

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

Part 2:

Interpretation of Dimensionality Reduction Results

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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



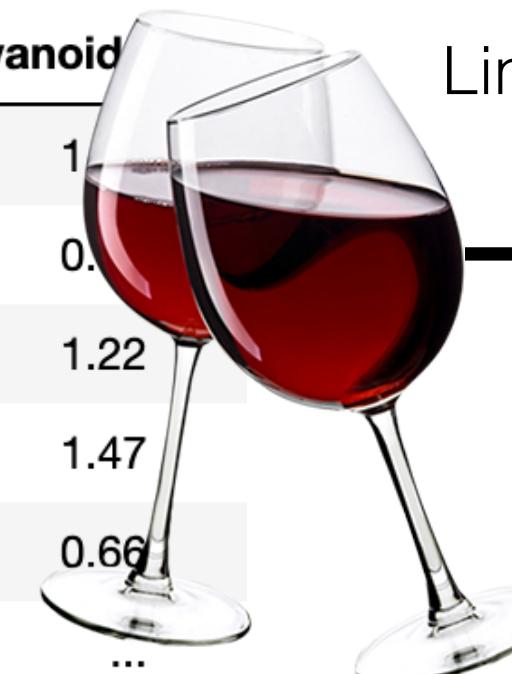
<https://hyeonword.com/dr-tutorial/>

Interpretation of dimensionality reduction (DR) results

Wine dataset (13D)

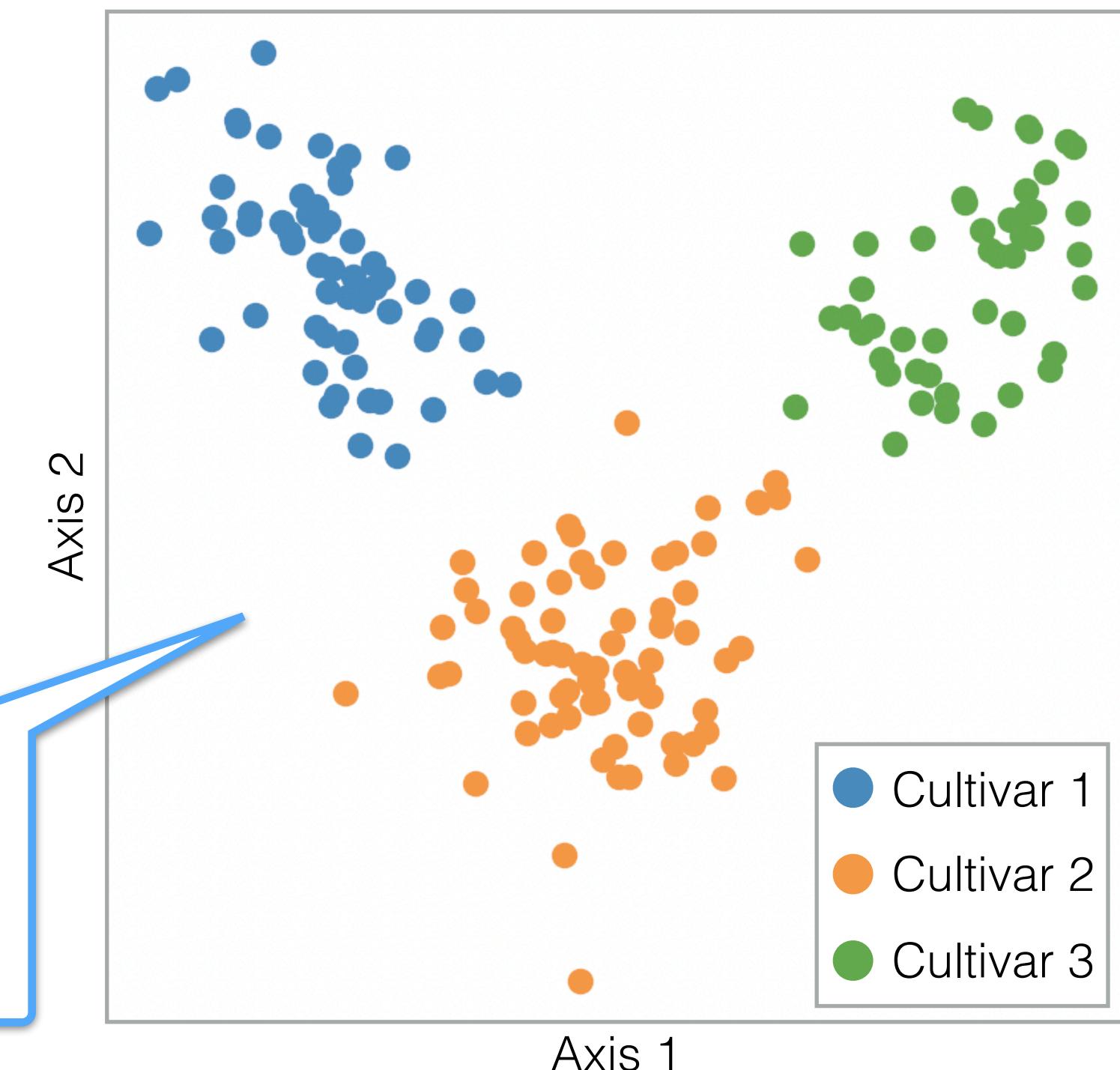
	alchol	malic_acid	ash	alcalinity_ash	magnesium	total_phenols	flavanoid
0	1.52	-0.56	0.23	-1.17	1.91	0.81	1.00
1	0.25	-0.50	-0.83	-2.49	0.02	0.57	0.00
2	0.20	0.02	1.11	-0.27	0.09	0.81	1.22
3	1.69	-0.35	0.49	-0.81	0.93	2.49	1.47
4	0.30	0.23	1.84	0.45	1.28	0.81	0.66
...

*displayed values are after the standardization



Linear discriminant analysis
LDA

How are they separated?
What are their differences?



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

Linear DR
Nonlinear DR
Nonlinear DR

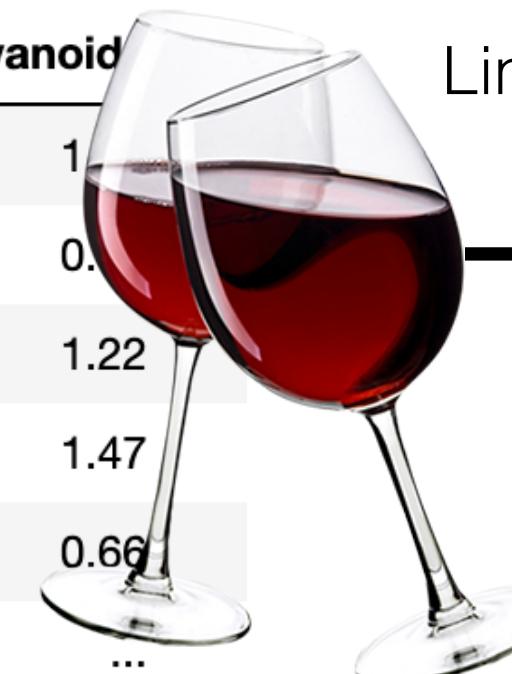
No single best way for the interpretation so far (especially, for nonlinear DR)

Interpretation of dimensionality reduction (DR) results

Wine dataset (13D)

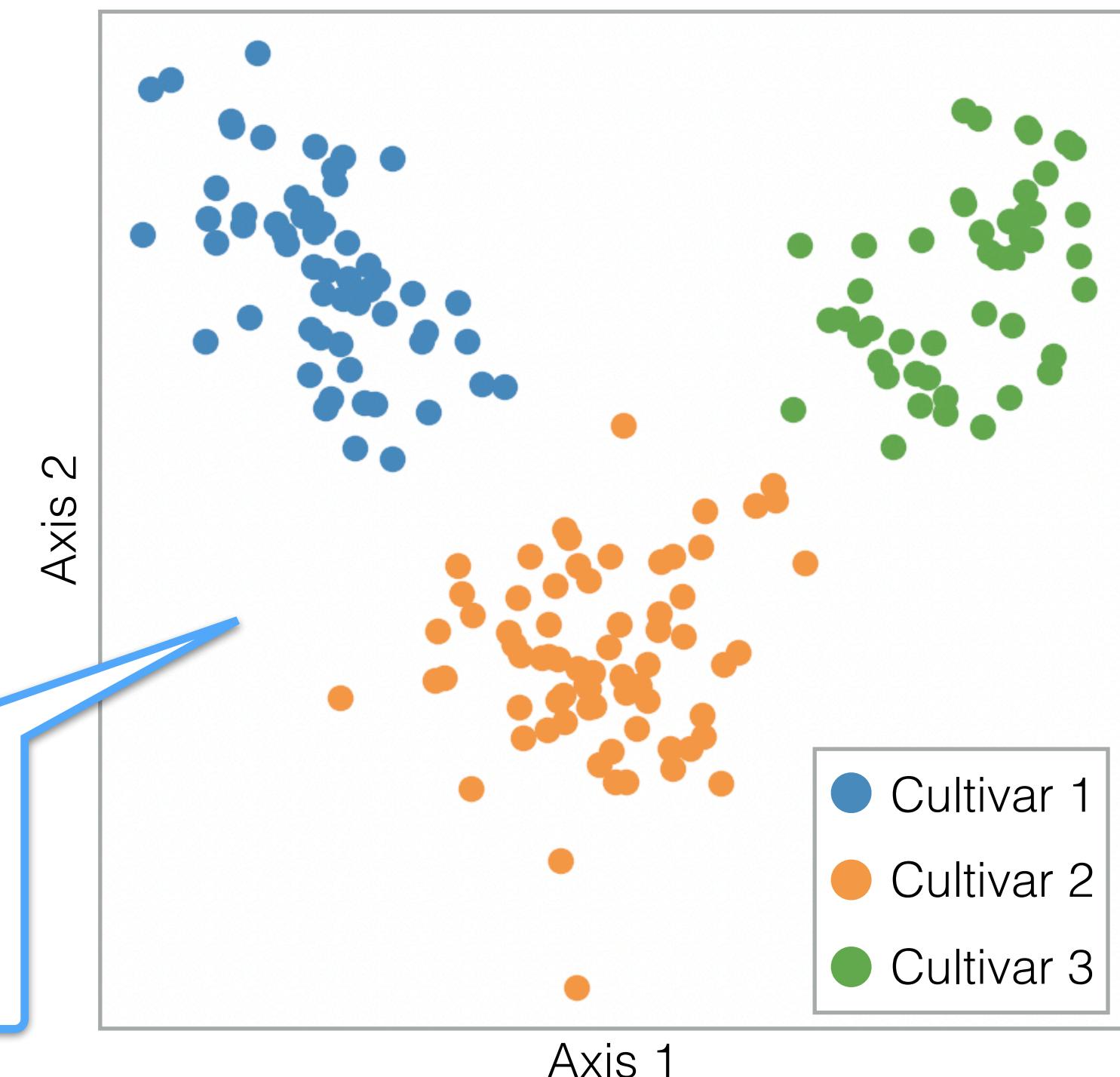
	alchol	malic_acid	ash	alcalinity_ash	magnesium	total_phenols	flavanoid
0	1.52	-0.56	0.23	-1.17	1.91	0.81	1.00
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How are they separated?
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- Interpreting a **lower-dimensional space**

Linear DR

- Interpreting based on **observed patterns** (e.g., clusters) **Nonlinear DR**

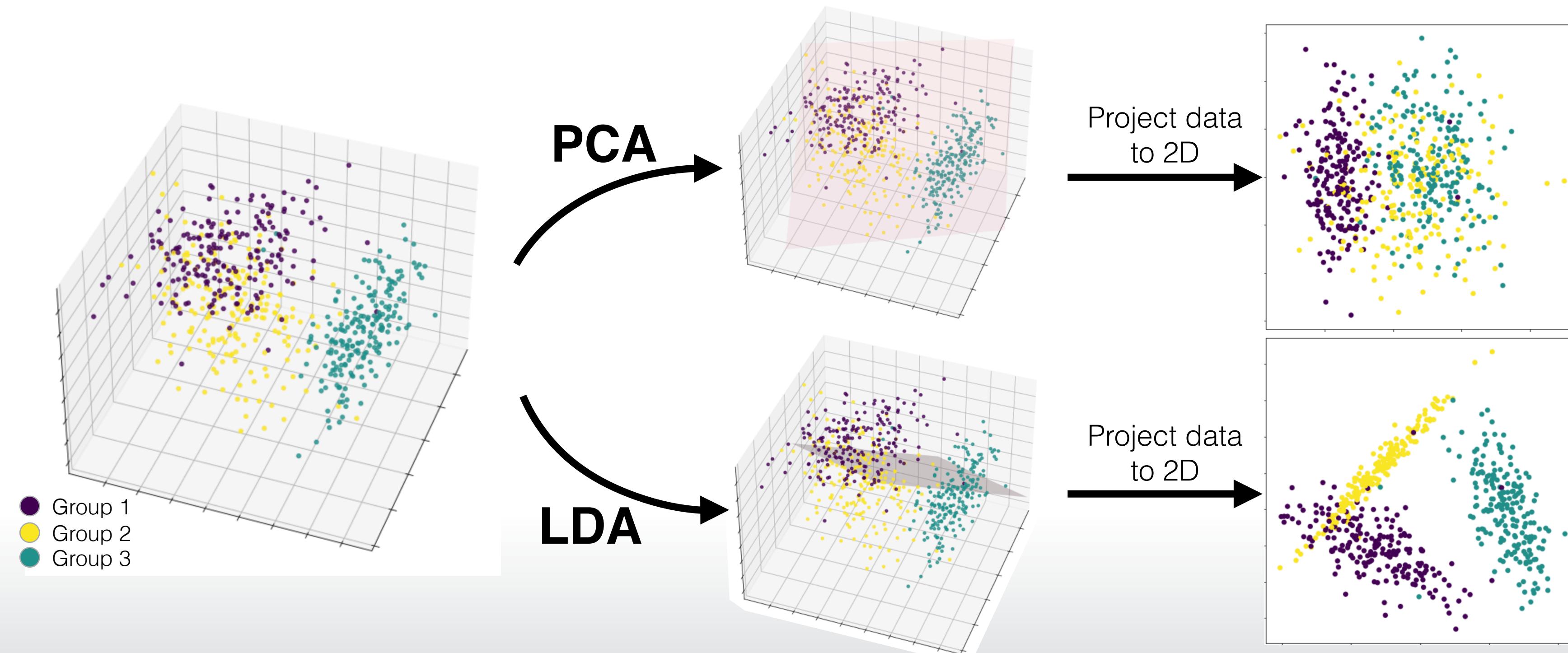
- Interpreting from a DR **model/mechanism** level

Nonlinear DR

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

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	
...	

Linear dimensionality reduction

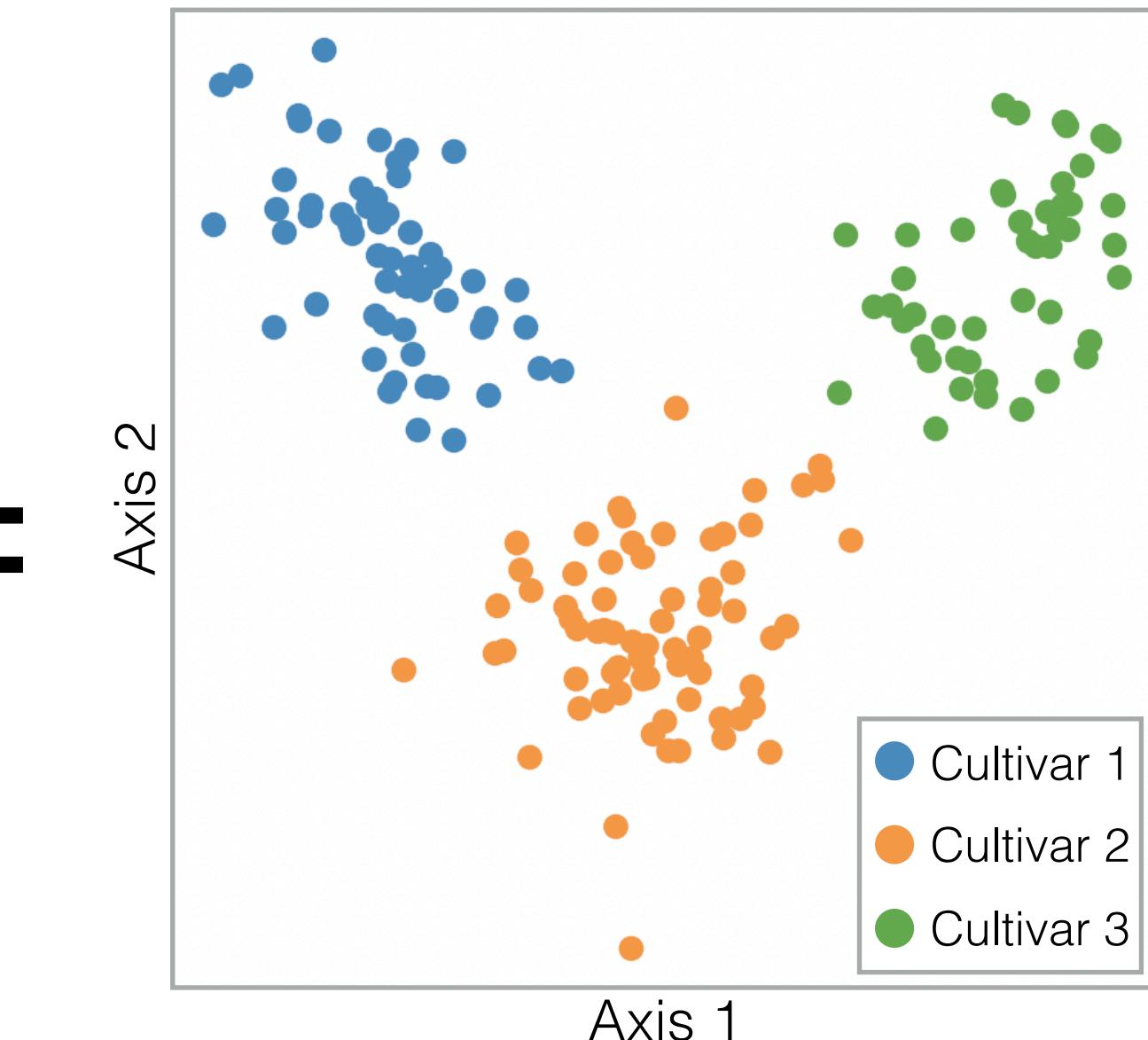
$$X \cdot P = Y$$

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 ...

