

Reliable Visual Analytics with Dimensionality Reduction: Quality Evaluation and Interpretation of Projections

Part 2:

Interpretation of Dimensionality Reduction Results

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3 – Linnaeus University

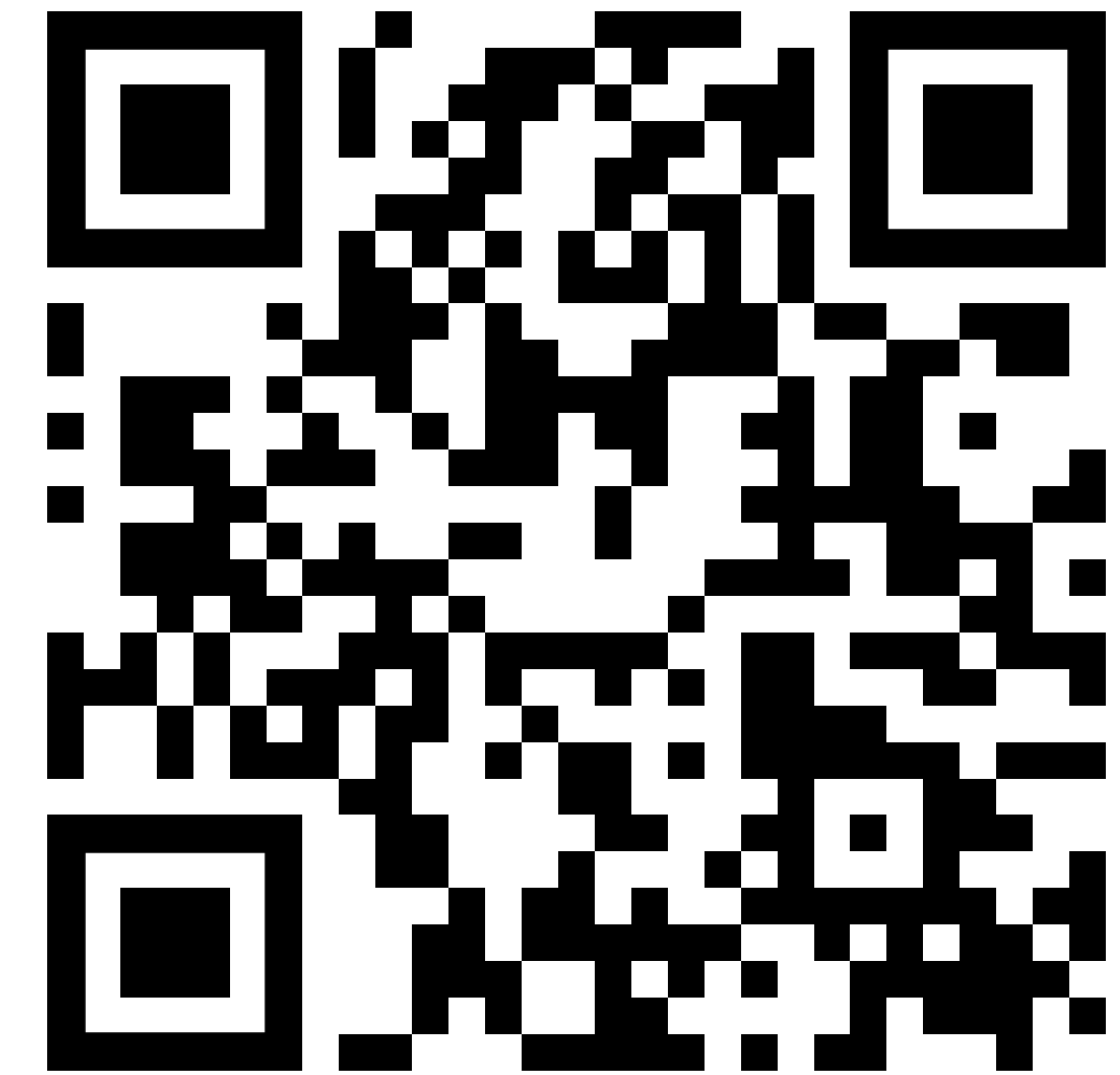
EuroVis 2025 Tutorial

EUROVIS 2025
LUXEMBOURG

What you will learn today

- Fundamentals: Interpretation of dimensionality reduction (DR) results
 - Linear DR
 - **Axis level**
 - Nonlinear DR
 - **Observed-pattern level**
 - Univariate focus
 - Composite variable focus
 - Classifier-based
 - Local pattern correlation
 - **Model-mechanism level**
 - Gradient-based
 - Parametric nonlinear DR
- Practices: Interpretations with existing libraries

Tutorial Materials



<https://hyeonword.com/dr-tutorial/>

Interpretation of dimensionality reduction (DR) results

Wine dataset (13D)

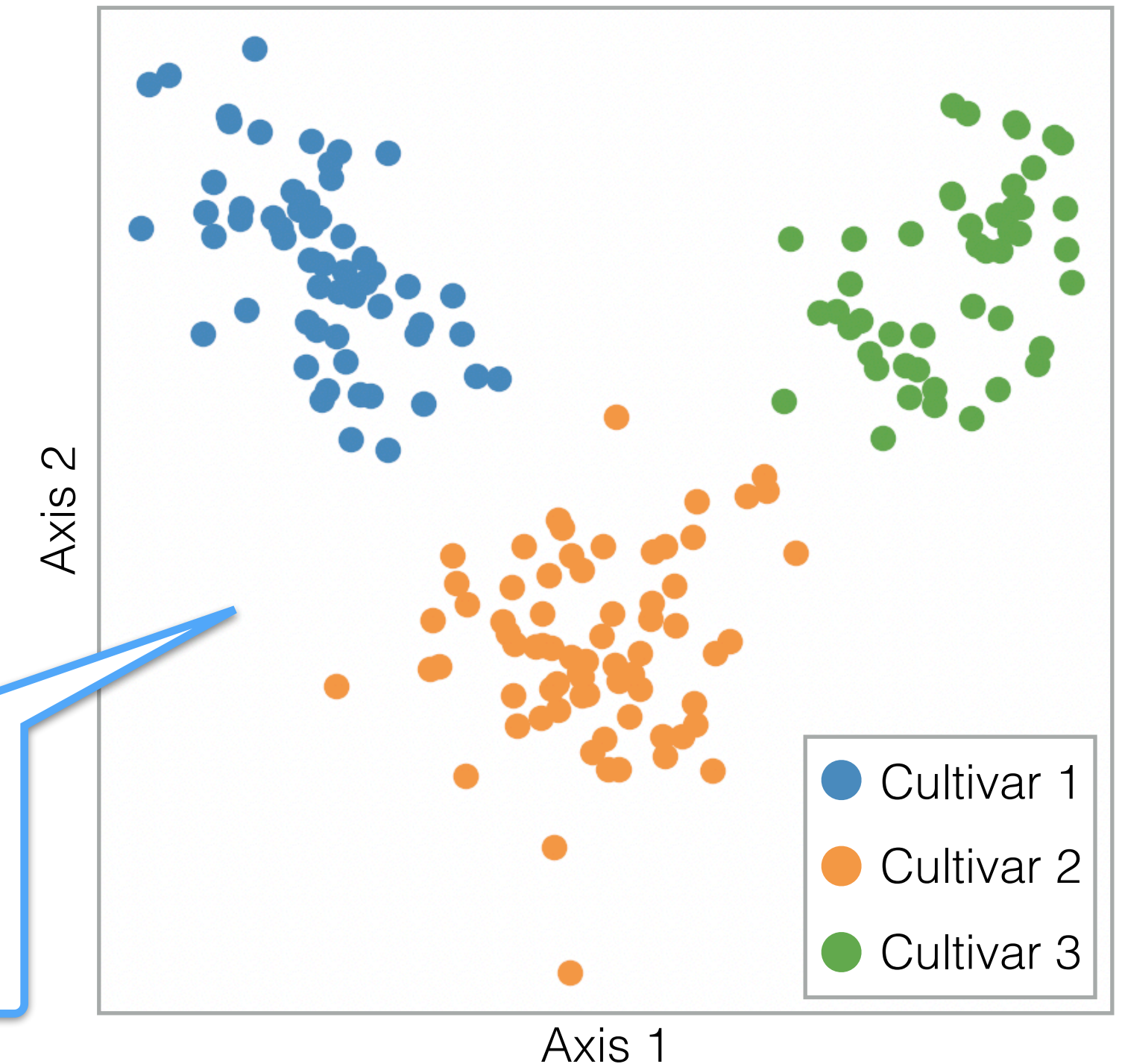
	alcohol	malic_acid	ash	alcalinity_ash	magnesium	total_phenols	flavanoid
0	1.52	-0.56	0.23	-1.17	1.91	0.81	1.01
1	0.25	-0.50	-0.83	-2.49	0.02	0.57	0.49
2	0.20	0.02	1.11	-0.27	0.09	0.81	1.22
3	1.69	-0.35	0.49	-0.81	0.93	2.49	1.47
4	0.30	0.23	1.84	0.45	1.28	0.81	0.66
...

*displayed values are
after the standardization



Linear discriminant analysis
LDA

How are they separated?
What are their differences?



- Interpreting a **lower-dimensional space** **Linear DR**
- Interpreting based on **observed patterns** (e.g., clusters) **Nonlinear DR**
- Interpreting from a DR **model/mechanism** level **Nonlinear DR**

No single best way for the interpretation so far (especially, for nonlinear DR)

Interpretation of dimensionality reduction (DR) results

Wine dataset (13D)

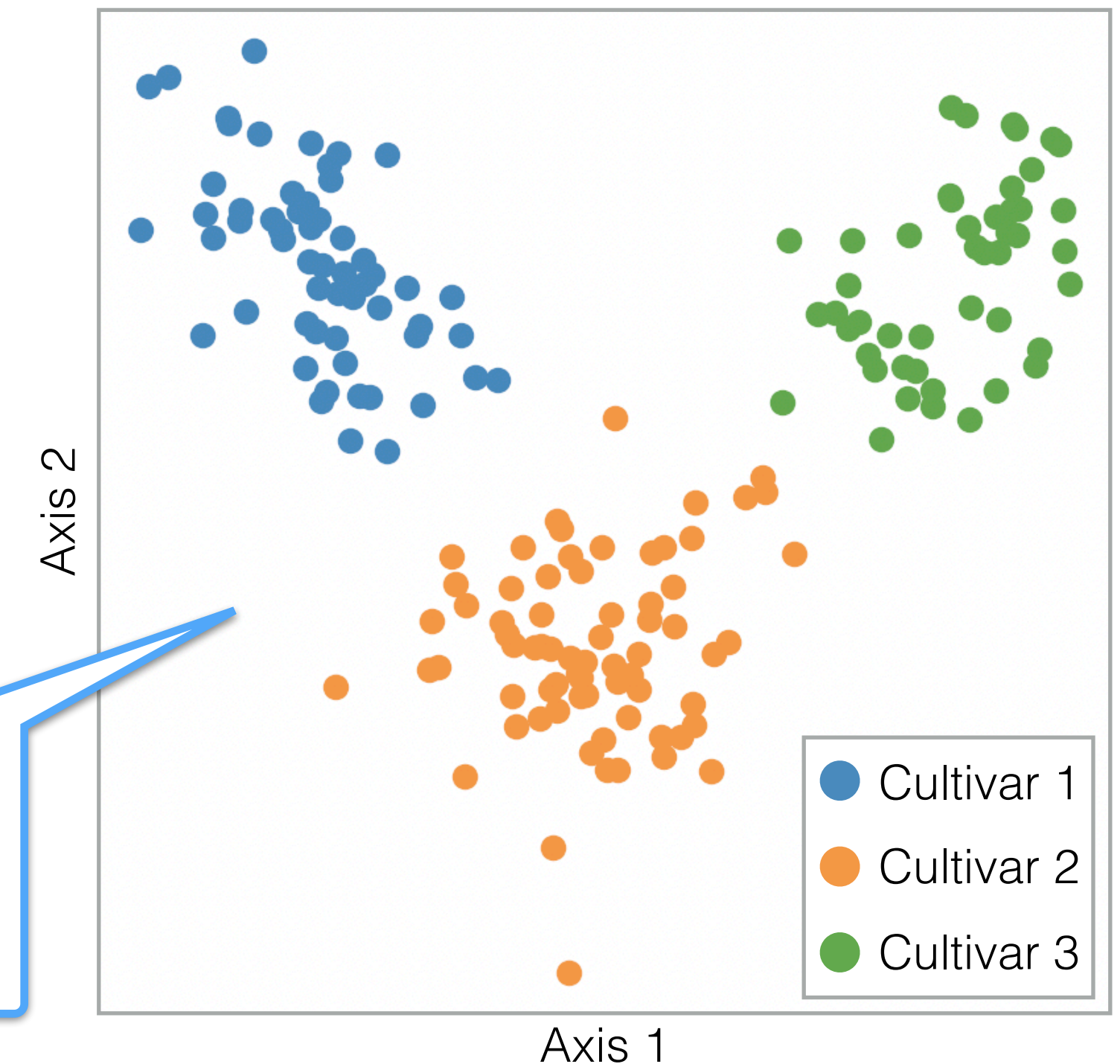
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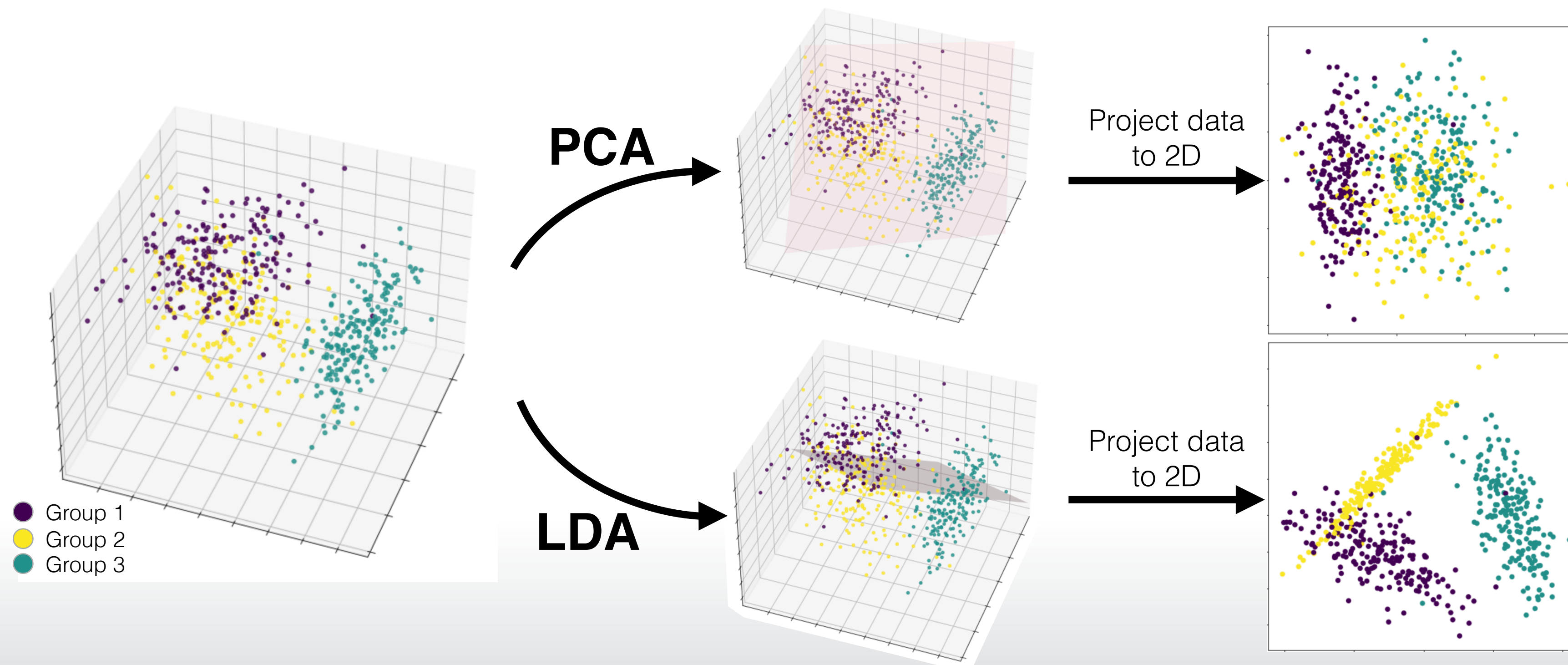
Linear DR

- Finds a linear projection from the original dimensions to low-dimensional axes

$\mathbf{X} \cdot \mathbf{P} = \mathbf{Y}$ $\mathbf{X} \in \mathbb{R}^{n \times d}$: original data, $\mathbf{P} \in \mathbb{R}^{d \times d'}$: projection matrix, $\mathbf{Y} \in \mathbb{R}^{n \times d'}$: projected data,
(n : # of instances, d : # of original dimensions, d' : # of dimensions after projection)

- Representative methods

- Principal component analysis (PCA) [Pearson, 1901]: Preserves data **variance** as much as possible
- Linear discriminant analysis (LDA) [Fisher, 1936]: Maximizes the **separation** of predefined groups



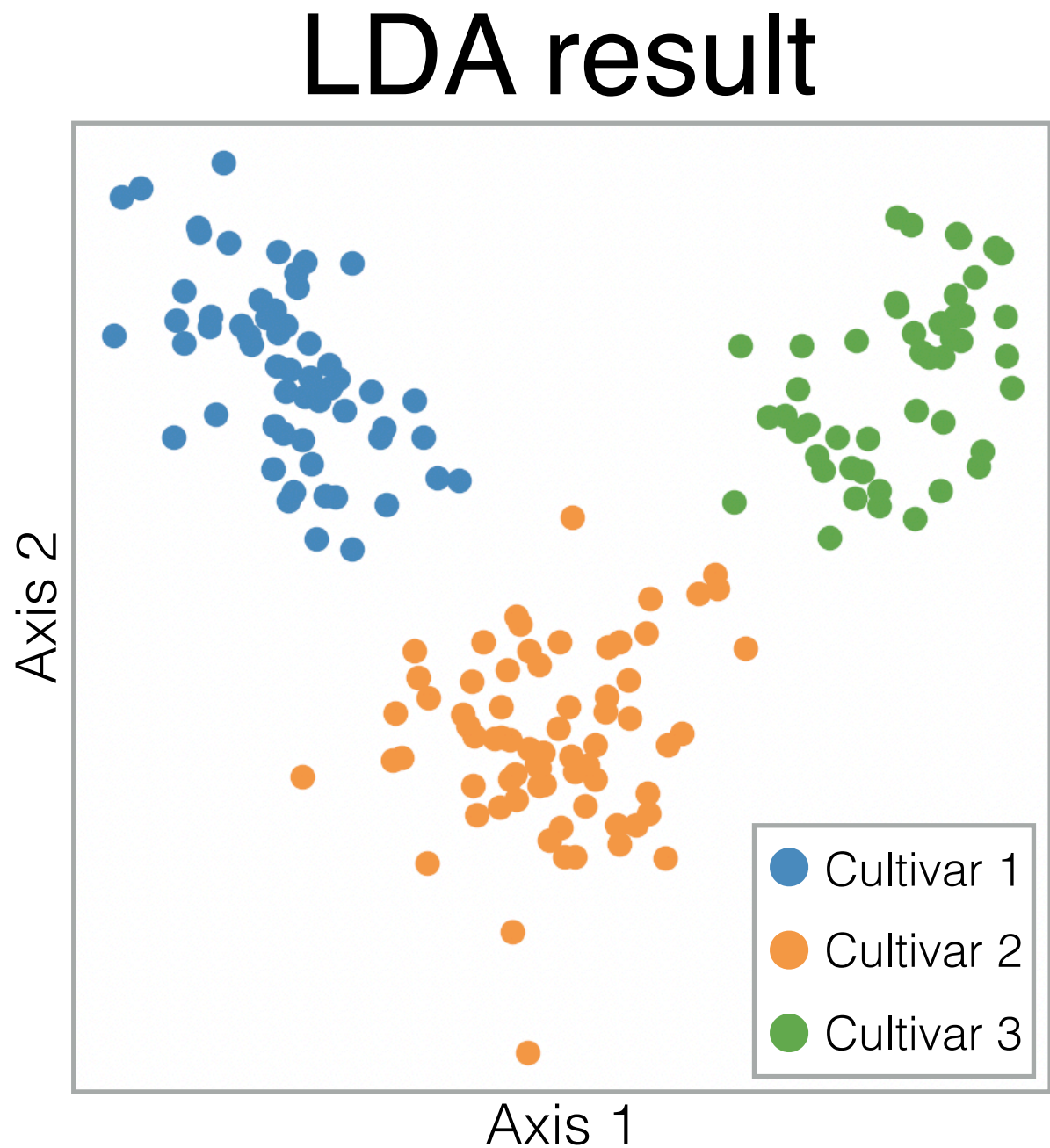
Interpreting the axes

Wine dataset (13D)

	alchol	malic_acid	ash	alcalinity_ash	magnesium	total_phenols	flavanoids	no
0	1.52	-0.56	0.23	-1.17	1.91	0.81	1.03	
1	0.25	-0.50	-0.83	-2.49	0.02	0.57	0.73	
2	0.20	0.02	1.11	-0.27	0.09	0.81	1.22	
3	1.69	-0.35	0.49	-0.81	0.93	2.49	1.47	
4	0.30	0.23	1.84	0.45	1.28	0.81	0.66	
...	

	axis 1	axis 2
alchol	-0.20	0.79
malic_acid	0.11	0.38
ash	-0.06	0.72
alcalinity_ash	0.31	-0.54
magnesium	-0.02	-0.01
total_phenols	0.23	-0.02
flavanoids	-1.00	-0.55
nonflav_phenols	-0.11	-0.23
proanthocyanins	0.05	-0.20
color_intensity	0.50	0.65
hue	-0.11	-0.39
od280/od315	-0.50	0.04
proline	-0.51	1.00

=



Linear dimensionality reduction

X

•

P

=

Y

The projection matrix contains the information of the axes

For example, Axis 1 is generated by
-0.20 alcohol + 0.11 malic_acid - 0.06 ash ...

