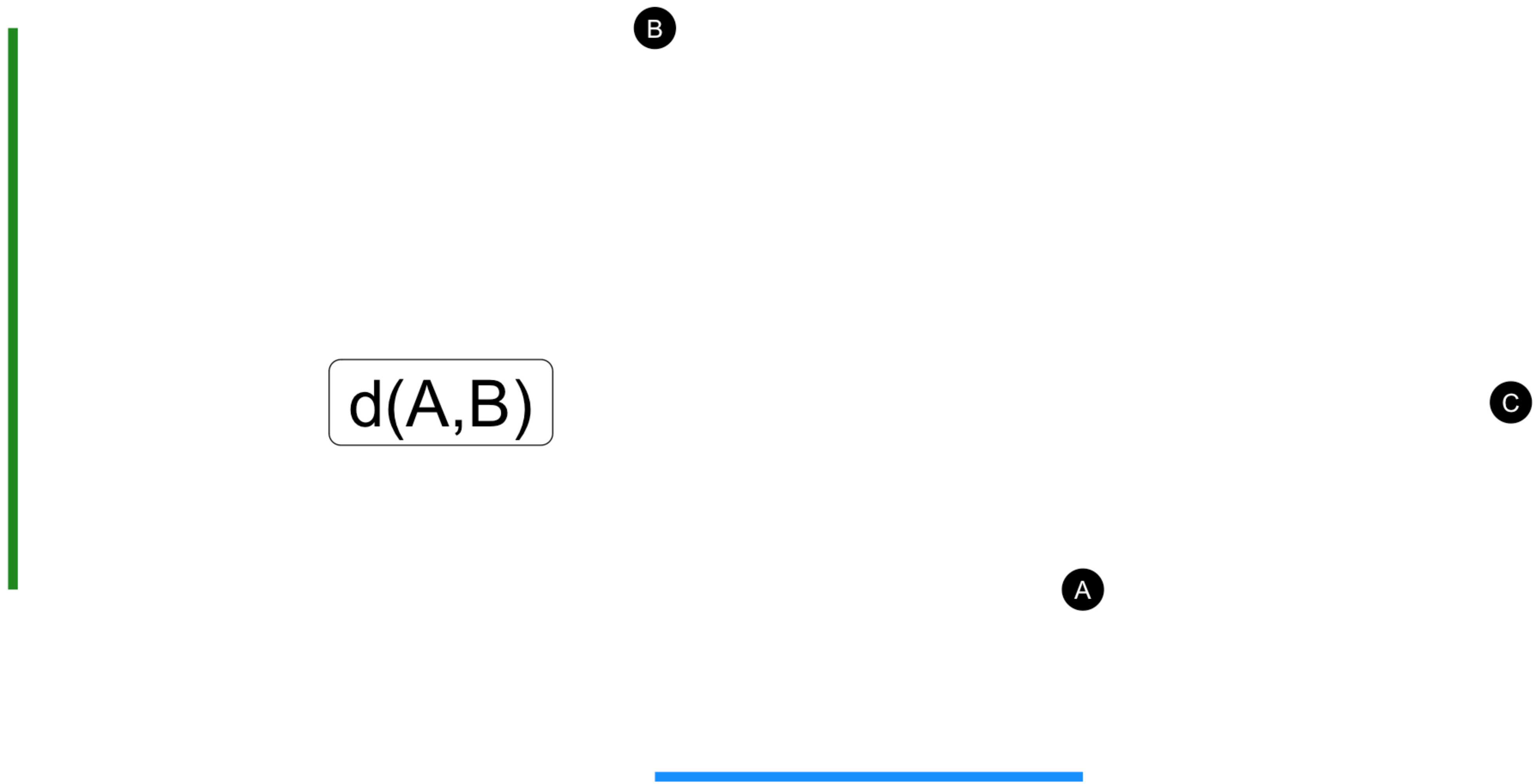

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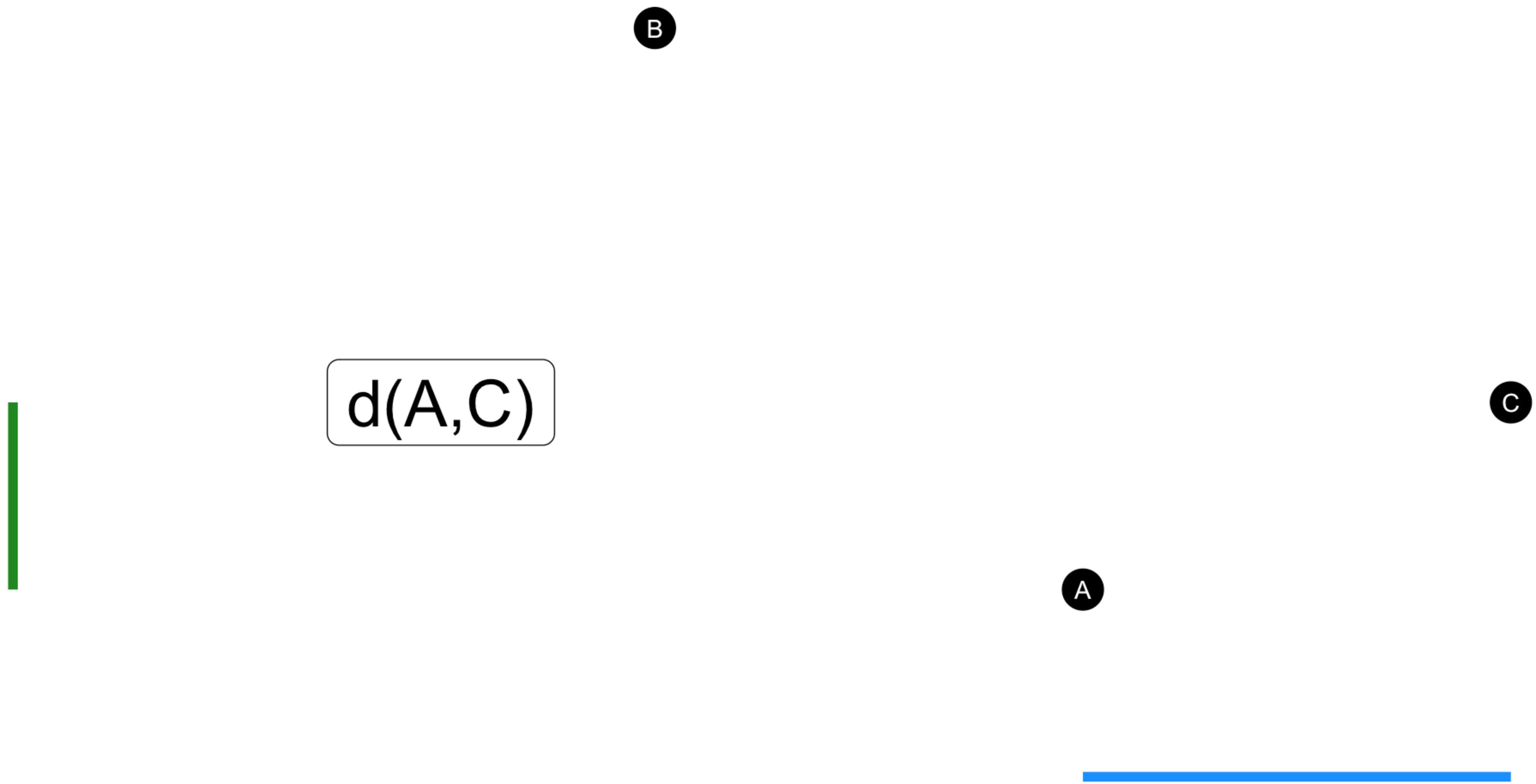