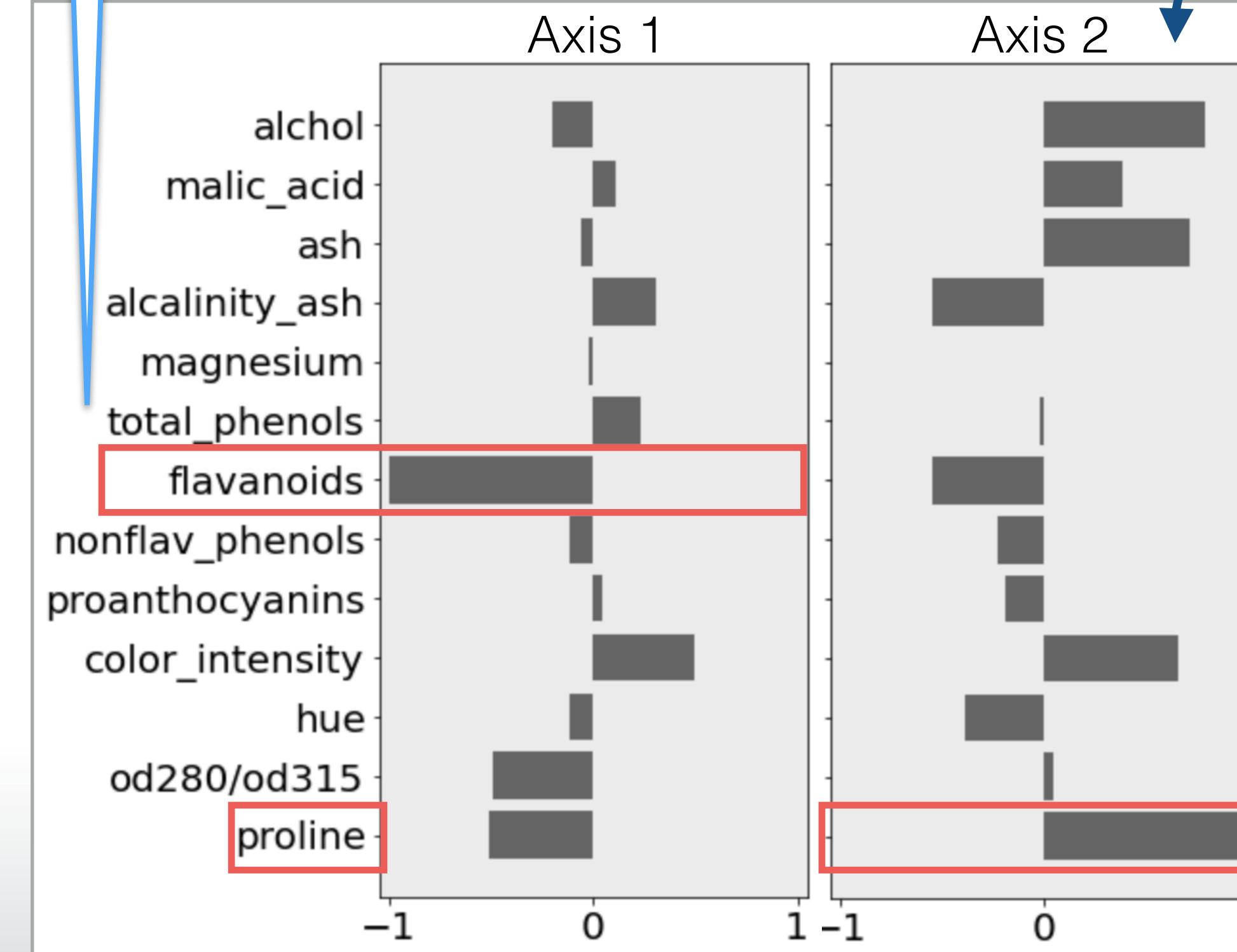
	axis 1	axis 2
alchol	-0.20	0.79
malic_acid	0.11	0.38
ash	-0.06	0.72
alcalinity_ash	0.31	-0.54
magnesium	-0.02	-0.01
total_phenols	0.23	-0.02
flavanoids	-1.00	-0.55
nonflav_phenols	-0.11	-0.23
proanthocyanins	0.05	-0.20
color_intensity	0.50	0.65
hue	-0.11	-0.39
od280/od315	-0.50	0.04
proline	-0.51	1.00



Interpreting the axes

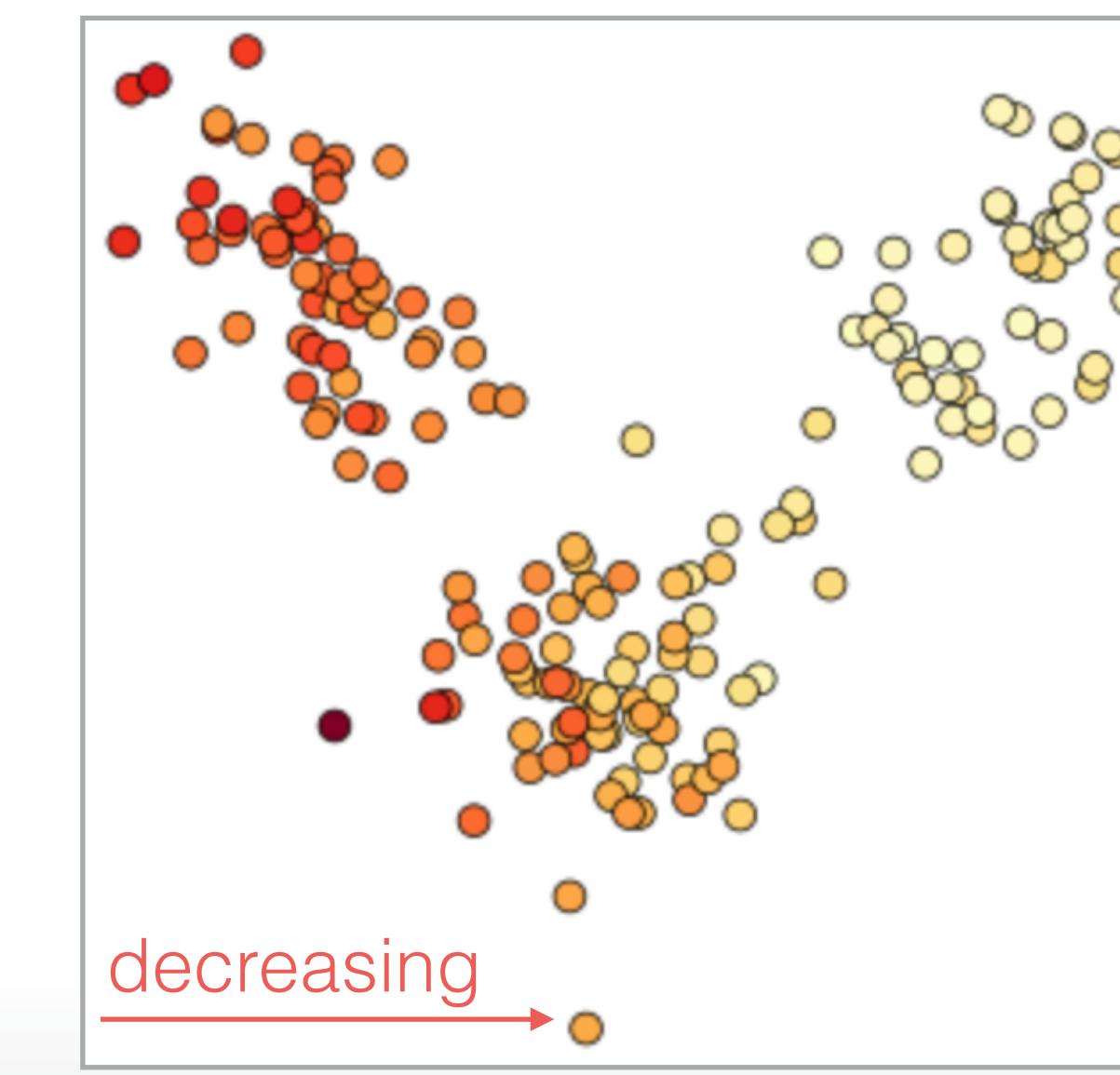
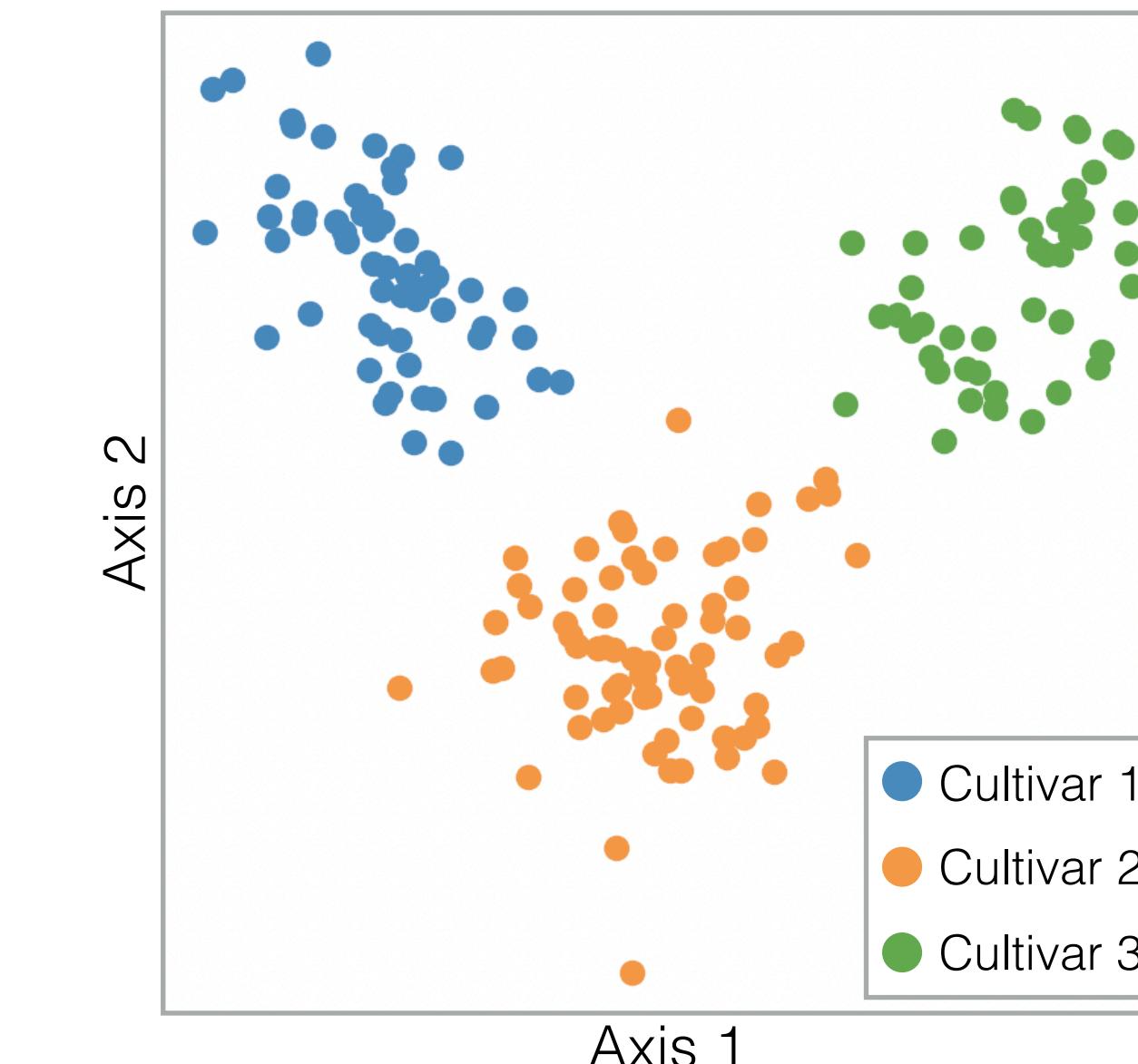
Axes 1 and 2 should be highly influenced by **flavanoids** and **proline**, respectively

Visualize

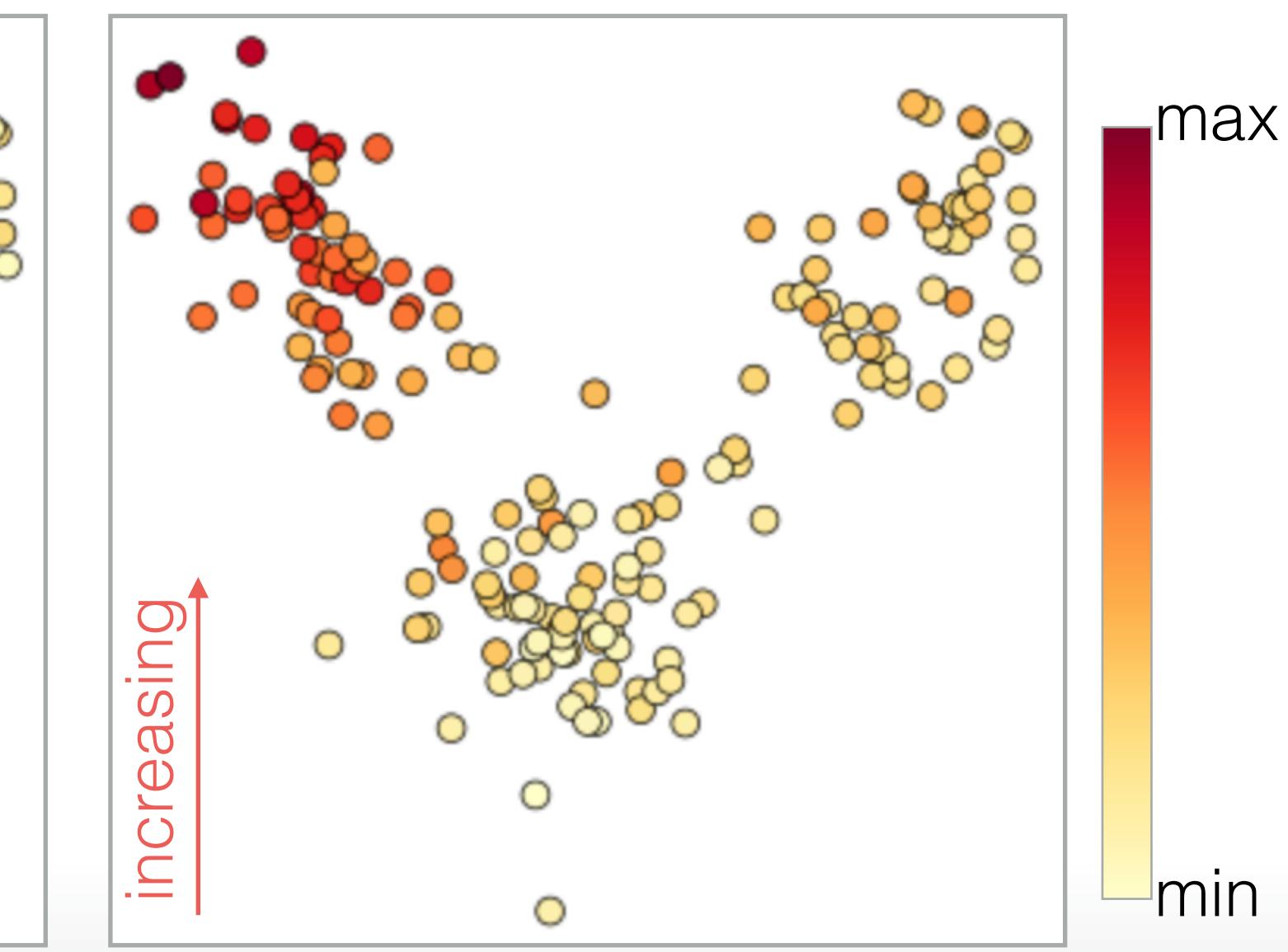


	axis 1	axis 2
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nonflav_phenols	-0.11	-0.23
proanthocyanins	0.05	-0.20
color_intensity	0.50	0.65
hue	-0.11	-0.39

LDA result

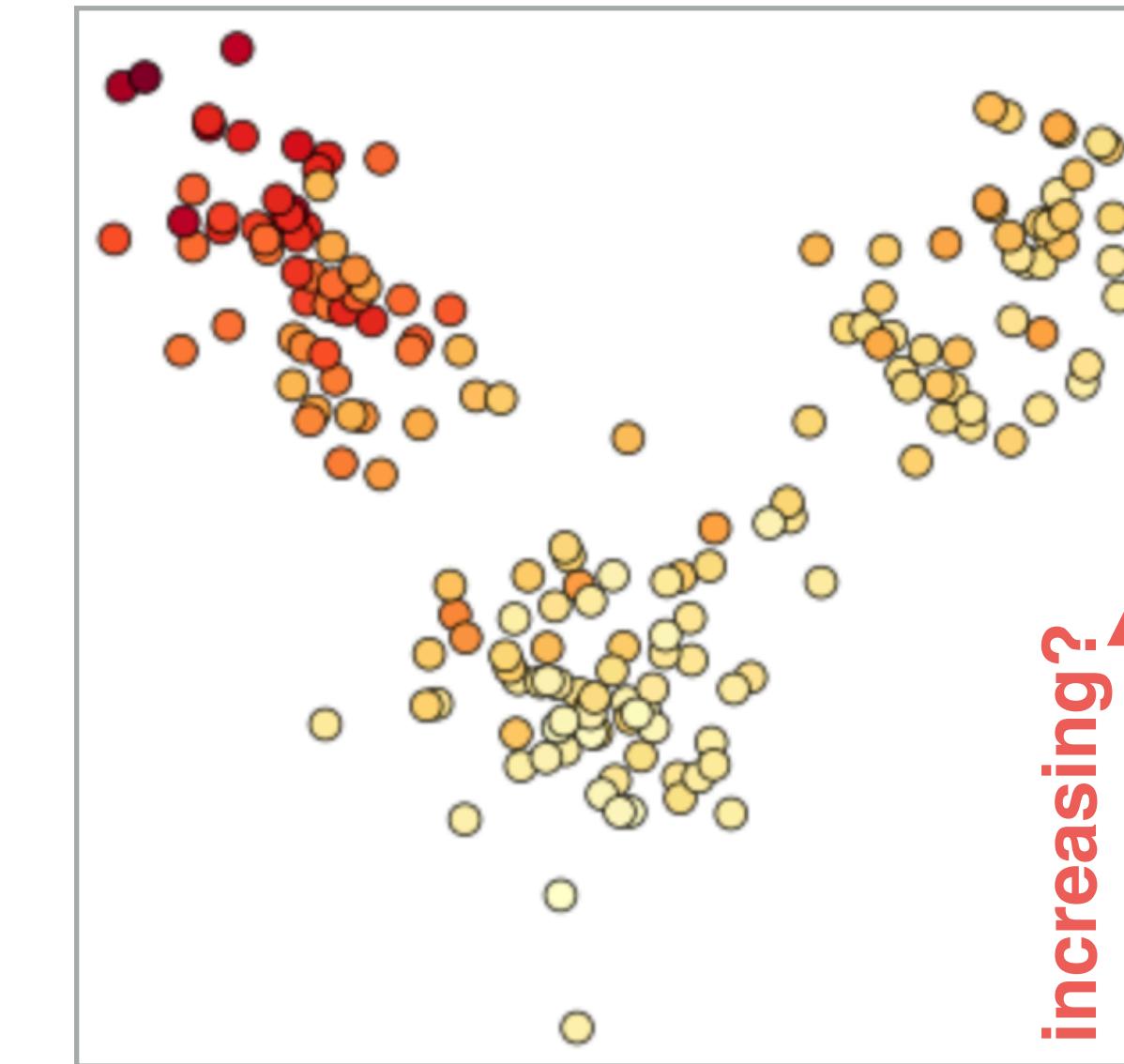
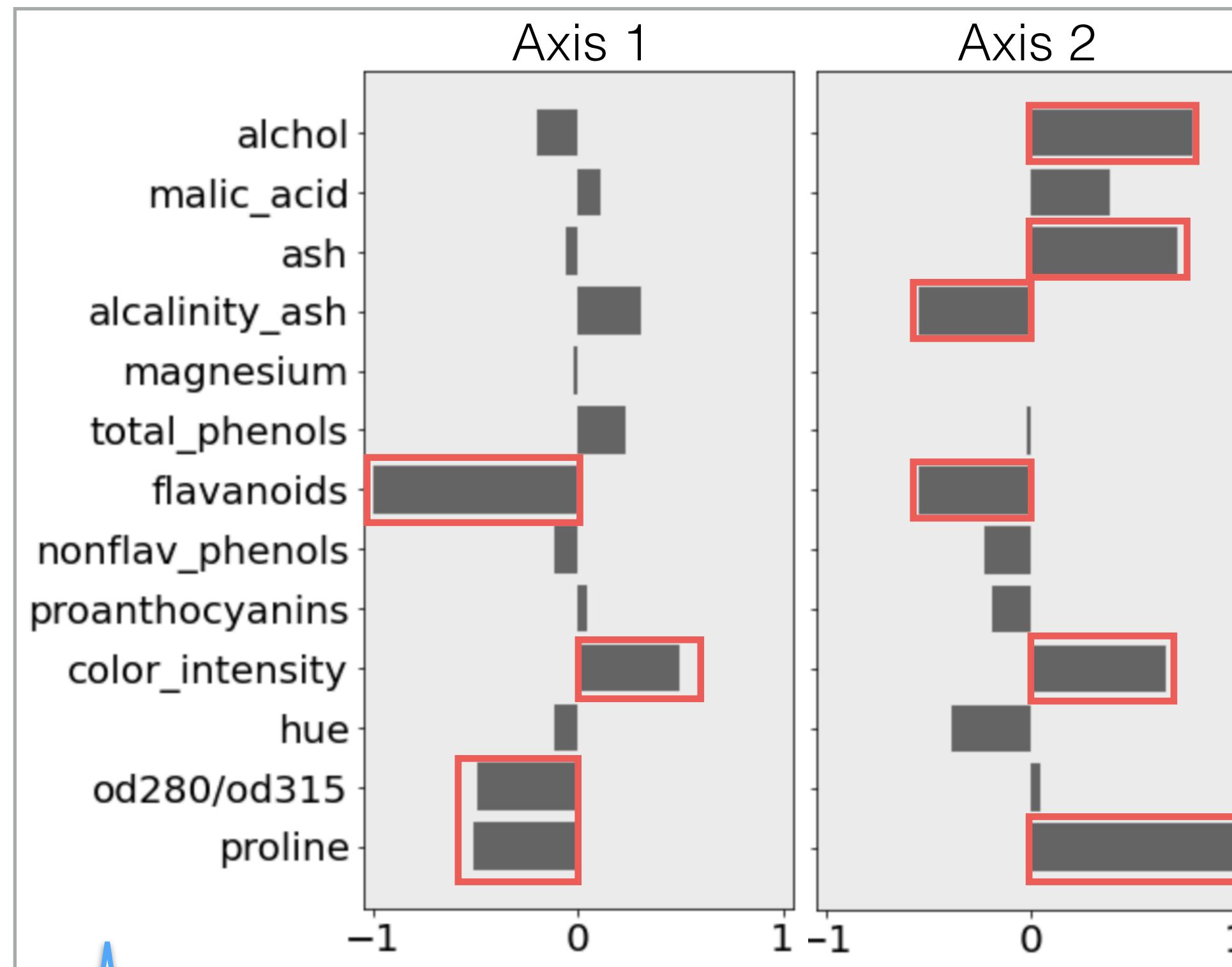