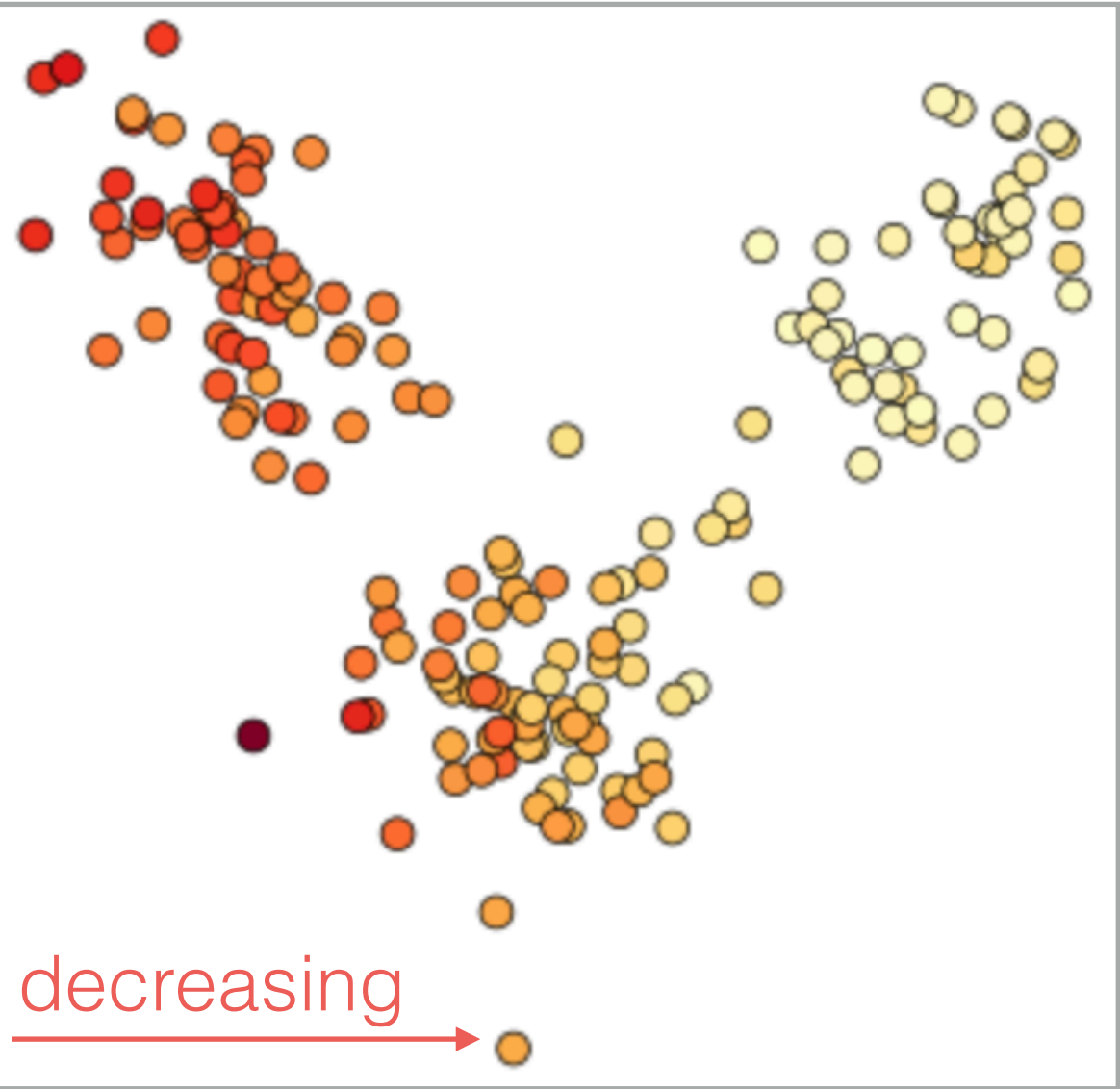
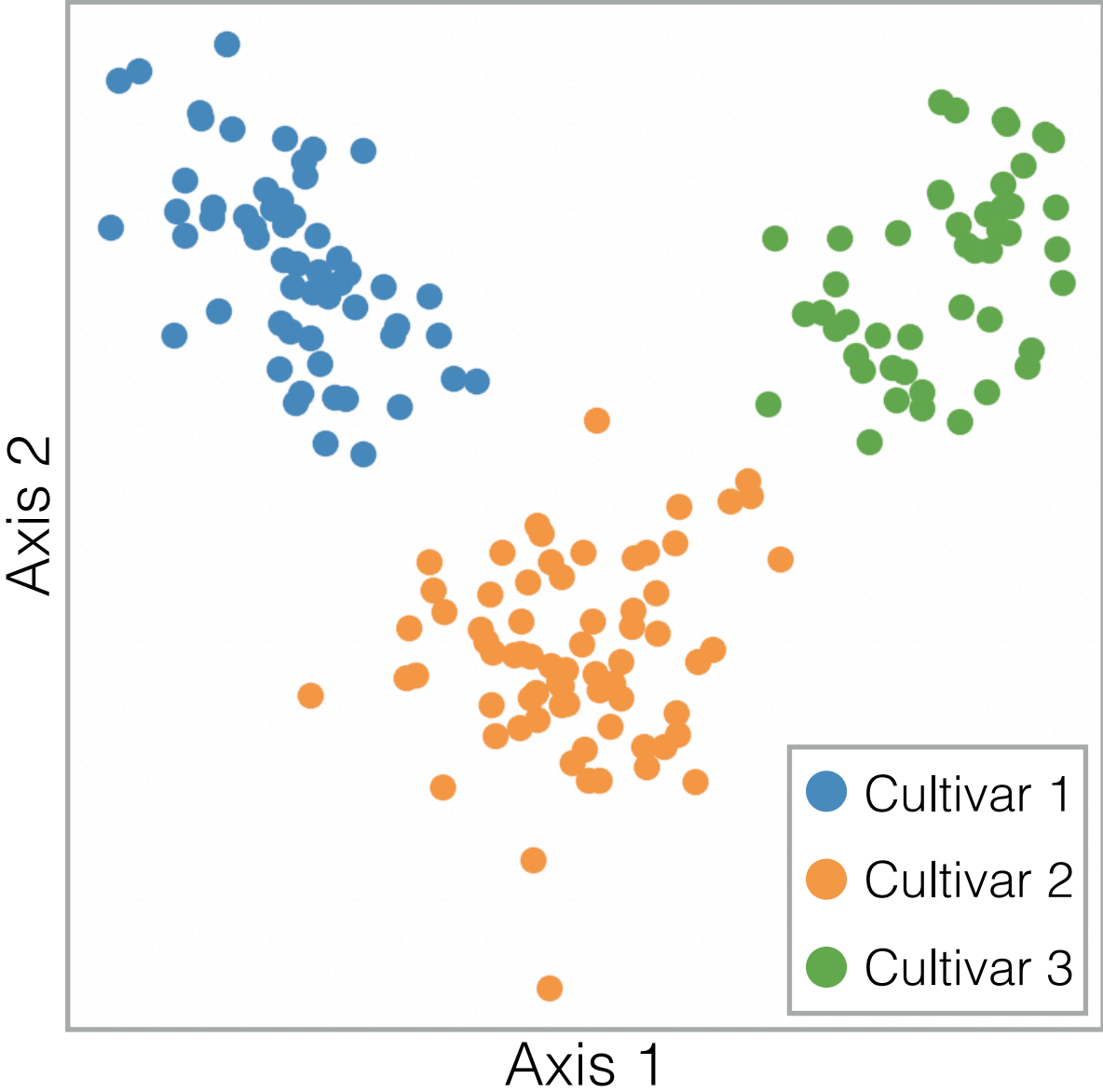
Interpreting the axes

Axes 1 and 2 should be highly influenced by **flavanoids** and **proline**, respectively

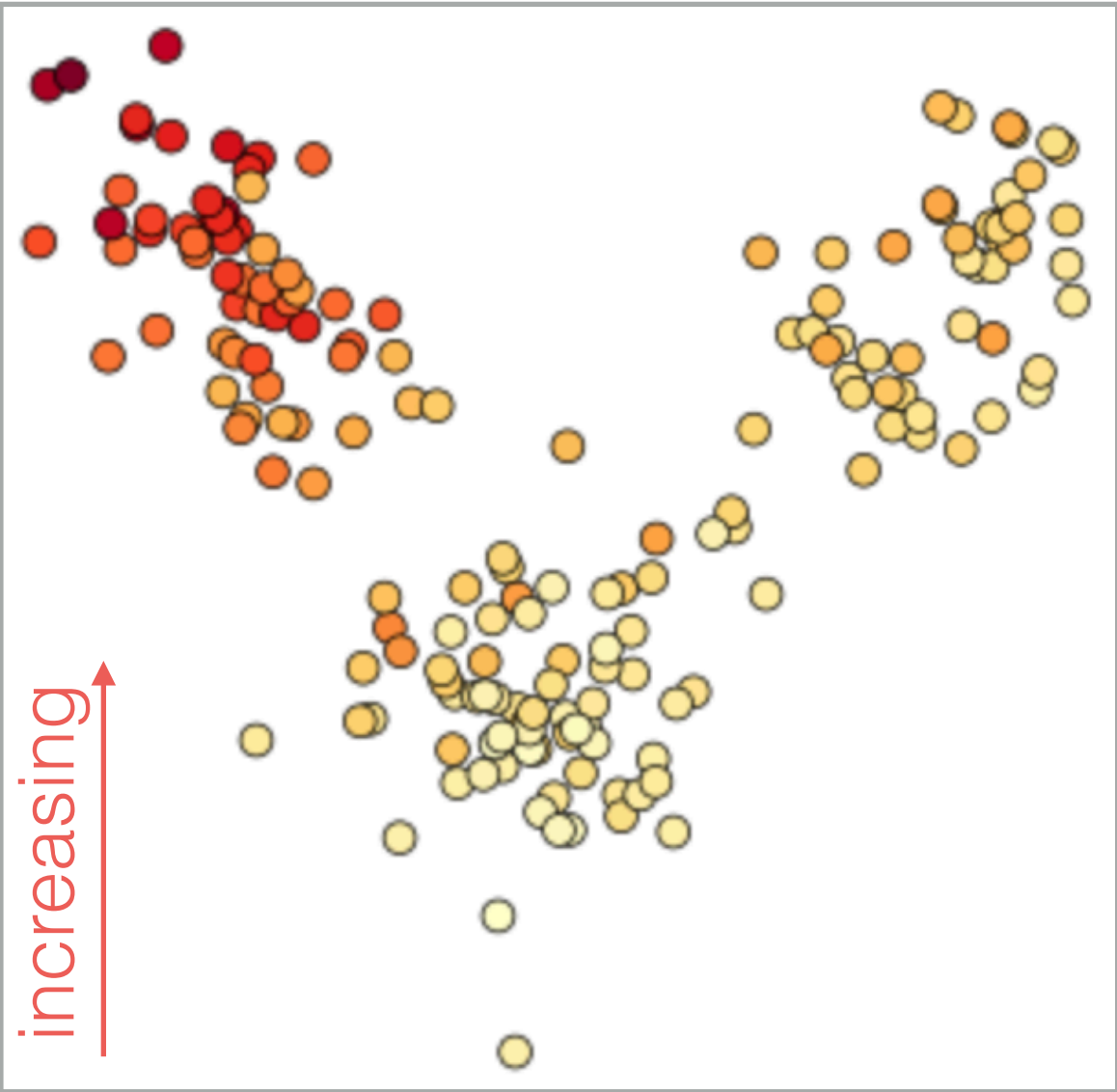
Visualize

	axis 1	axis 2
alchol	-0.20	0.79
malic_acid	0.11	0.38
ash	-0.06	0.72
alcalinity_ash	0.31	-0.54
magnesium	-0.02	-0.01
total_phenols	0.23	-0.02
flavanoids	-1.00	-0.55
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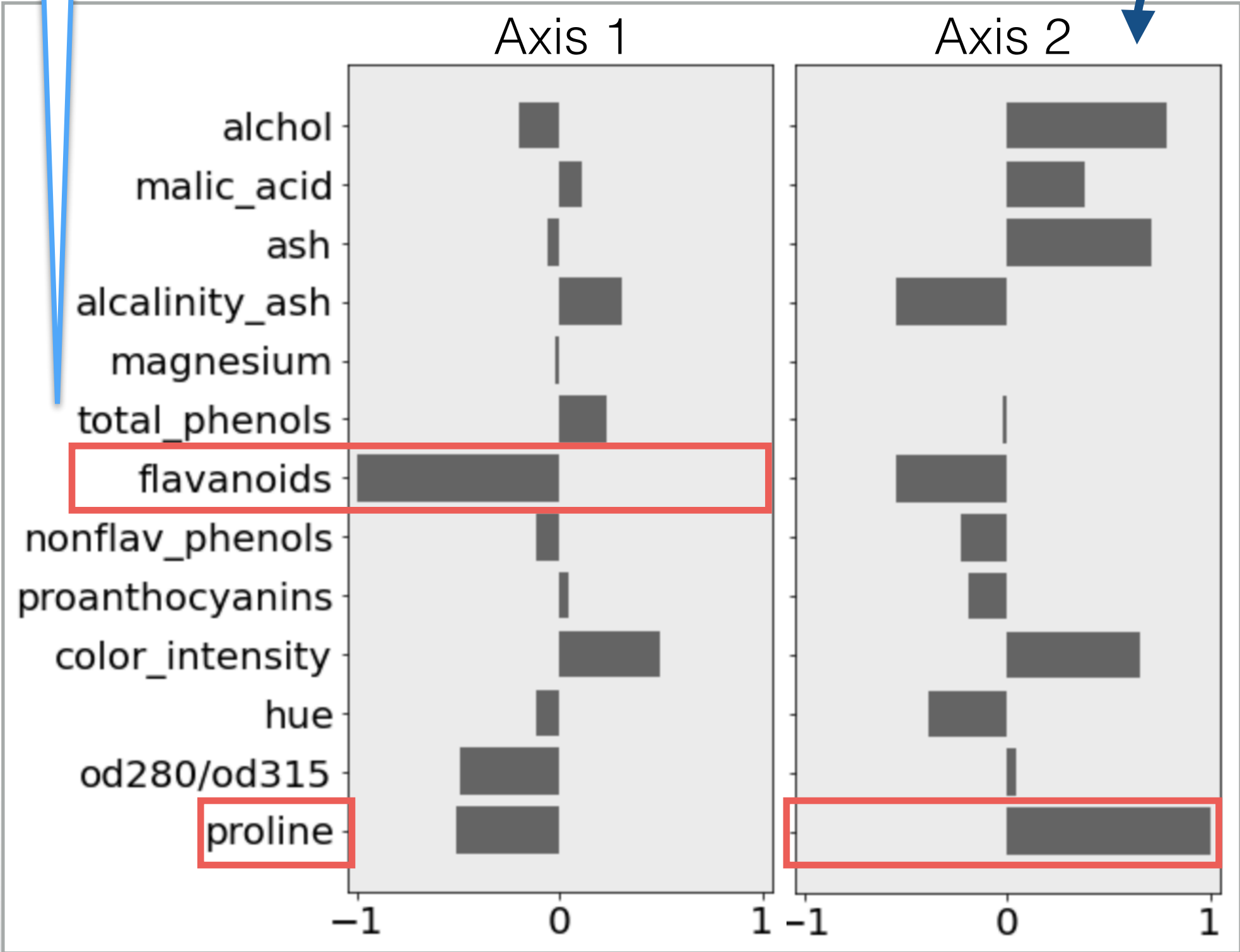
LDA result



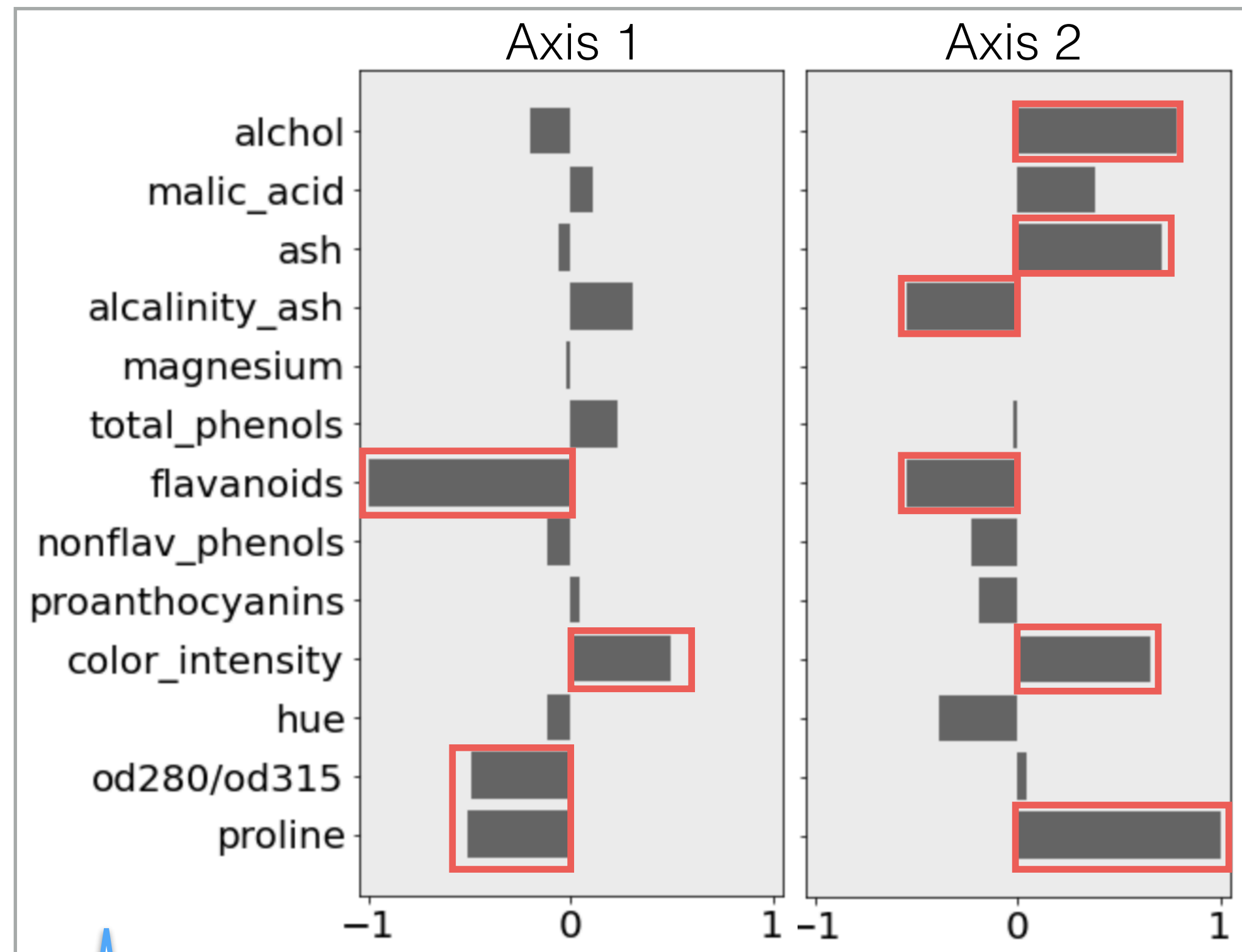
Colored by flavanoids



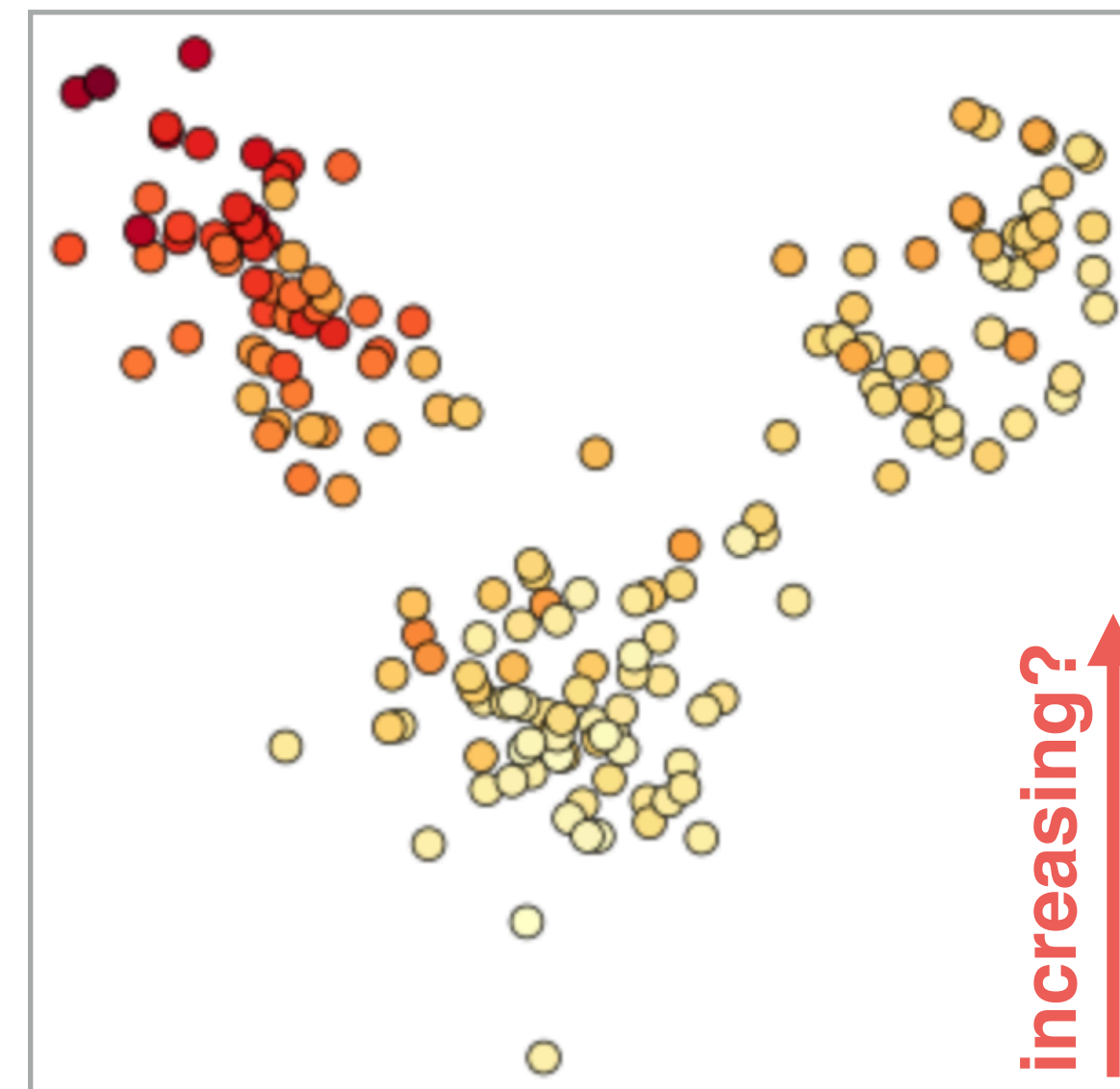
Colored by proline



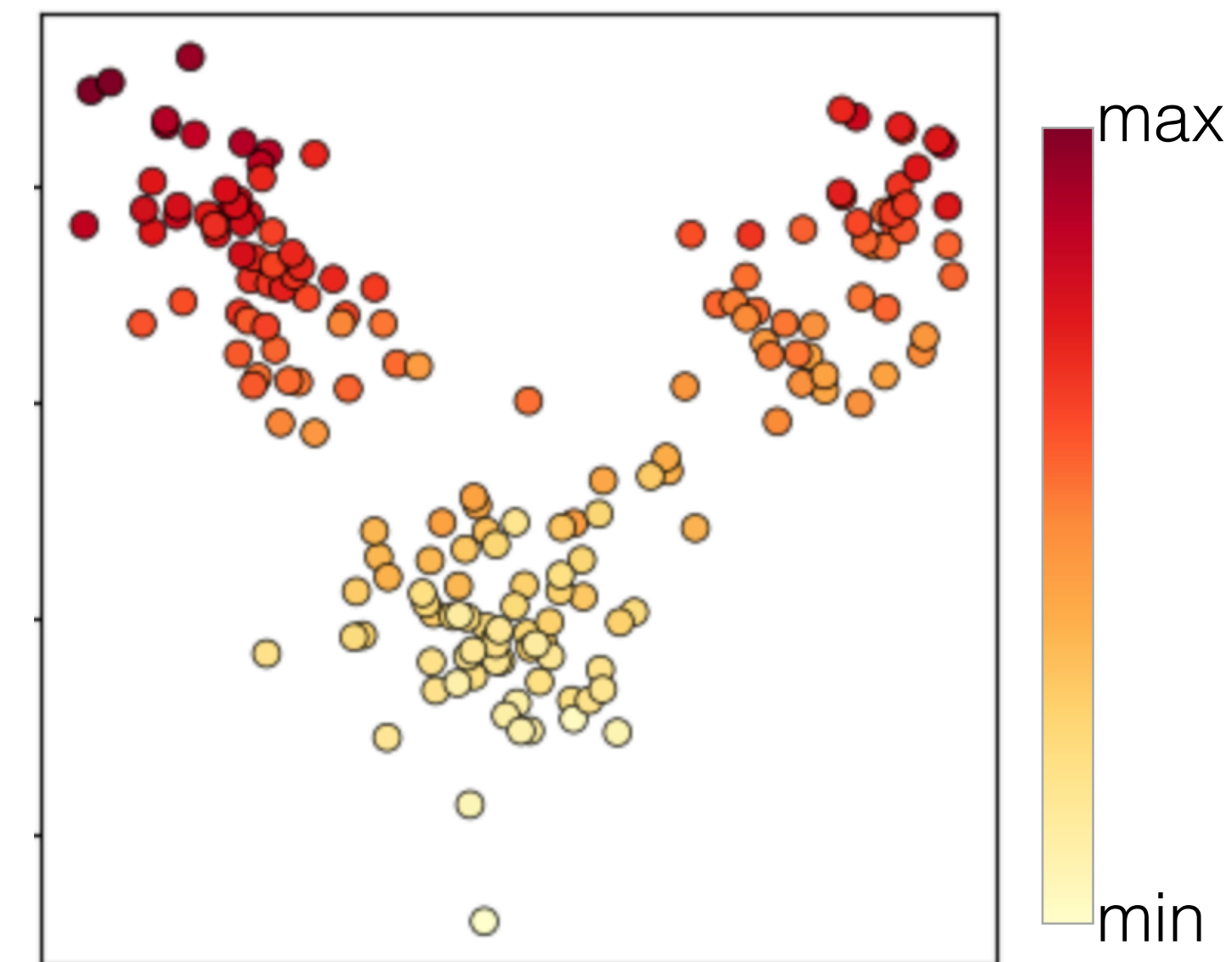
Interpreting the axes



To better understand the axes, we should consider relationships of multiple attributes



Colored by proline
(univariate)



Colored by
 $0.8 \text{ alcohol} + 0.7 \text{ ash} - 0.5 \text{ alcalinity_ash}$
 $- 0.5 \text{ flavanoids} + 0.7 \text{ color_intensity} + \text{proline}$
(composite variable)