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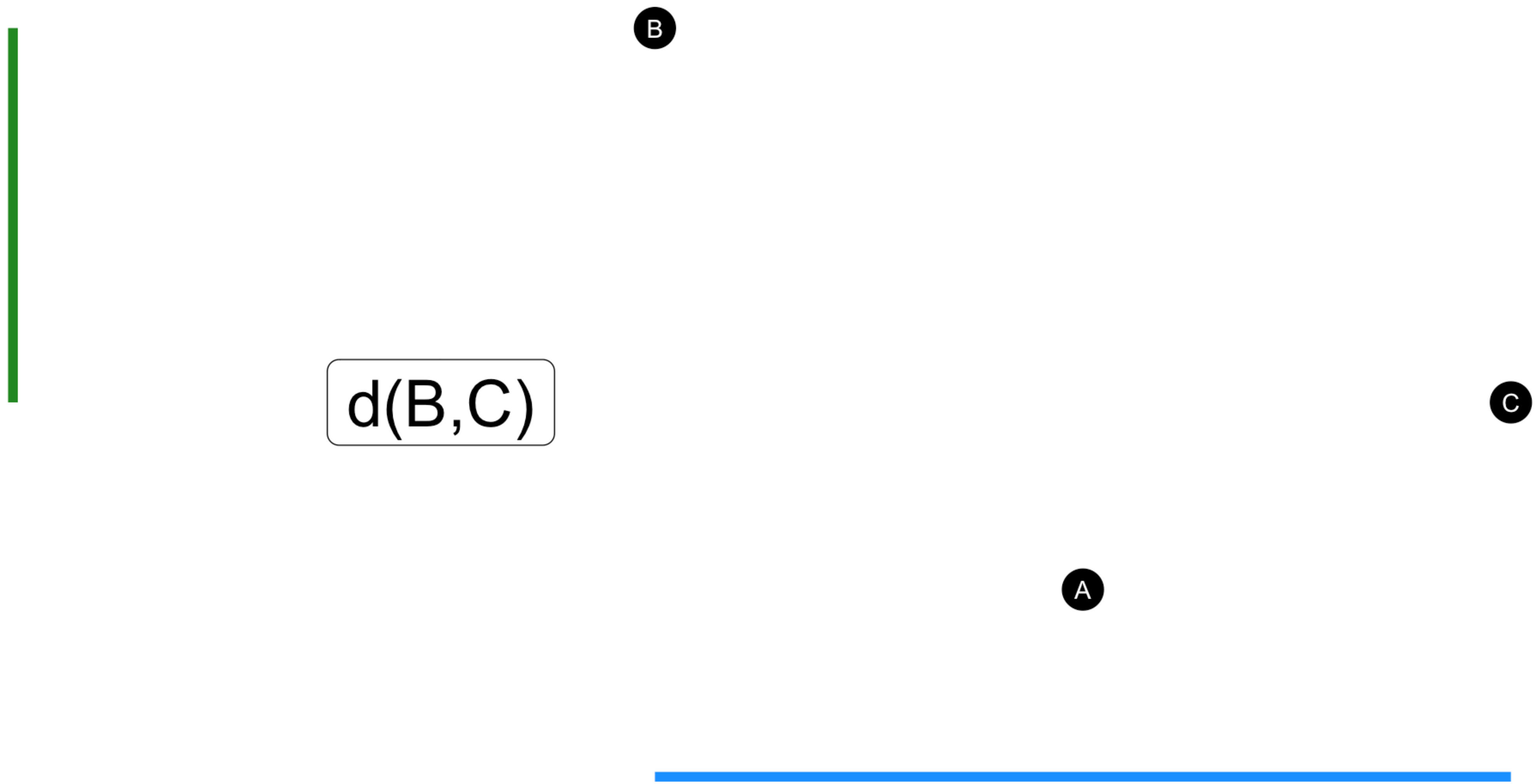
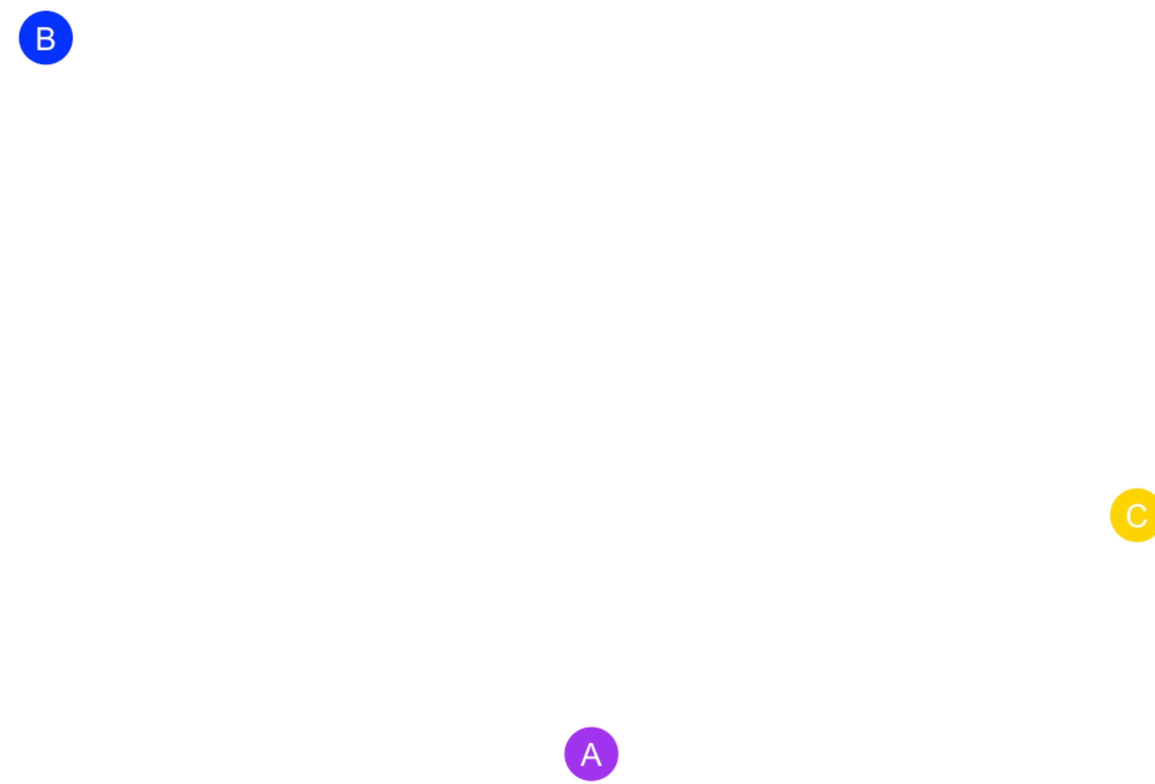


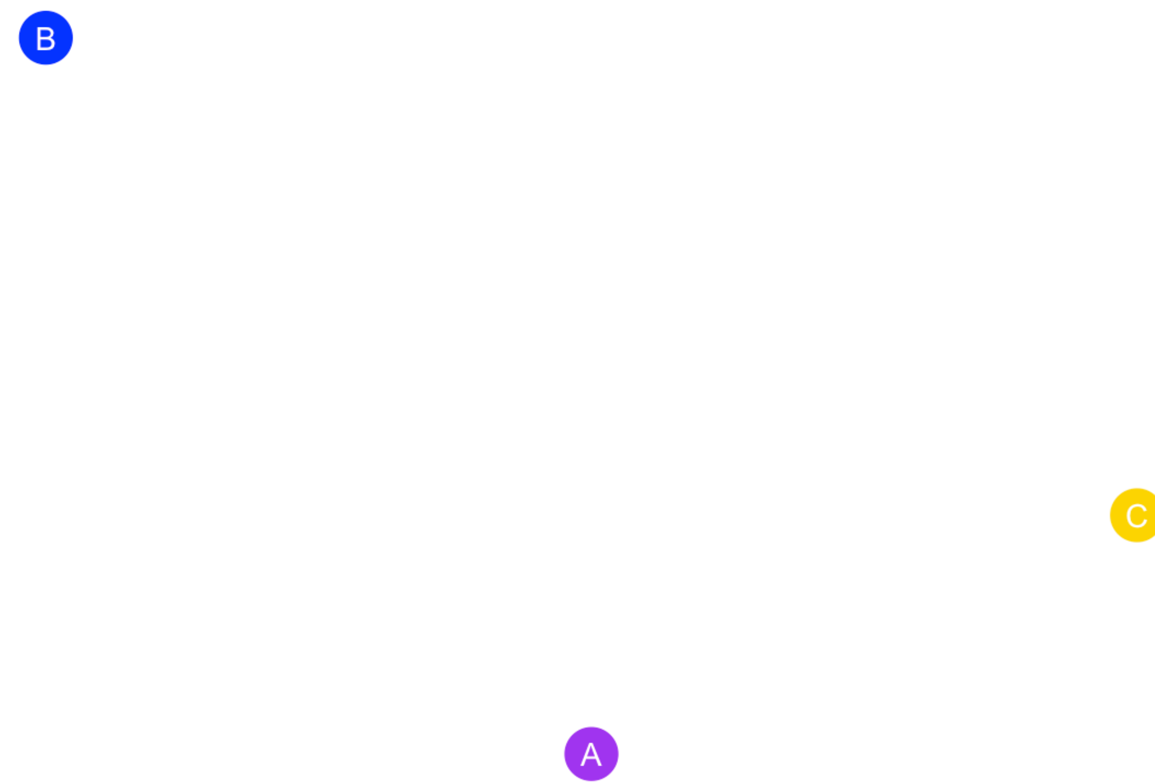
intuition

2 continuous and 1 categorical variables



intuition

one might consider purple and blue *closer* than e.g. purple and yellow



independence-based

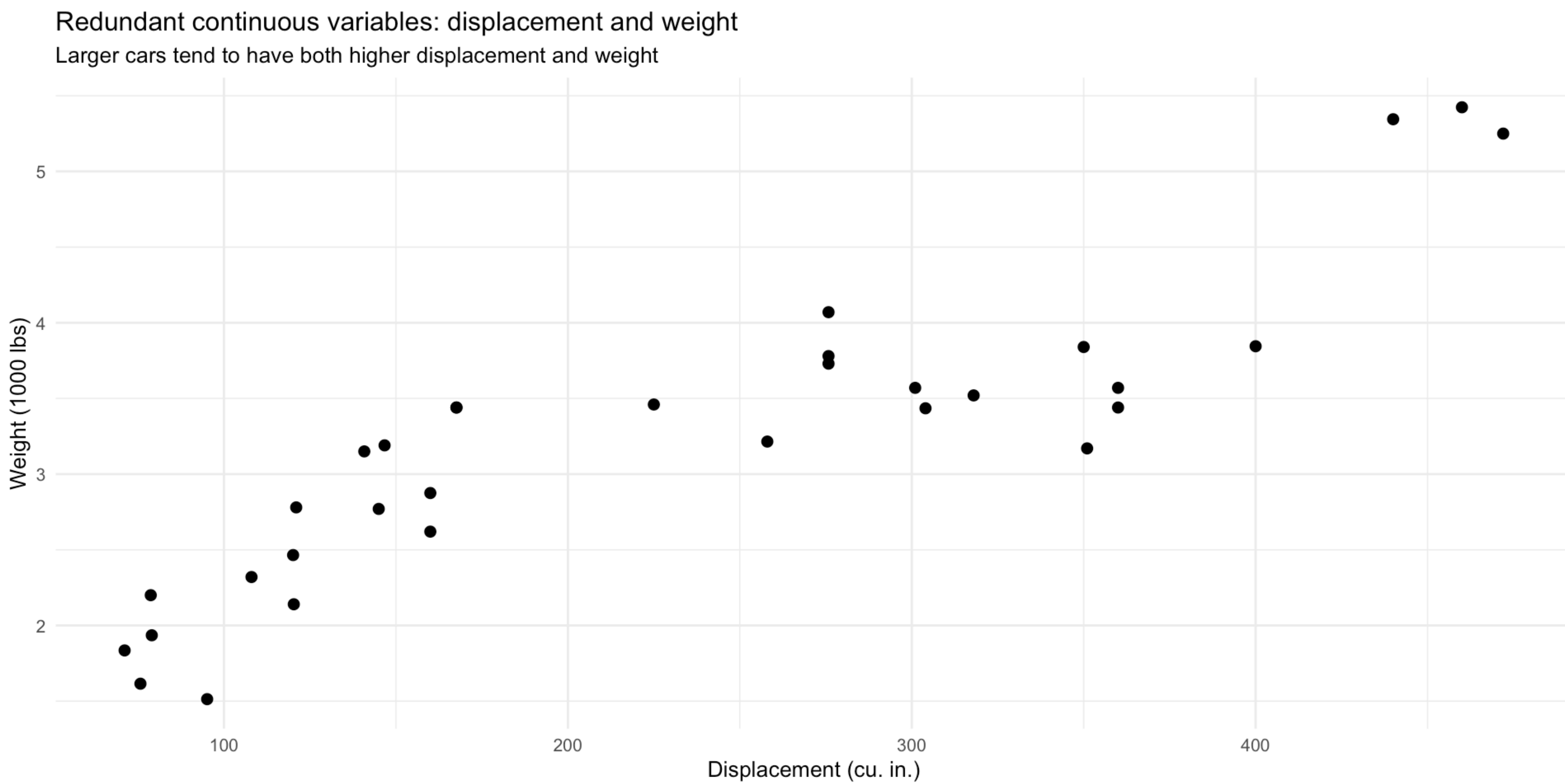
Most commonly used dissimilarity (or, distance) measures are based on by-variable differences that are then added together

- in the continuous case: Euclidean or Manhattan distances
- in the categorical case: Hamming (matching) distance (among MANY others)
- in the mixed data case: Gower dissimilarity index

no inter-variable relations are considered $\rightarrow$ independence-based

independence-based

- When variables are correlated or associated, shared information is effectively counted multiple times
- inflated dissimilarities may cause potential distortions in downstream unsupervised learning tasks.