Colored by flavanoids

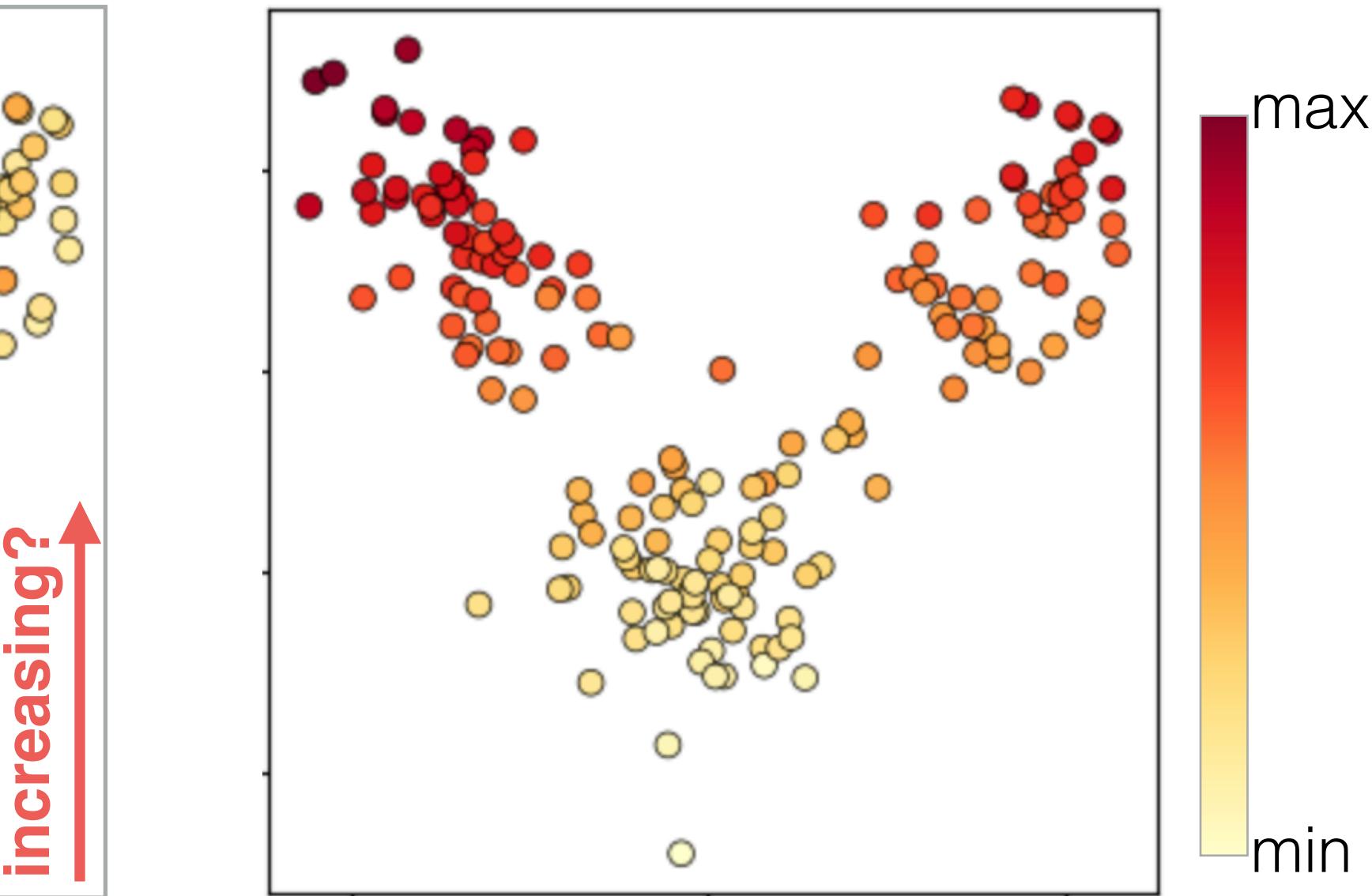


Colored by proline

Interpreting the axes



Colored by proline
(univariate)



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

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

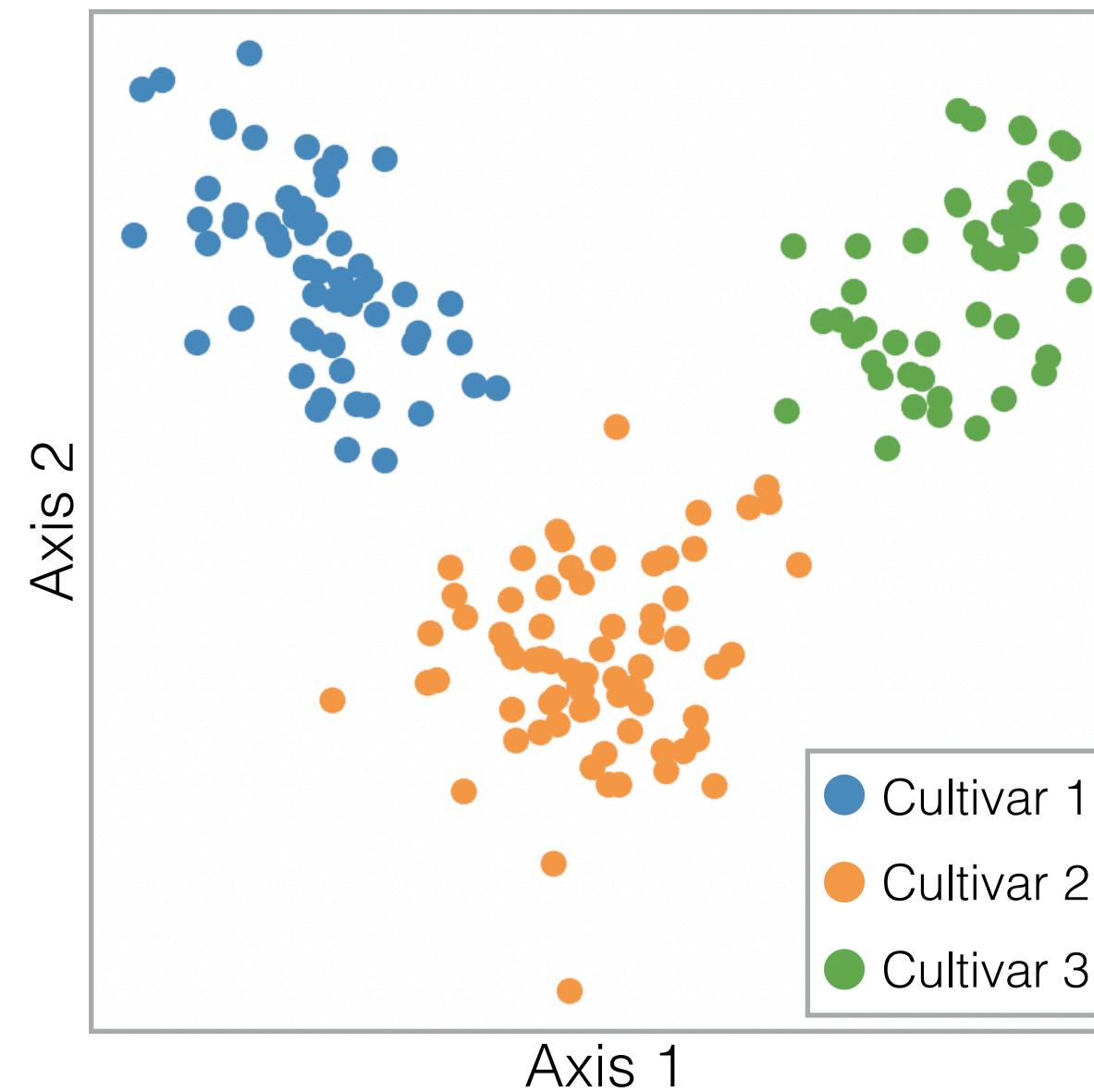
Do you think linear DR is still explainable if there are many attributes (e.g., 100)?

Sparse linear DR

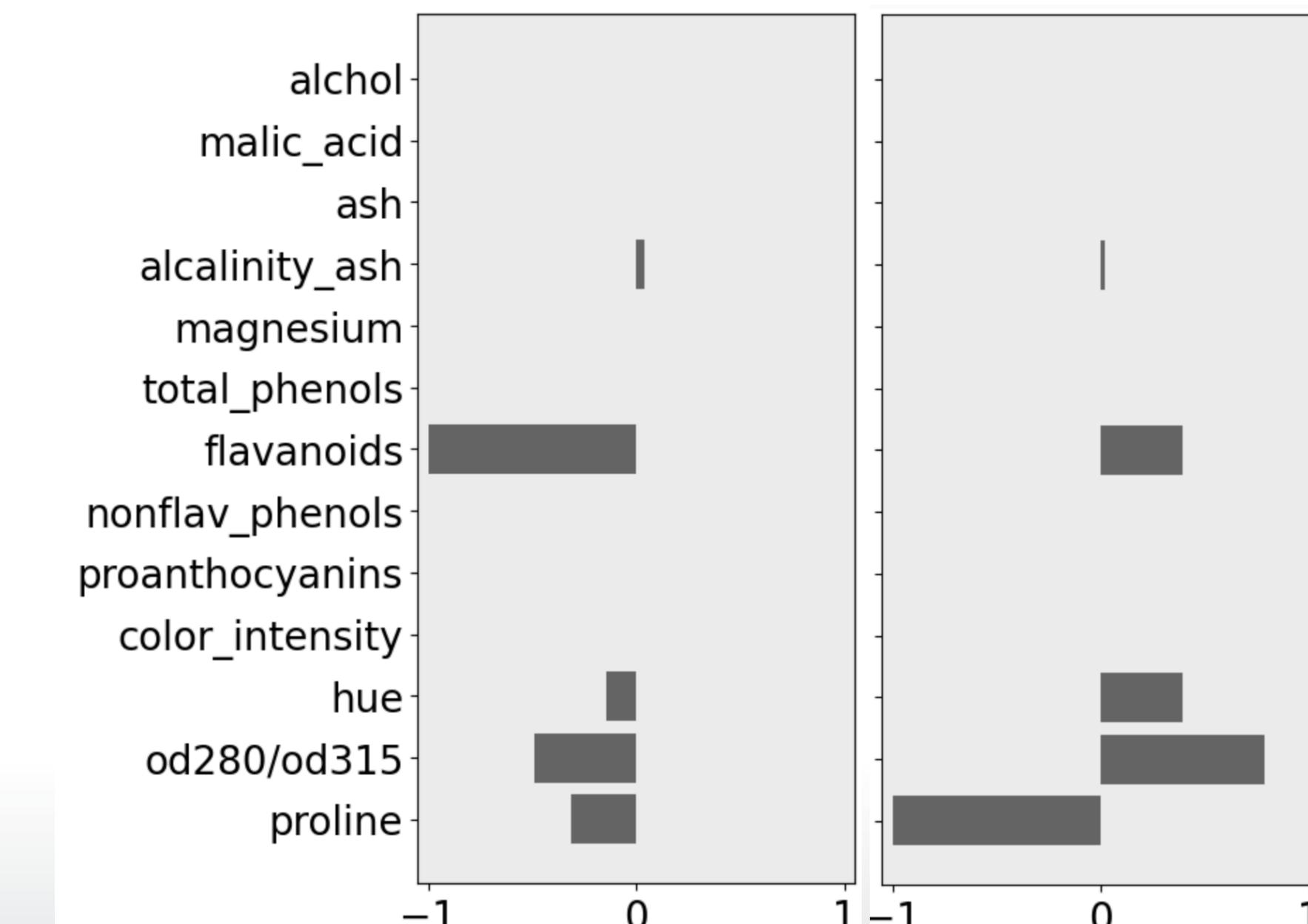
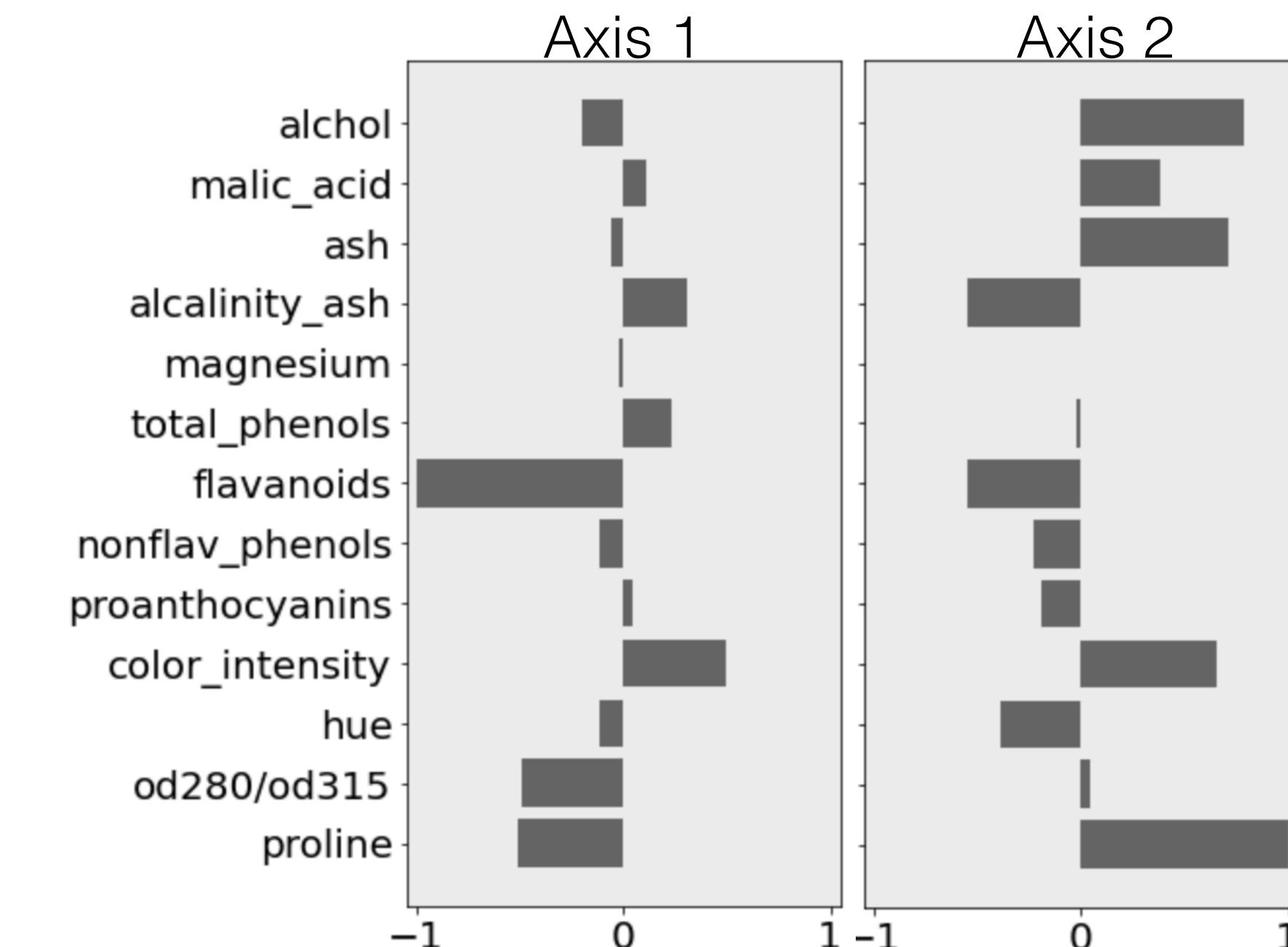
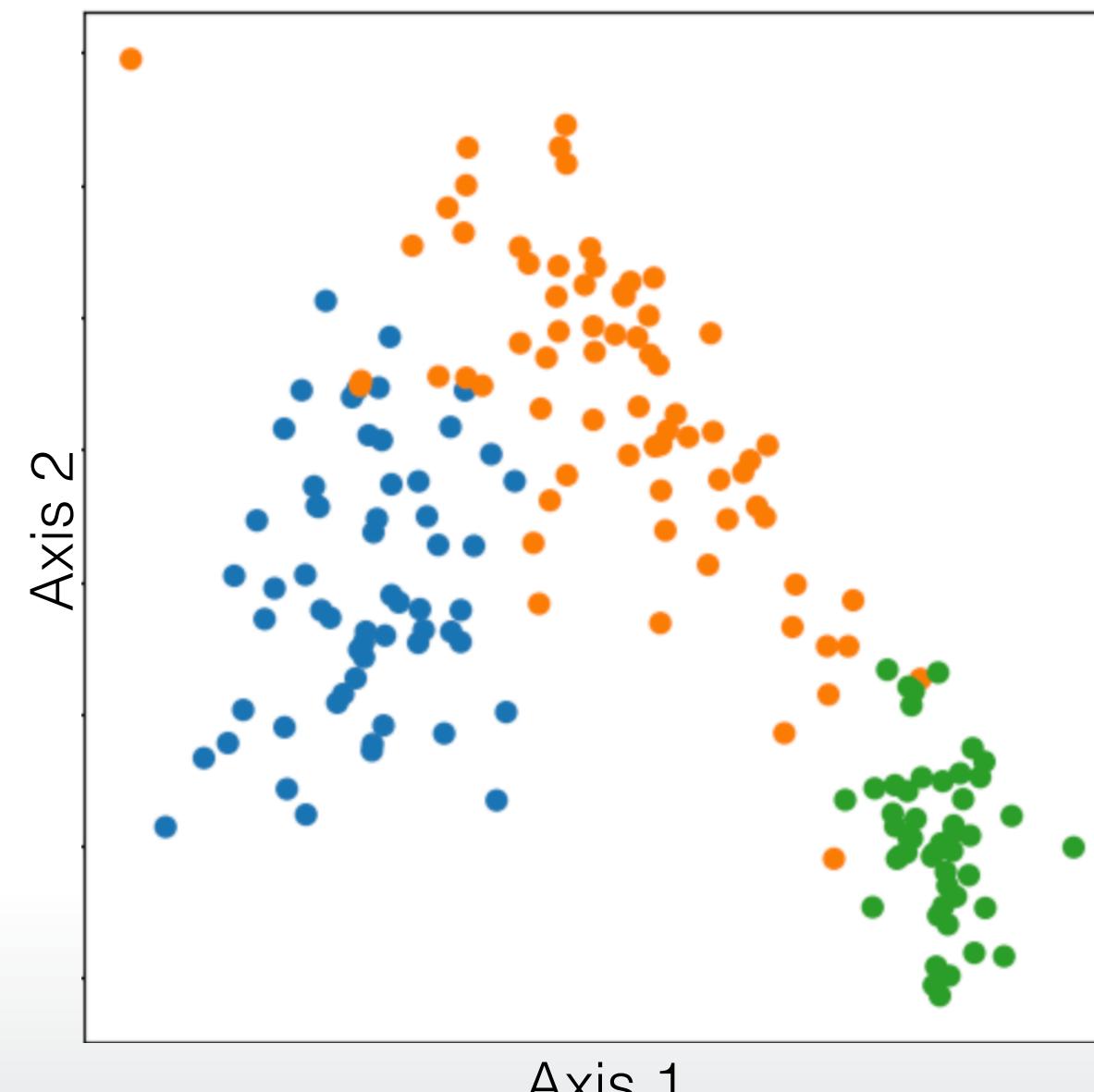
- Finds a linear projection, \mathbf{P} , that has a **small number of nonzero** elements
 - $\mathbf{X} \cdot \mathbf{P} = \mathbf{Y}$ $\mathbf{X} \in \mathbb{R}^{n \times d}$: original data, $\mathbf{P} \in \mathbb{R}^{d \times d'}$: projection matrix, $\mathbf{Y} \in \mathbb{R}^{n \times d'}$: projected data, (n : # of instances, d : # of original dimensions, d' : # of dimensions after projection)
- 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