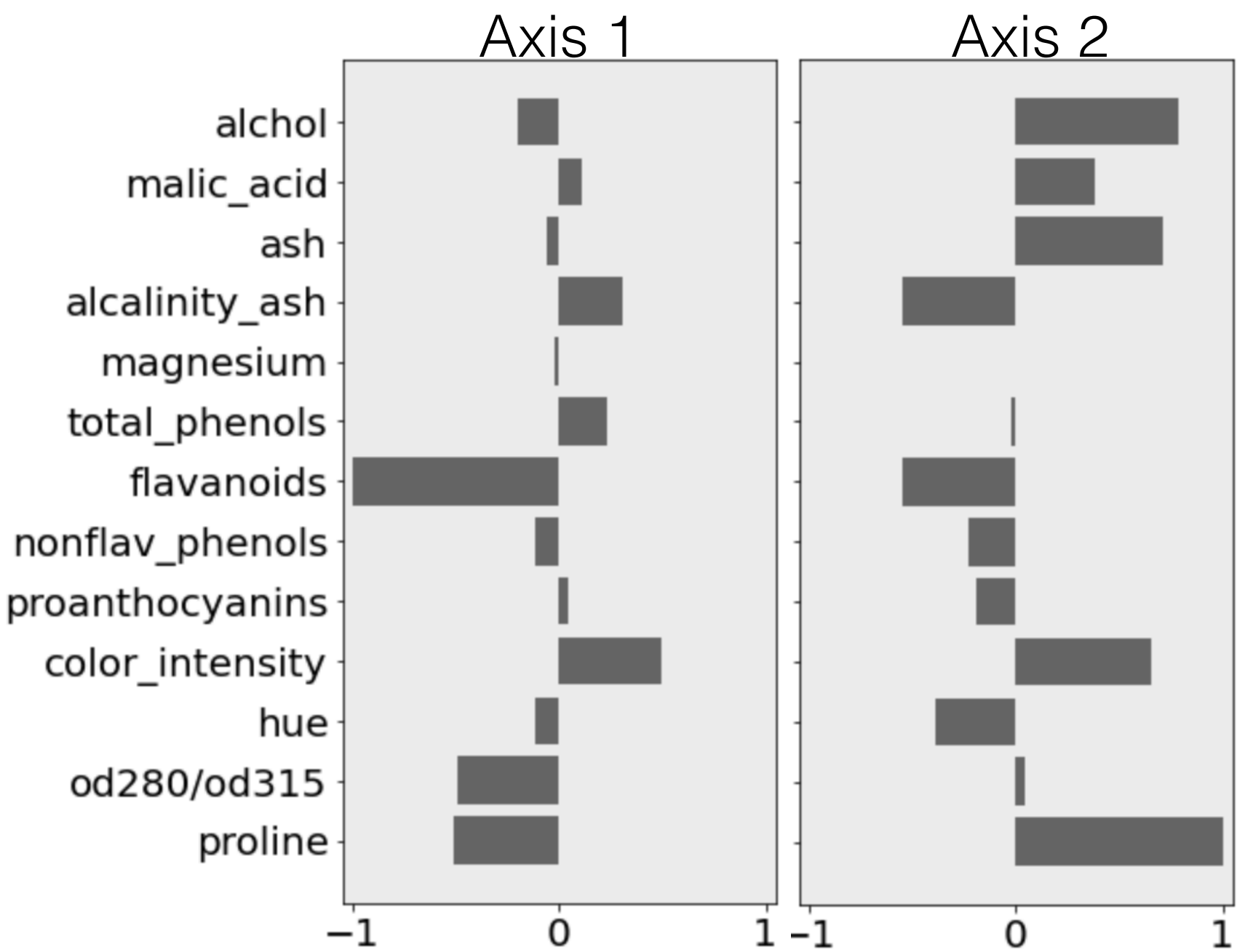
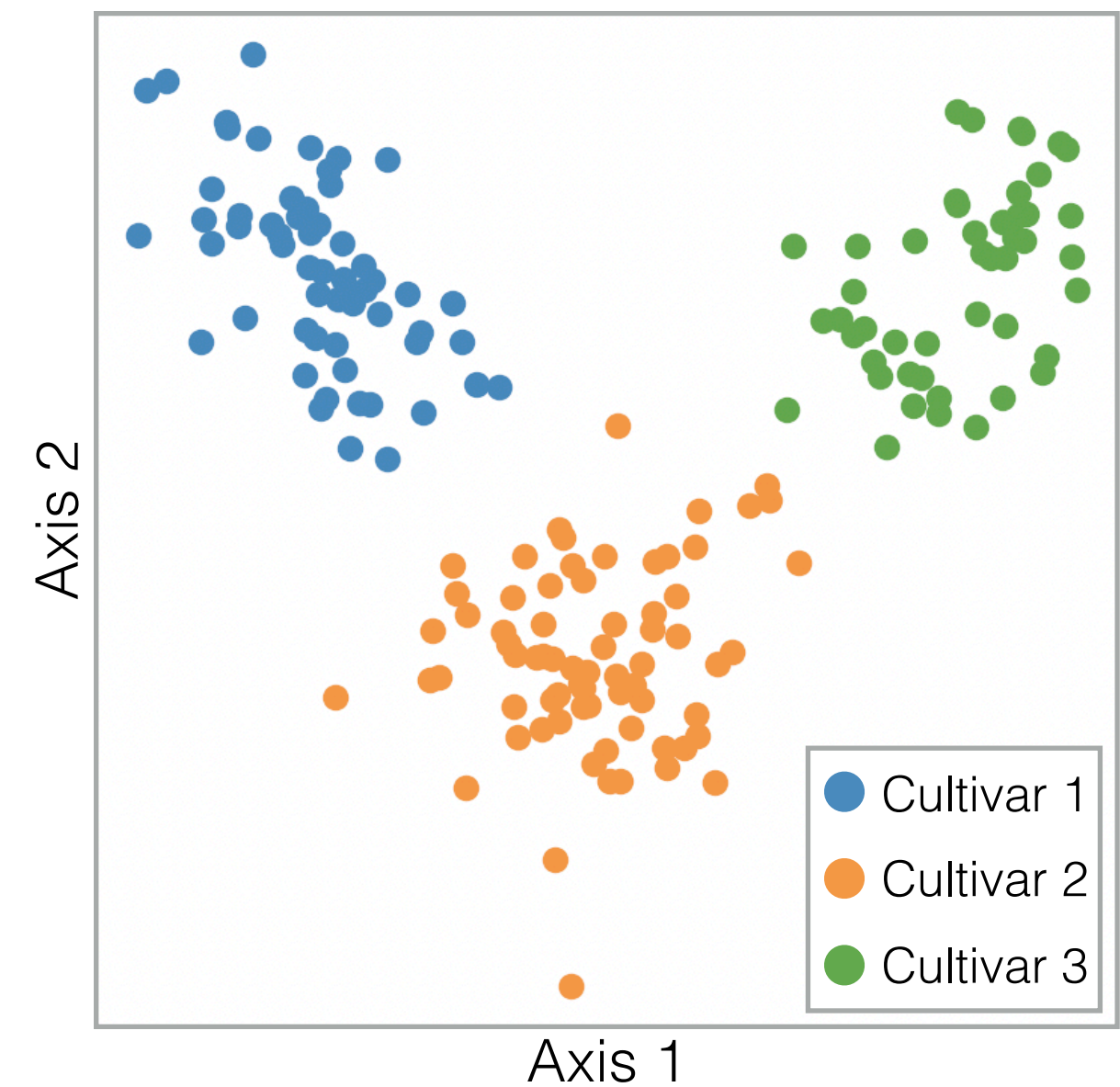
Do you think linear DR is still explainable if there are many attributes (e.g., 100)?

Sparse linear DR

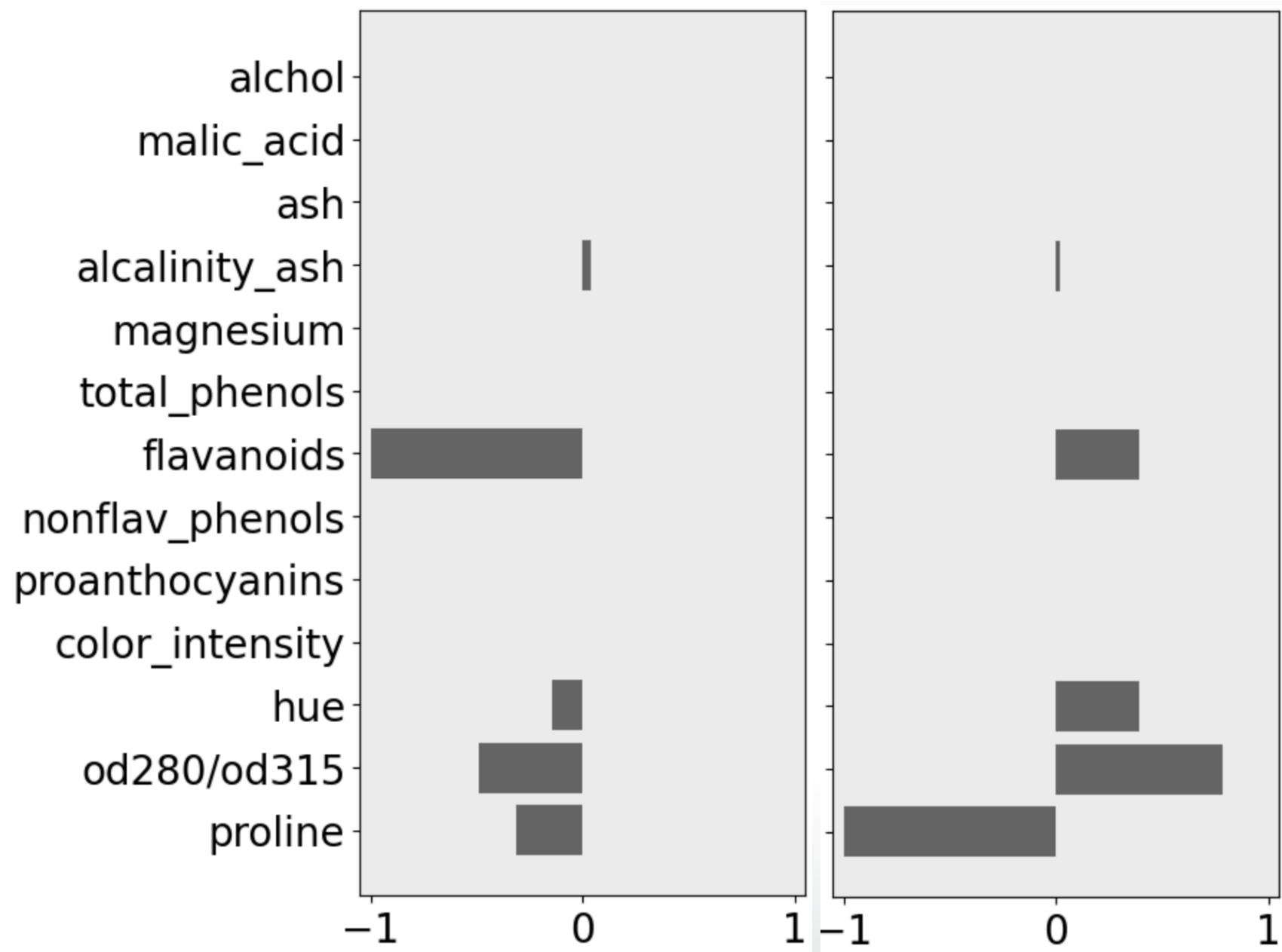
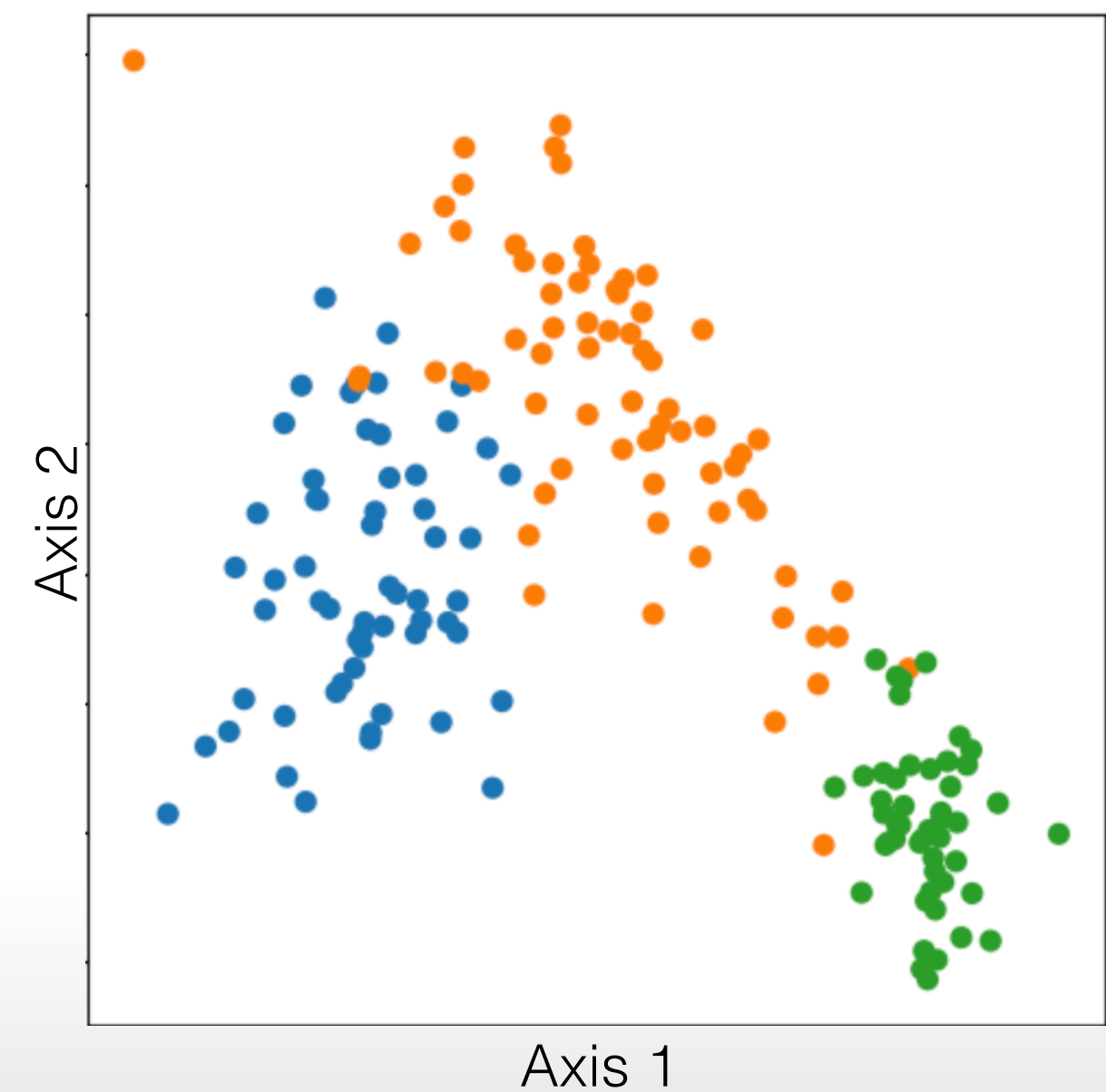
- Finds a linear projection, \mathbf{P} , that has a **small number of nonzero elements**
 - $\mathbf{X} \cdot \mathbf{P} = \mathbf{Y}$ $\mathbf{X} \in \mathbb{R}^{n \times d}$: original data, $\mathbf{P} \in \mathbb{R}^{d \times d'}$: projection matrix, $\mathbf{Y} \in \mathbb{R}^{n \times d'}$: projected data,
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- Representative methods
 - Sparse PCA
(e.g., Zou et al., “Sparse principal component analysis.” *J. Comput. Graph. Stat.*, 2006.)
 - Sparse LDA
(e.g., Wen et al., “Robust sparse linear discriminant analysis.” *IEEE Trans. Circuits Syst. Video Technol.*, 2018.)

Sparse linear DR

LDA



Sparse LDA



Interpretation of dimensionality reduction results

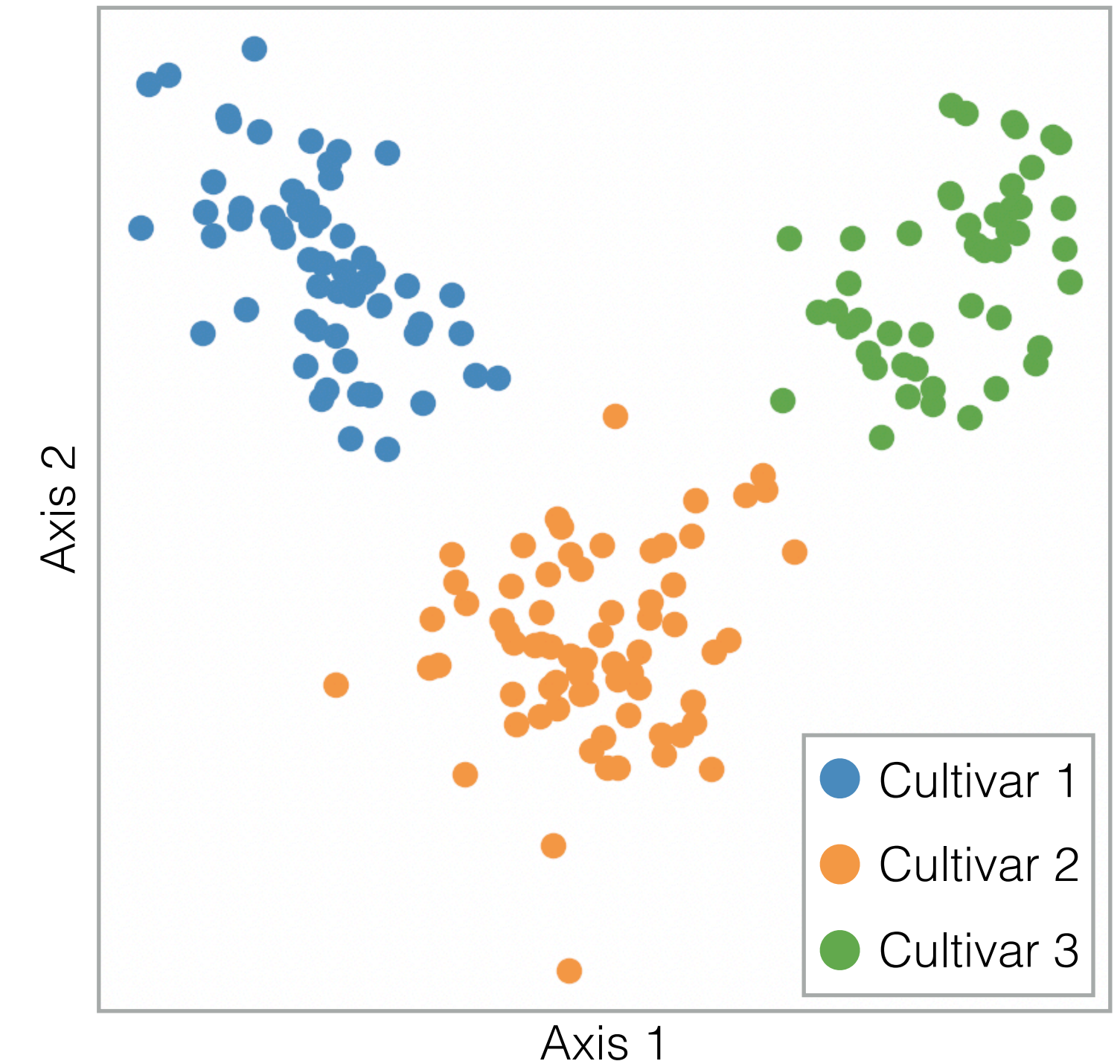
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- Interpreting from a DR **model/mechanism** level

Linear DR

Nonlinear DR

Nonlinear DR

Nonlinear DR

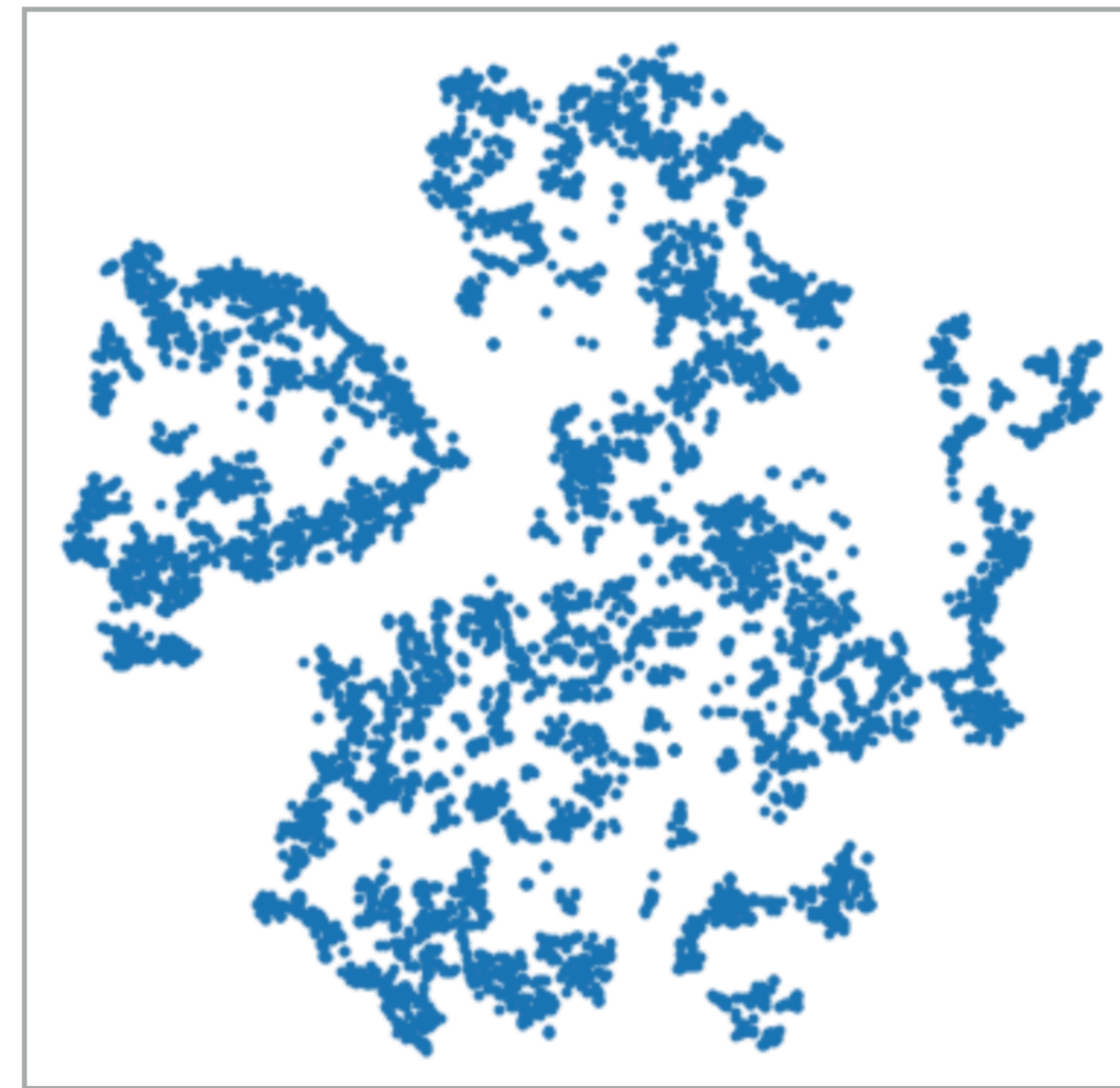
- Does not produce a linear projection from the original to the low-dimensional space
- Many commonly used nonlinear methods such as UMAP, t-SNE, Metric MDS do not provide a **parametric mapping** from the original to the low-dimensional space
 - Parametric mapping $f_{\theta} : \mathbf{X} \rightarrow \mathbf{Y}$ where θ are parameters
 - Without the parametric mapping, we do not have the information how the original data is projected onto the low-dimensional space.