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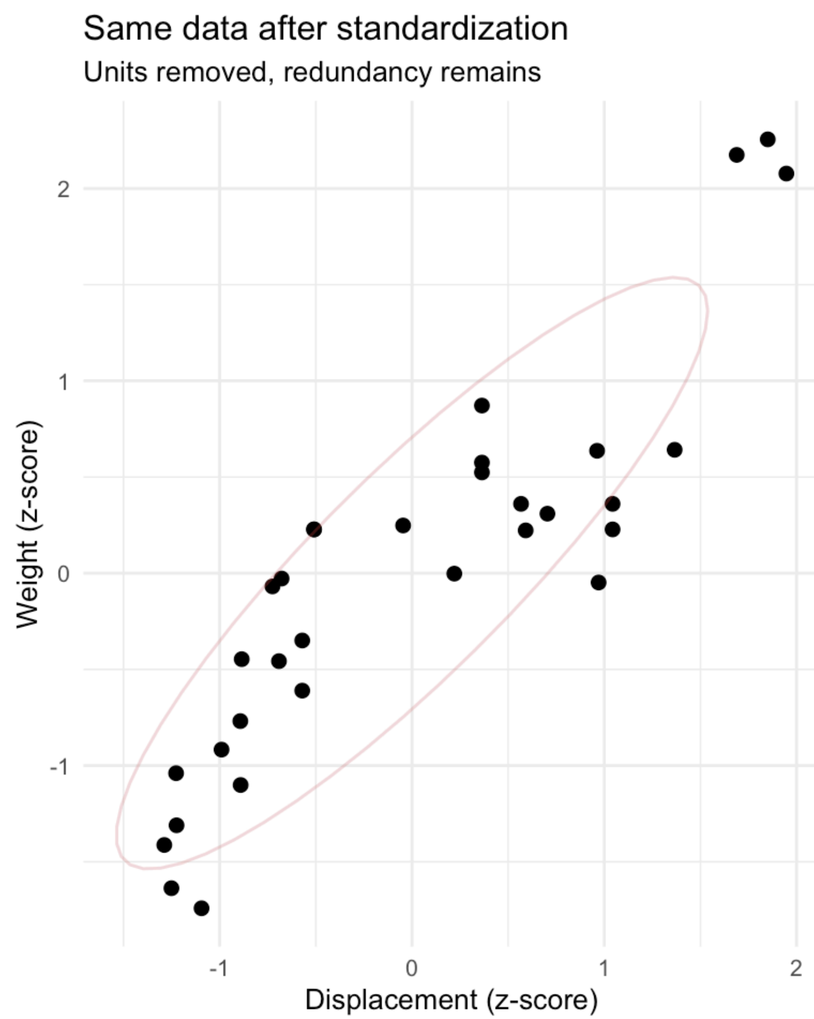
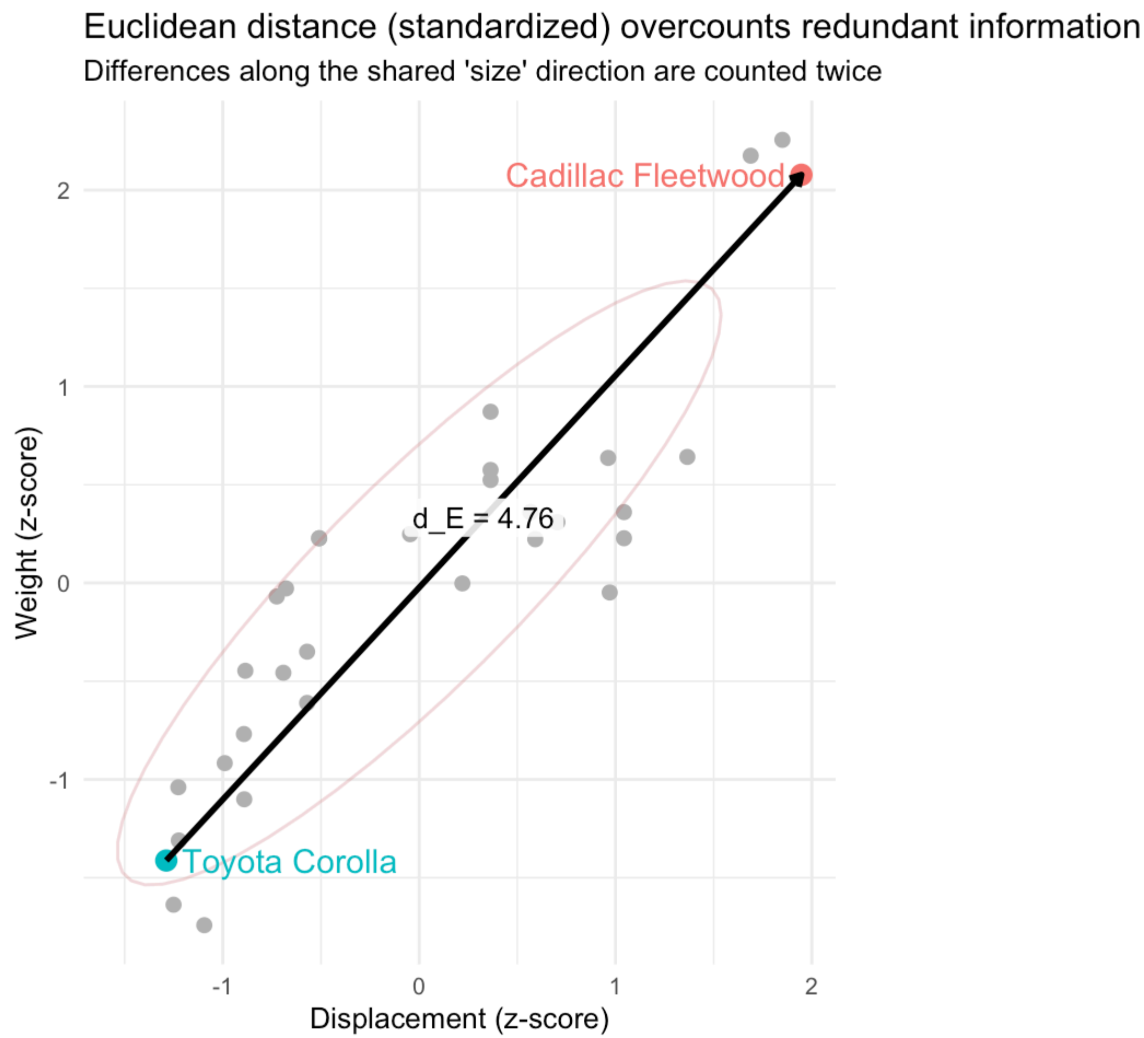


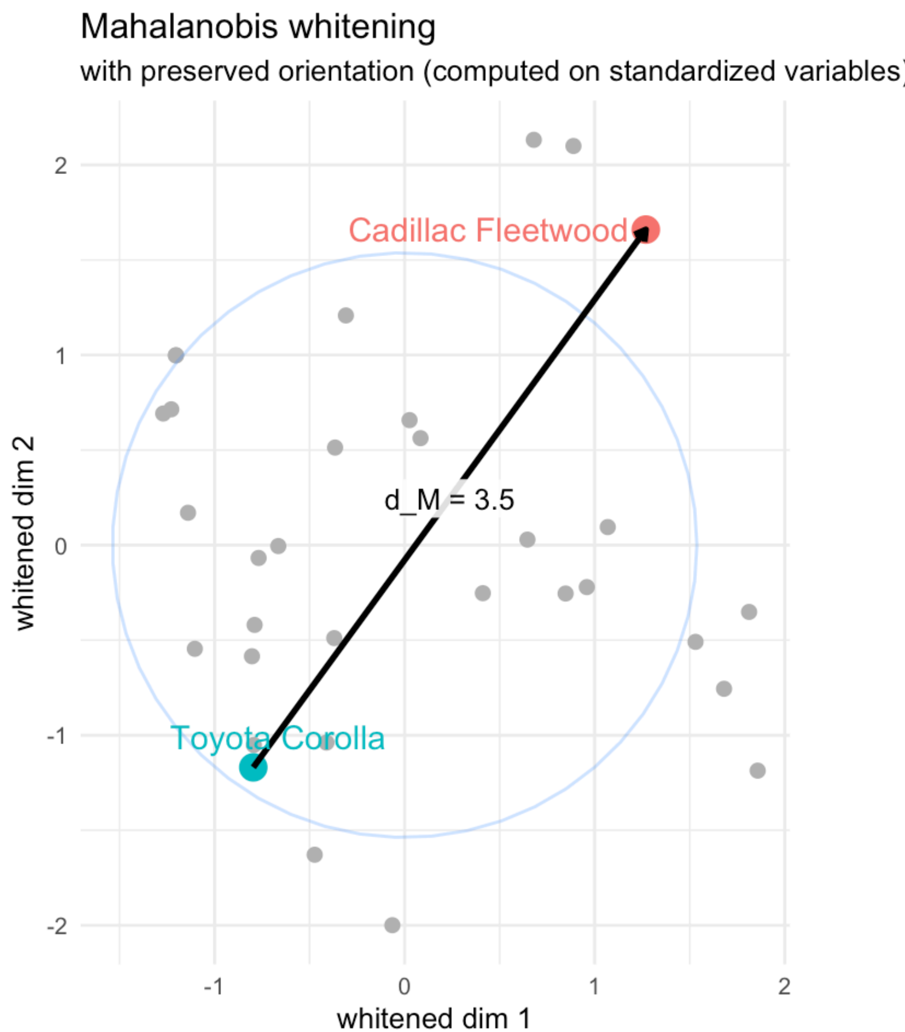
independence-based

The Euclidean distance ⟶ shared information is over-counted



association-based

The Mahalanobis distance $\longrightarrow$ shared information is not over-counted



this is an association-based distance for continuous data

association-based pairwise distance

- differences in line with the inter-variables association/correlation are down-weighted