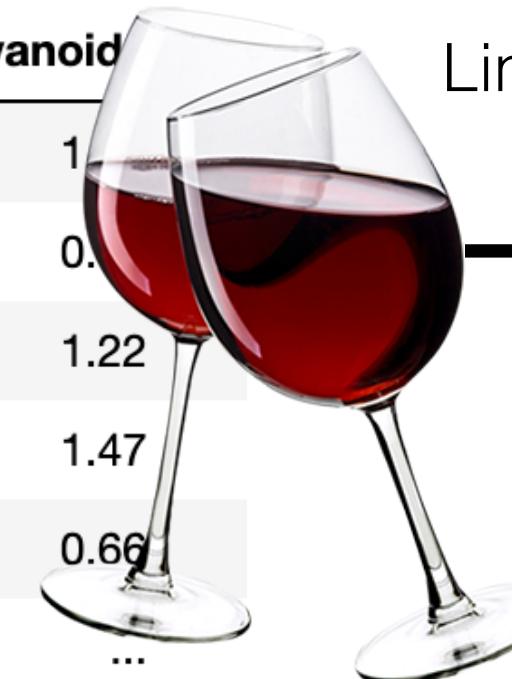


Interpretation of dimensionality reduction results

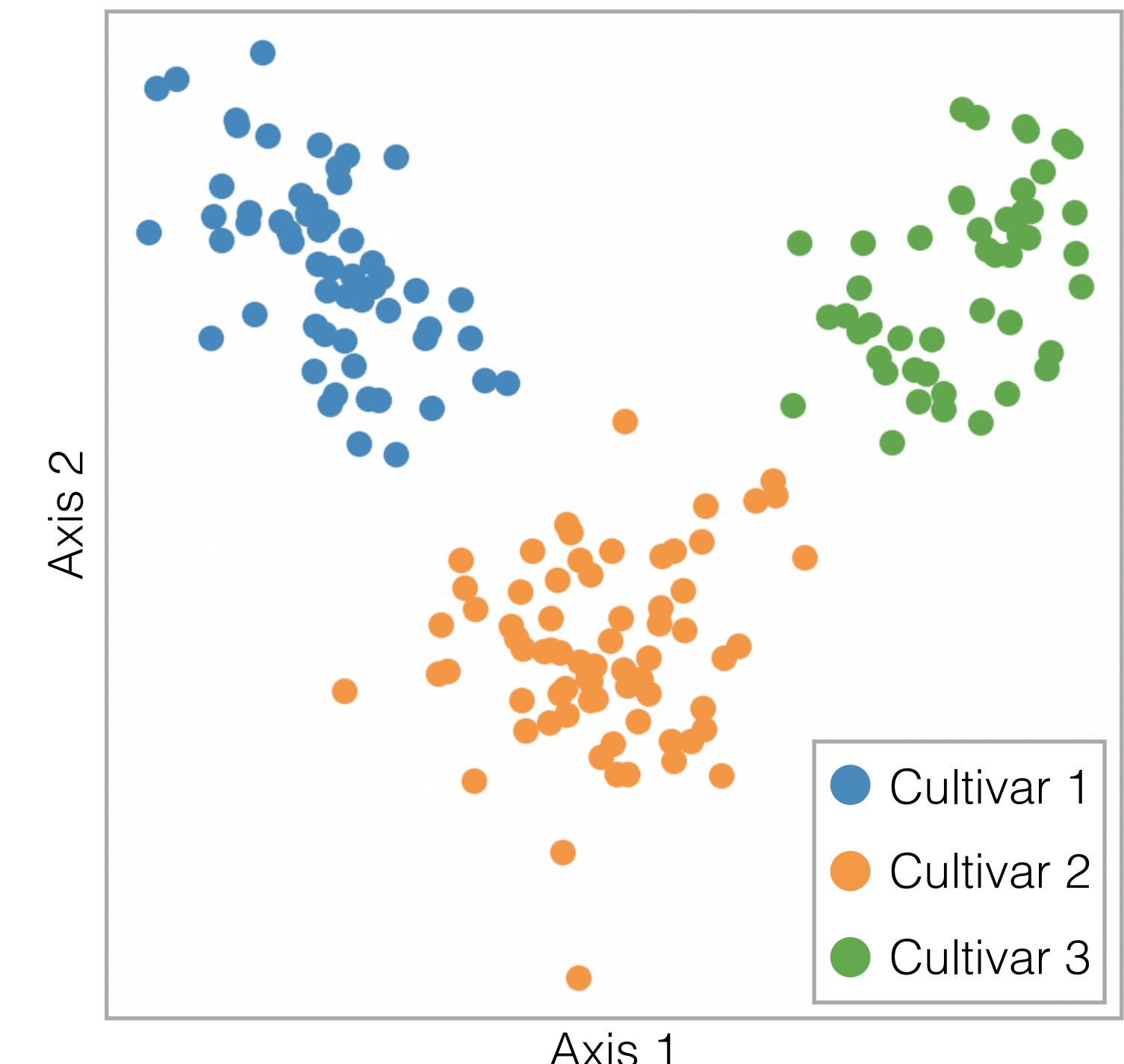
Wine dataset (13D)

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Linear discriminant analysis
LDA



- 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**

Nonlinear DR

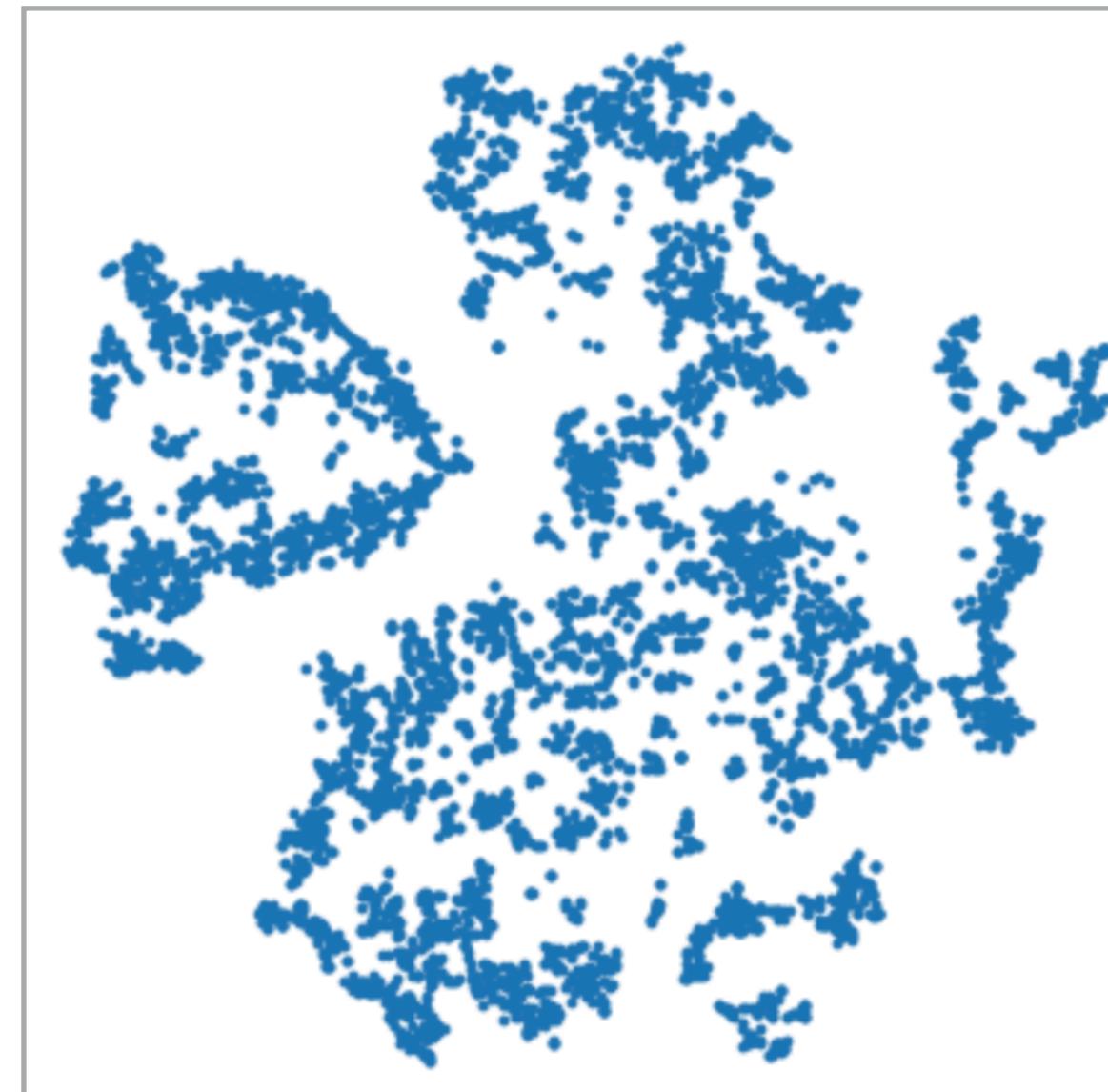
- Does not produce a linear projection from the original to the low-dimensional space
- Many commonly used nonlinear methods such as UMAP, t-SNE, Metric MDS do not provide a **parametric mapping** from the original to the low-dimensional space
 - Parametric mapping $f_{\theta} : \mathbf{X} \rightarrow \mathbf{Y}$ 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.



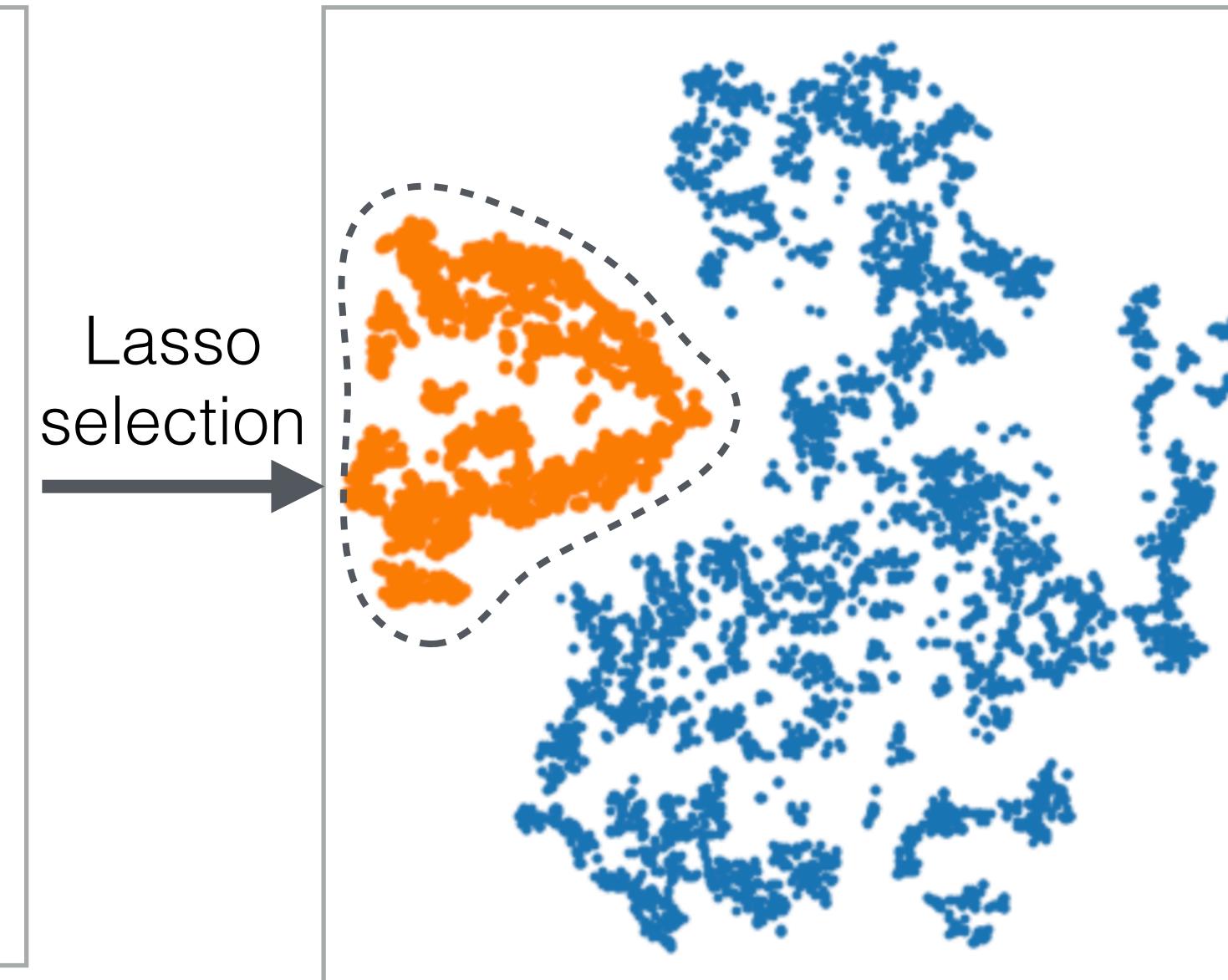
Instead of understanding the low-dimensional axes, we can try to perform the interpretation based on visual patterns appeared in a DR result

Interpreting by comparing groups/clusters

Food nutrition dataset (12D)