Instead of understanding the low-dimensional axes, we can try to perform the interpretation based on visual patterns appeared in a DR result

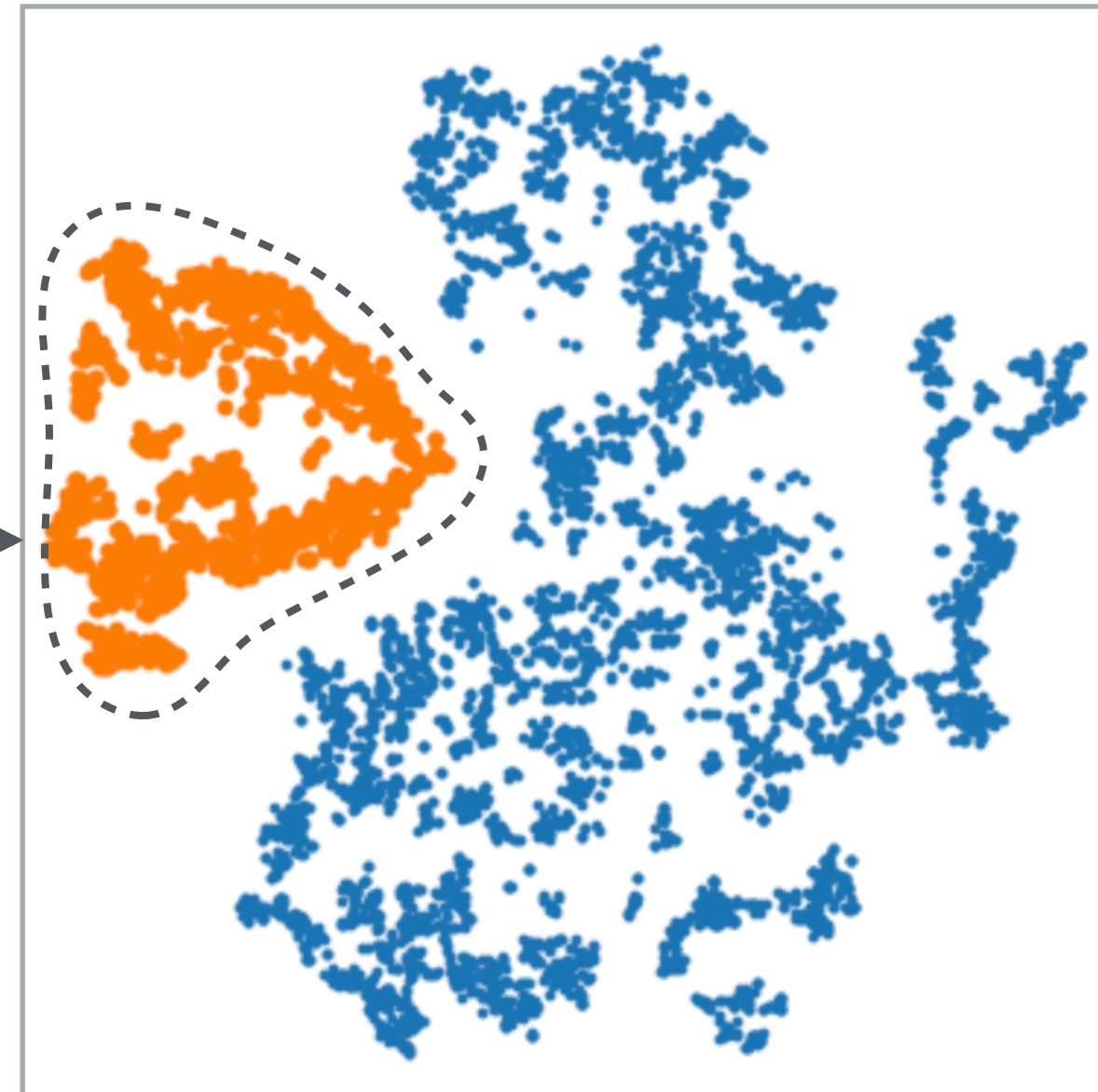
Interpreting by comparing groups/clusters

Food nutrition dataset (12D)



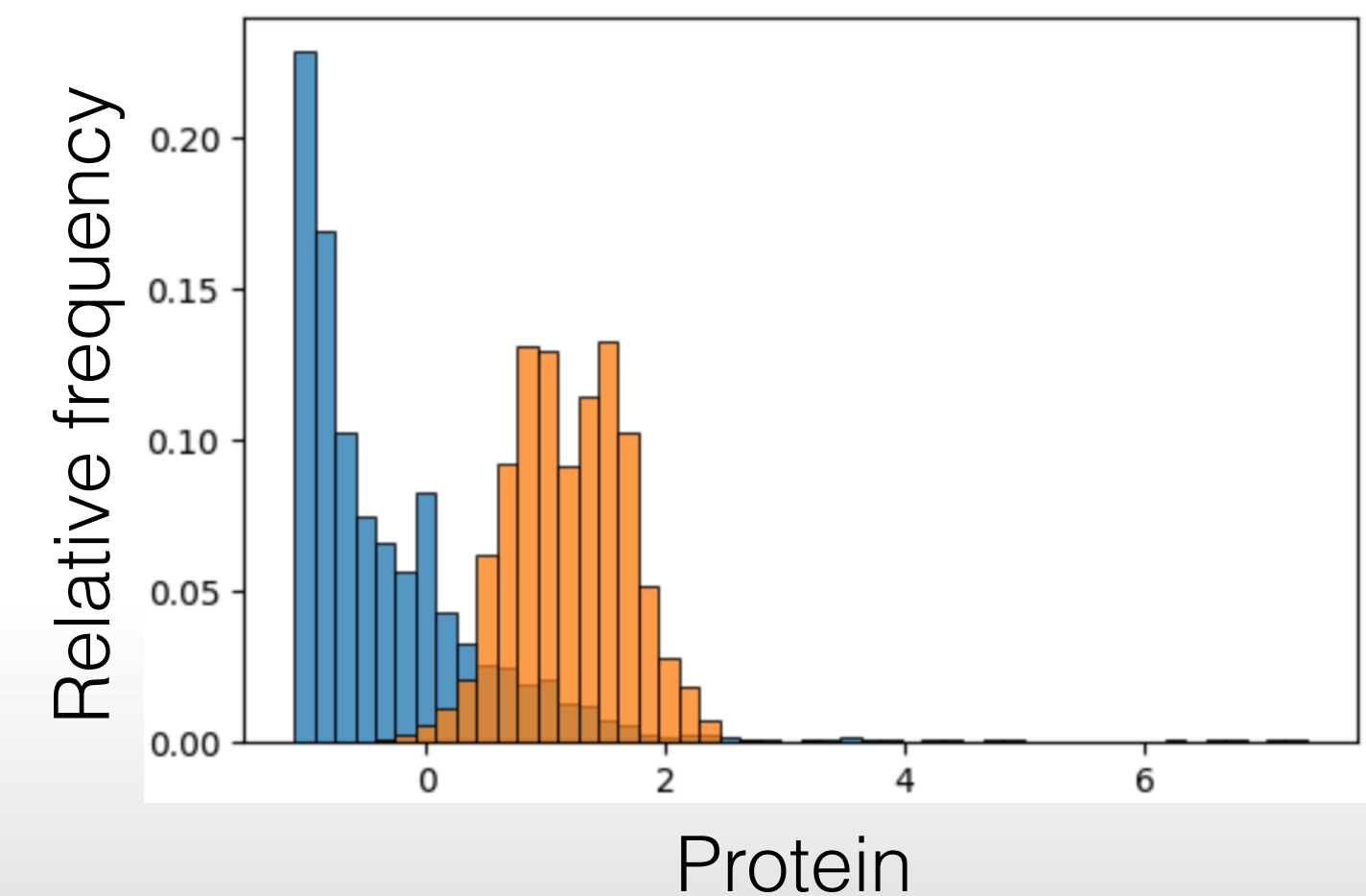
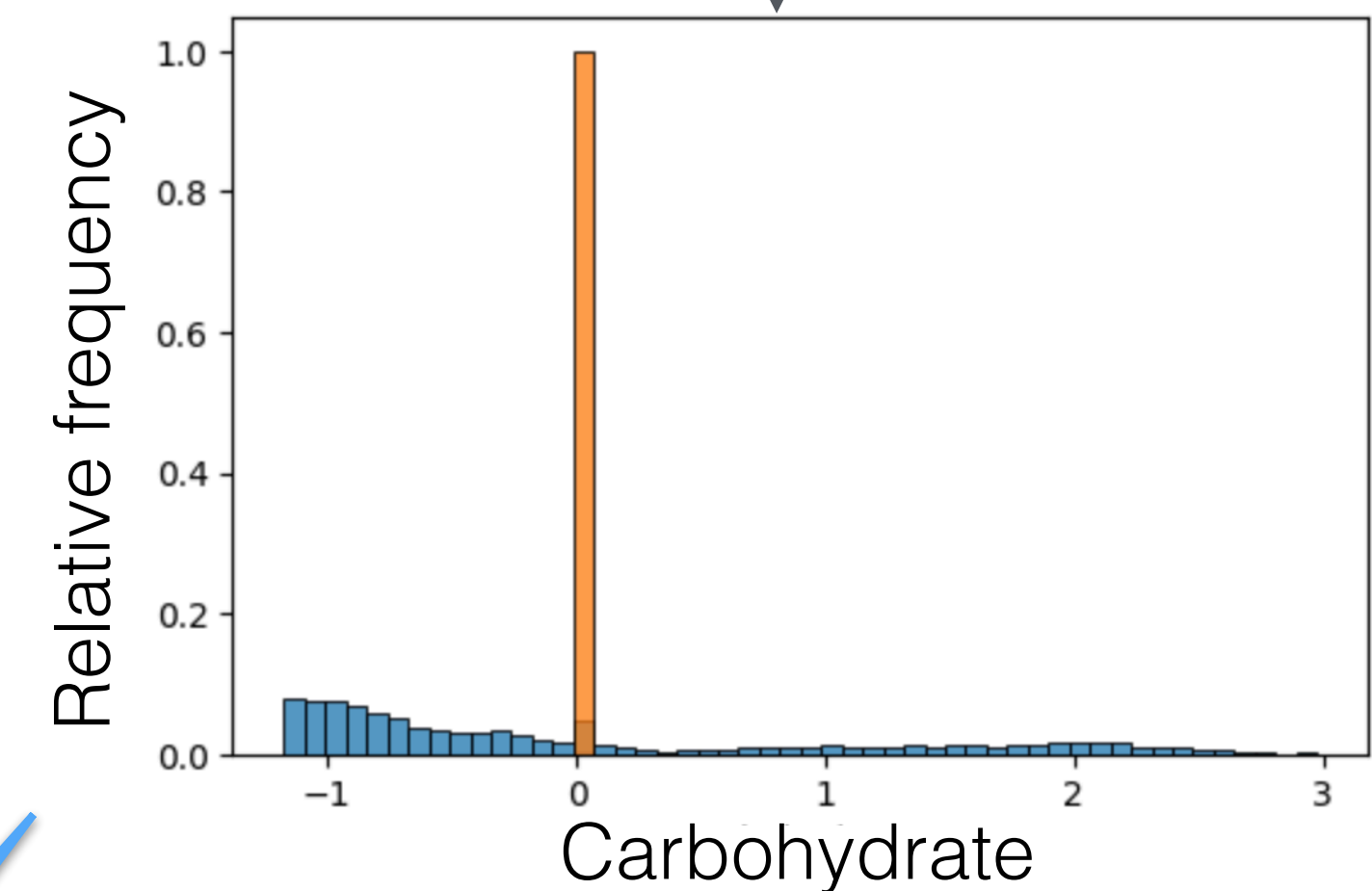
t-SNE result

Lasso
selection



One cluster is selected

Select attributes with statistical measures (e.g., t-test, histogram intersection, LDA); then, visualize them with histograms, etc.



Selected foods have a medium level of carbohydrate but have a lot of protein

Existing approaches for comparing groups/clusters

- Univariate focus

- e.g., t-student test-based attribute selection

Marcílio-Jr et al., “Contrastive analysis for scatterplot-based representations of dimensionality reduction.” *C&G*, 2021.

- Composite variable focus

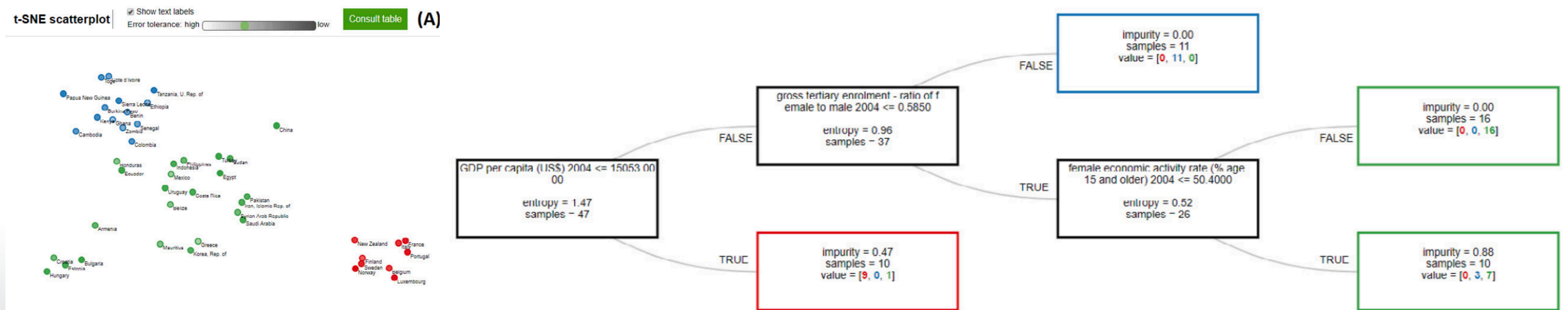
- e.g., comparative analysis using linear DR

Fujiwara et al., “Supporting analysis of dimensionality reduction results with contrastive learning.” *IEEE TVCG*, 2020.

- Classifier-based

- e.g., building a simple model that classifies clusters in a DR result

Bibal et al., “IXVC: An interactive pipeline for explaining visual clusters in dimensionality reduction visualizations with decision trees.” *Array*, 2021.



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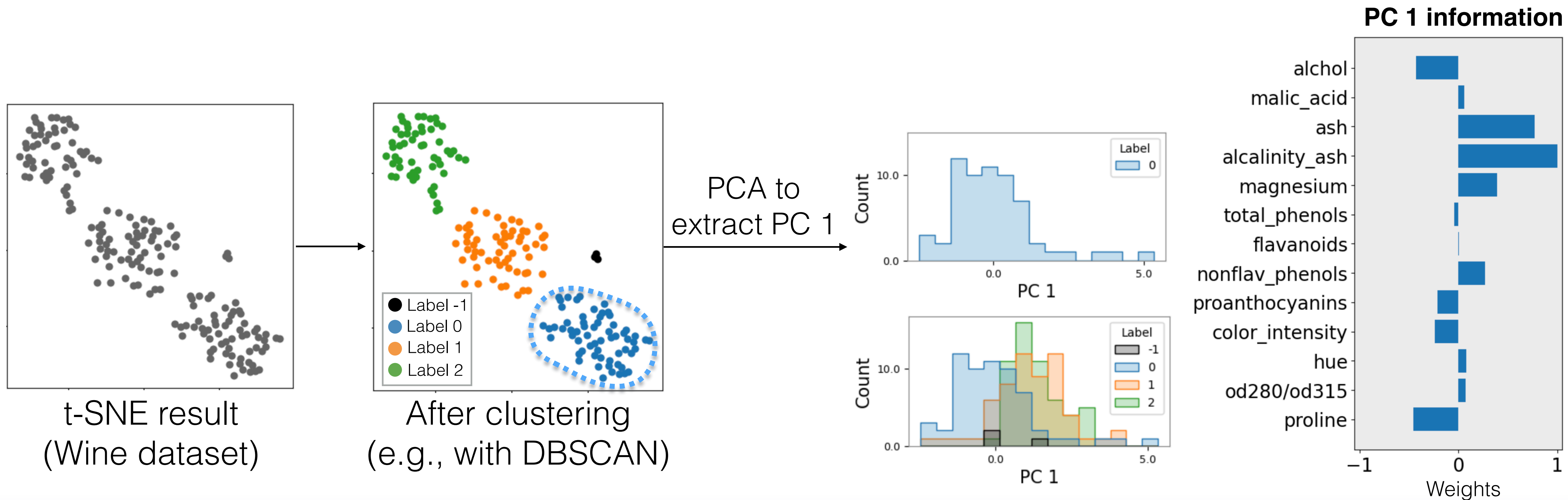
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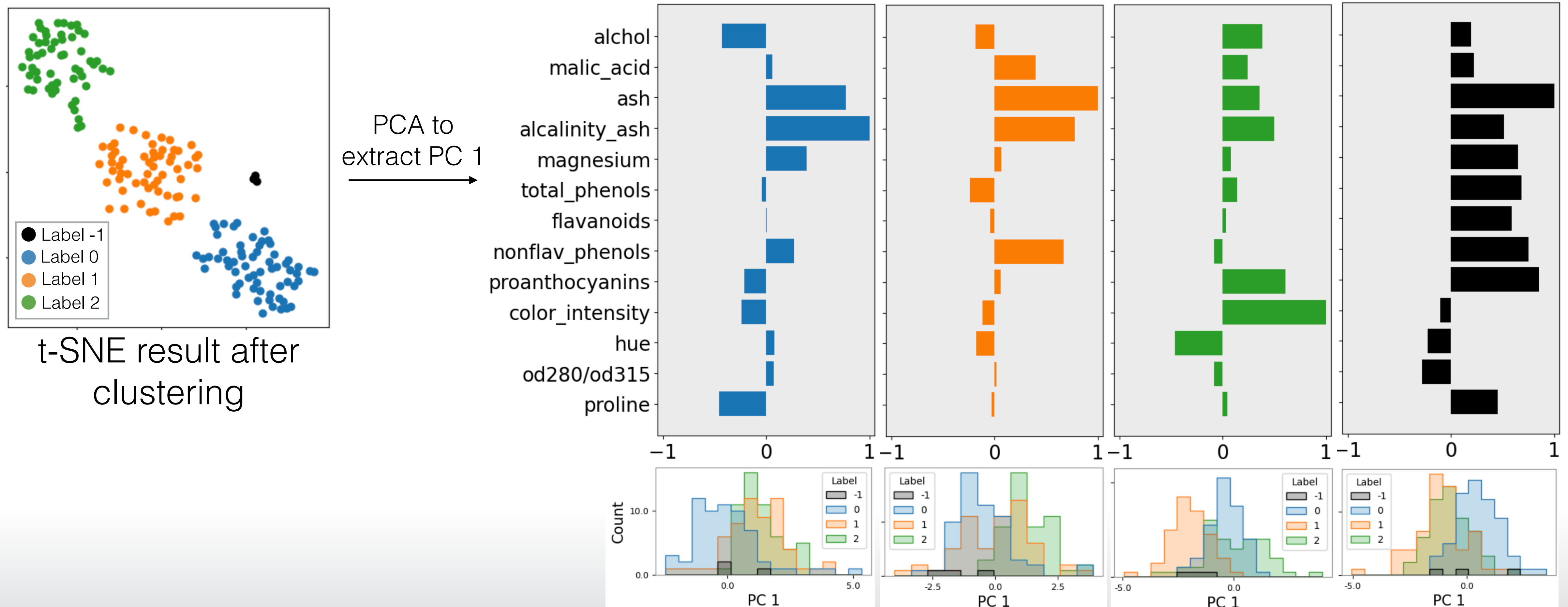
Comparing clusters/groups using linear DR: PCA-based

- Applying **PCA** for each cluster
(e.g., `PCA(n_components=1).fit(data[label==0])`)
 - Extract variance-related information of each cluster—**variety factors**



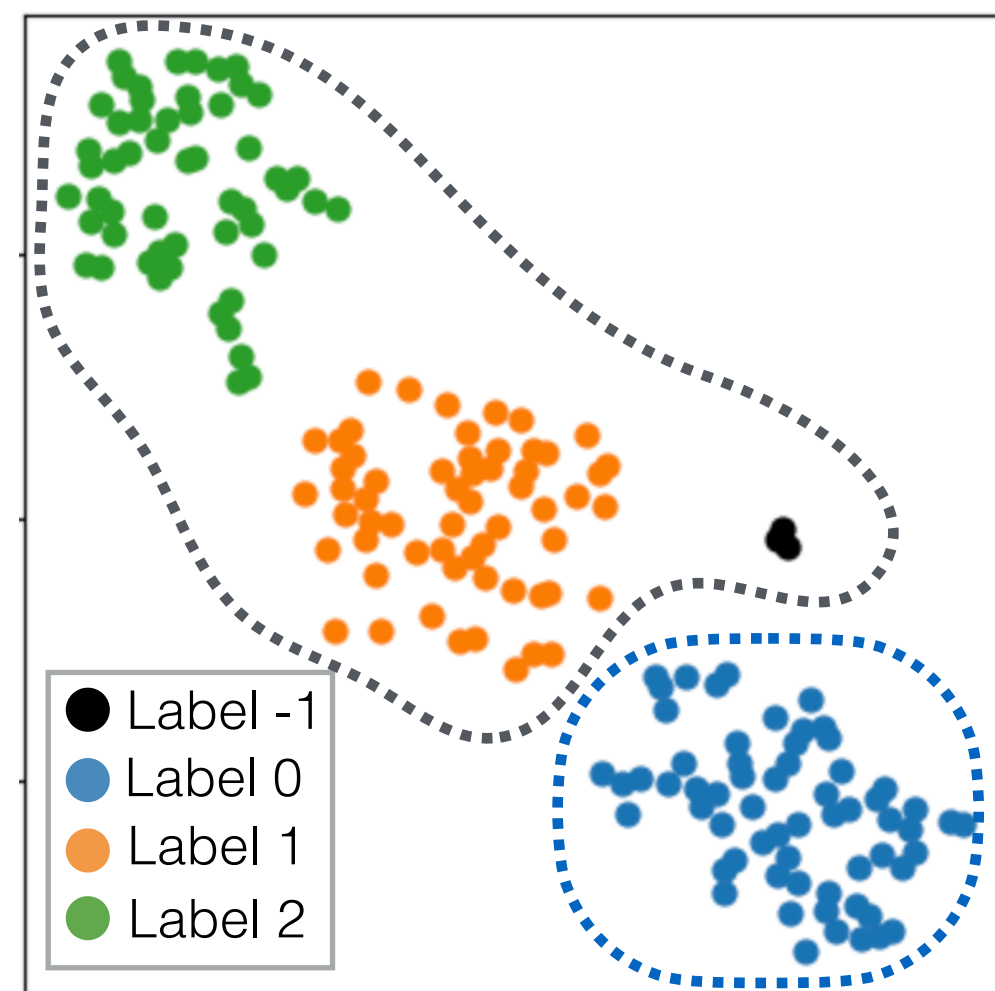
Comparing clusters/groups using linear DR: PCA-based

- Applying **PCA** for each cluster
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 - Extract variance-related information of each cluster—**variety factors**
 - But, there is no consideration of differences between one cluster and others



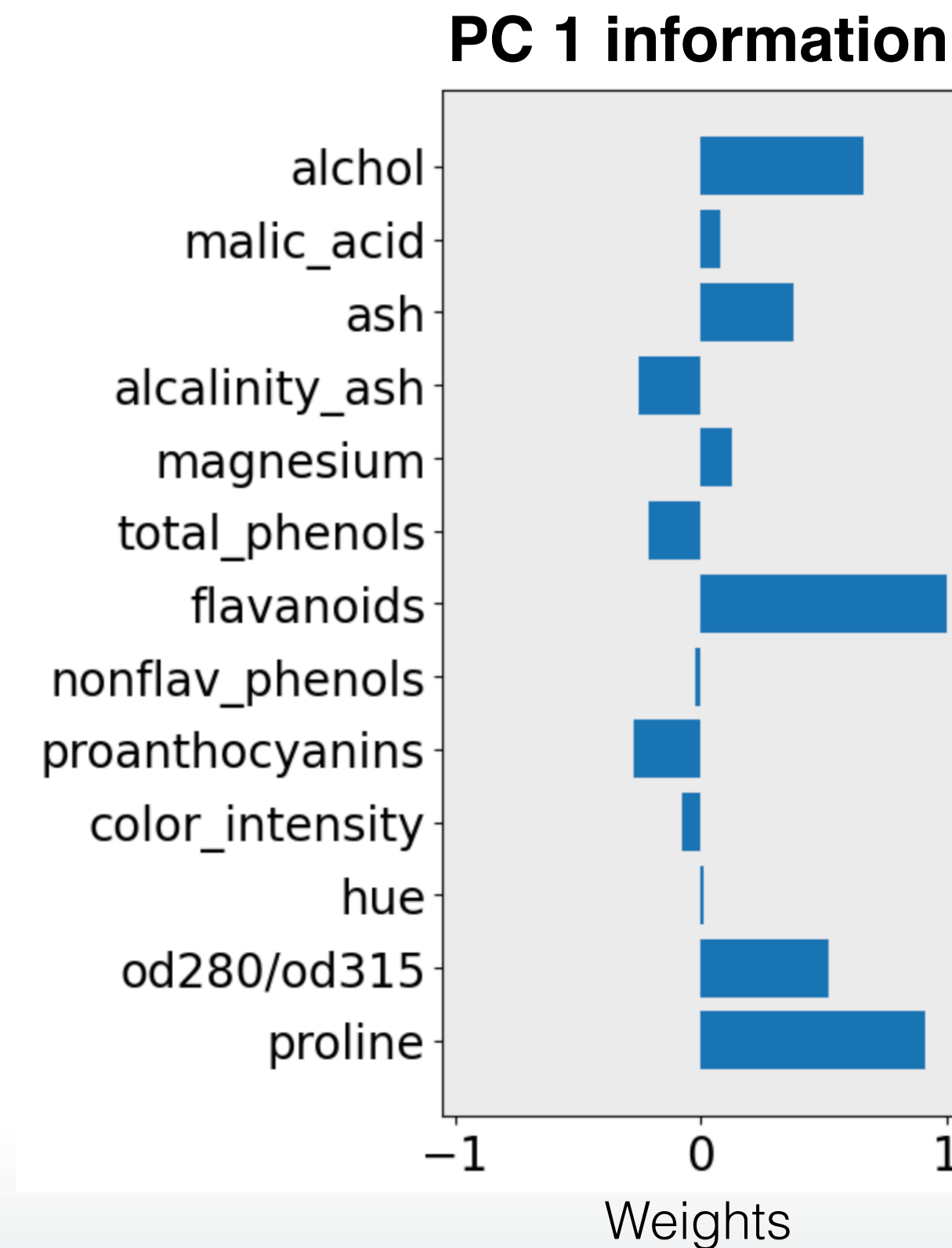
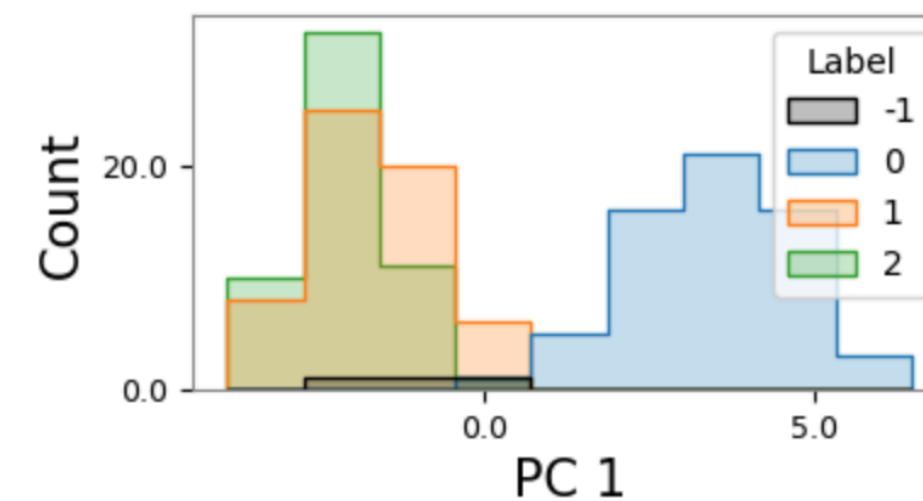
Comparing clusters/groups using linear DR: LDA-based