Association-based for continuous: Mahalanobis distance

Let $\mathbf{X}_{con}$ be $n \times Q_d$ a data matrix of n observations described by Q_d continuous variables, and let $\mathbf{S}$ the sample covariance matrix, the Mahalanobis distance matrix is

$$\mathbf{D}_{mah} = \left[\text{diag}(\mathbf{G})\,\mathbf{1}_n^\mathsf{T} + \mathbf{1}_n\ \text{diag}(\mathbf{G})^\mathsf{T} - 2\mathbf{G}\right]^{\odot 1/2}$$

where

- $[\cdot]^{\odot 1/2}$ denotes the element-wise square root
- $\mathbf{G} = (\mathbf{C}\mathbf{X}_{con})\mathbf{S}^{-1}(\mathbf{C}\mathbf{X}_{con})^\mathsf{T}$ is the Mahalanobis Gram matrix
- $\mathbf{C} = \mathbf{I}_n - \frac{1}{n}\mathbf{1}_n\mathbf{1}_n^\mathsf{T}$ is the centering operator

association-based pairwise distance

- differences in line with the inter-variables association/correlation are down-weighted

Association-based for categorical: total variation distance (TVD)[1]

To distance matrix $\mathbf{D}_{tvd}$ is defined using the so-called delta framework[2] a general way to define categorical data distances.

Let $\mathbf{X}_{cat}$ be $n \times Q_c$ a data matrix of n observations described by Q_c categorical variables.

$$\mathbf{D} = \mathbf{Z}\Delta\mathbf{Z}^{\mathsf{T}} = \begin{bmatrix}\mathbf{Z}_1 & \dots & \mathbf{Z}_{Q_c}\end{bmatrix} \begin{bmatrix}\mathbf{\Delta}_1 & & \\ & \ddots & \\ & & \mathbf{\Delta}_{Q_c}\end{bmatrix} \begin{bmatrix}\mathbf{Z}_1^{\mathsf{T}} \\ \vdots \\ \mathbf{Z}_{Q_c}^{\mathsf{T}}\end{bmatrix}$$

- where $\mathbf{Z} = [\mathbf{Z}_1, \dots, \mathbf{Z}_{Q_c}]$ is the super-indicator matrix, with $Q^* = \sum_{j=1}^{Q_c} q_j$

- Δ_j is the category dissimilarity matrix for variable j, i.e., the jth diagonal block of the block-diagonal matrix Δ.
- setting Δ_j determines the categorical distance measure of choice (independent- or association-based)

association-based pairwise distance

- differences in line with the inter-variables association/correlation are down-weighted

Association-based for categorical: total variation distance (TVD)[1] (2)

Consider the empirical joint probability distributions stored in the off-diagonal blocks of $\mathbf{P}$:

$$\mathbf{P} = \frac{1}{n}\begin{bmatrix} \mathbf{Z}_1^\top\mathbf{Z}_1 & \mathbf{Z}_1^\top\mathbf{Z}_2 & \cdots & \mathbf{Z}_1^\top\mathbf{Z}_{Q_c} \\ \vdots & \ddots & \vdots & \vdots \\ \mathbf{Z}_{Q_c}^\top\mathbf{Z}_1 & \mathbf{Z}_{Q_c}^\top\mathbf{Z}_2 & \cdots & \mathbf{Z}_{Q_c}^\top\mathbf{Z}_{Q_c} \end{bmatrix}.$$

We refer to the conditional probability distributions for each variable j given each variable i ($i, j = 1, \ldots, Q_c, i \neq j$), stored in the block matrix

$$\mathbf{R} = \mathbf{P}_z^{-1}(\mathbf{P} - \mathbf{P}_z).$$

where $\mathbf{P}_z = \mathbf{P} \odot \mathbf{I}_{Q^*}$, and $\mathbf{I}_{Q^*}$ is the $Q^* \times Q^*$ identity matrix.

association-based pairwise distance

- differences in line with the inter-variables association/correlation are down-weighted

Association-based for categorical: total variation distance (TVD)[1] (3)

Let $\mathbf{r}_a^{ji}$ and $\mathbf{r}_b^{ji}$ be the rows of $\mathbf{R}_{ji}$, the (j,i)th off-diagonal block of $\mathbf{R}$ The category dissimilarity between a and b for variable j based on the total variation distance (TVD) is defined as

$$\delta_{tvd}^j(a,b) = \sum_{i\neq j}^{Q_c} w_{ji}\Phi^{ji}(\mathbf{r}_a^{ji}, \mathbf{r}_b^{ji}) = \sum_{i\neq j}^{Q_c} w_{ji}\left[\frac{1}{2}\sum_{\ell=1}^{q_i}|\mathbf{r}_{a\ell}^{ji} - \mathbf{r}_{b\ell}^{ji}|\right],$$

where $w_{ji} = 1/(Q_c - 1)$ for equal weighting (can be user-defined).

TVD-based dissimilarity matrix is, therefore,

$$\mathbf{D}_{tvd} = \mathbf{Z}\Delta^{(tvd)}\mathbf{Z}^{\mathsf{T}}.$$

association-based for mixed?

association-based for mixed

A straightforward AB-distance for mixed data is given by the convex combination of Mahalanobis and TVD distances:

$$\mathbf{D}_{mix} = \frac{Q_d}{Q}\mathbf{D}_{mah} + \left(1 - \frac{Q_d}{Q}\right)\mathbf{D}_{tvd}.$$

- this distance only accounts for correlations or associations among variables of the same type
- no continuous–categorical interactions are considered.

how to measure interactions?

how to measure interactions

define $\mathbf{\Delta}^{int}$, that accounts for the interactions and augment $\mathbf{\Delta}^{tvd}$

- the dissimilarity measure becomes

$$\mathbf{D}_{mix}^{(int)} = \mathbf{D}_{mah} + \mathbf{D}_{cat}^{(int)}.$$

where

$$\mathbf{D}_{cat}^{(int)} = \mathbf{Z}\tilde{\mathbf{\Delta}}\mathbf{Z}^{\top}$$

and

$$\tilde{\mathbf{\Delta}} = (1-\alpha)\mathbf{\Delta}^{tvd} + \alpha\mathbf{\Delta}^{int}$$

where $\alpha = \frac{1}{Q_c}$.

how to measure interactions

What is Δ^{int}?

- the general entry for the j^{th} diagonal block is $\delta^{j}_{int}(a,b)$ accounts for the interaction by measuring how the continuous variables help in discriminating between the observations choosing category a and those choosing category b for the j^{th} categorical variable

- consider the computation of $\delta^{ij}_{int}(ab)$ as a two-class (a/b) classification problem, with the continuous variables as predictors
  - use a distance-based classifier: nearest-neighbors

Δ_j^{int}

- consider $\mathbf{D}_{mah}$ and sort it to identify the neighbors for each observation.
- set a proportion of neighbors to consider, say $\hat{\pi}_{nn} = 0.1$
- for each pair of categories $(a, b), a, b = 1, \ldots, q_j, a \neq b$ of the j^{th} categorical variable:
- classify the observations using the prior corrected[1] decision rule

$$\text{if } i \text{ is such that } \quad \frac{\hat{\pi}_{nn}(a)}{\hat{\pi}(a)} \geq \frac{\hat{\pi}_{nn}(b)}{\hat{\pi}(b)} \quad \text{then assign } i \text{ to class } a \text{ else to class } b$$

- compute the balanced accuracy[2] (average of class-wise sensitivities)

$$\delta_{int}^{j}(a,b) = \frac{1}{2}\left(\frac{\texttt{true}\ a}{\texttt{true}\ a + \texttt{false}\ a} + \frac{\texttt{true}\ b}{\texttt{true}\ b + \texttt{false}\ b}\right)$$

well separated or not

Building Δ_j^{int}

for the general categorical variable j with q_j you compute the quantities for $\frac{q_j(q_j-1)}{2}$ pairs

$$\Delta_{int} = \begin{pmatrix} 0 & \cdot & \cdot & \cdot \\ \cdot & 0 & \cdot & \cdot \\ \cdot & \cdot & 0 & \cdot \\ \cdot & \cdot & \cdot & 0 \end{pmatrix}$$

Building Δ_j^{int}

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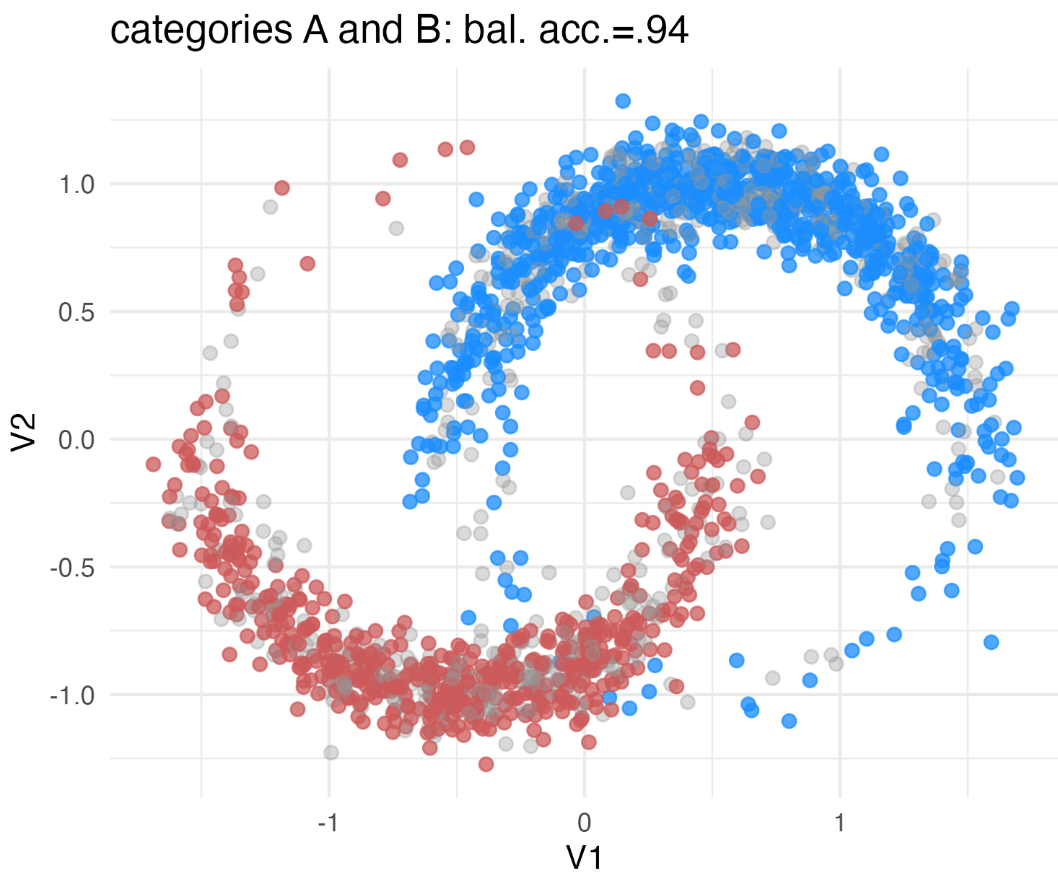