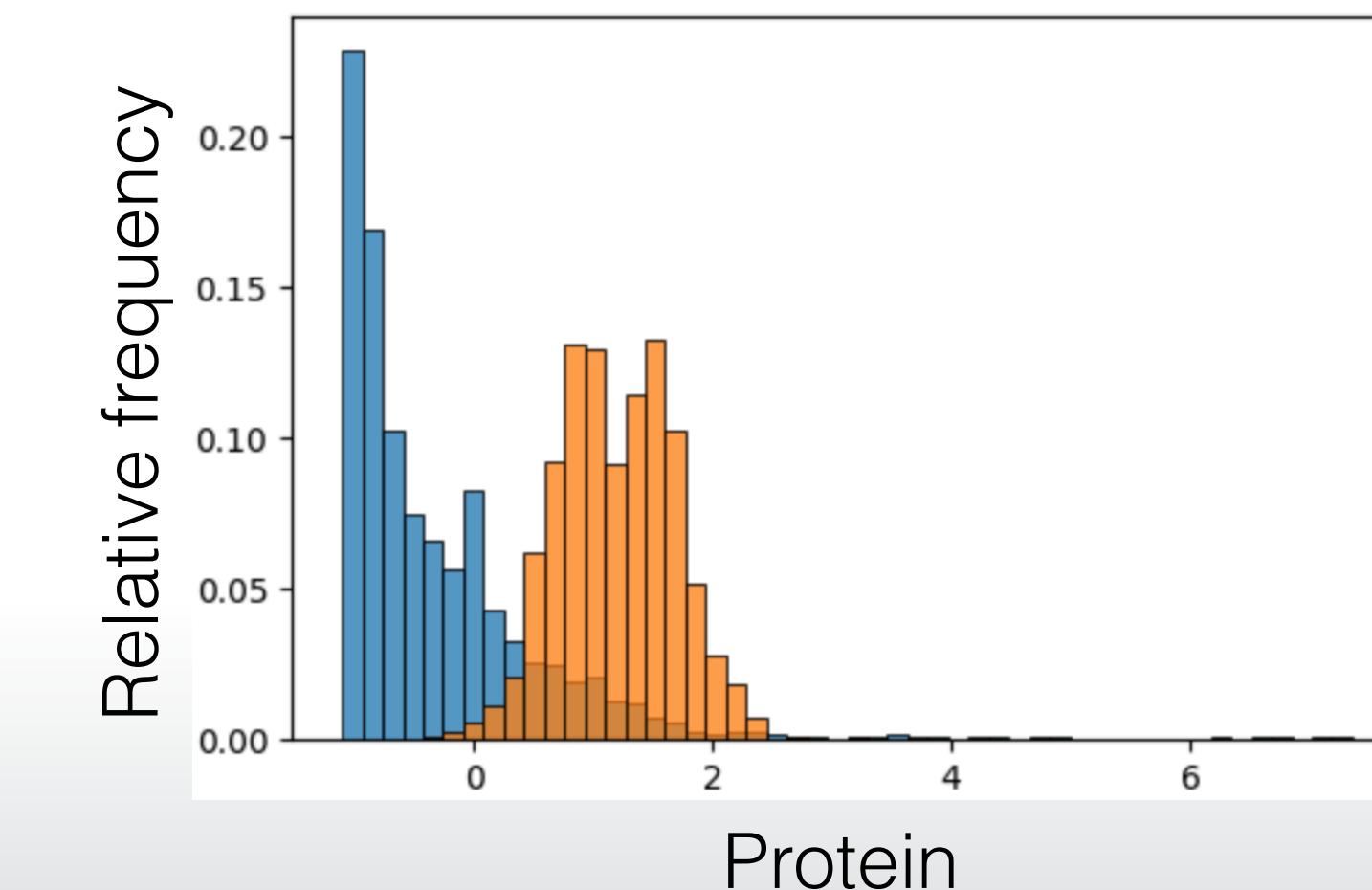
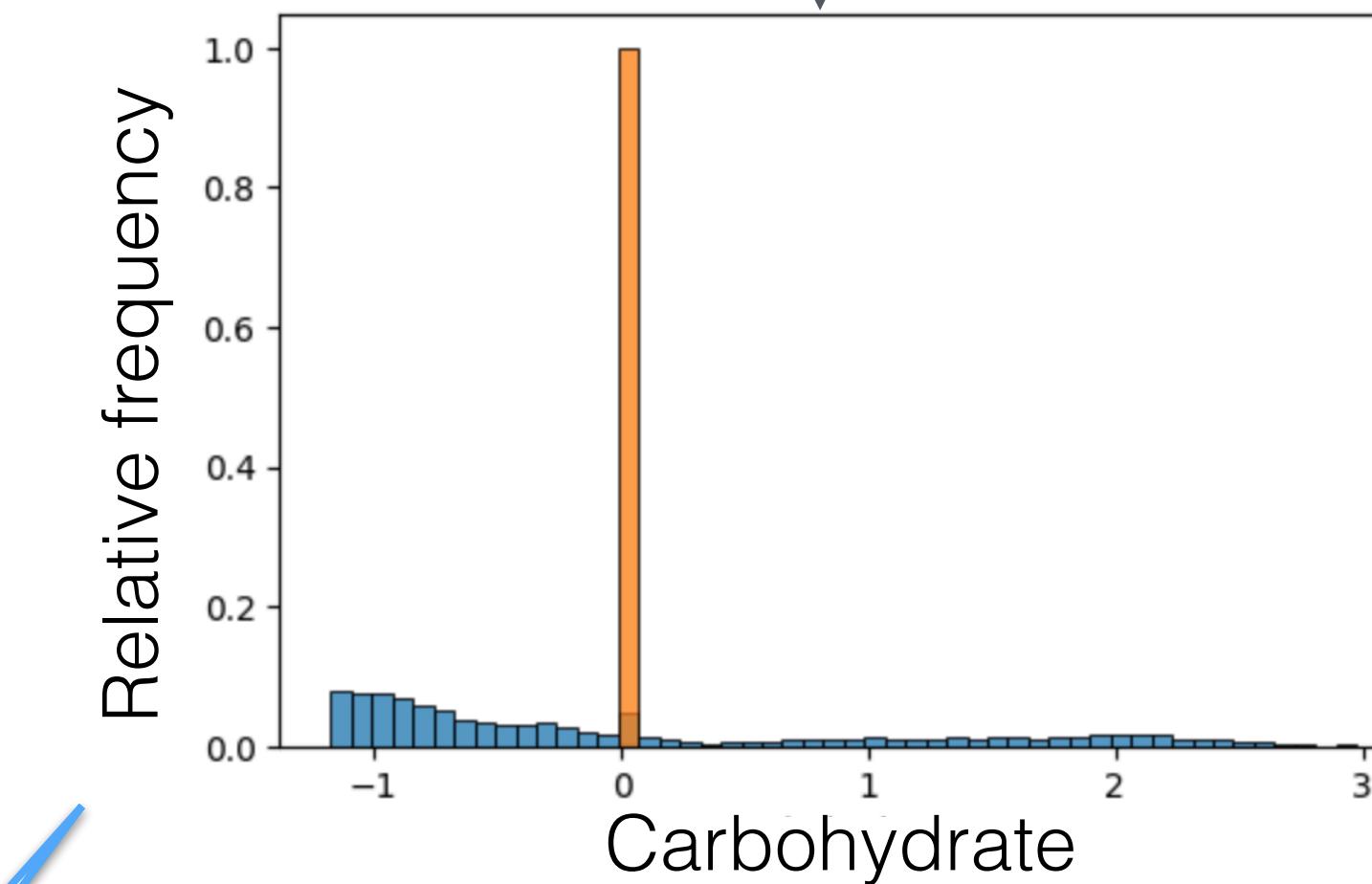
t-SNE result



One cluster is selected

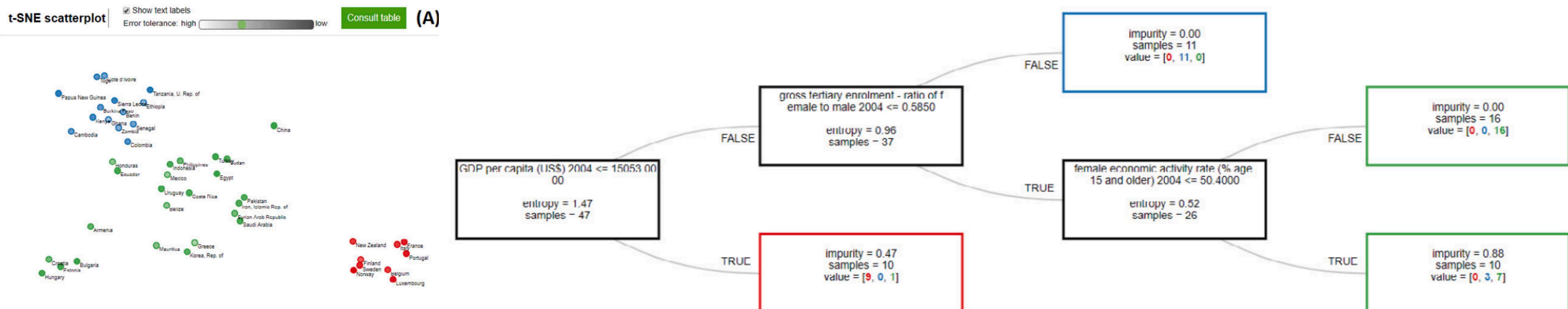
Selected foods have a medium level of carbohydrate but have a lot of protein

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



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.

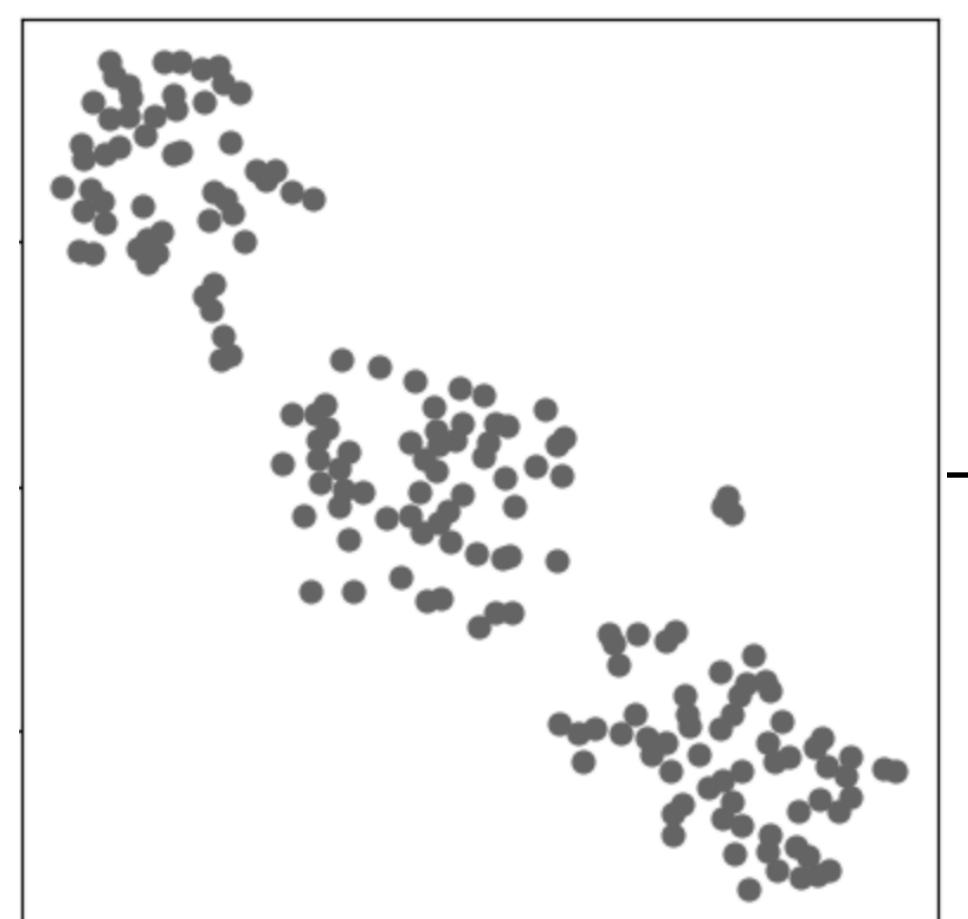


Existing approaches for comparing groups/clusters

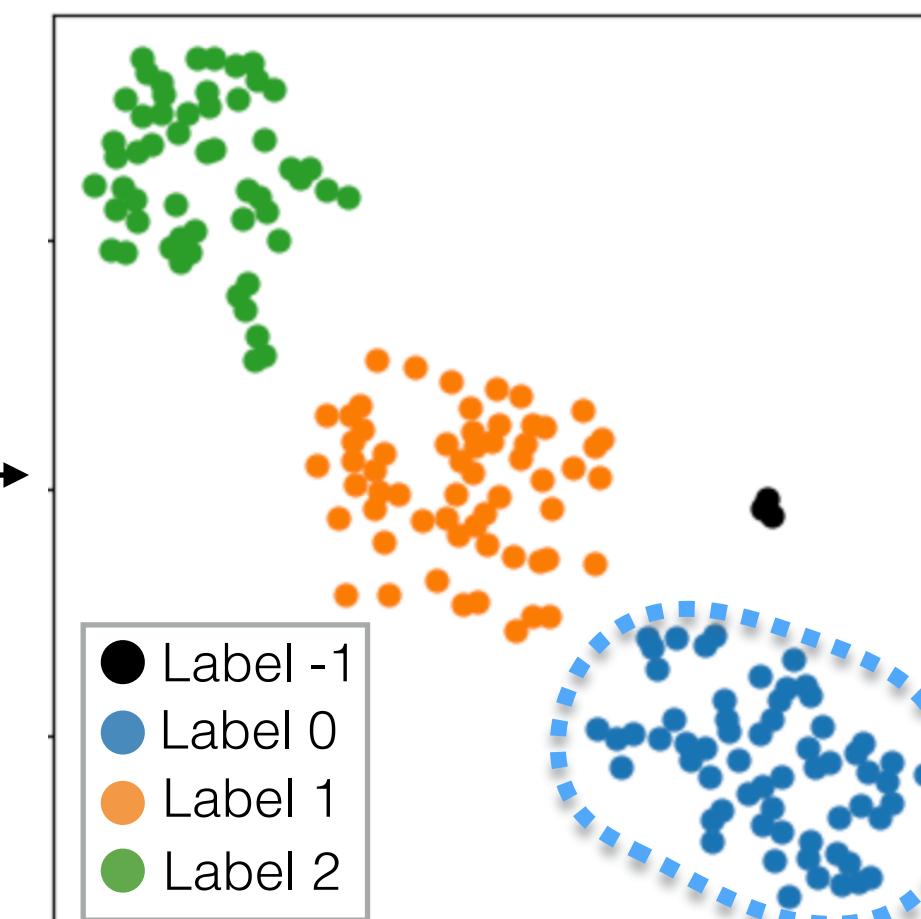
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 - e.g., building a simple model that classifies clusters in a DR result
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Comparing clusters/groups using linear DR: PCA-based

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

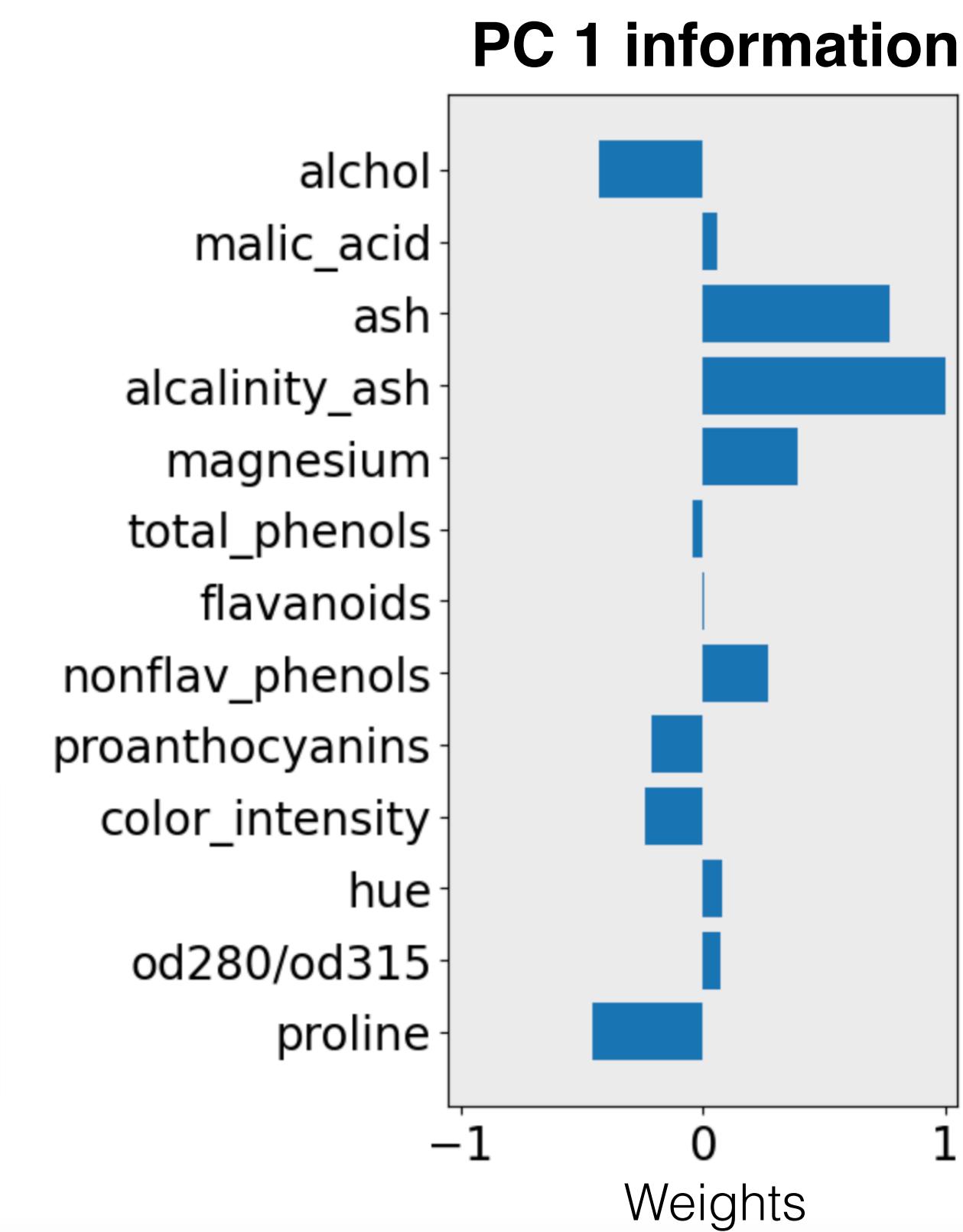
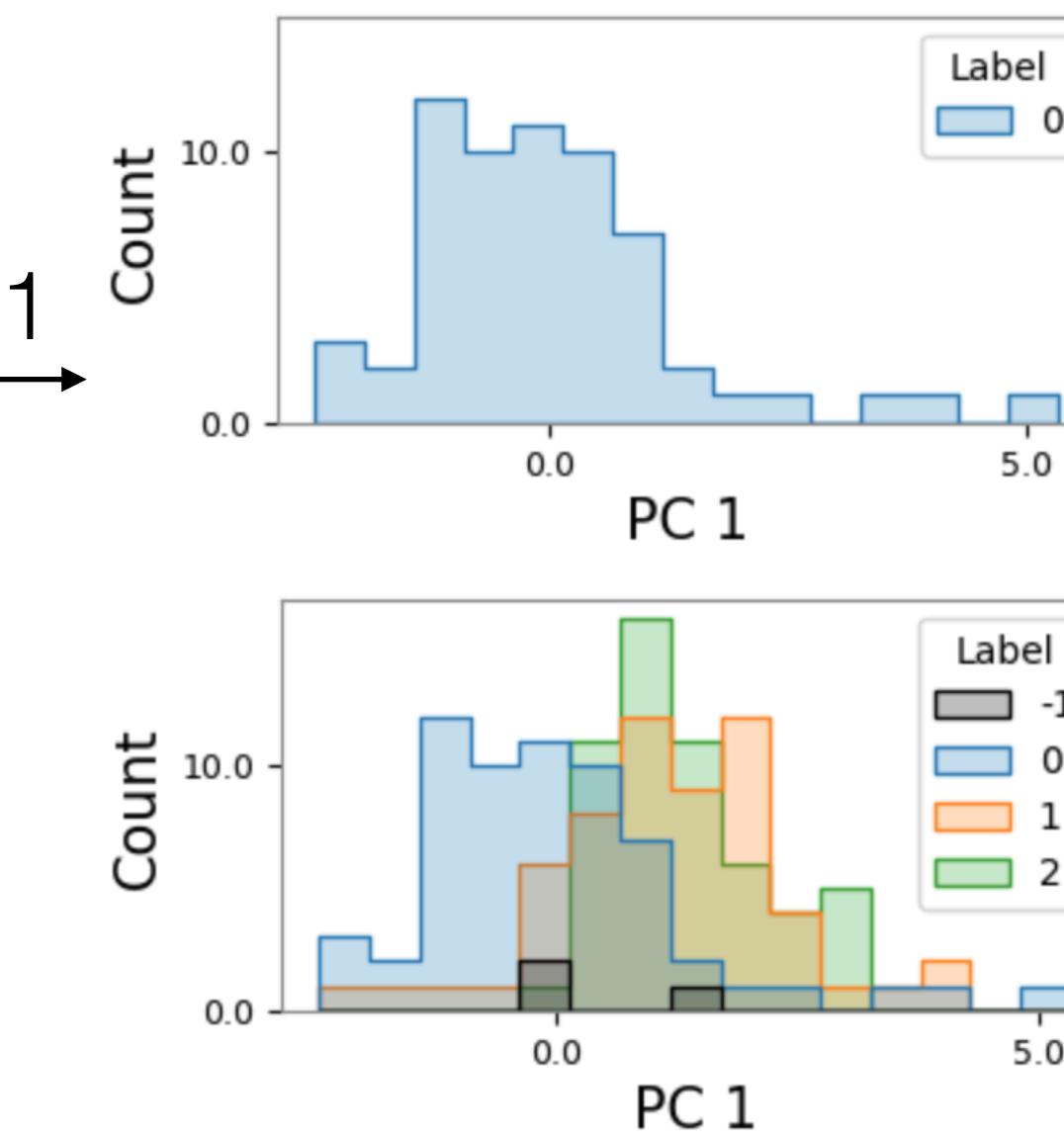


t-SNE result
(Wine dataset)