- Applying linear discriminant analysis (**LDA**) to distinguish one cluster and others (e.g., `LDA(n_components=1).fit(data, label==0)`)
 - Find differences between one cluster and others—**differentiating factors**



t-SNE result after clustering

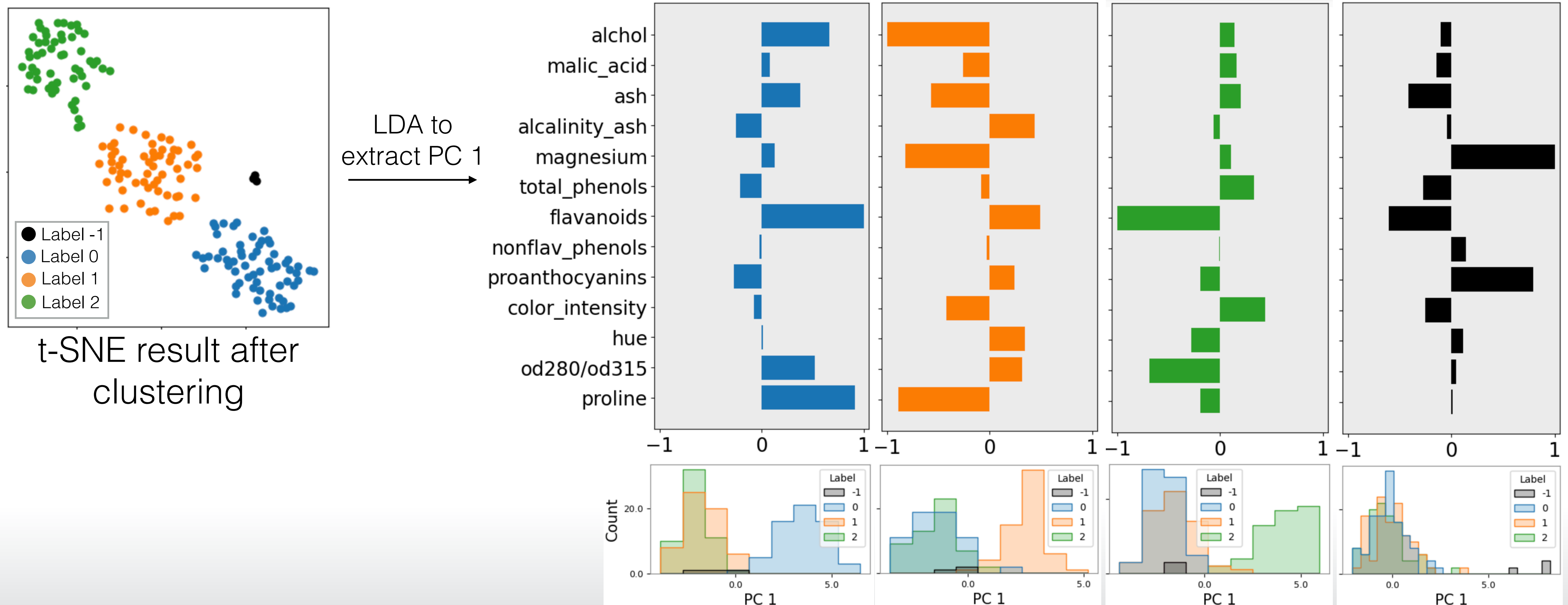
Classification
Label 0 and **others**
with LDA and then
extraction of PC 1



[demo script](#)

Comparing clusters/groups using linear DR: PCA-based

- Applying linear discriminant analysis (**LDA**) to distinguish one cluster and others (e.g., `LDA(n_components=1).fit(data, label==0)`)
 - Find differences between one cluster and others—**differentiating factors**
 - **But, may lose overall/variance information related each cluster**



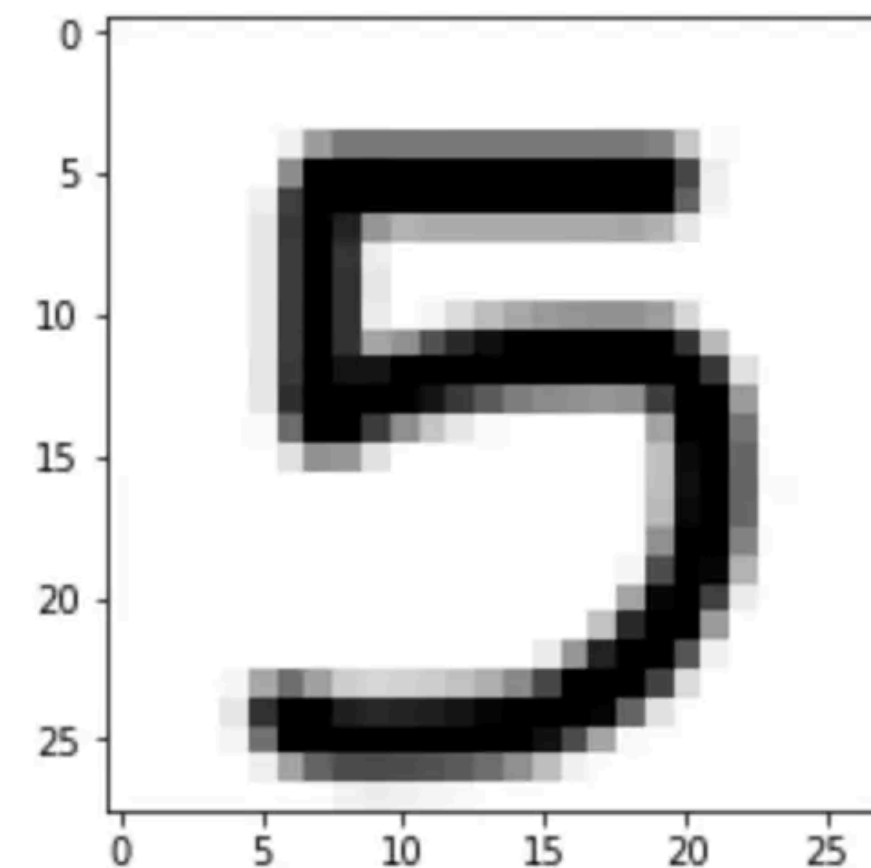
ccPCA: Contrasting clusters in PCA

Fujiwara et al., “Supporting analysis of dimensionality reduction results with contrastive learning.” *IEEE TVCG*, 2020.

- Extract salient factors in one group relative to others while considering their distinction—**characterizing factors**

MNIST Dataset

70,000
hand-written digits



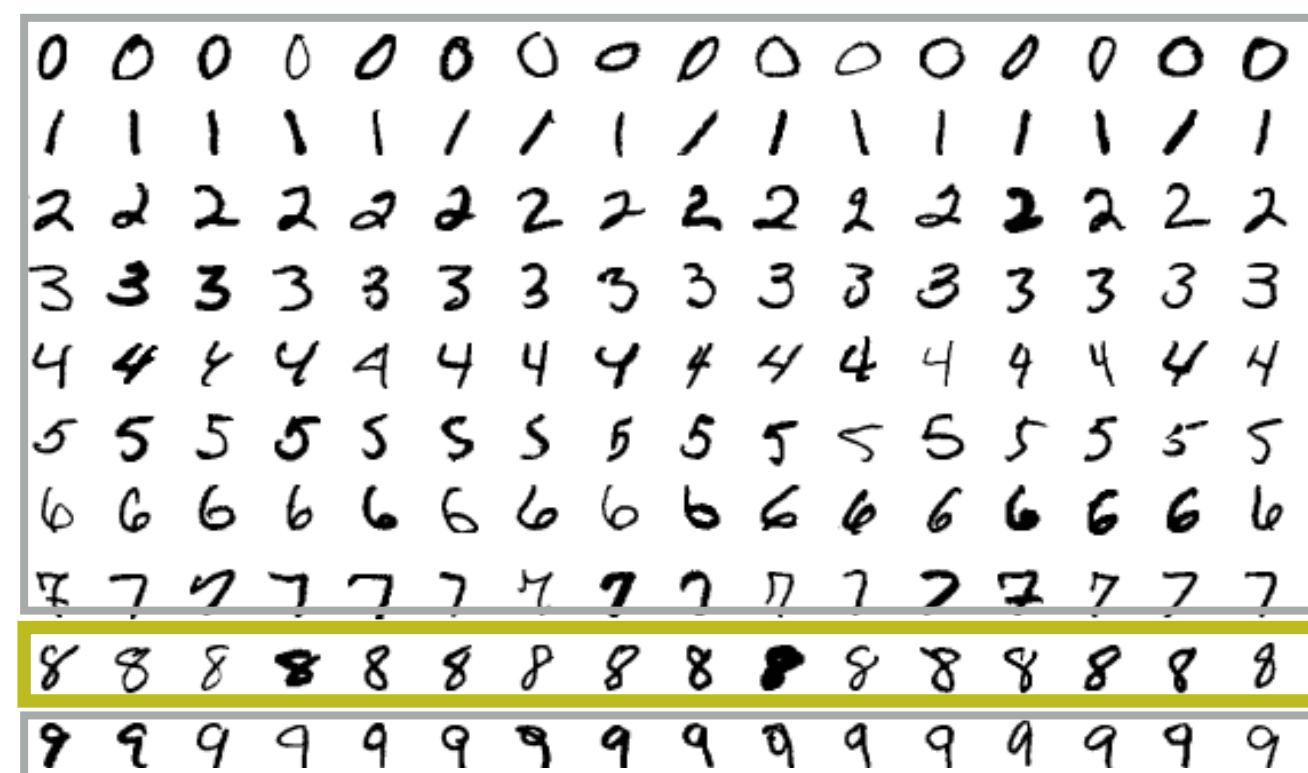
28 pixels x 28 pixels
= 784 dimensions

ccPCA: Contrasting clusters in PCA

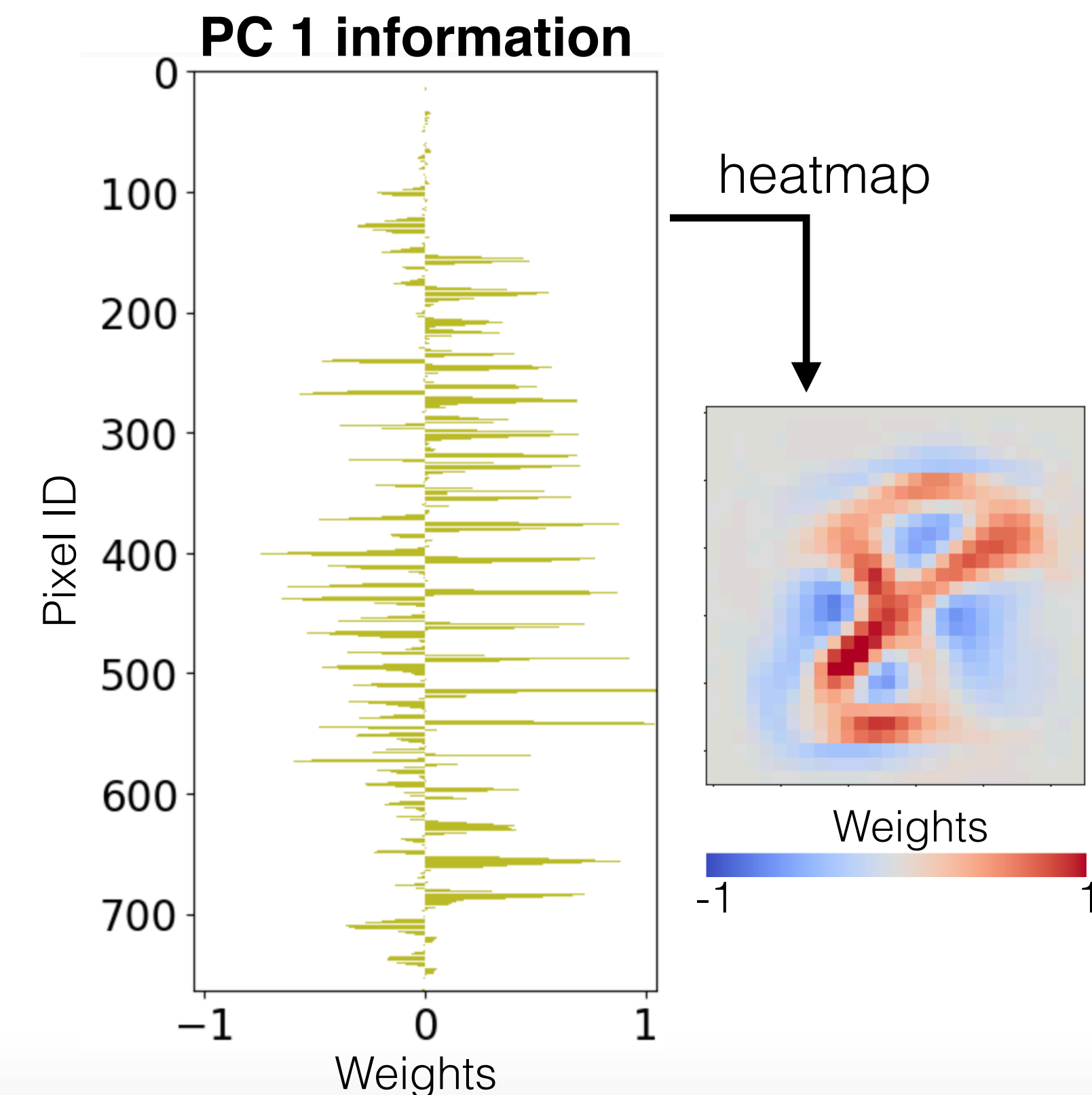
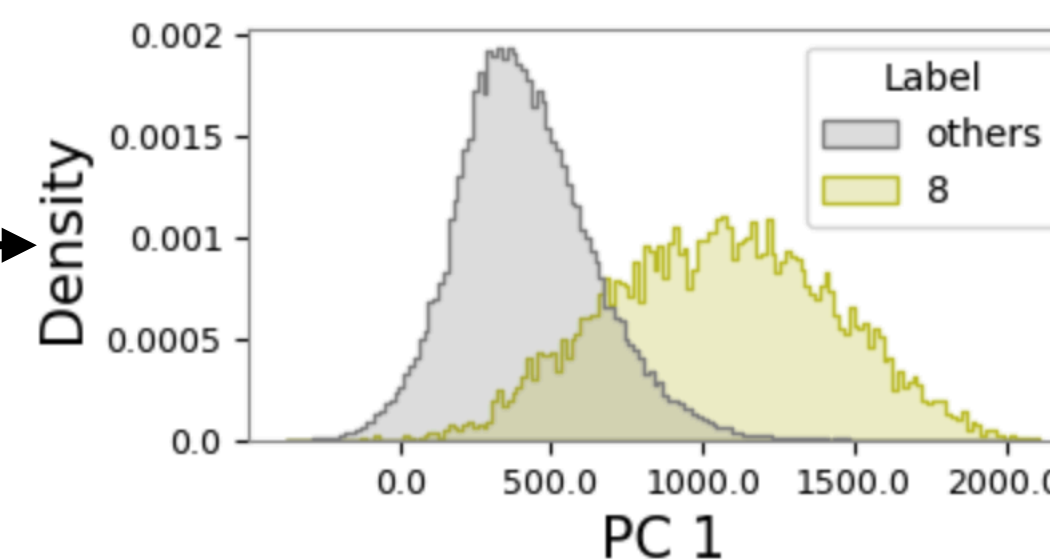
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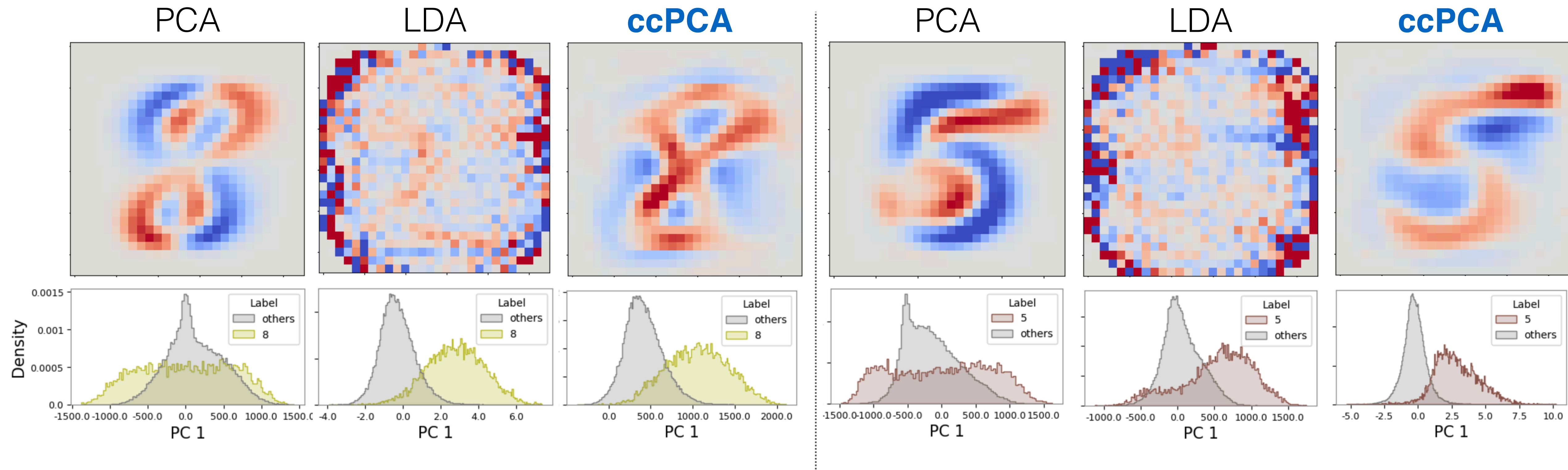
ccPCA
784D to 1D



ccPCA: Contrasting clusters in PCA

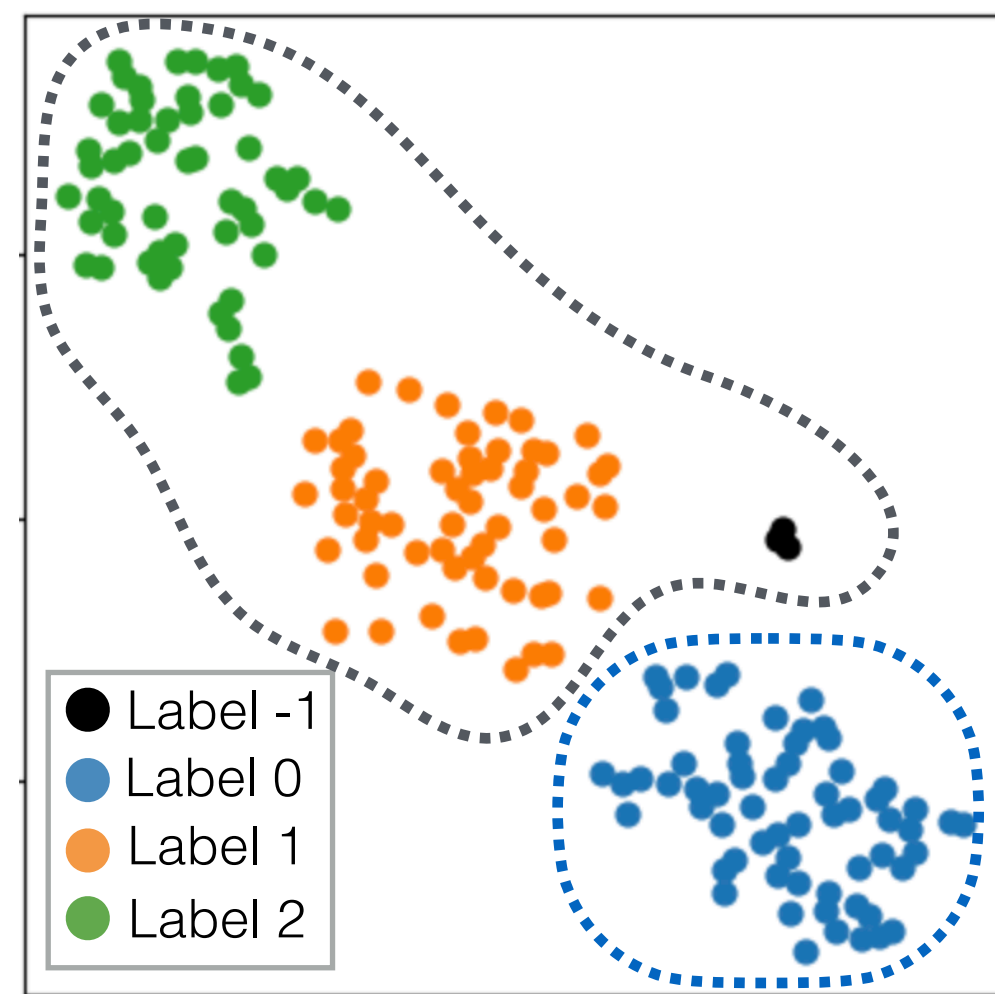
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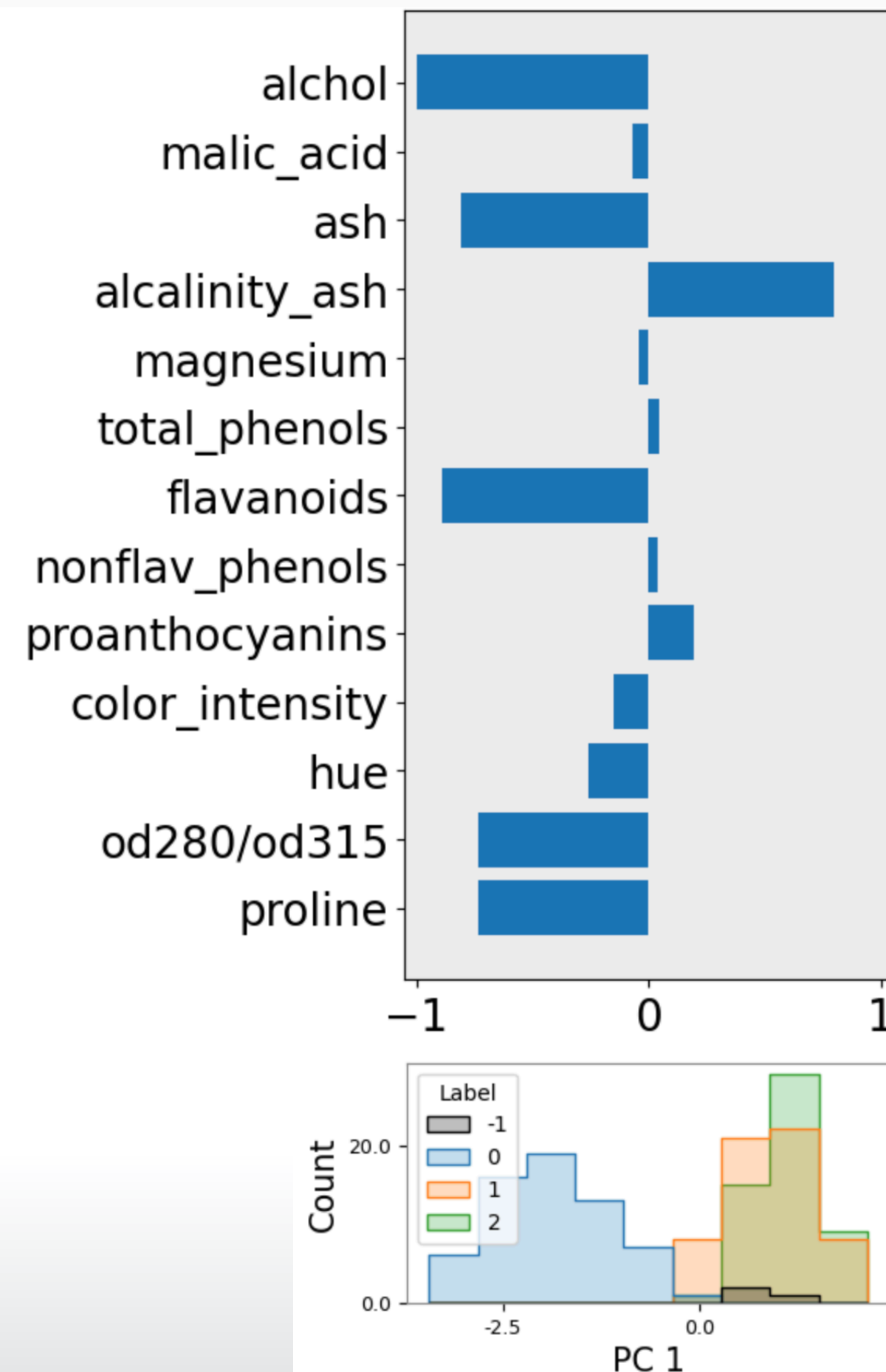
Comparing clusters/groups using linear DR: ccPCA-based