$$\Delta_{int} = \begin{pmatrix} 0 & 0.94 & \cdot & \cdot \\ 0.94 & 0 & \cdot & \cdot \\ \cdot & \cdot & 0 & \cdot \\ \cdot & \cdot & \cdot & 0 \end{pmatrix}$$

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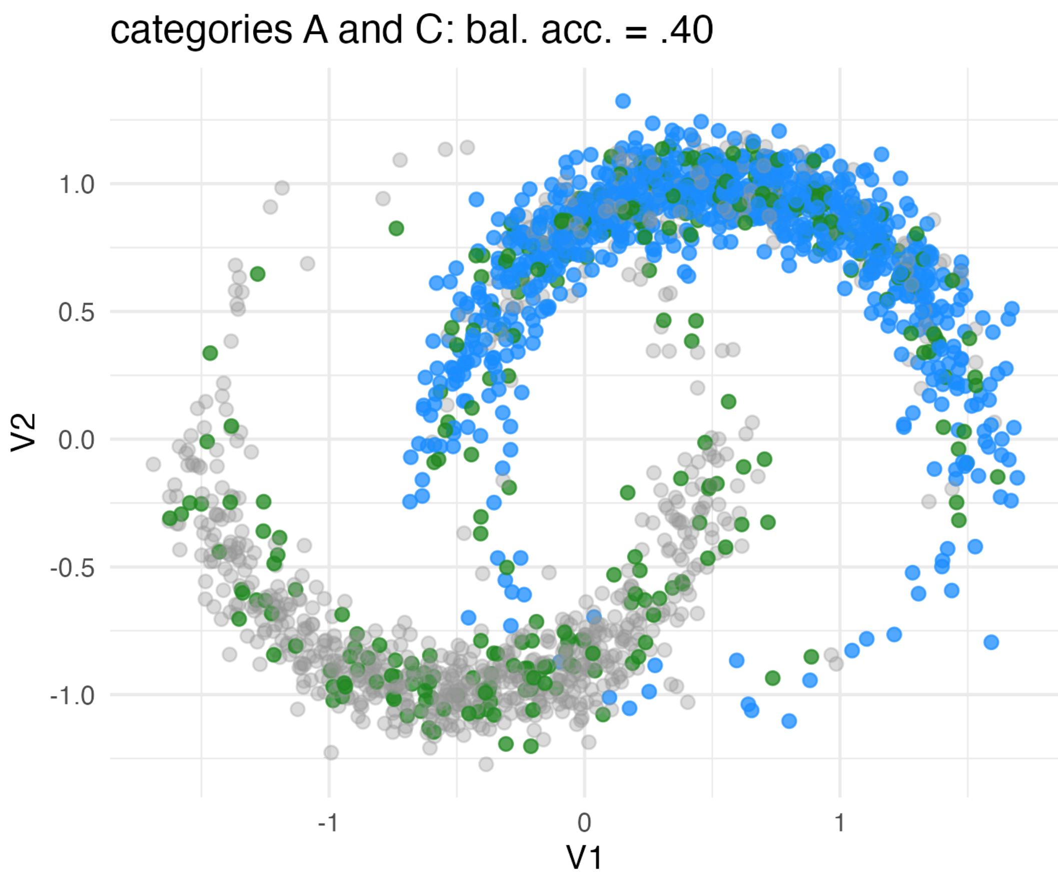

$$\Delta_{int} = \begin{pmatrix} 0 & 0.94 & \color{red}{0.4} & \cdot \\ 0.94 & 0 & \cdot & \cdot \\ \color{red}{0.4} & \cdot & 0 & \cdot \\ \cdot & \cdot & \cdot & 0 \end{pmatrix}$$

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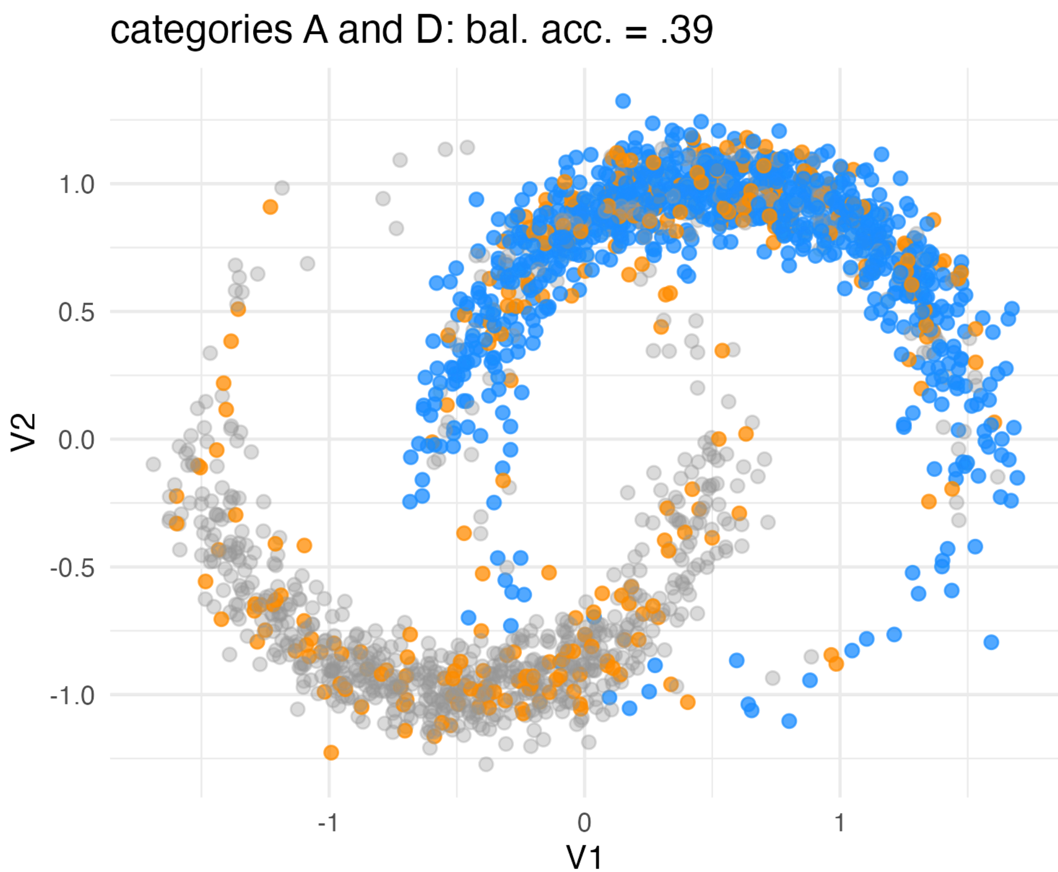

$$\Delta_{int} = \begin{pmatrix} 0 & 0.94 & 0.4 & 0.39 \\ 0.94 & 0 & \cdot & \cdot \\ 0.4 & \cdot & 0 & \cdot \\ 0.39 & \cdot & \cdot & 0 \end{pmatrix}$$

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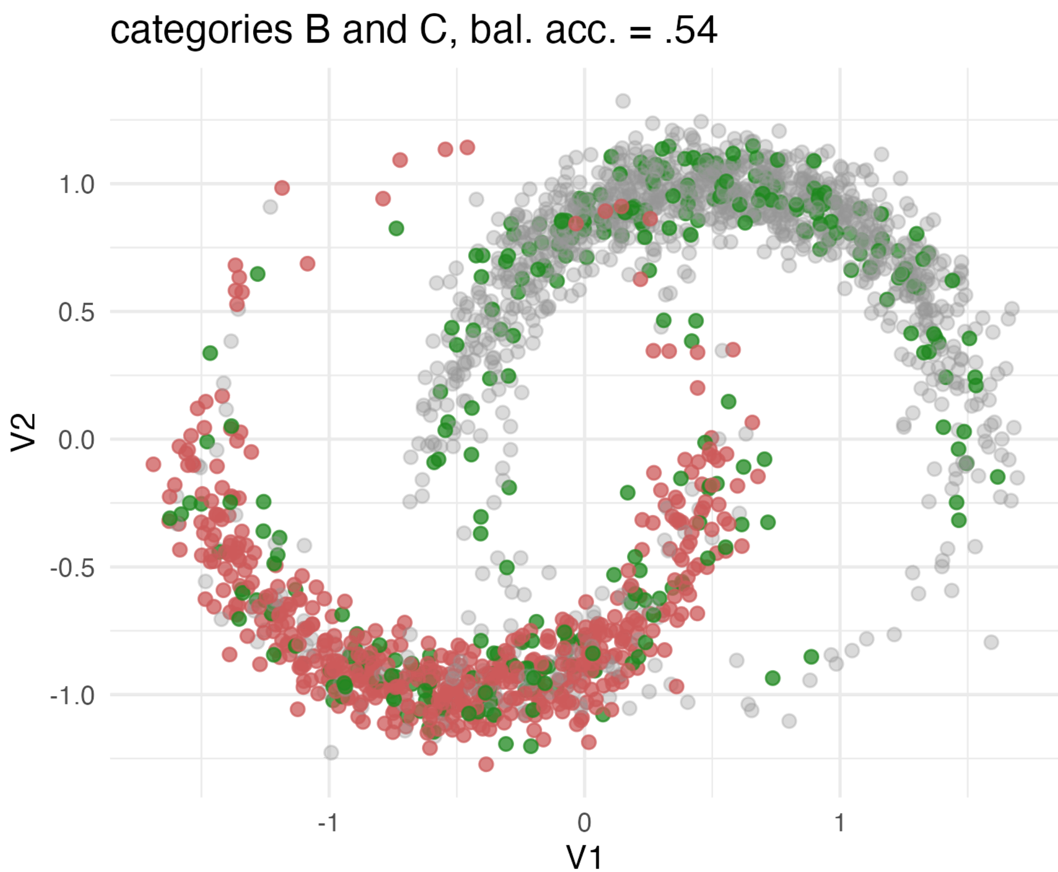

$$\Delta_{int} = \begin{pmatrix} 0 & 0.94 & 0.4 & 0.39 \\ 0.94 & 0 & 0.54 & \cdot \\ 0.4 & 0.54 & 0 & \cdot \\ 0.39 & \cdot & \cdot & 0 \end{pmatrix}$$