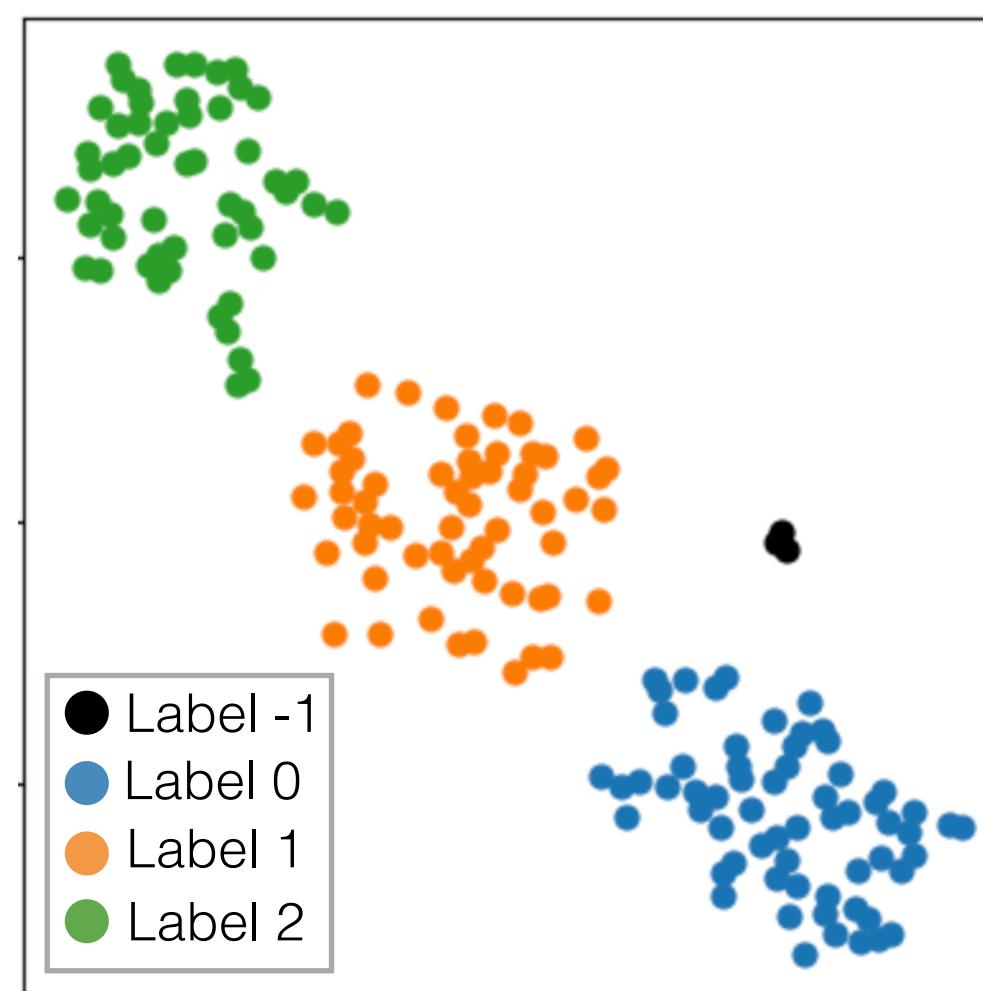
After clustering
(e.g., with DBSCAN)

PCA to
extract PC 1

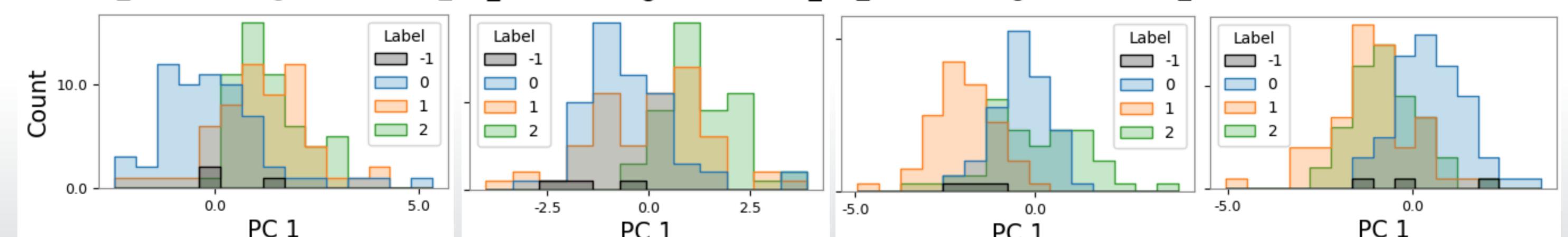
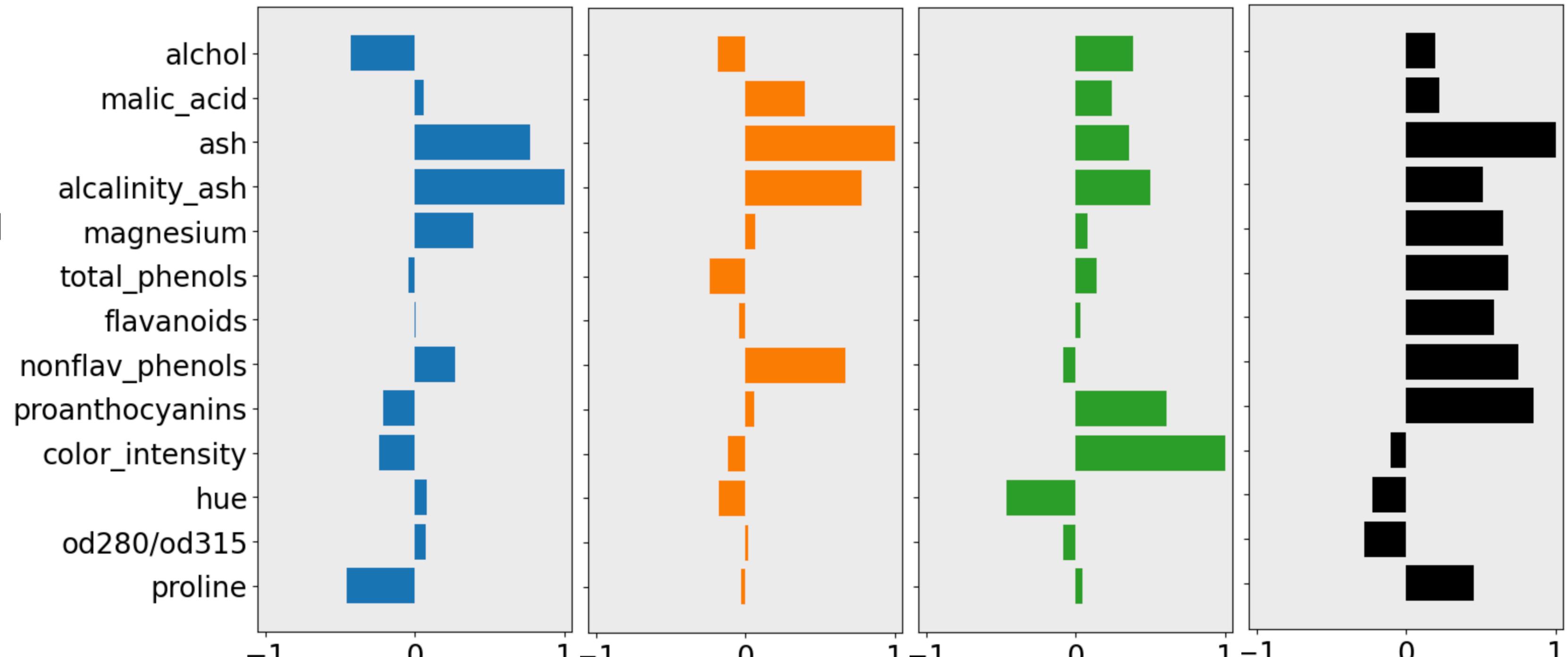


Comparing clusters/groups using linear DR: PCA-based

- Applying **PCA** for each cluster
(e.g., `PCA(n_components=1).fit(data[label==0])`)
 - Extract variance-related information of each cluster—**variety factors**
 - But, there is no consideration of differences between one cluster and others

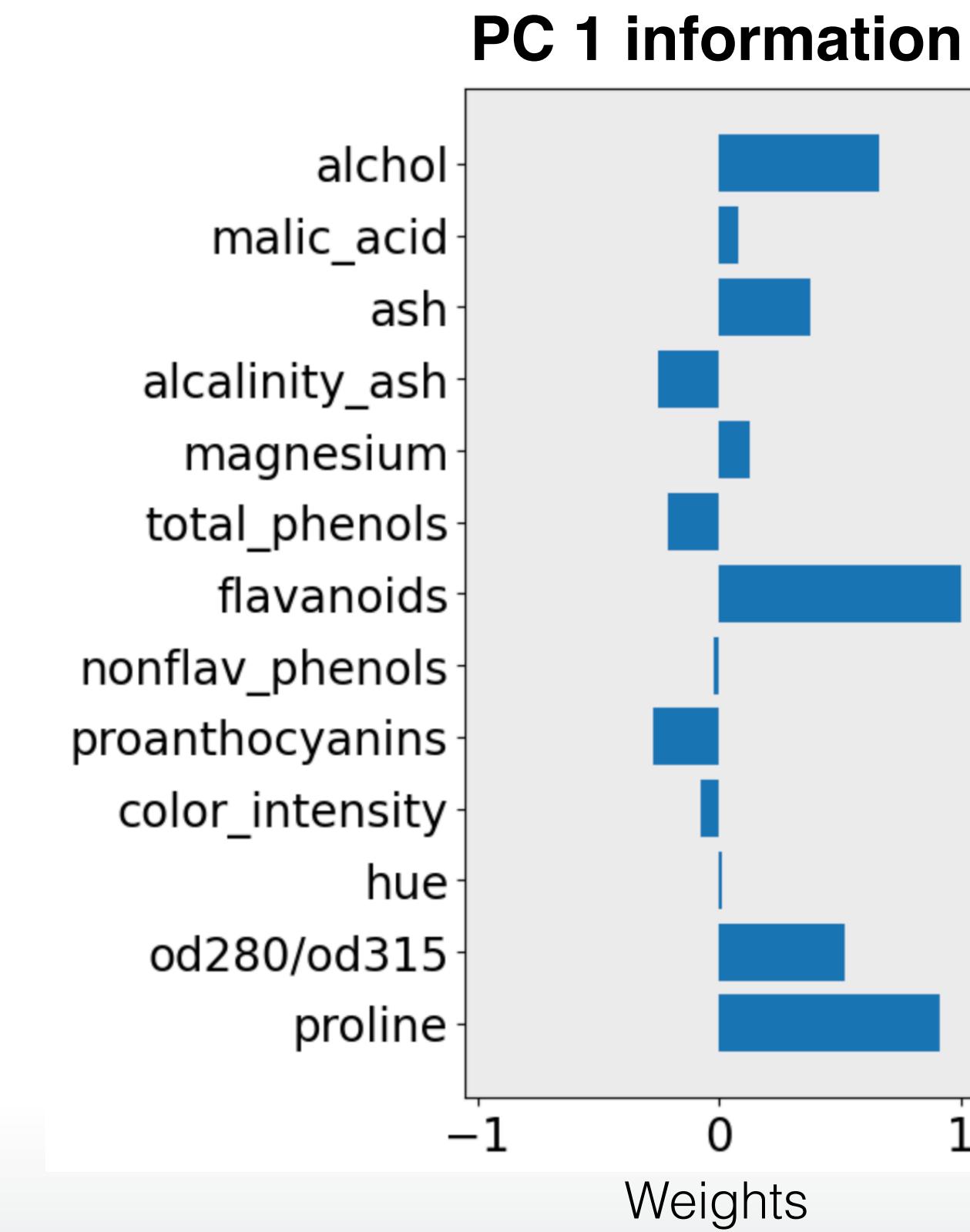
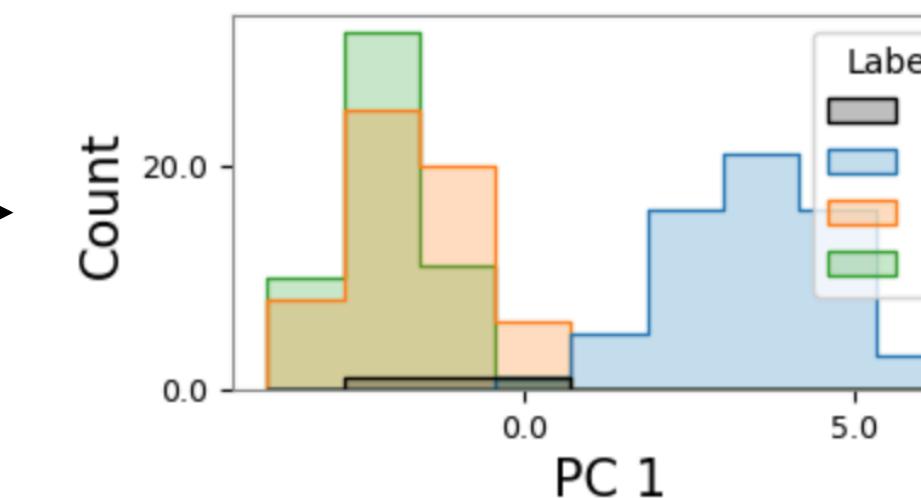
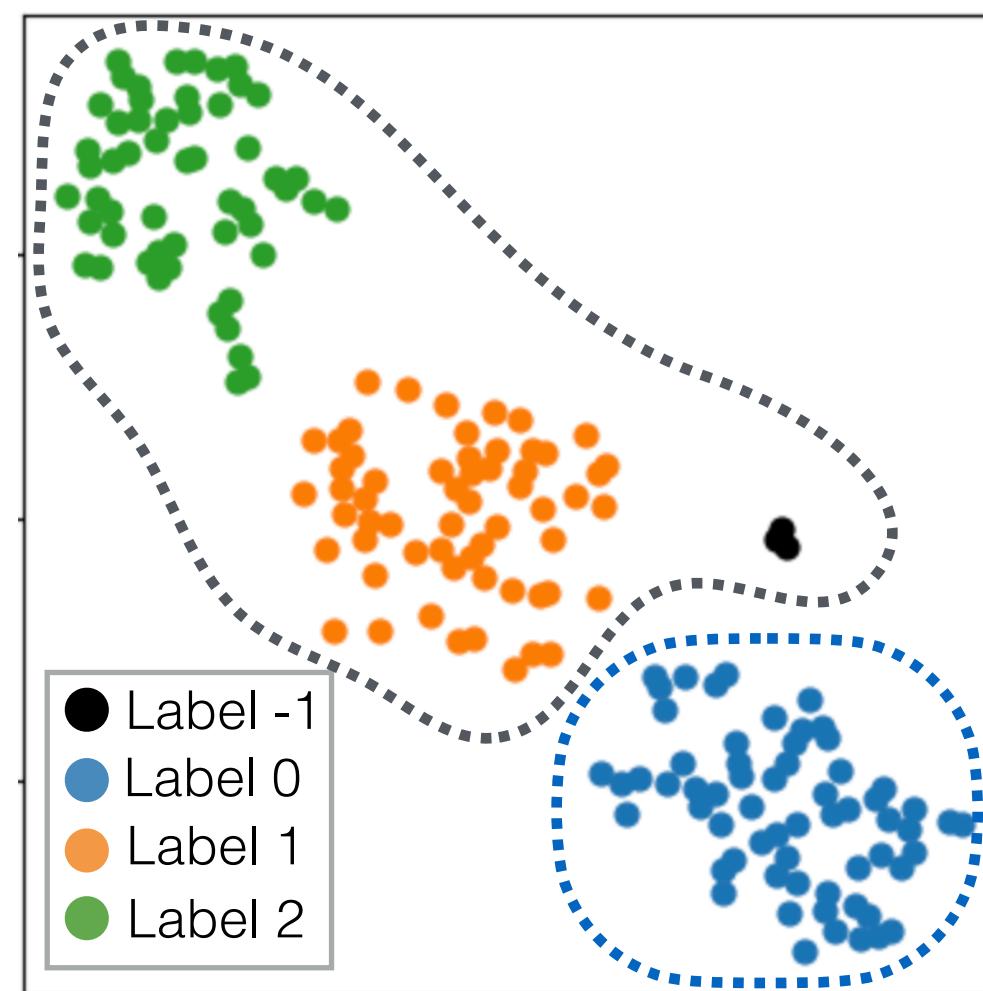


PCA to
extract PC 1



Comparing clusters/groups using linear DR: LDA-based

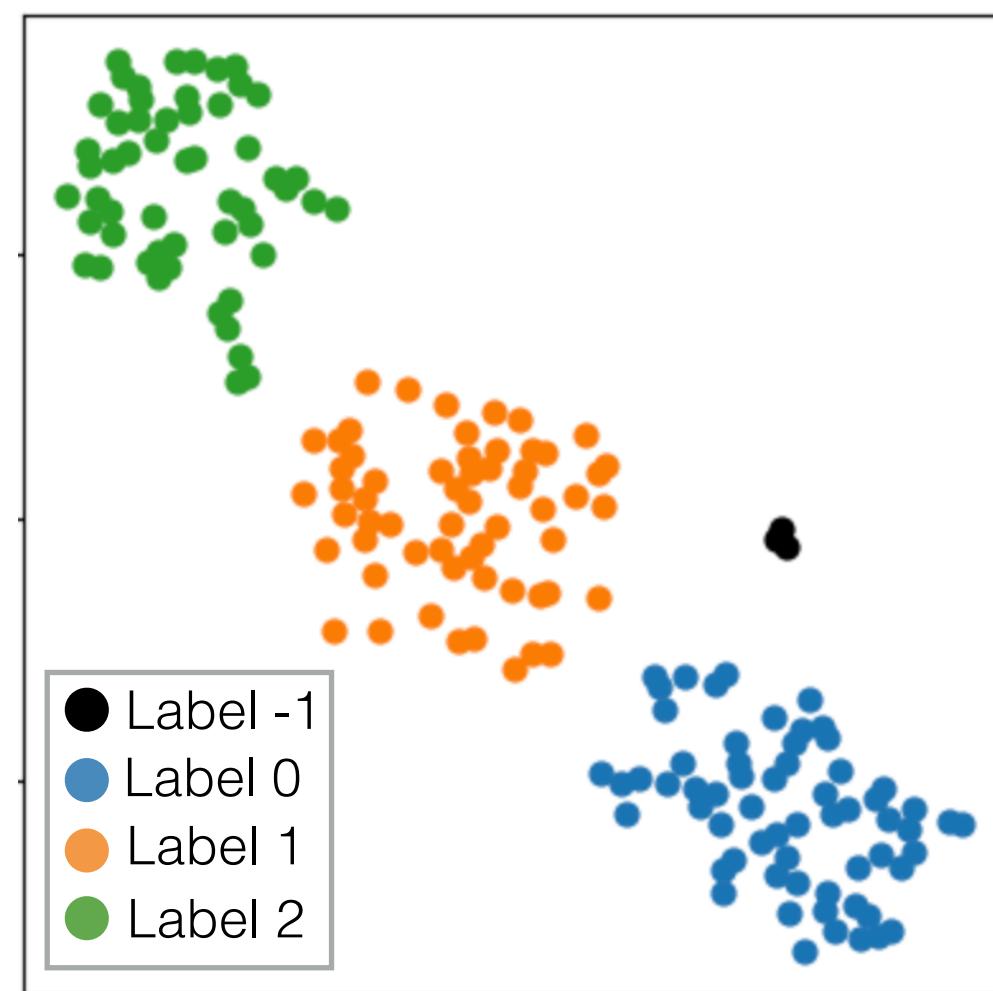
- Applying linear discriminant analysis (**LDA**) to distinguish one cluster and others (e.g., `LDA(n_components=1).fit(data, label==0)`)
 - Find differences between one cluster and others—**differentiating factors**