- Applying **ccPCA** to contrast one cluster with others
(e.g., `CCPCA(n_components=1).fit(data[label==0], data[label!=0])`)
 - Balance the preservation of variance within a cluster and the distinction from others
 - better match with t-SNE and UMAP's algorithms



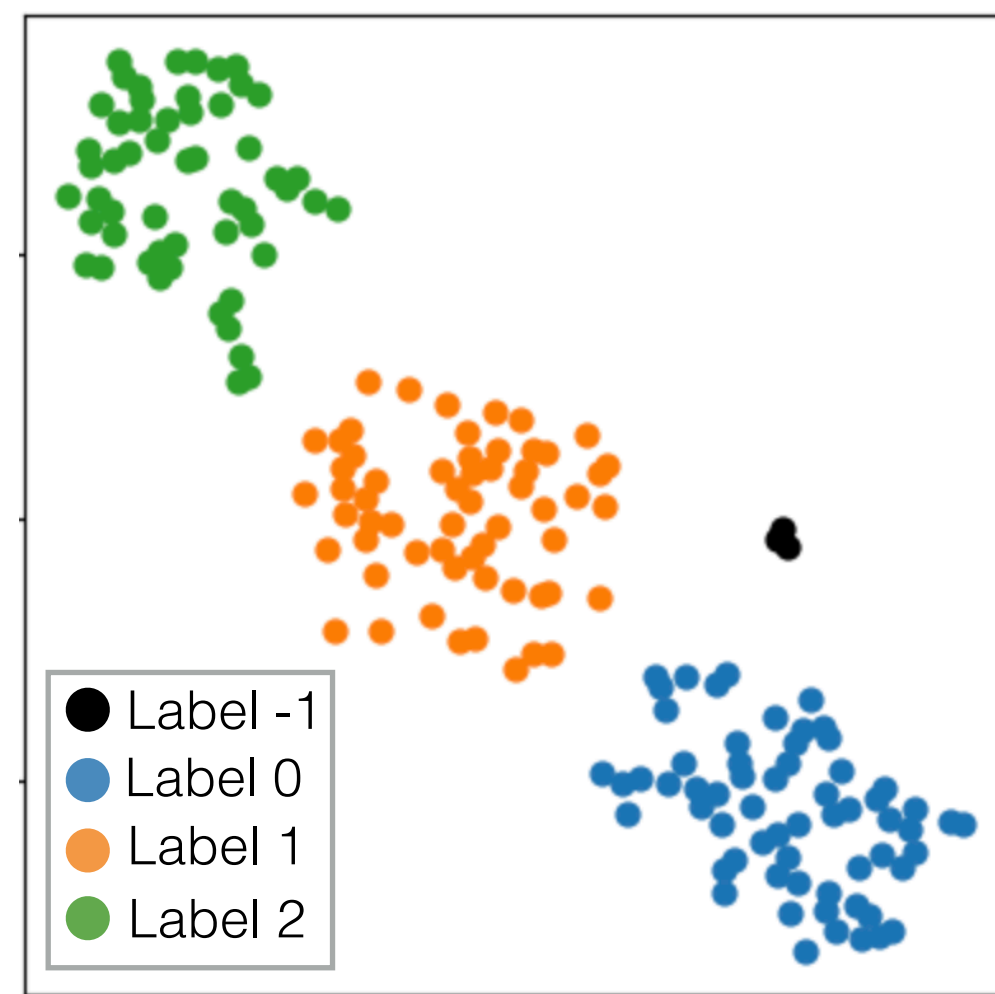
t-SNE result after clustering

ccPCA to
extract PC

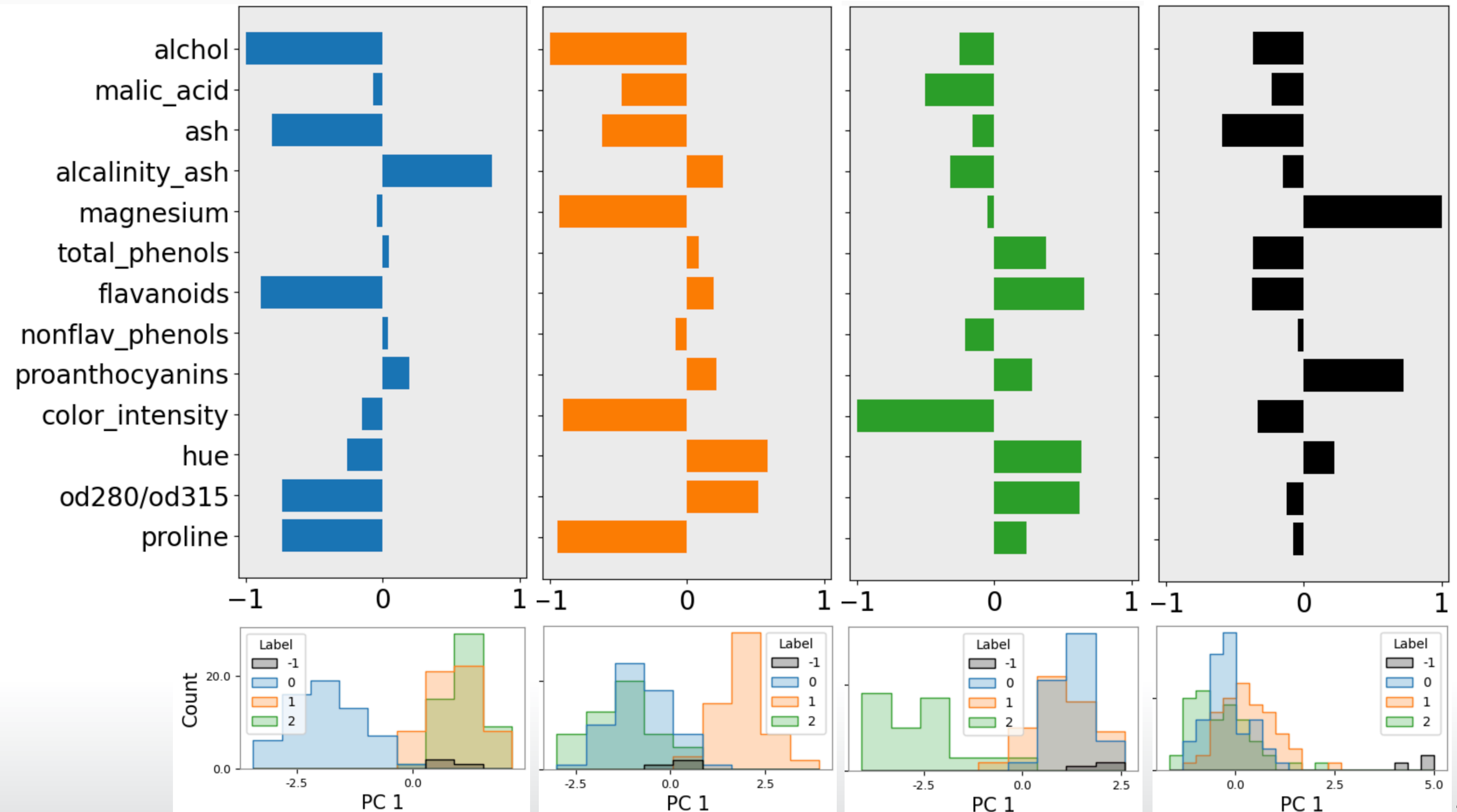


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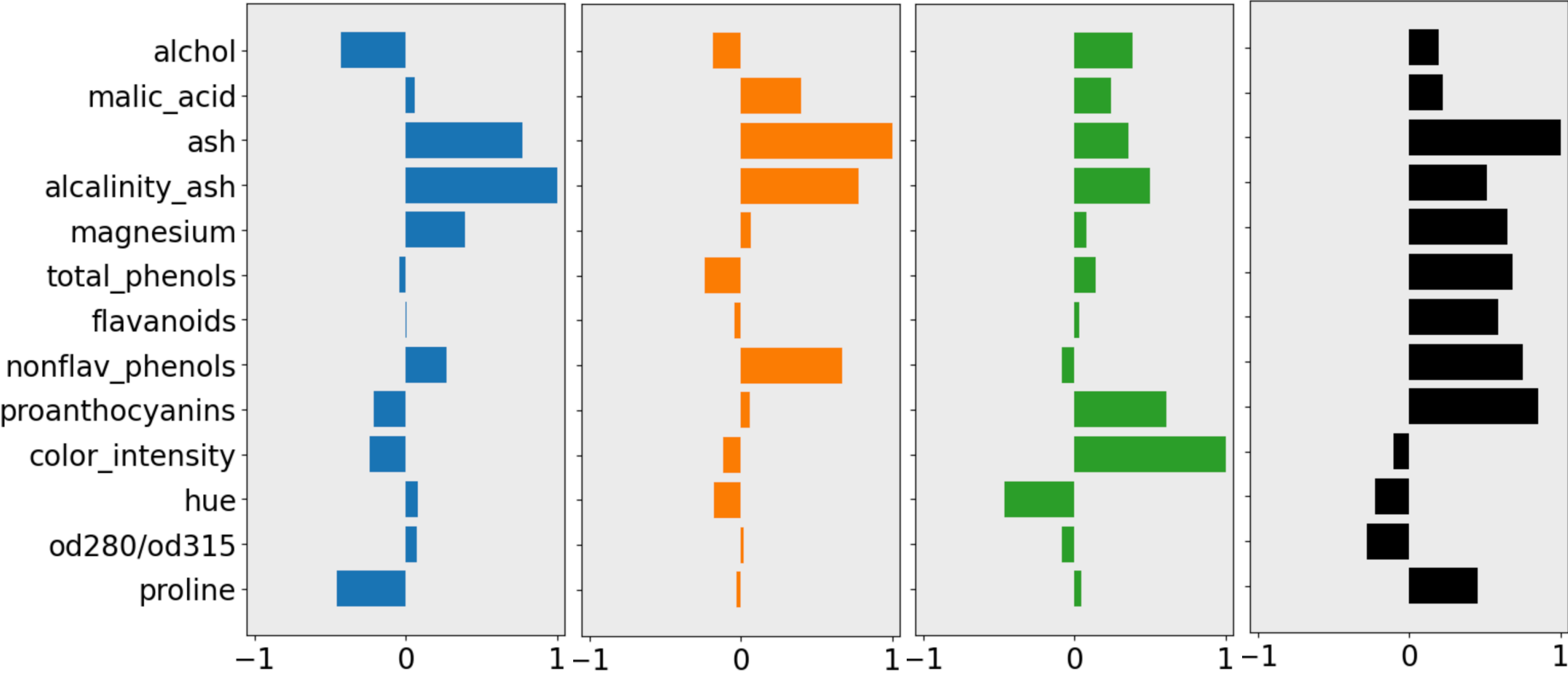


ccPCA to
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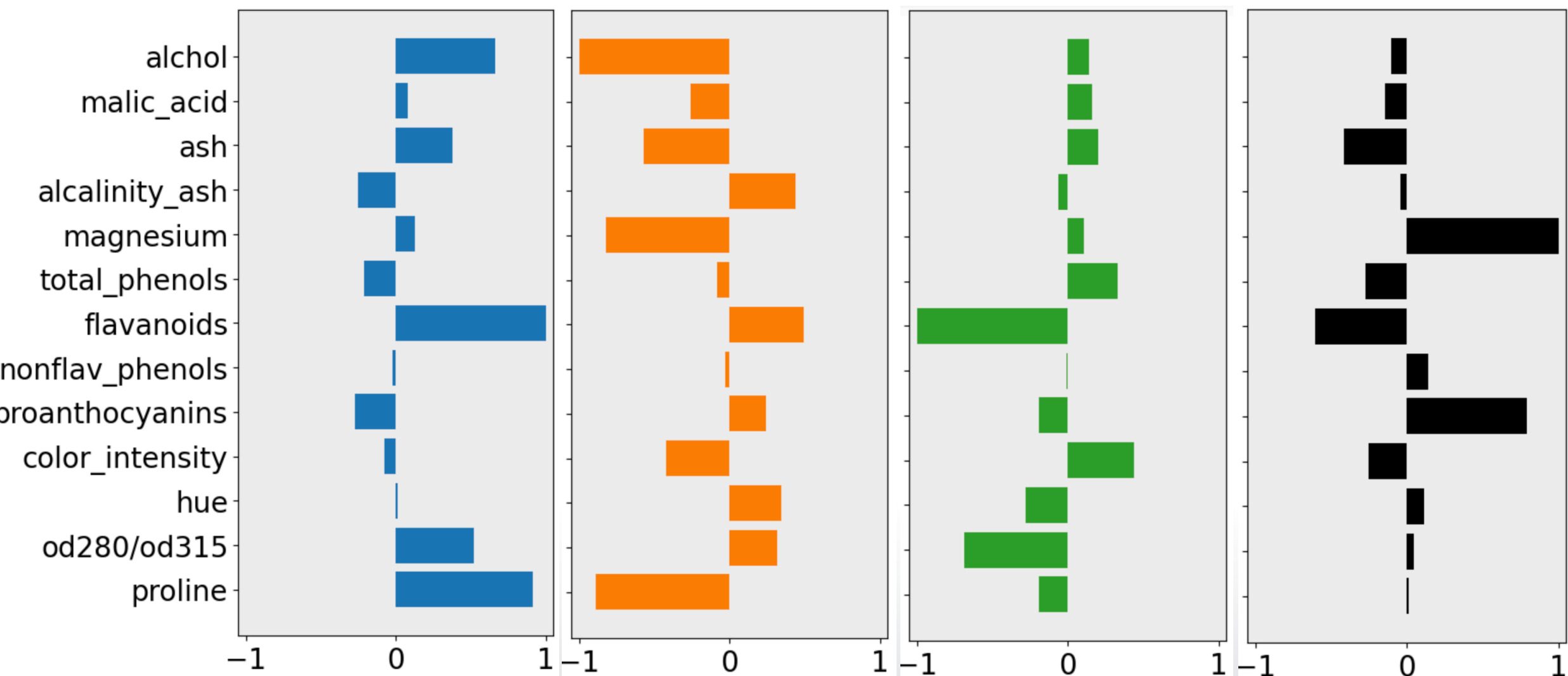


Comparing clusters/groups using linear DR

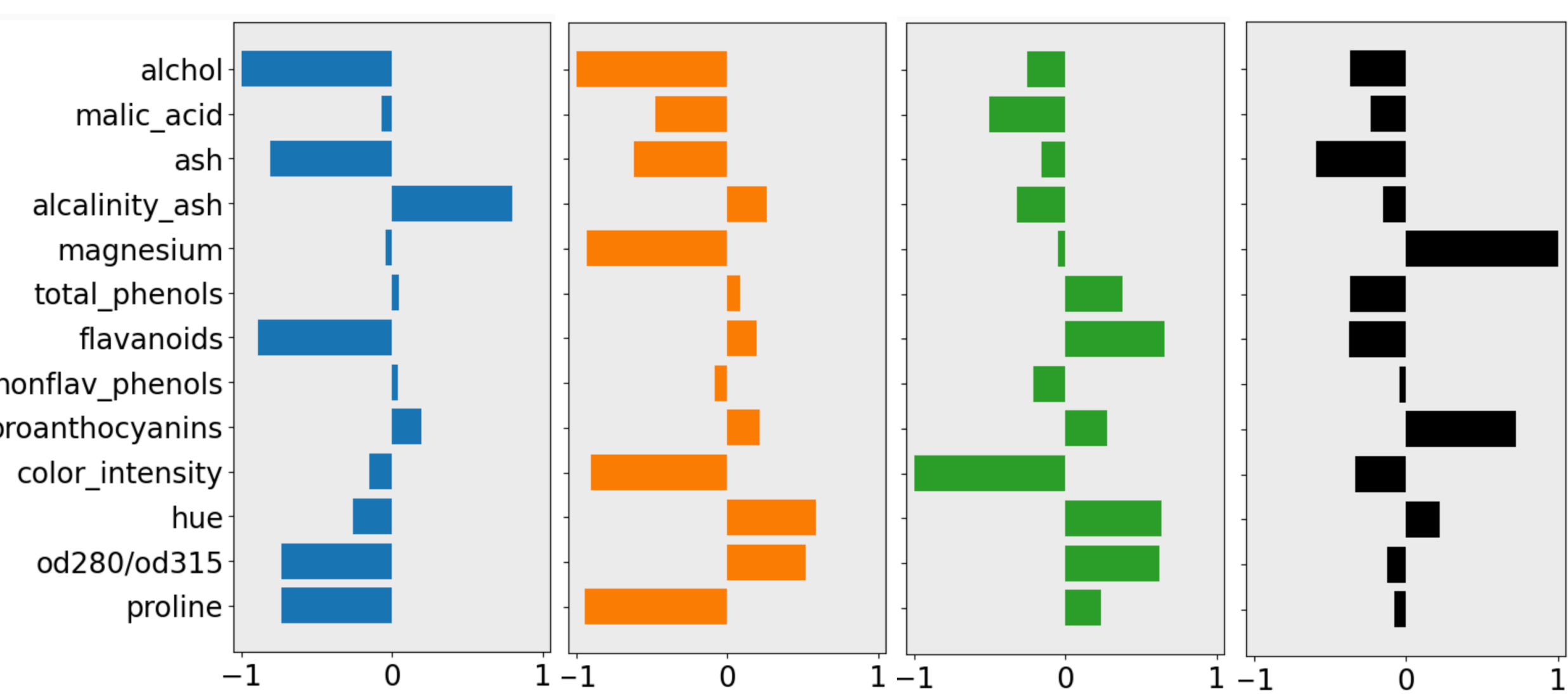
PCA



LDA



ccPCA



Coding exercise (20 minutes)

- Colab notebook link: <http://bit.ly/3ZF0oqv>
- Select one dataset
- Apply t-SNE or UMAP
- Label instances shown in the DR result (manually or apply clustering)
- Try multiple different interpretation approaches
 1. Univariate statistics-based attribute selection/ranking
 2. PCA
 3. LDA
 4. ccPCA
- Compare outcomes from the above approaches



More flexible comparison

- Unified linear comparative analysis (ULCA)

Fujiwara et al., “Interactive dimensionality reduction for comparative analysis.” *IEEE TVCG*, 2022.

<https://github.com/takanori-fujiwara/ulca>

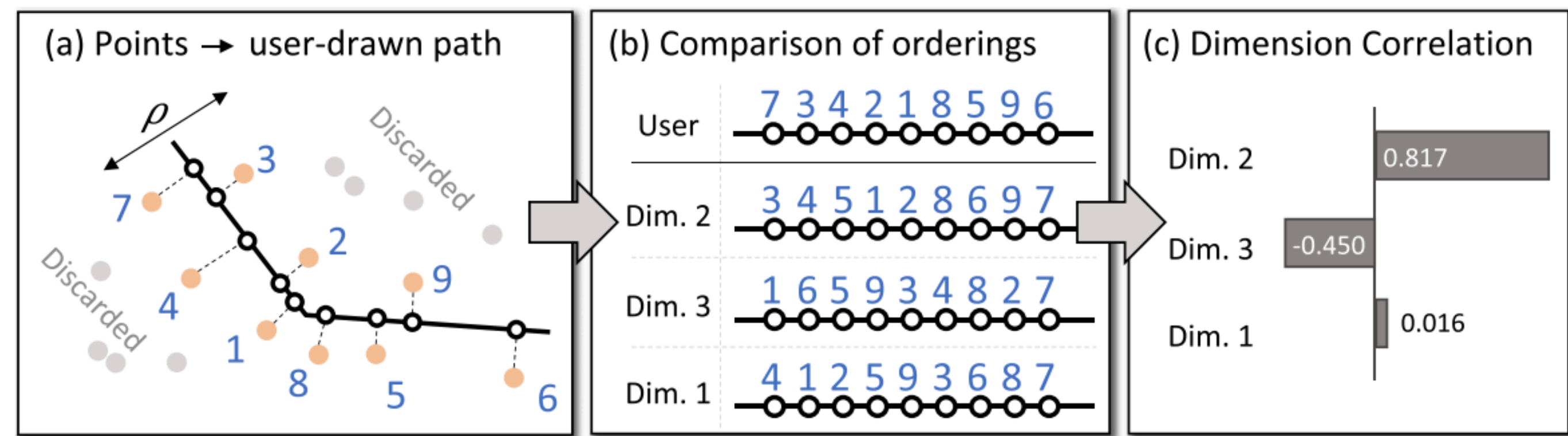
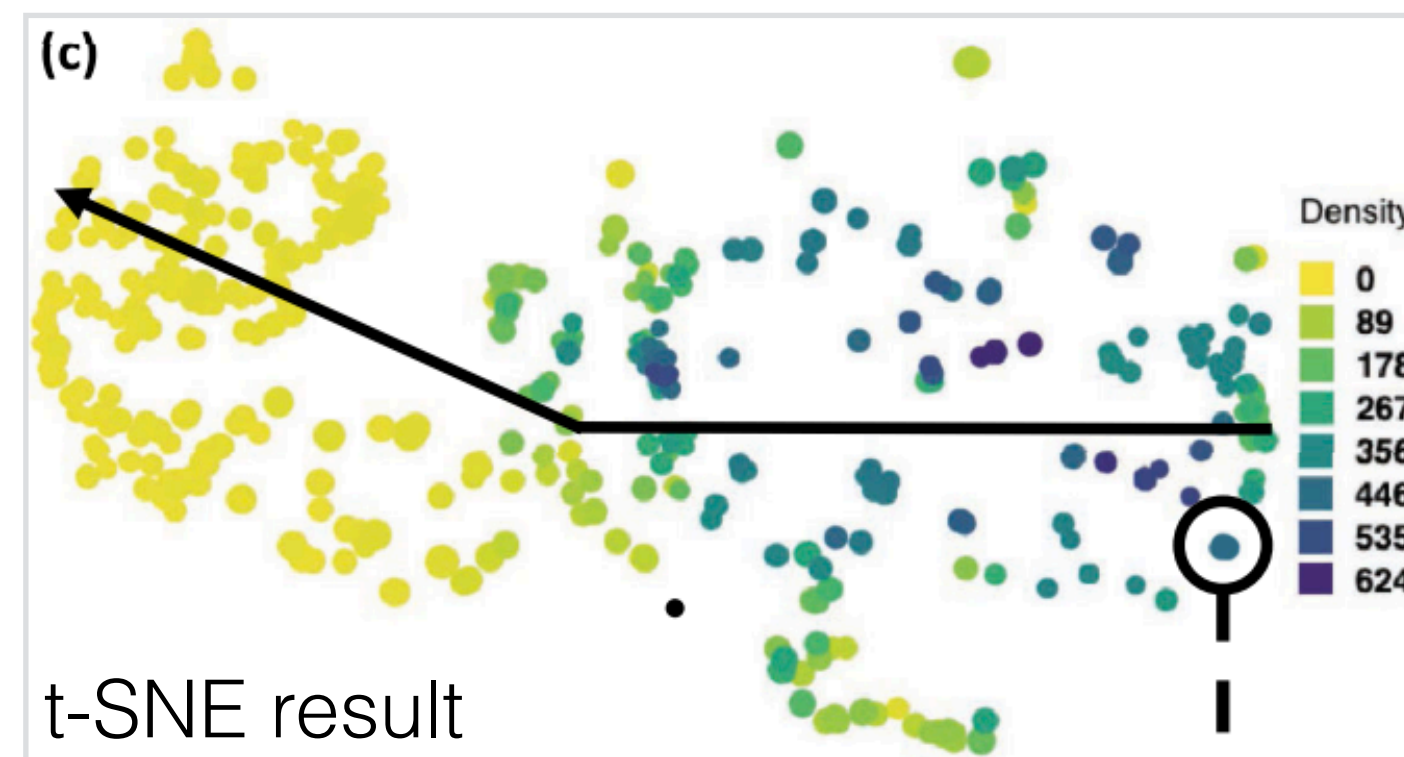
- More explicitly control of how strongly linear DR **separates** groups and **preserves/eliminates variance** of each group

Other interpretation approach based on observed patterns

- Local direction/path

- e.g., checking a correlation between a user-drawn path and each attribute

Chatzimpampas et al., “t-viSNE: Interactive assessment and interpretation of t-SNE projections.” *IEEE TVCG*, 2020.