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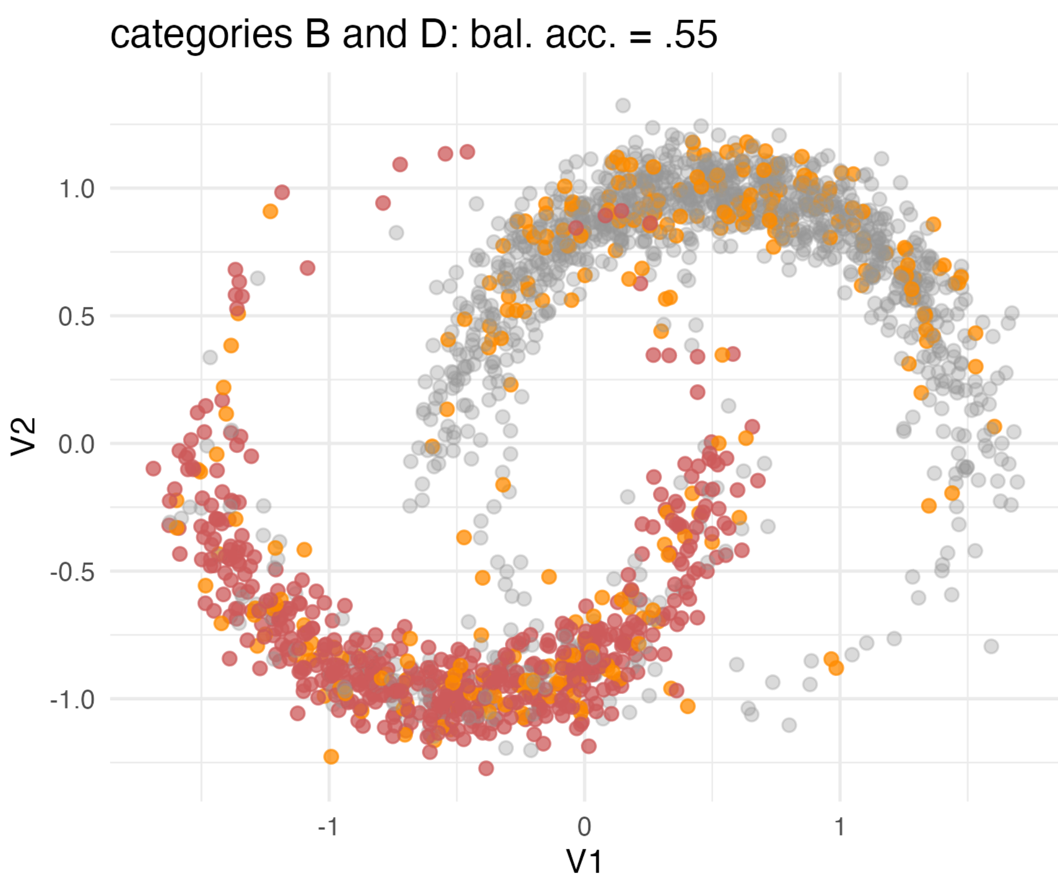

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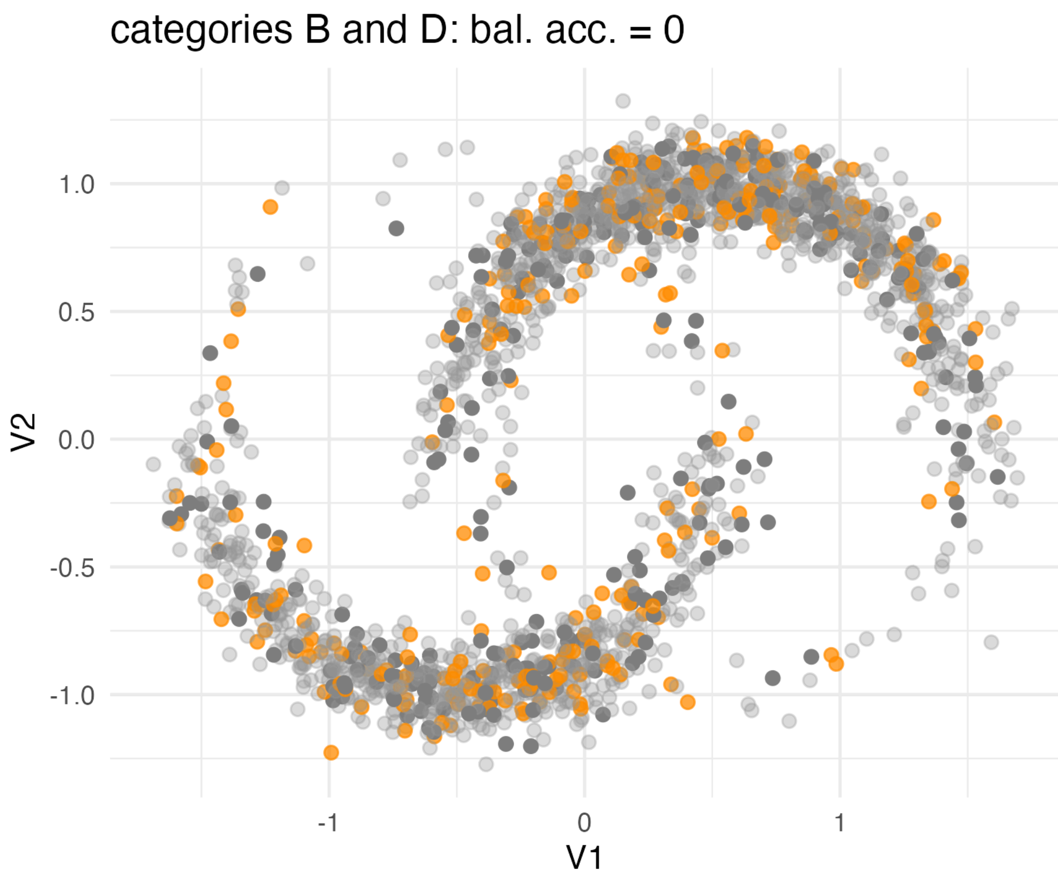

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Just one-way interaction?

Just one-way interaction?

Let $\mathbf{X} = [\mathbf{X}_{con}\mathbf{X}_{cat}]$ be a mixed data matrix with n observations described by Q_d continuous and Q_c categorical variables, respectively, and let $\mathbf{x}_i = [\mathbf{x}_{i_{con}}\mathbf{x}_{i_{cat}}]$ the i^{th} observation

We build upon the following results

result A

The distribution of $\mathbf{x}_i$ can be written as

$$f(\mathbf{x}_{i_{con}}, \mathbf{x}_{i_{cat}}) = f(\mathbf{x}_{i_{con}})f(\mathbf{x}_{i_{cat}} \mid \mathbf{x}_{i_{con}})$$

result B

According to Hennig *et al.* (2019)[1], starting from an arbitrary distance $d(x, c_k)$ from a prototype, it possible to construct a probabilistic clustering model[2] as $f(x; c_k, s_k) = g(c_k, s_k)exp(-s_k d(x, c_k))$, where s_k is a concentration parameter.

Then if $f(\cdot) \sim N(\mathbf{c}_k, \mathbf{S}_k)$, and $d(\cdot, \cdot)$ the Mahalanobis distance, it results that

$$f(\mathbf{x}_i; \mathbf{c}_k, \mathbf{S}_k) = g(\mathbf{c}_k, \mathbf{S}_k) \exp\left[-d(\mathbf{x}_i, \mathbf{c}_k,)\right]$$

where $g(\mathbf{c}_k, \mathbf{S}_k)$ is a normalization constant to make sure $f(\mathbf{x}_i; \mathbf{c}_k, \mathbf{S}_k)$ is a density function.

Just one-way interaction?

result C

the dissimilarity between $\mathbf{x}_{i_{con}}$ and a generic cluster k with center $\mathbf{c}_k$ and covariance matrix $\mathbf{S}_k$ is[1]

$$d(\mathbf{x}_{i_{con}}, \mathbf{c}_k) = \log(M_k f(\mathbf{x}_{i_{con}}; \mathbf{c}_k, \mathbf{S}_k)^{-1})$$

- $f(\cdot)$ a symmetric probability density function
- M_k is the maximum of the density function
- that is, if $\mathbf{x}_{i_{con}} = \mathbf{c}_k$ then $d(\mathbf{x}_{i_{con}}, \mathbf{c}_k) = 0$.

replace $\mathbf{c}_k$ with a generic observation i', the above becomes

$$d(\mathbf{x}_{i_{con}}, \mathbf{x}_{i'_{con}}) = \log(M f(\mathbf{x}_{i_{con}}; \mathbf{x}_{i'_{con}}, \mathbf{S})^{-1})$$

where M is the maximum of the density function.