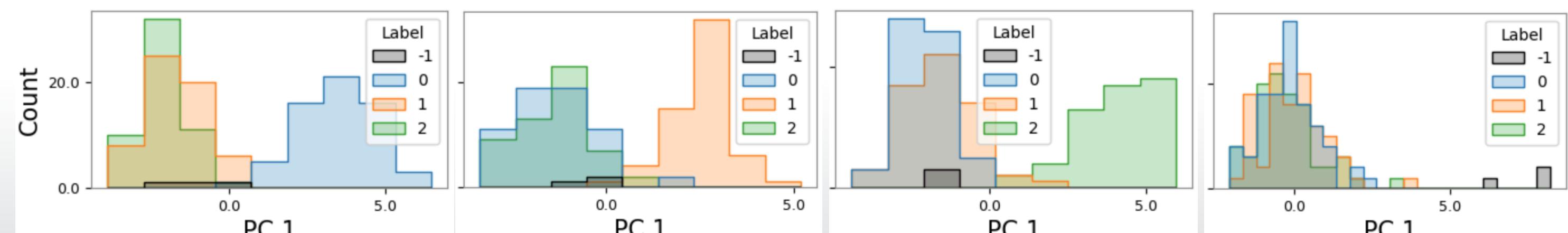
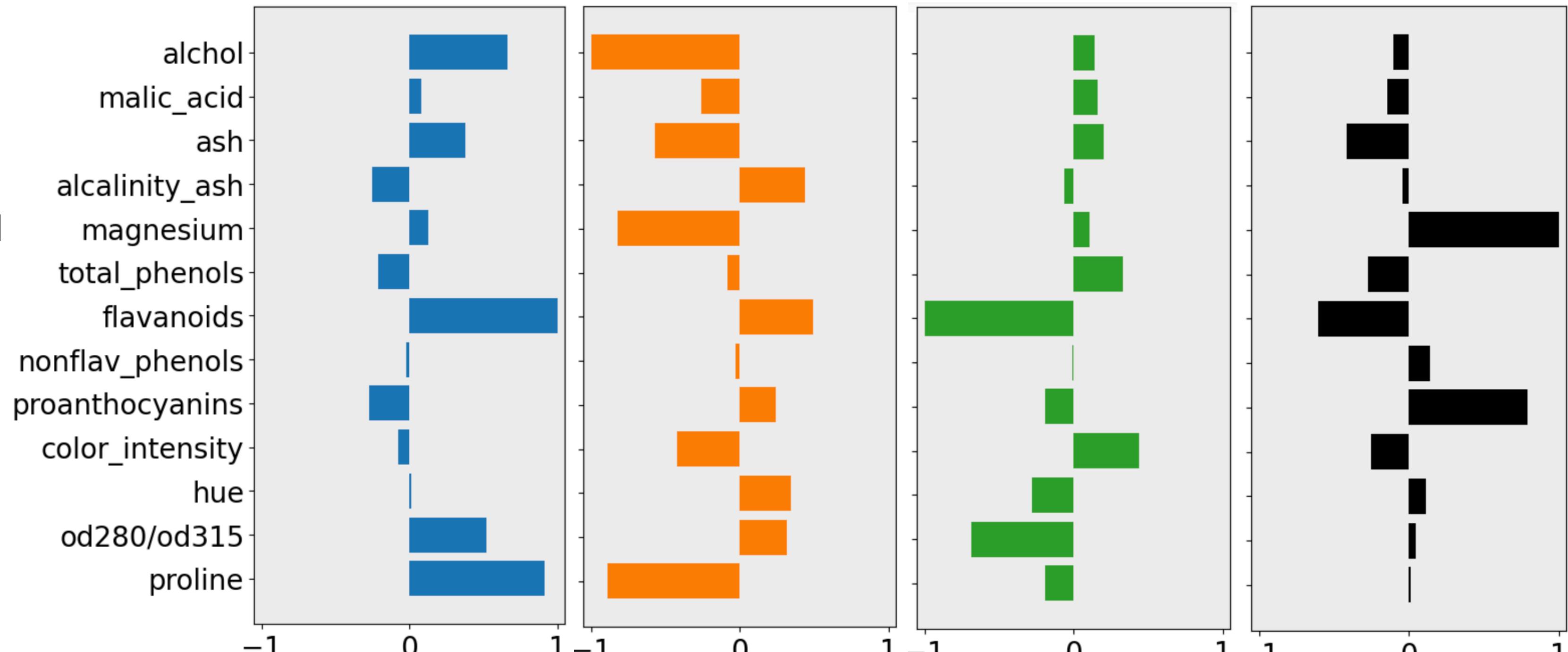
[demo script](#)

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



LDA to
extract PC 1

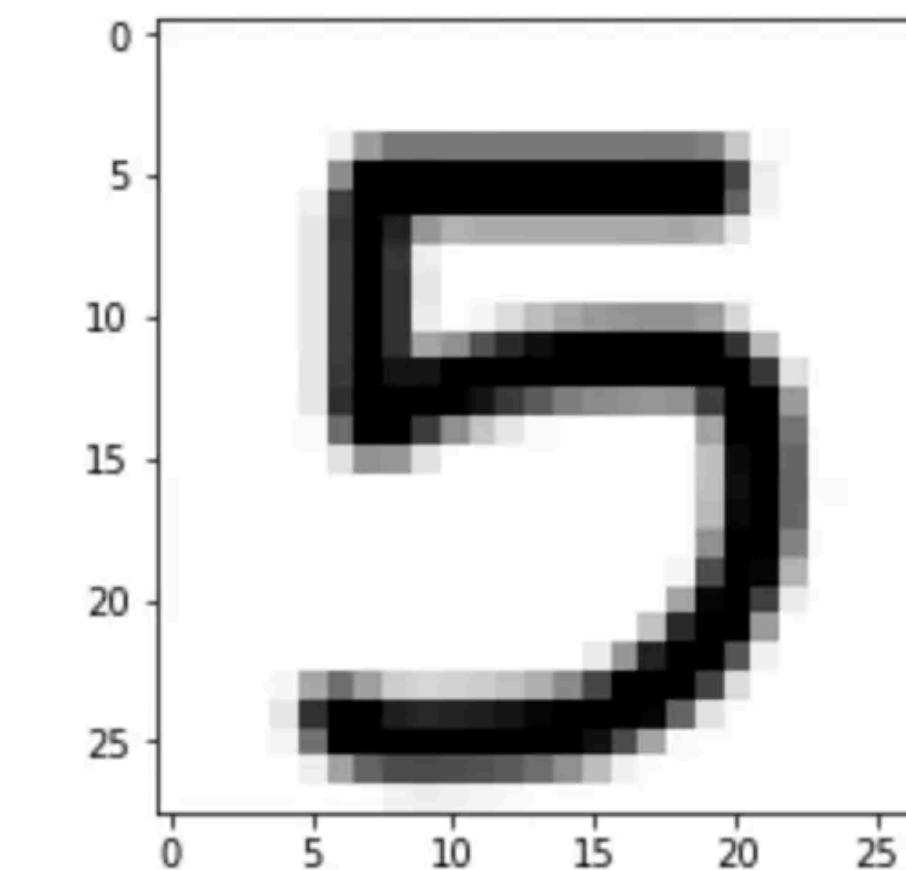


ccPCA: Contrasting clusters in PCA

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



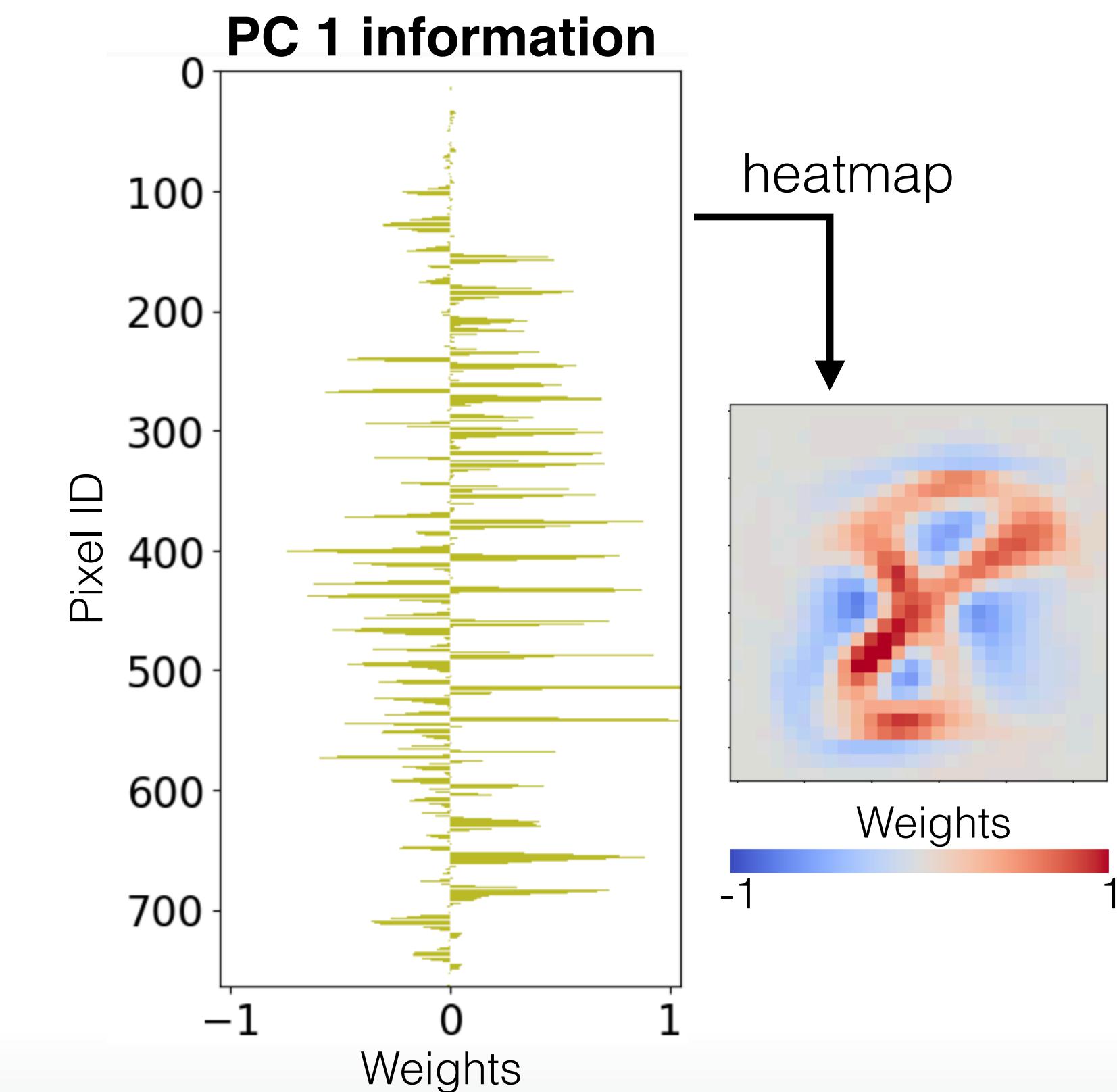
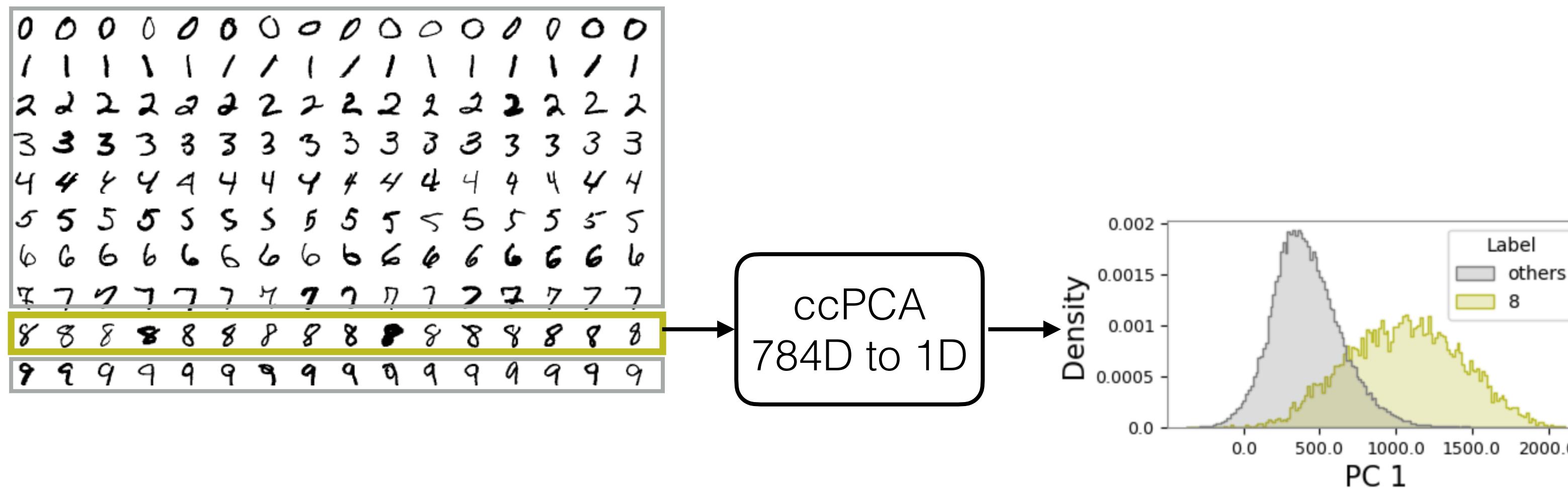
28 pixels x 28 pixels
= 784 dimensions

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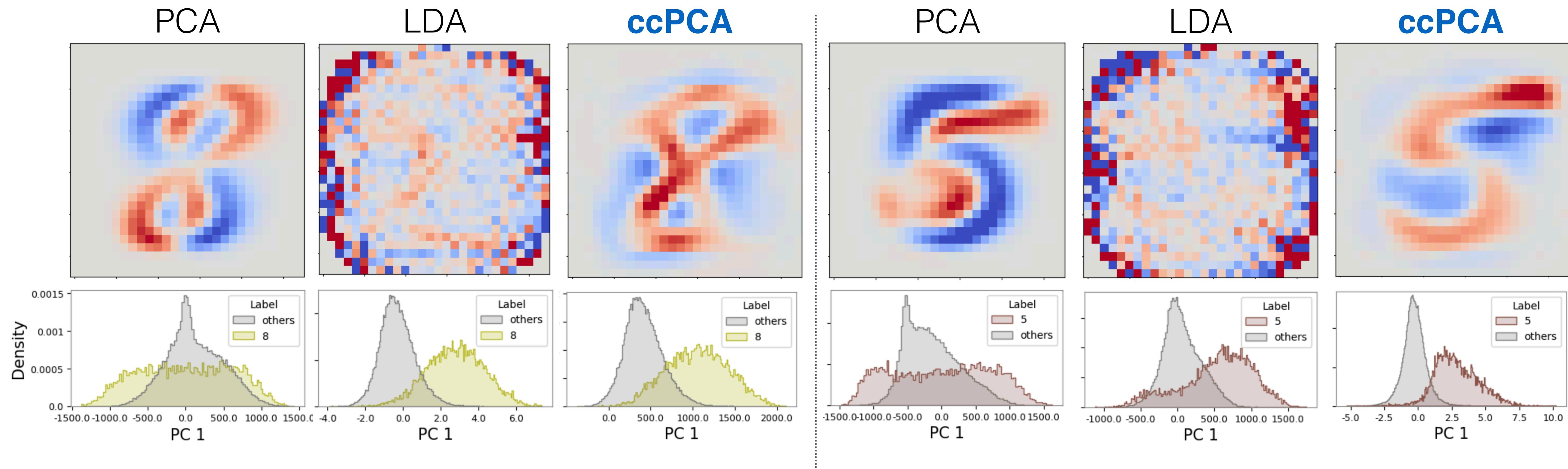
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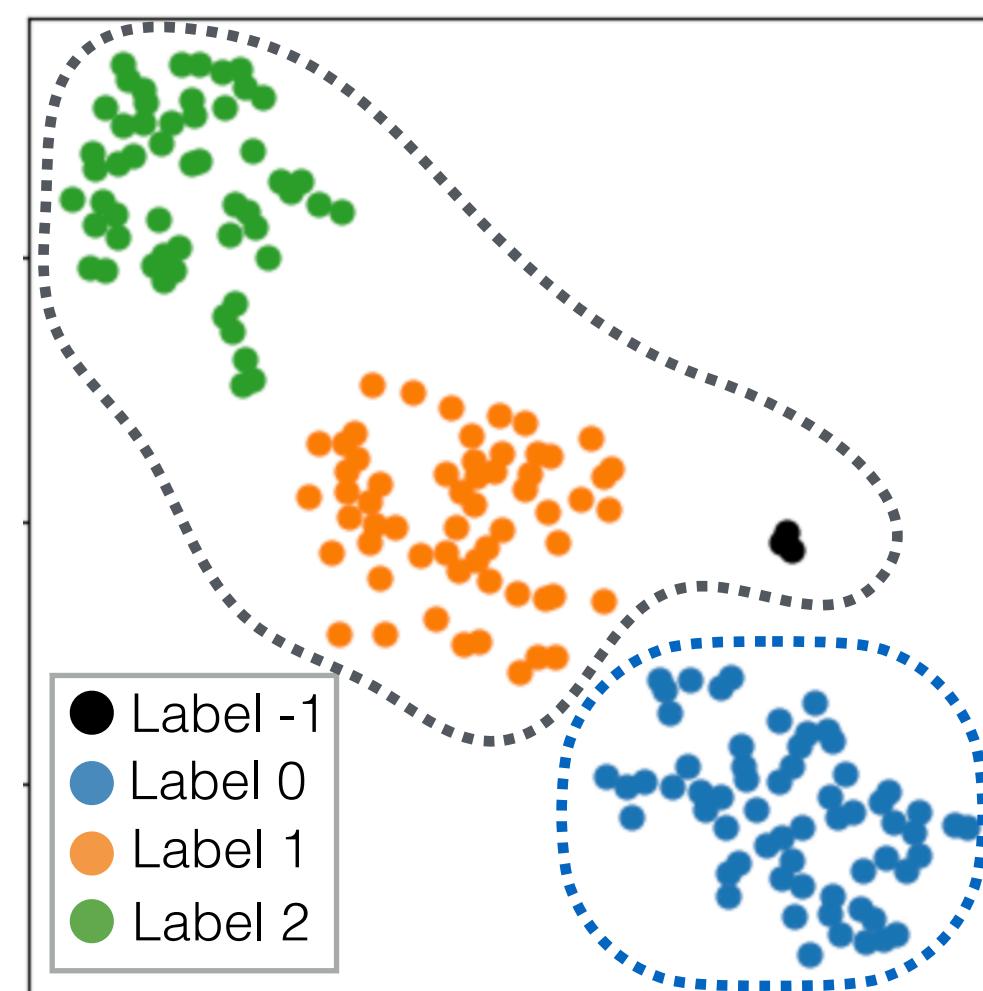
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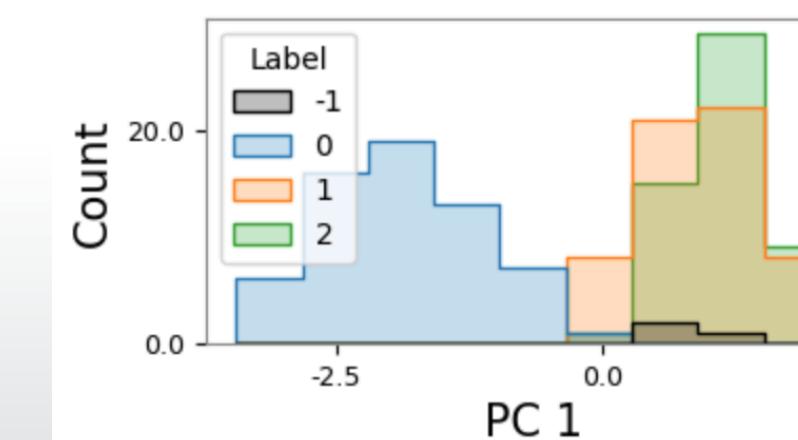
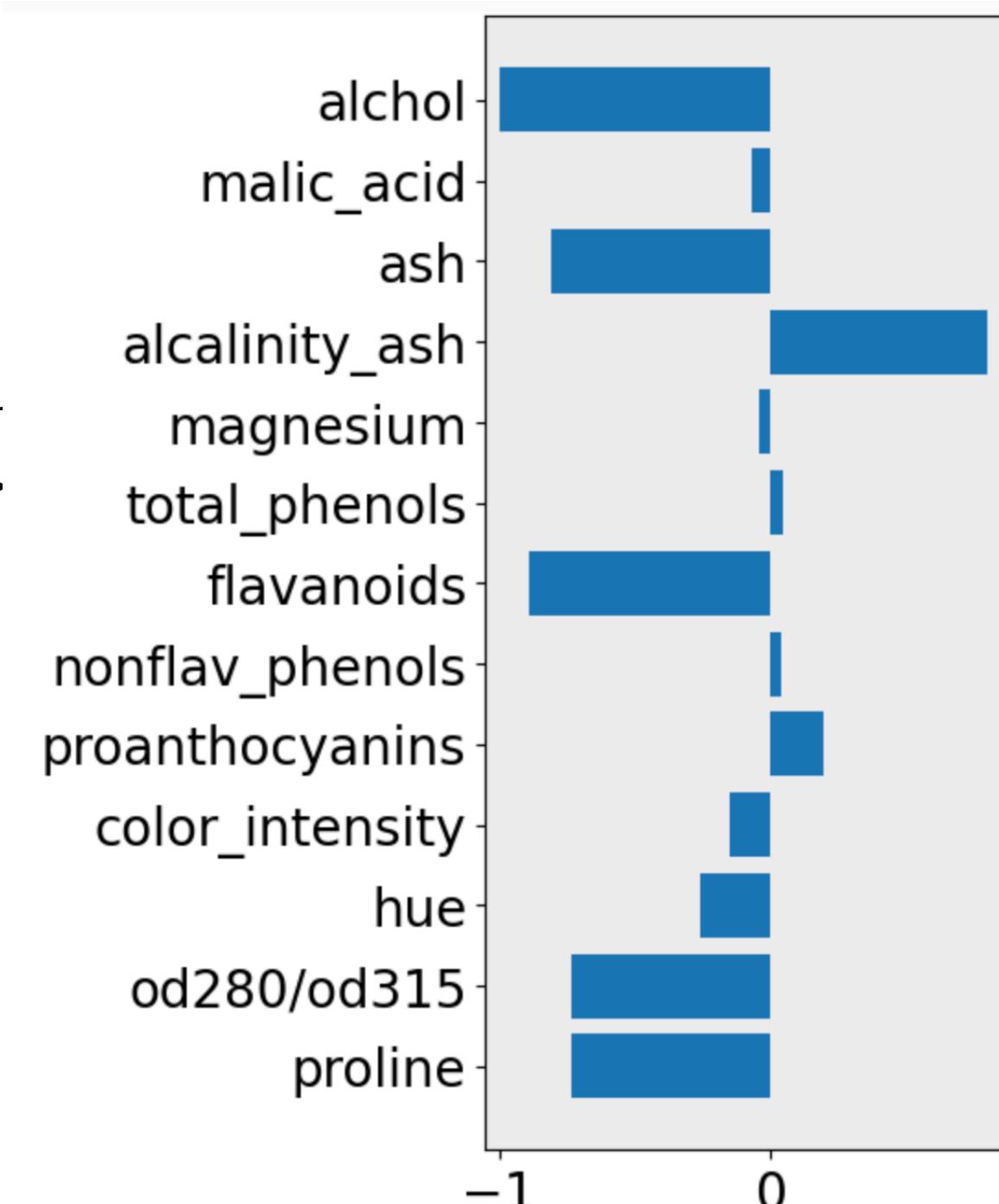