Interpretation of dimensionality reduction results

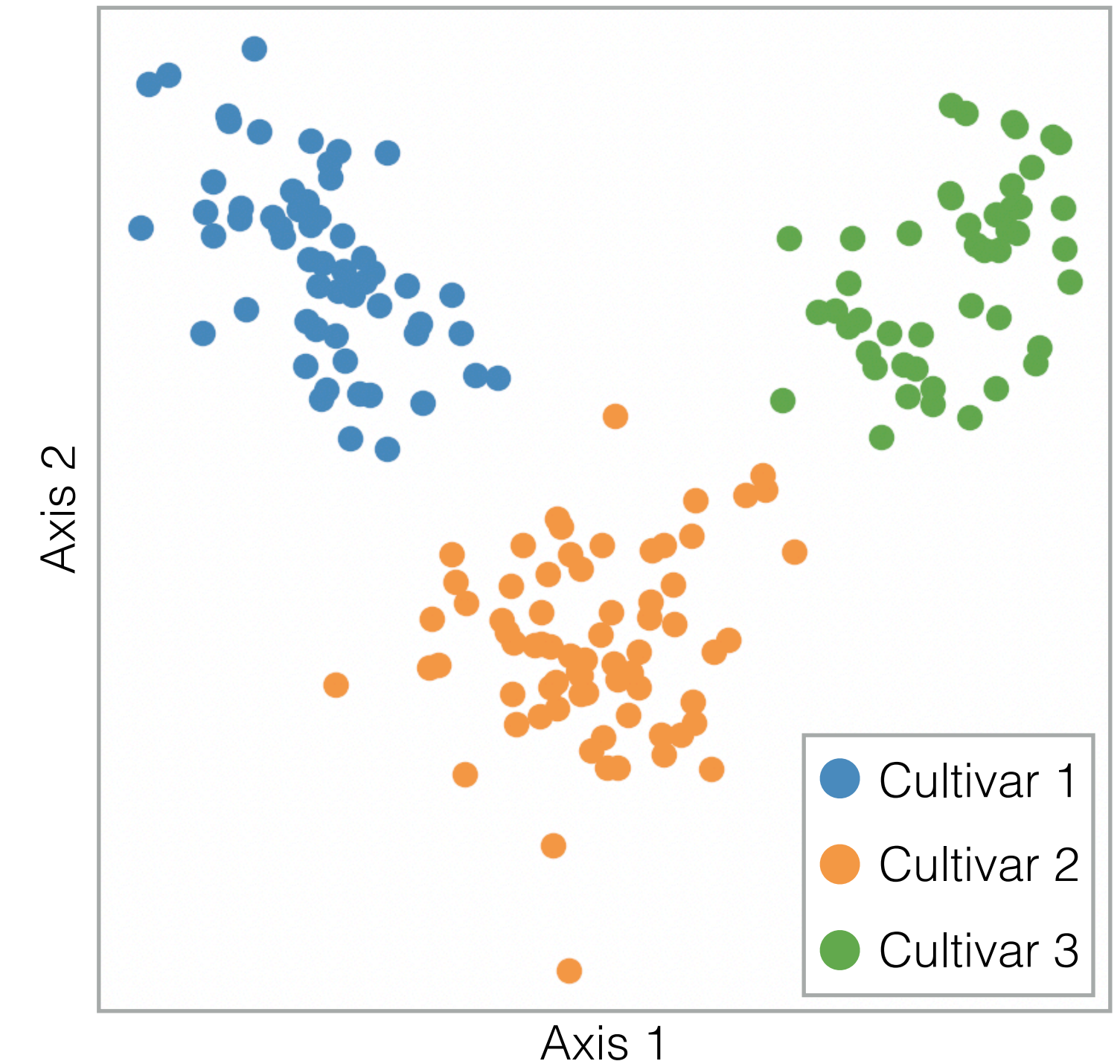
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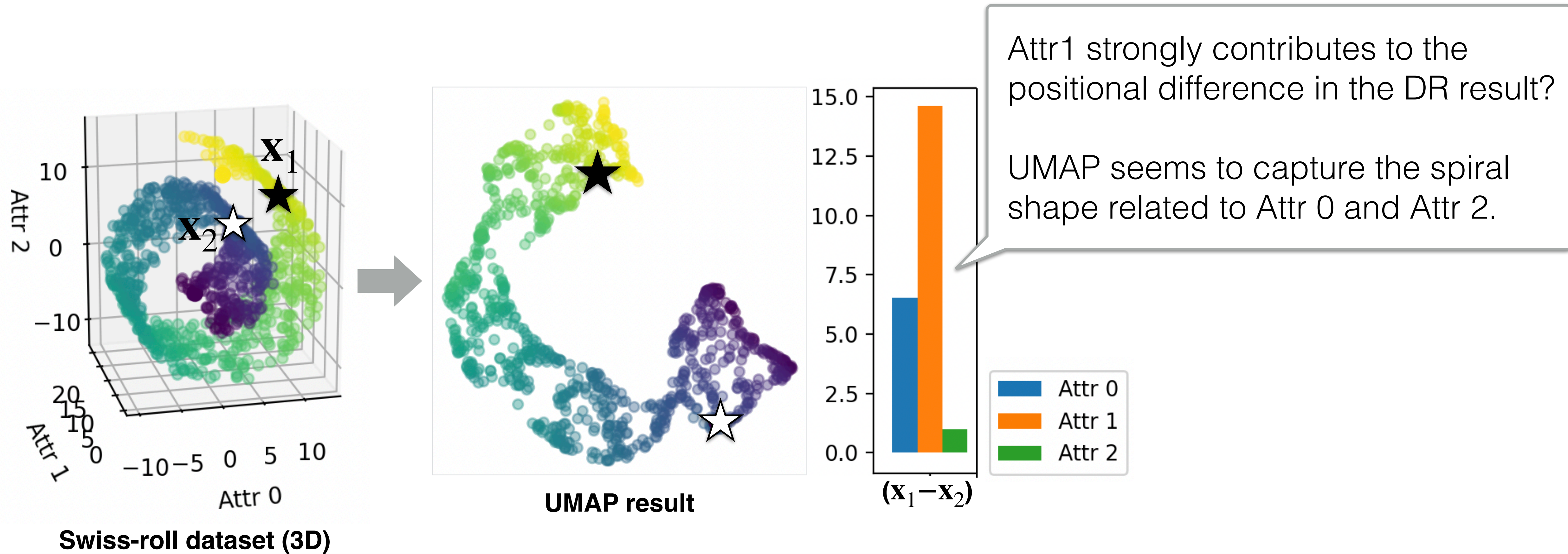
Linear discriminant analysis
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- Interpreting a **lower-dimensional space** **Linear DR**
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Critical problem of observed-level interpretations

- Comparing (groups of) instances in a DR result does not consider how the DR method projected the instances



Existing approaches for DR model/mechanism-level interpretations

- Gradient-based

- Approximately derive **gradient** of each low-dimensional coordinate with respect to their high-dimensional coordinate and use the gradient to understand the DR result
e.g., Corbugy et al., “Gradient-based explanation for non-linear non-parametric dimensionality reduction.” *Data Mining and Knowledge Discovery*, 2024.
Faust et al., “DimReader: Axis lines that explain non-linear projections.” *IEEE TVCG*, 2019.

- Parametric nonlinear DR

- Use **neural networks-based DR** optimization to produce a parametric mapping ($f_{\theta} : \mathbf{X} \rightarrow \mathbf{Y}$) and then interpret results based on the mapping
e.g., Zang et al., “DMT-EV: An explainable deep network for dimension reduction.” *IEEE TVCG*, 2024.
- Build a **substitute parametric model** that mimics a mapping from the original to low-dimensional space or from the low-dimensional to original space
e.g., Espadoto et al., “UnProjection: Leveraging inverse-projections for visual analytics of high-dimensional data.” *IEEE TVCG*, 2023.

Existing approaches for DR model/mechanism-level interpretations

- Gradient-based

- Approximately derive **gradient** of each low-dimensional coordinate with respect to their high-dimensional coordinate and use the gradient to understand the DR result
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Gradient-based interpretation

Corbugy et al., “Gradient-based explanation for non-linear non-parametric dimensionality reduction.”
Data Mining and Knowledge Discovery, 2020.

- t-SNE’s objective function

$$\arg \min_{\mathbf{Y}} \text{KL-Divergence}(\mathbf{P}, \mathbf{Q})$$

\mathbf{P} : Similarities in the original space

\mathbf{Q} : Similarities in the low-dimensional space

$$p_{ij} = \frac{1}{2n}(p_{i|j} + p_{j|i})$$

$$p_{j|i} = \frac{e^{-\frac{1}{2}\|\mathbf{x}_i - \mathbf{x}_j\|_2^2 \sigma_i^{-2}}}{\sum_{\ell \neq i} e^{-\frac{1}{2}\|\mathbf{x}_i - \mathbf{x}_\ell\|_2^2 \sigma_i^{-2}}}$$

$$q_{ij} = \frac{(1 + \|\mathbf{y}_i - \mathbf{y}_j\|_2^2)^{-1}}{\sum_{r=1}^n \sum_{\ell \neq r} (1 + \|\mathbf{y}_r - \mathbf{y}_\ell\|_2^2)^{-1}}$$

- Apply Gould et al.’s approximation formula to derive the gradient of the low-dimensional coordinate, \mathbf{y}_i , with respect to the original data, \mathbf{x}_i

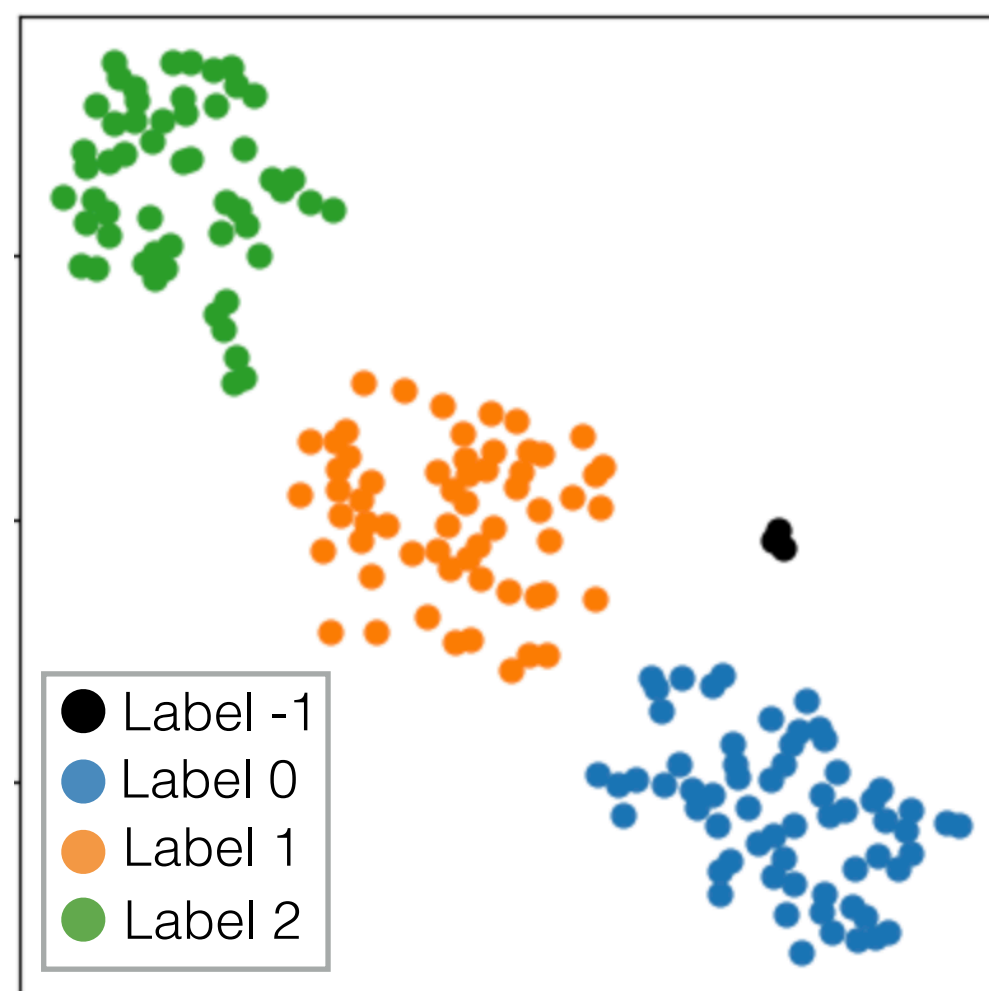
Gould et al., “On differentiating parameterized argmin and argmax problems with application to bi-level optimization.” *arXiv*, 2016.

$$\nabla_{\mathbf{y}_i} f(\mathbf{x}_i, \mathbf{y}_i) = 4 \sum_{j \neq i} (p_{ij} - q_{ij})(1 + \|\mathbf{y}_i - \mathbf{y}_j\|_2^2)^{-1} (\mathbf{y}_i - \mathbf{y}_j)$$

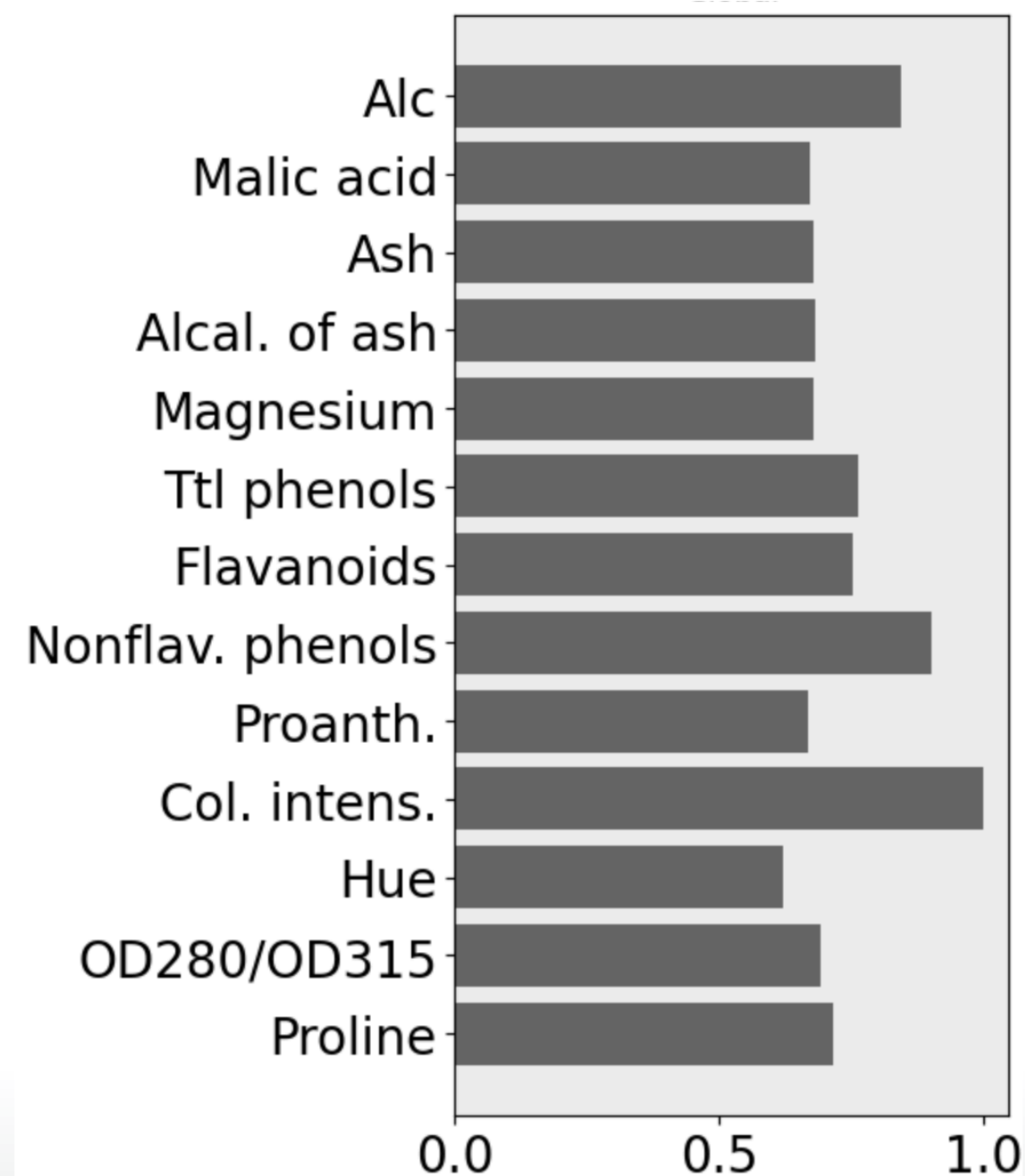
Gradient-based interpretation

Corbugy et al., “Gradient-based explanation for non-linear non-parametric dimensionality reduction.”
Data Mining and Knowledge Discovery, 2020.

- Complementary tools
 - Global feature importance
 - Compute attribute importances by summing the lengths of the gradient vectors at the coordinates of all instances in the DR result



t-SNE result

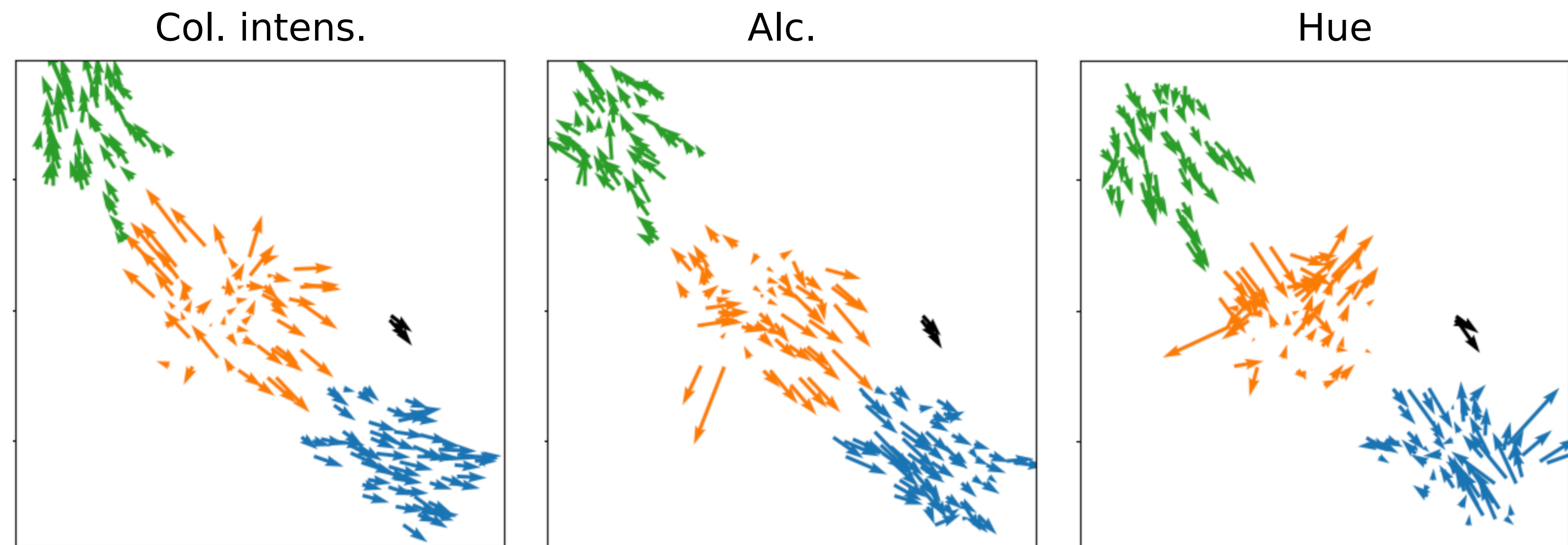
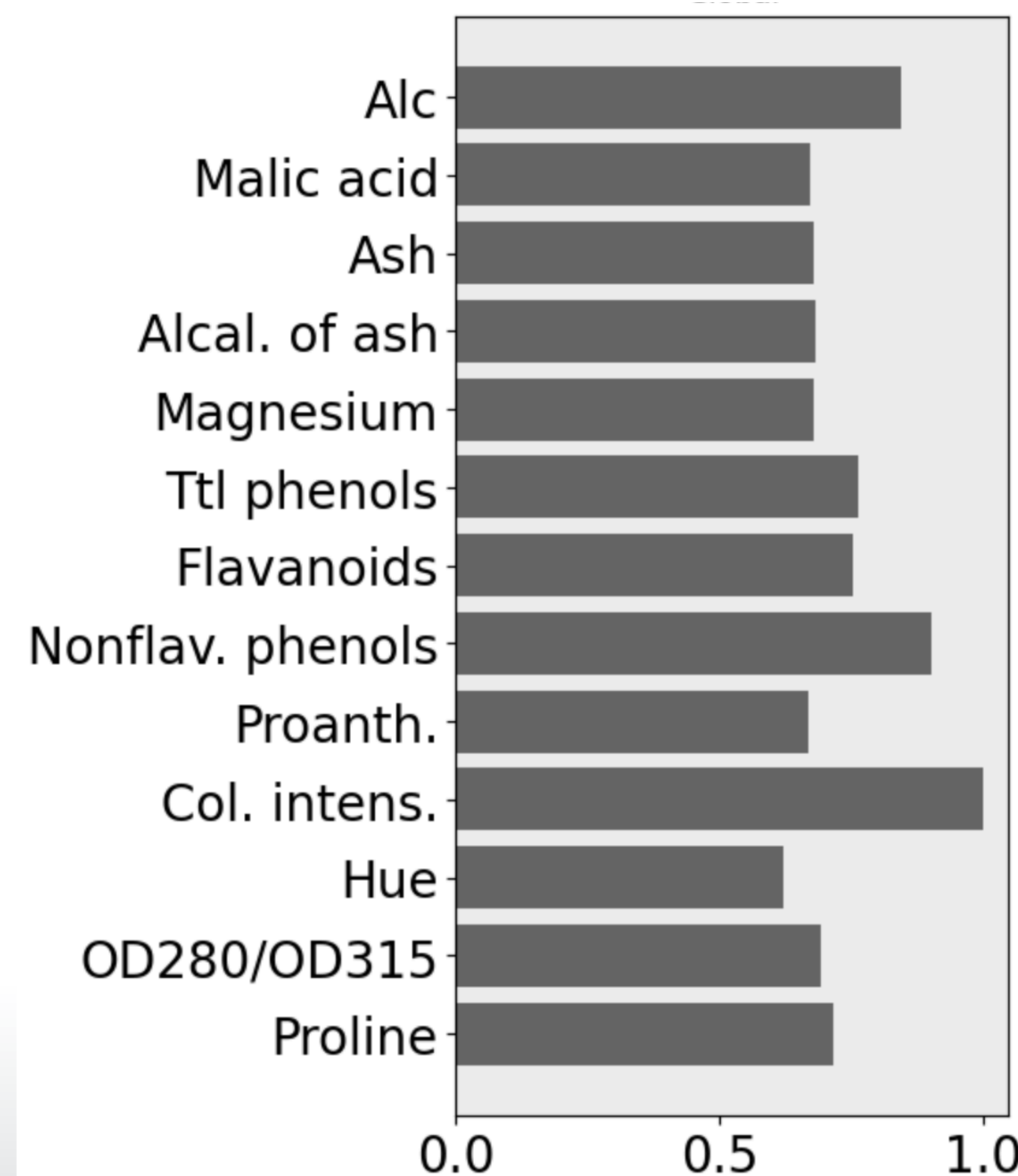


Global feature importance

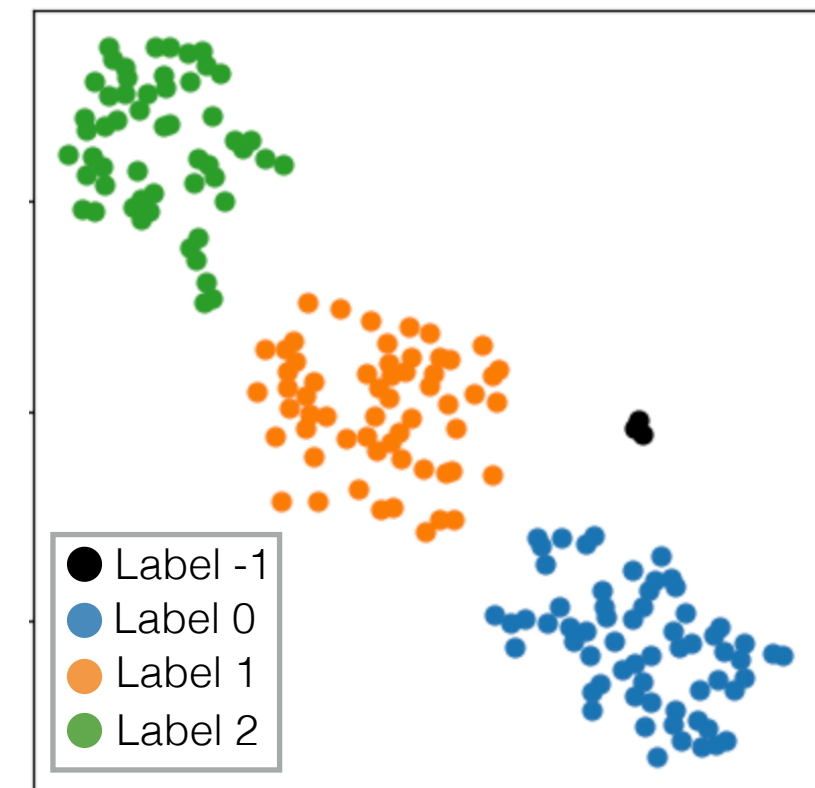
Gradient-based interpretation

Corbugy et al., “Gradient-based explanation for non-linear non-parametric dimensionality reduction.”
Data Mining and Knowledge Discovery, 2020.