Just one-way interaction…

Using the result C, it can be shown that

$$d(\mathbf{x}_{i_{con}}, \mathbf{x}_{i'_{con}}) = \frac{1}{2}(\mathbf{x}_{i_{con}} - \mathbf{x}_{i'_{con}})\mathbf{S}^{-1}(\mathbf{x}_{i_{con}} - \mathbf{x}_{i'_{con}})^{\mathsf{T}}$$

categorical analogue

consider the Q_{cat}-dimensional categorical vector $\mathbf{x}_{i_{cat}}$, it results, for its j^{th} element, that

$$p(x_{ij_{cat}} = a | x_{i'j_{cat}} = b) = \left[\delta^j(a,b)\right]^{-1}$$

where a and b are two general categories of the jth variable

For the whole vector it results

$$p(\mathbf{x}_{ij_{cat}}; \mathbf{x}_{i'j_{cat}}) = \prod_{j=1}^{Q_c} p(x_{ij_{cat}} = a_j; x_{i'j_{cat}} = b_j) = \prod_{j=1}^{Q_c} \left[\delta^j(a_j, b_j)\right]^{-1}$$

Just one-way interaction… (wrap-up)

using the previous results, it is possible to define the dissimilarity between two mixed-data observations

$\mathbf{x}_i$ and $\mathbf{x}_{i'}$

$$d(\mathbf{x}_i, \mathbf{x}_{i'}) = \frac{1}{2}(\mathbf{x}_{i_{con}} - \mathbf{x}_{i'_{con}})\mathbf{S}^{-1}(\mathbf{x}_{i_{con}} - \mathbf{x}_{i'_{con}})^{\mathsf{T}} - \log(p(\mathbf{x}_{i_{cat}}|\mathbf{x}_{i_{con}}; \mathbf{x}_{i'_{cat}}, \mathbf{x}_{i'_{con}}))$$

that takes into account correlations, associations and cross-type interactions and is a equivalent to the genral entry of the previously defined

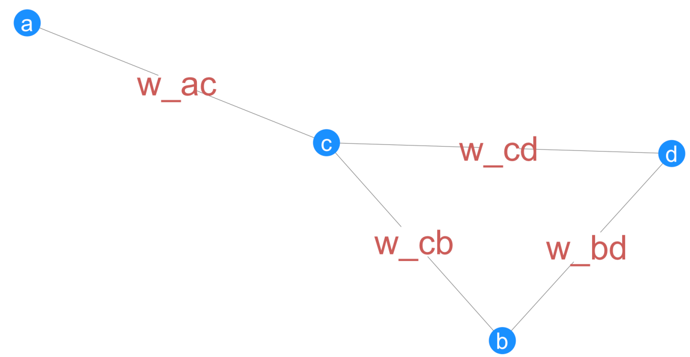
$$\mathbf{D}_{mix}^{(int)} = \mathbf{D}_{mah} + \mathbf{D}_{cat}^{(int)}.$$

spectral clustering in a nutshell

Spectral clustering: a graph partitioning problem

Graph representation

a graph representation of the data matrix $\mathbf{X}$: the aim is then to cut it into K groups (clusters)



the affinity matrix $\mathbf{A}$

the elements $\mathbf{w_{ij}}$ of $\mathbf{A}$ are high (low) if i and j are in the same (different) groups

.	a	b	c	d
a	0	0	w_ac	0
b	0	0	w_cb	w_bd
c	w_ca	w_cb	0	w_cd
d	0	w_db	w_dc	0

Spectral clustering: making the graph easy to cut

An approximated solution to the graph partitioning problem:

- spectral decomposition of the graph Laplacian matrix, that is a normalized version of the affinity matrix $\mathbf{A}$:

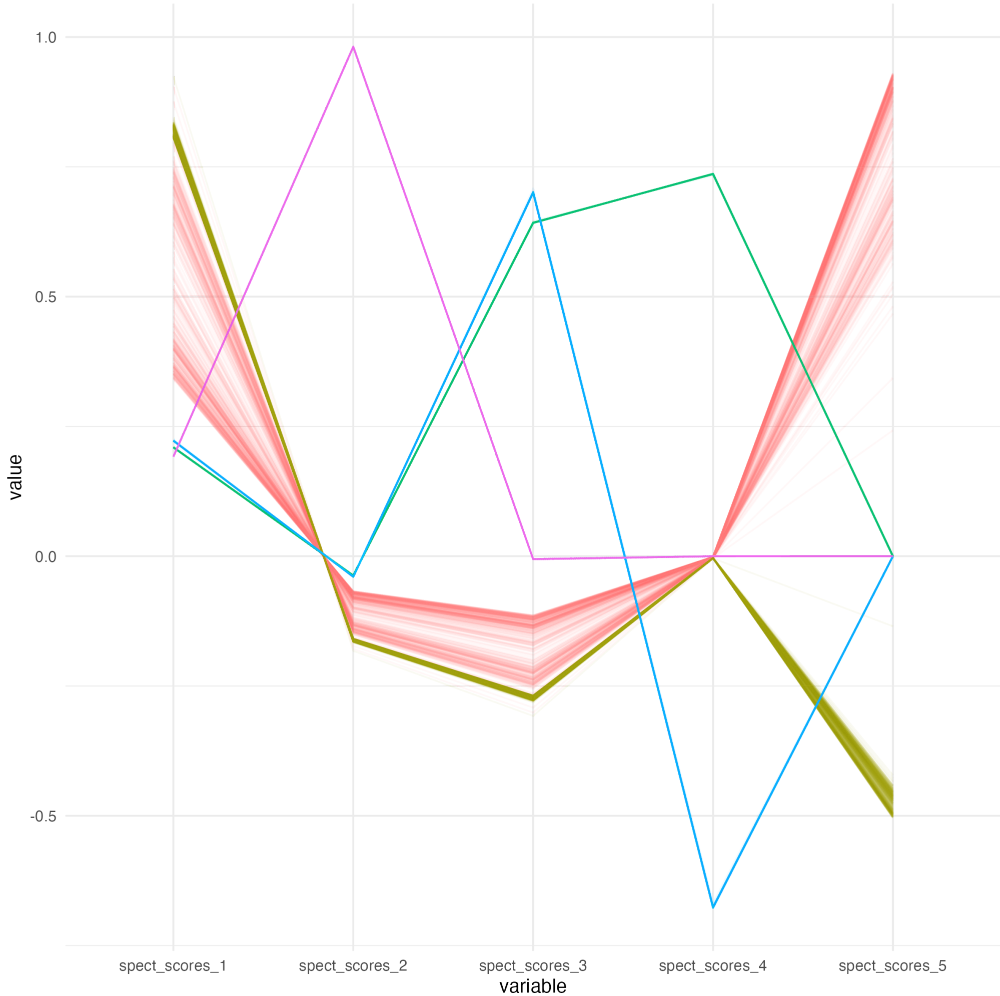
$$\mathbf{L} = \mathbf{D}_r^{-1/2} \underbrace{exp(-\mathbf{D}^2(2\sigma^2)^{-1})}_{\text{affinity matrix } \mathbf{A}} \mathbf{D}_r^{-1/2} = \mathbf{Q}\Lambda\mathbf{Q}^\mathsf{T}$$

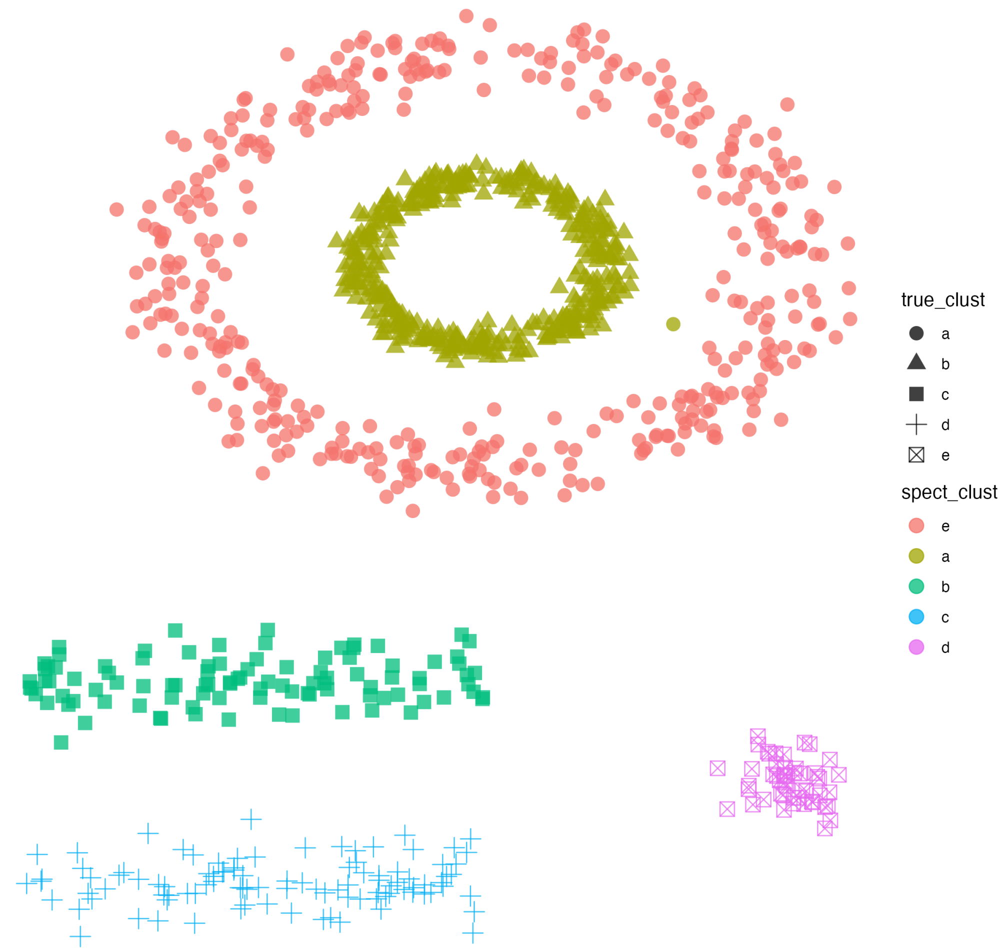
- $\mathbf{D}$ be the $n \times n$ matrix of pairwise distances
- the σ parameter dictates the number of neighbors each observation is linked to (rule of thumb: median distance to the 20th nearest neighbor)
- diagonal terms of $\mathbf{A}$ are set to zero: $a_{ii} = 0$, $i = 1, \dots, n$
- $\mathbf{D}_r = diag(\mathbf{r})$, $\mathbf{r} = \mathbf{A1}$ and $\mathbf{1}$ is an n-dimensional vector of 1's