- Complementary tools
 - Global feature importance
 - Vector field visualization for a selected attribute



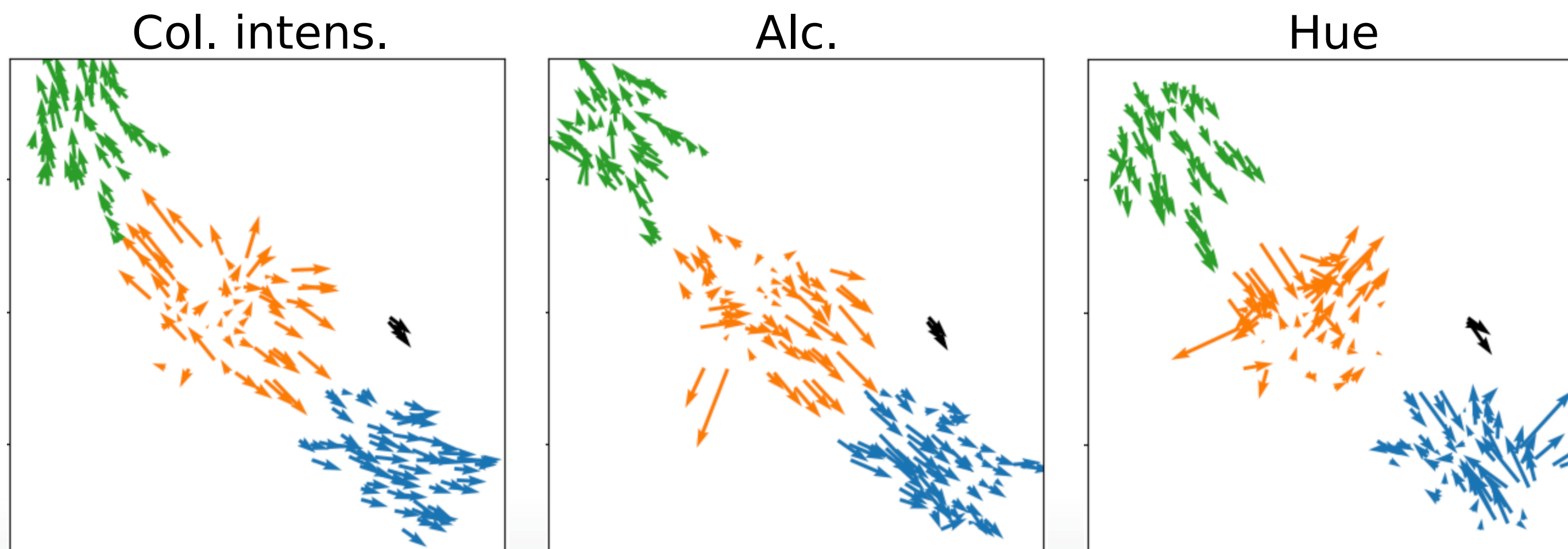
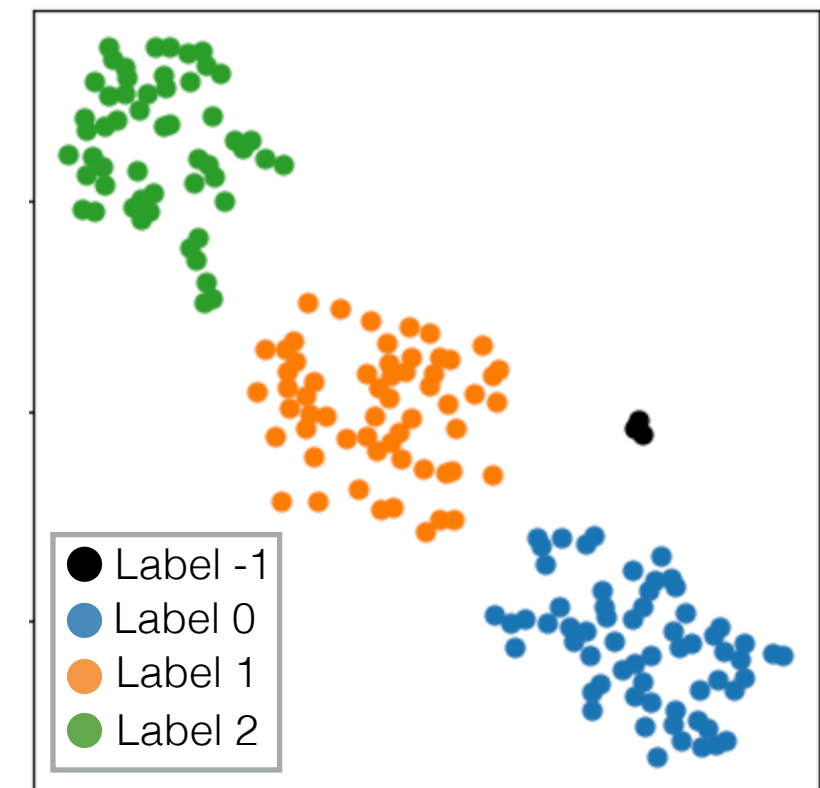
Vector field visualizations



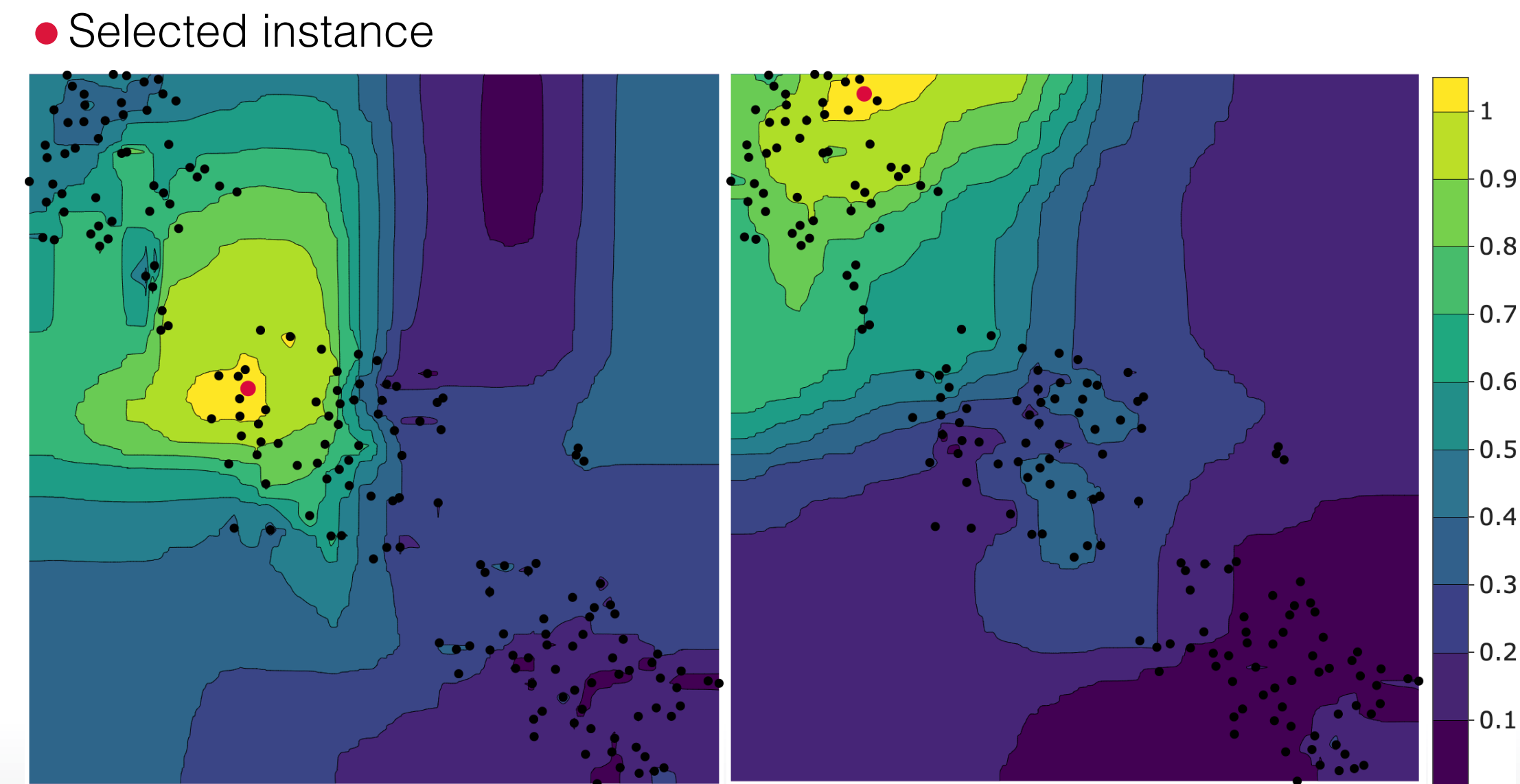
Gradient-based interpretation

Corbugy et al., “Gradient-based explanation for non-linear non-parametric dimensionality reduction.”
Data Mining and Knowledge Discovery, 2020.

- Complementary tools
 - Global feature importance
 - Vector field visualization for a selected attribute
 - Explanation scope from a selected instance
 - Based on similarities of the gradient vectors



Vector field visualizations

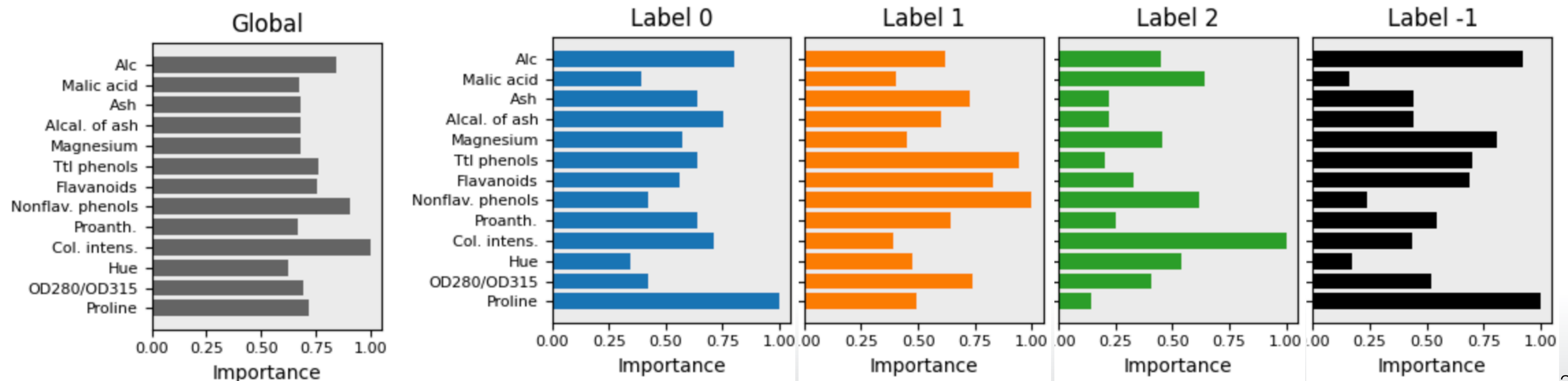
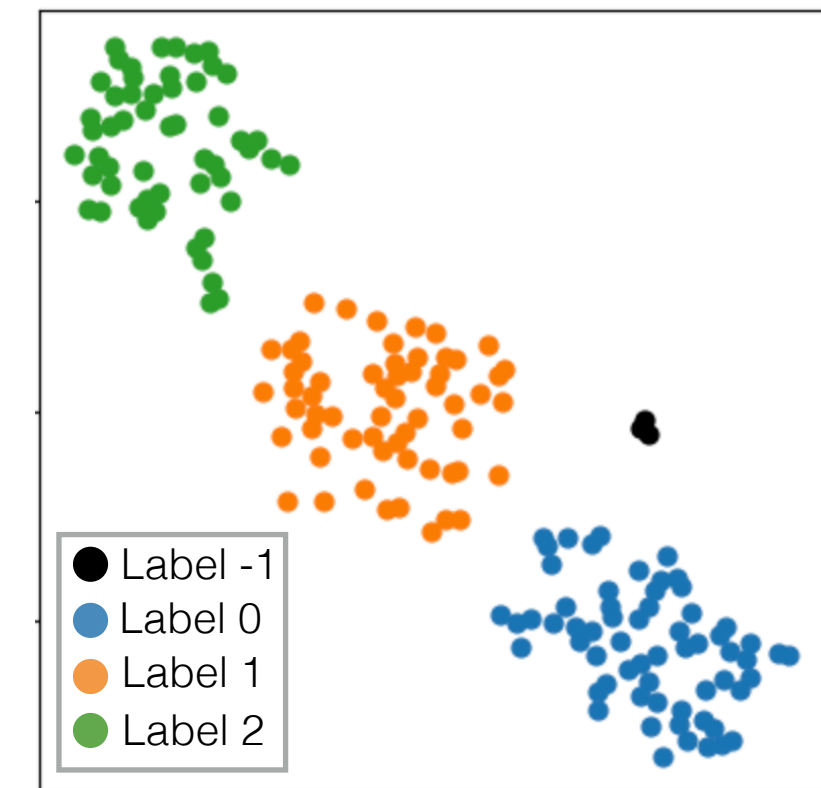


Explanation scope visualizations

Gradient-based interpretation

Corbugy et al., “Gradient-based explanation for non-linear non-parametric dimensionality reduction.”
Data Mining and Knowledge Discovery, 2020.

- Complementary tools
 - Global feature importance
 - Vector field visualization for a selected attribute
 - Explanation scope from a selected instance
 - Cluster-level feature importance (newly made for this tutorial)
 - The sum of each cluster's gradient vector lengths



Coding exercise (20 minutes)

- Colab notebook link: <https://bit.ly/4kCNPWD>
- Select one dataset
- Apply t-SNE
- Apply the gradient-based interpretation method
- Use the complementary visualizations to interpret the t-SNE result
- Compare the interpretation result with the previous coding exercise results (e.g., PCA)



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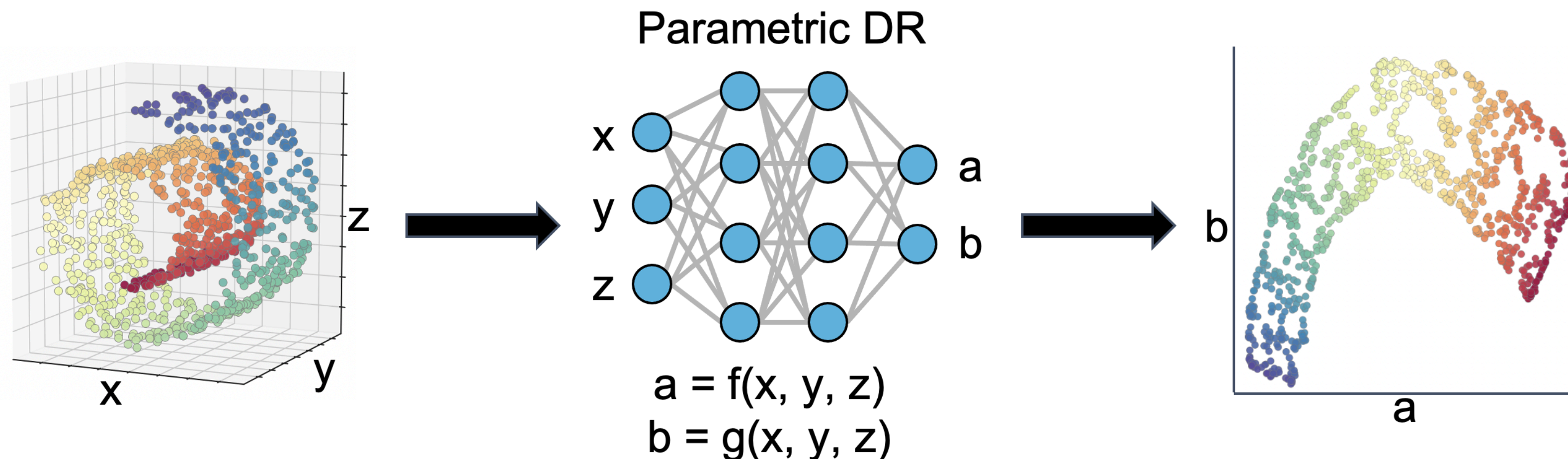
Parametric nonlinear DR

- (typically) uses neural networks to have a parametric mapping from the original space to the low-dimensional space
 - Parametric UMAP, parametric t-SNE, etc.

Sainburg et al., “Parametric UMAP embeddings for representation and semisupervised learning.” *Neural Computation*, 2021.

Van der Maaten, “Learning a parametric embedding by preserving local structure.” *PMLR*, 2009.

Hinterreiter et al., “ParaDime: A framework for parametric dimensionality reduction.” *CGF*, 2023.



- Due to the parametric mapping, we can apply various existing interpretation methods designed for deep learning
 - e.g., integrated gradients Sundararajan et al., “Axiomatic Attribution for Deep Networks.” *arXiv*, 2017

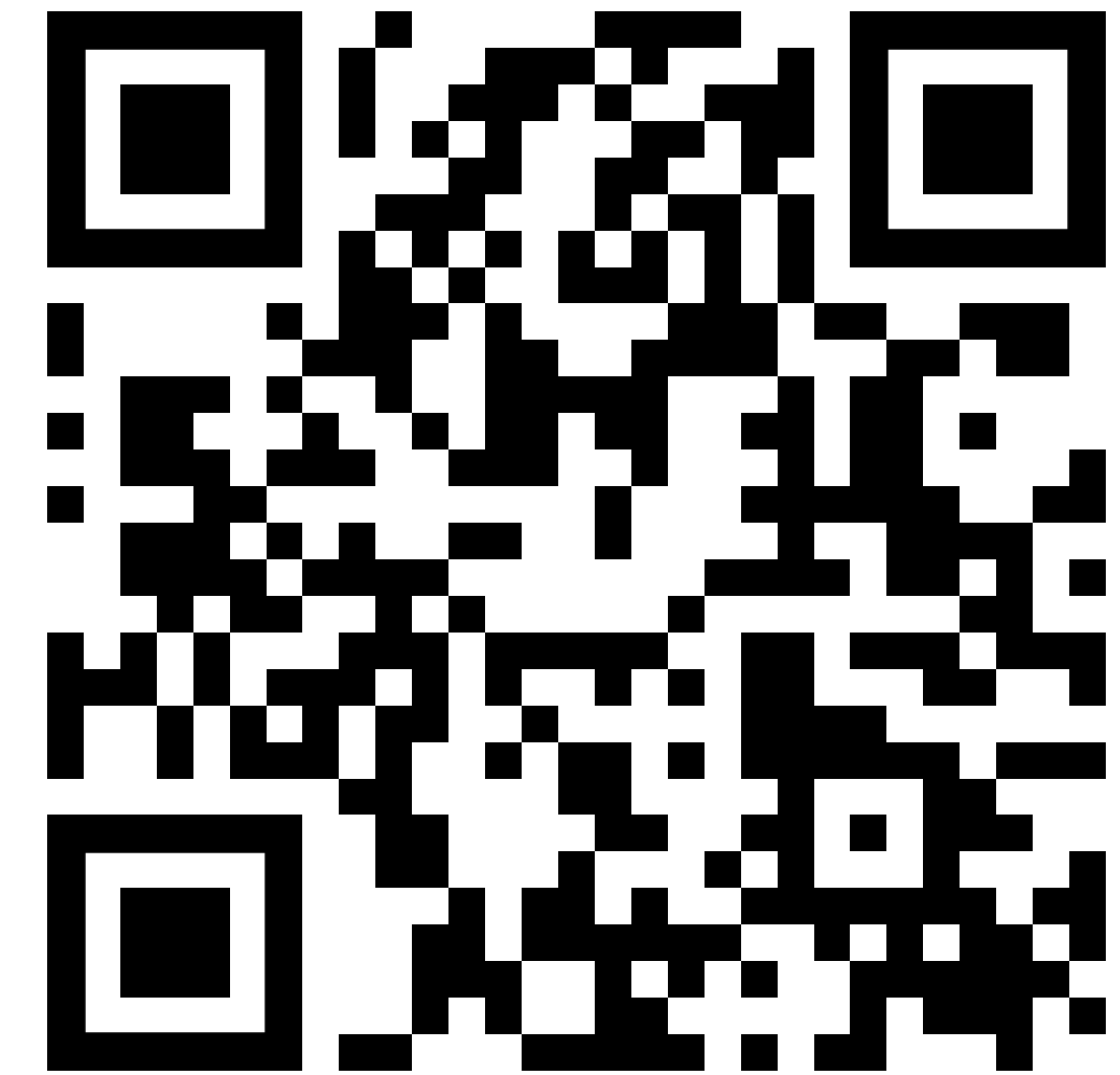
Remaining challenges

- Evaluation
 - How can we say which interpretation methods are better than others?
 - How can we ensure that we interpret a DR result well?
- Limited existing work on the DR model/mechanism-level interpretations
- Limited availability of source code
(no source code, too old to install, no documentation/examples, etc.)
- Many more...

What you learned today

- Fundamentals: Interpretation of dimensionality reduction (DR) results
 - Linear DR
 - **Axis level**
 - Nonlinear DR
 - **Observed-pattern level**
 - Univariate focus
 - Composite variable focus
 - Classifier-based
 - Local pattern correlation
 - **Model-mechanism level**
 - Gradient-based
 - Parametric nonlinear DR
- Practices: Interpretations with existing libraries

Tutorial Materials



<https://hyeonword.com/dr-tutorial/>

References

Python libraries

- PCA, LDA, t-SNE: Scikit-learn <https://scikit-learn.org/>
- ccPCA: <https://github.com/takanori-fujiwara/ccpca>
- ULCA: <https://github.com/takanori-fujiwara/ulca>
- DimVis: <https://github.com/parisa-salmanian/DimVis>
- t-SNE gradients explanation: https://github.com/sady410/tsne_gradients_explanation

Referred papers in today's slides

- Bibal et al., “IXVC: An interactive pipeline for explaining visual clusters in dimensionality reduction visualizations with decision trees.” *Array*, 2021.
- Chatzimpampas et al., “t-viSNE: Interactive Assessment and Interpretation of t-SNE Projections.” *IEEE TVCG*, 2020.
- Corbugy et al., “Gradient-based explanation for non-linear non-parametric dimensionality reduction.” *Data Mining and Knowledge Discovery*, 2020.
- Espadoto et al., “UnProjection: Leveraging inverse-projections for visual analytics of high-dimensional data.” *IEEE TVCG*, 2023.
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- Fujiwara et al., “Supporting analysis of dimensionality reduction results with contrastive learning.” *IEEE TVCG*, 2020.
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- Hinterreiter et al., “ParaDime: A framework for parametric dimensionality reduction.” *CGF*, 2023.
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- Van der Maaten, “Learning a parametric embedding by preserving local structure.” *PMLR*, 2009.
- Sundararajan et al., “Axiomatic Attribution for Deep Networks.” *arXiv*, 2017.
- Wen et al., “Robust sparse linear discriminant analysis.” *IEEE Trans. Circuits Syst. Video Technol.*, 2018.
- Zang et al., “DMT-EV: An explainable deep network for dimension reduction.” *IEEE TVCG*, 2024.
- Zou et al., “Sparse principal component analysis.” *J. Comput. Graph. Stat.*, 2006