- the spectral clustering of the n original objects is a K-means applied on the rows of the matrix $\tilde{\mathbf{Q}}$, containing the first K columns of $\mathbf{Q}$

Spectral clustering: solution and performance

SC works well, particularly in case of non-convex and overlapping clusters[1]





a toy experiment

toy experiment: data generation

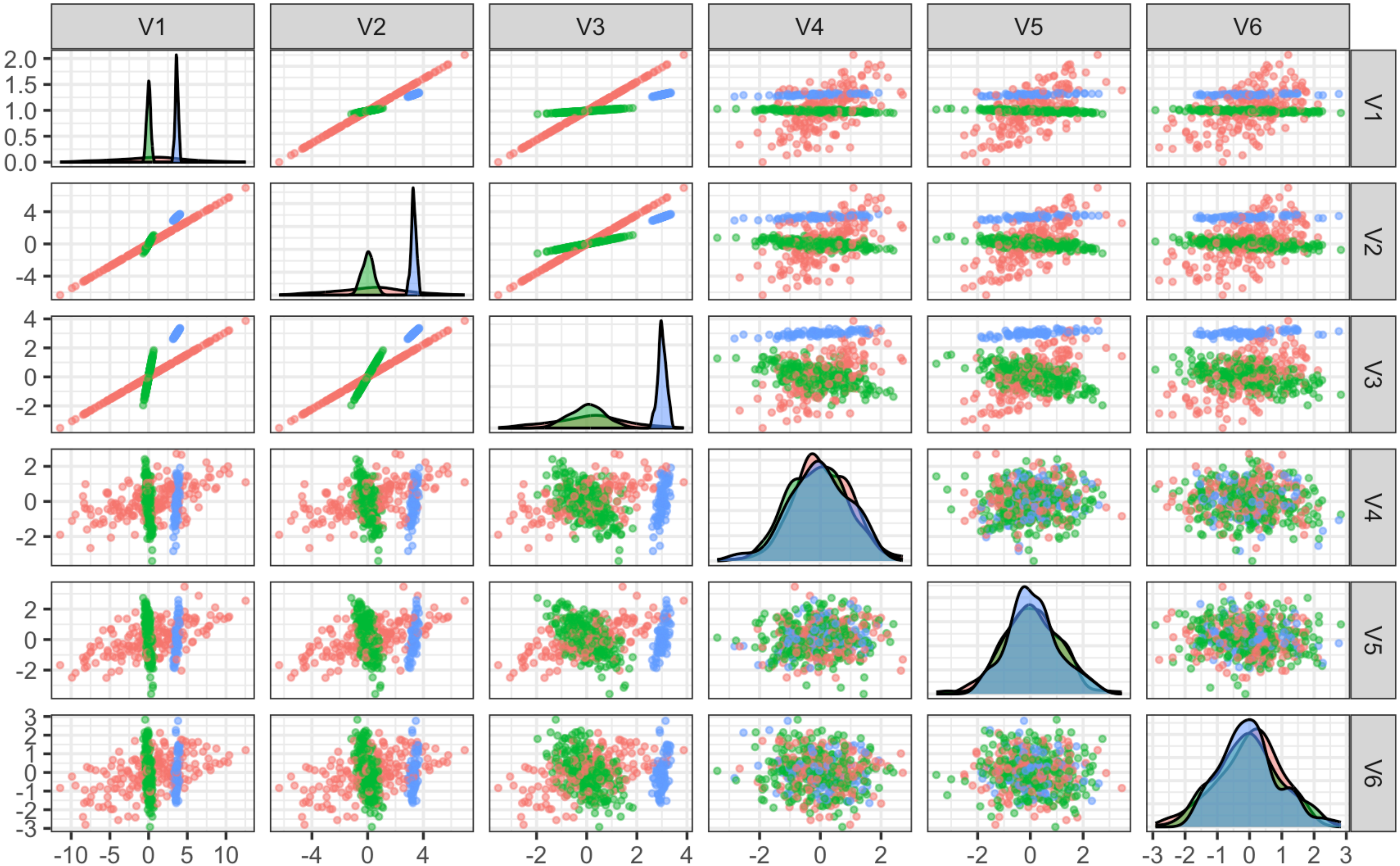
is $\delta^{j}_{int}(a,b)$ of help?

- three continuous signal, three continuous of Gaussian noise, three categorical variables (one noise)
- different dependence structures and location shifts in the signal continuous across the groups defined by the signal categorical variables.
- the continuous signal variables are generated conditionally on the signal categorical variables

$$X_j = \beta_{0,hq} + \sum_{k>j}^{6} \beta_{1,hq} X_k, \qquad j = 1, 2, 3$$

where $\beta_{1,hq}$ takes different values depending on the observed categories of the two signal categorical variables, h and q, respectively.

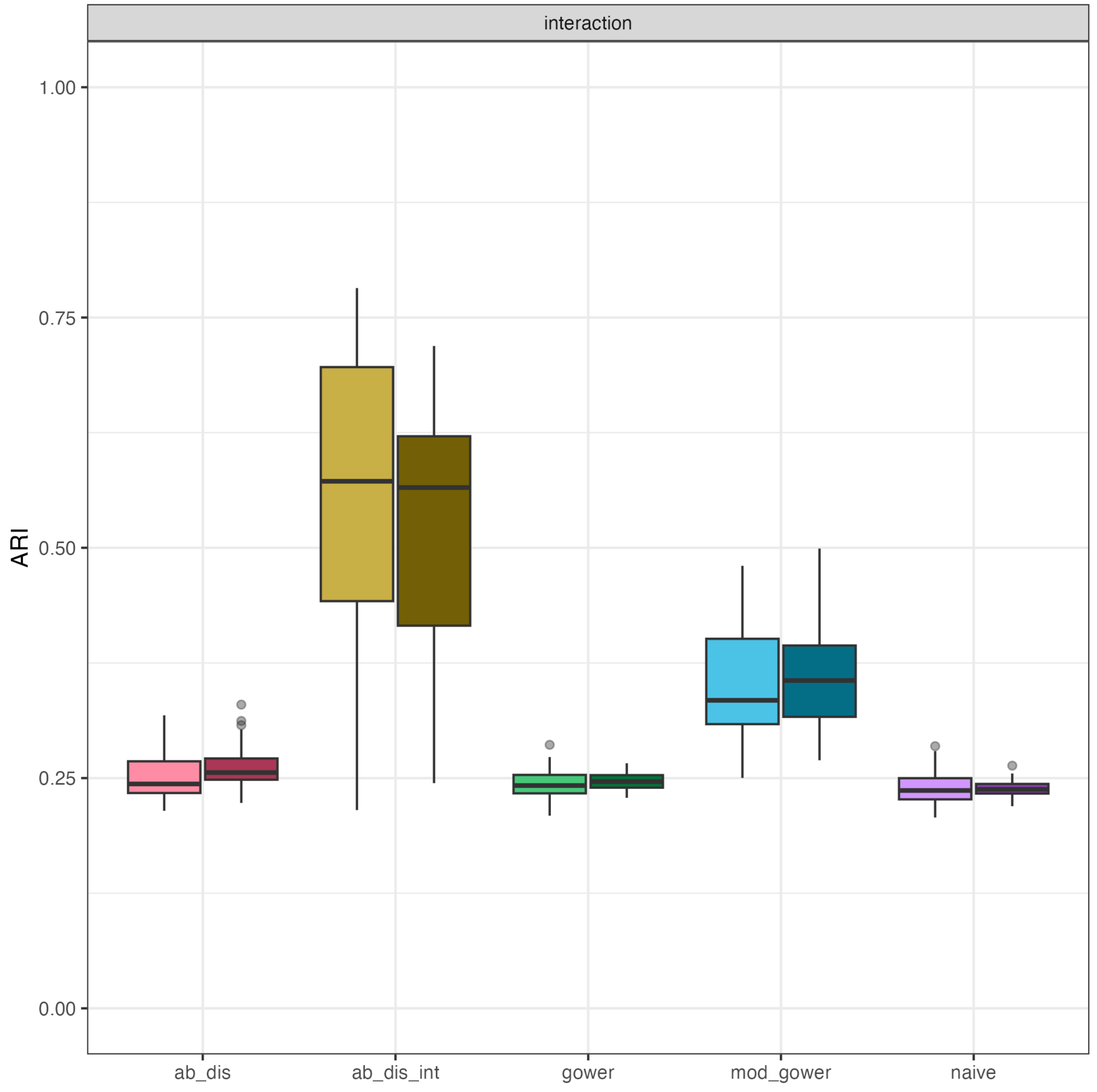
toy experiment



toy experiment: compared methods

- gower dissimilarity: a straightforward option
- naive [1]
- modified gower[2]
- association-based approach[3]: with and without interaction

toy experiment



Final considerations and future work

- association-based measures aim to go beyond match/mismatch of categories
- when the signal is limited to few variables, retrieving information from cont/cat interaction may be useful
- measuring interactions via non-parametric approach NN-based approach is suitable for non-convex/oddly shaped clusters
- computationally demanding (but it can be made bearable)
- π_{nn} tuning, regularization of δ_{int}'s to reduce variability

an R package to compute distances: manydist!

manydist on CRAN (stable(-ish) version)

manydist on GitHub version (for the latest updates)

general features

The `manydist` package is designed around a modular distance-based workflow.

Component	Function / Interface	Role
Core distance constructor	`mdist()`	Computes a pairwise dissimilarity matrix for mixed-type data: different indipendence-based and association based are specified, fully customizable
Recipe step	`step_mdist()`	Preprocessing step that computes an `mdist` dissimilarity matrix within a `recipe`, for seamless integration in learning pipelines.
k-nearest neighbors	`mdist_knn()`	Model specification for k-NN using a precomputed `mdist` dissimilarity matrix as input. Supports `tune`
leave-one-variable-out	`lovo_mdist()`	LOVO dissimilarity computations to assess by-variable contributions

forthcoming features

Component	Function / Interface	Role
Partitioning around medoids	`mdist_pam()`	Model specification for PAM clustering based on `mdist` dissimilarities.
spectral clustering	`mdist_spectral()`	Model specification for spectral clustering based on `mdist` dissimilarities.

and more to come…

main references

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https://alfonsoiodicede.github.io/Workshop_Bologna_26_pres_SC_mix.html