Comparing clusters/groups using linear DR: ccPCA-based

- 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



ccPCA to extract PC

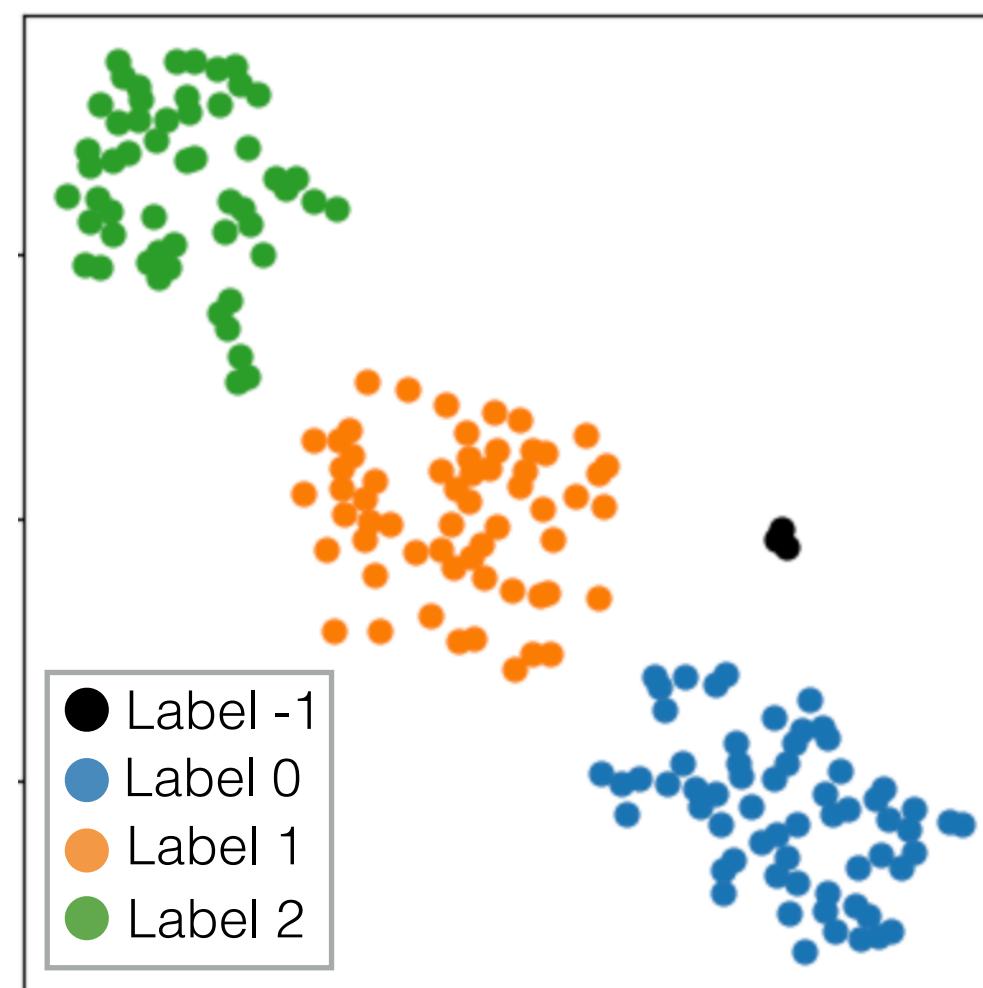


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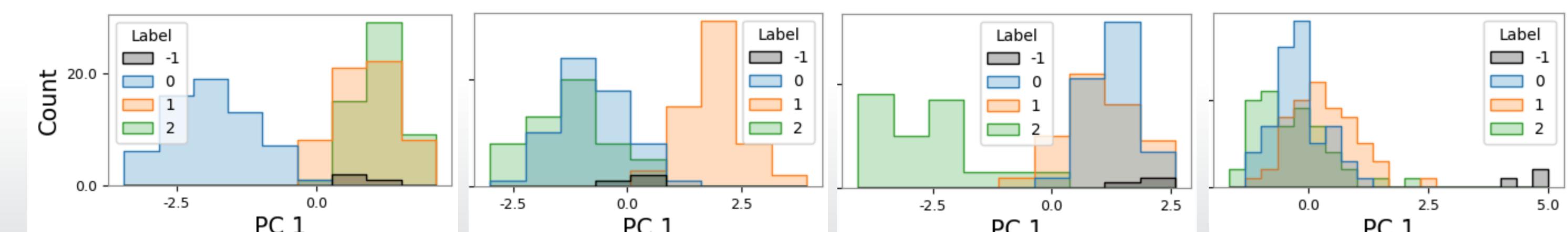
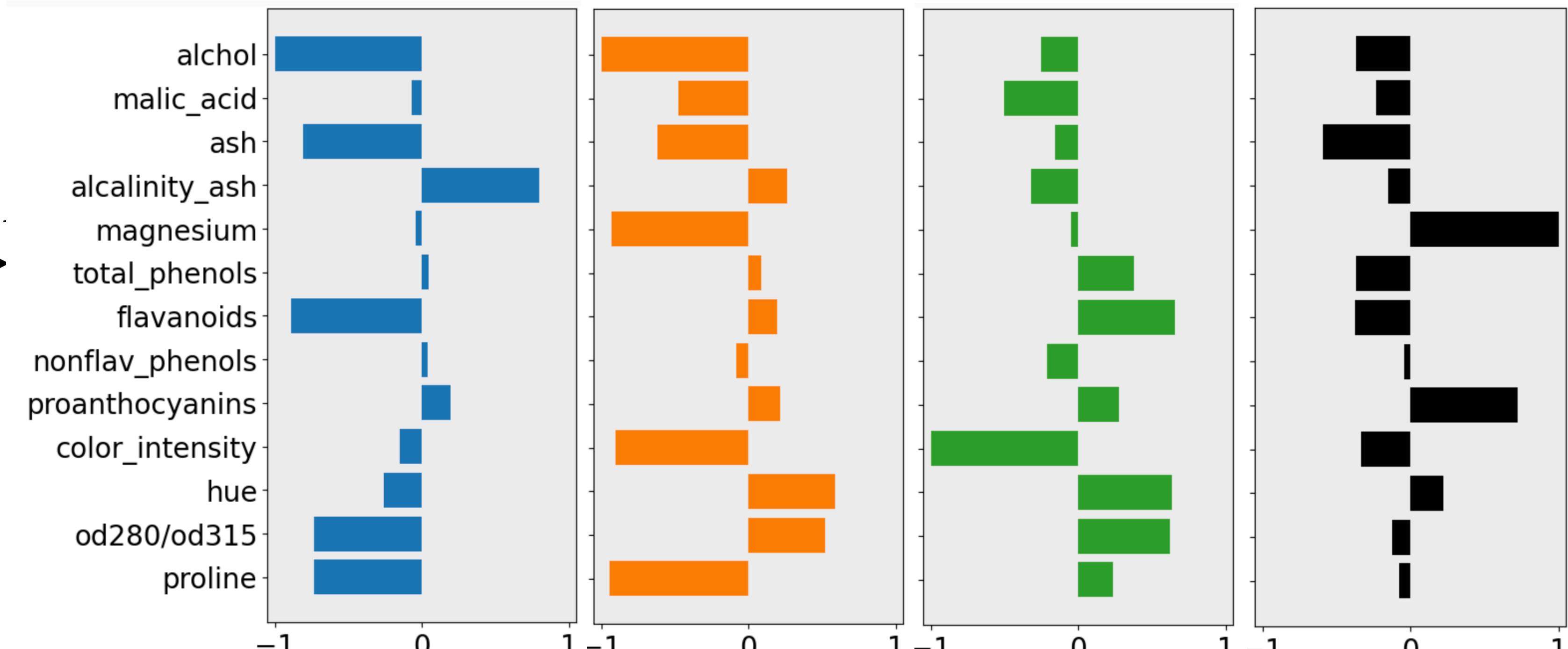
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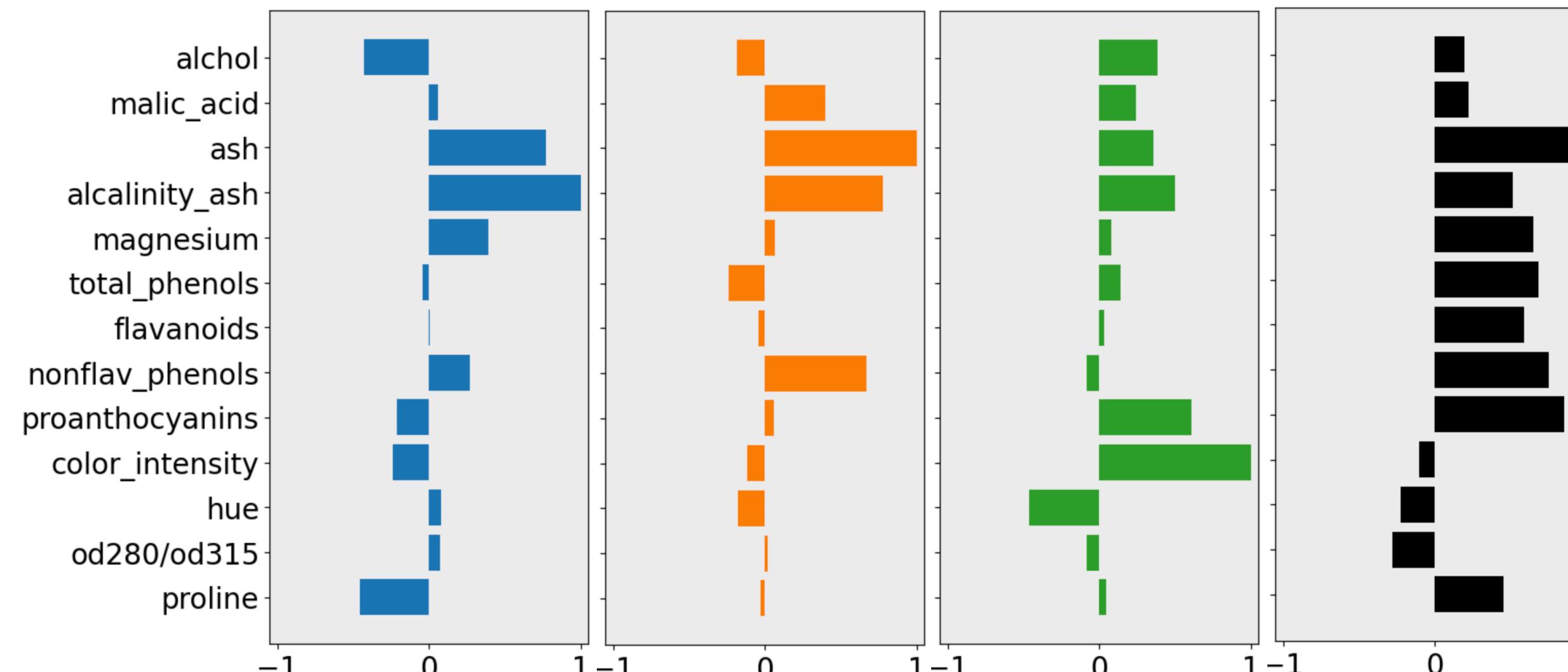


ccPCA to extract PC

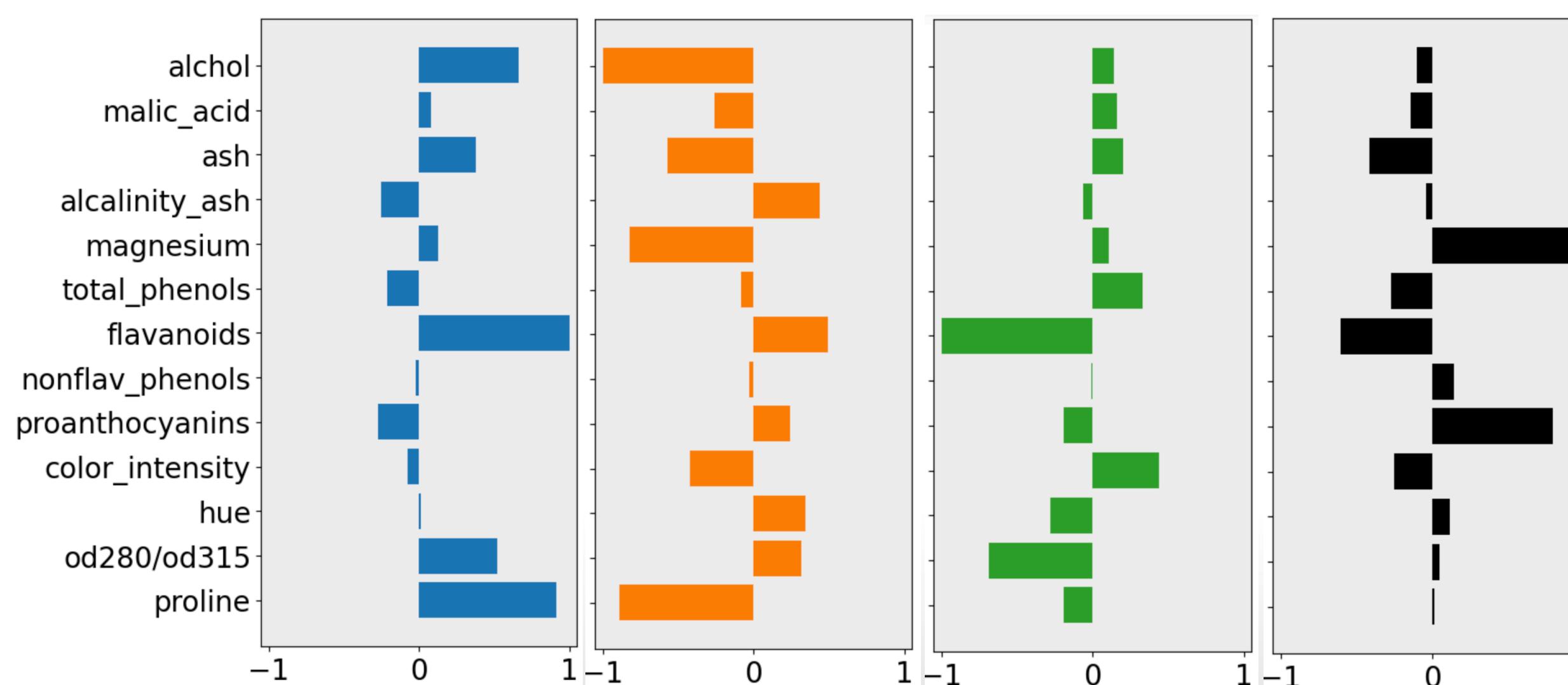


Comparing clusters/groups using linear DR

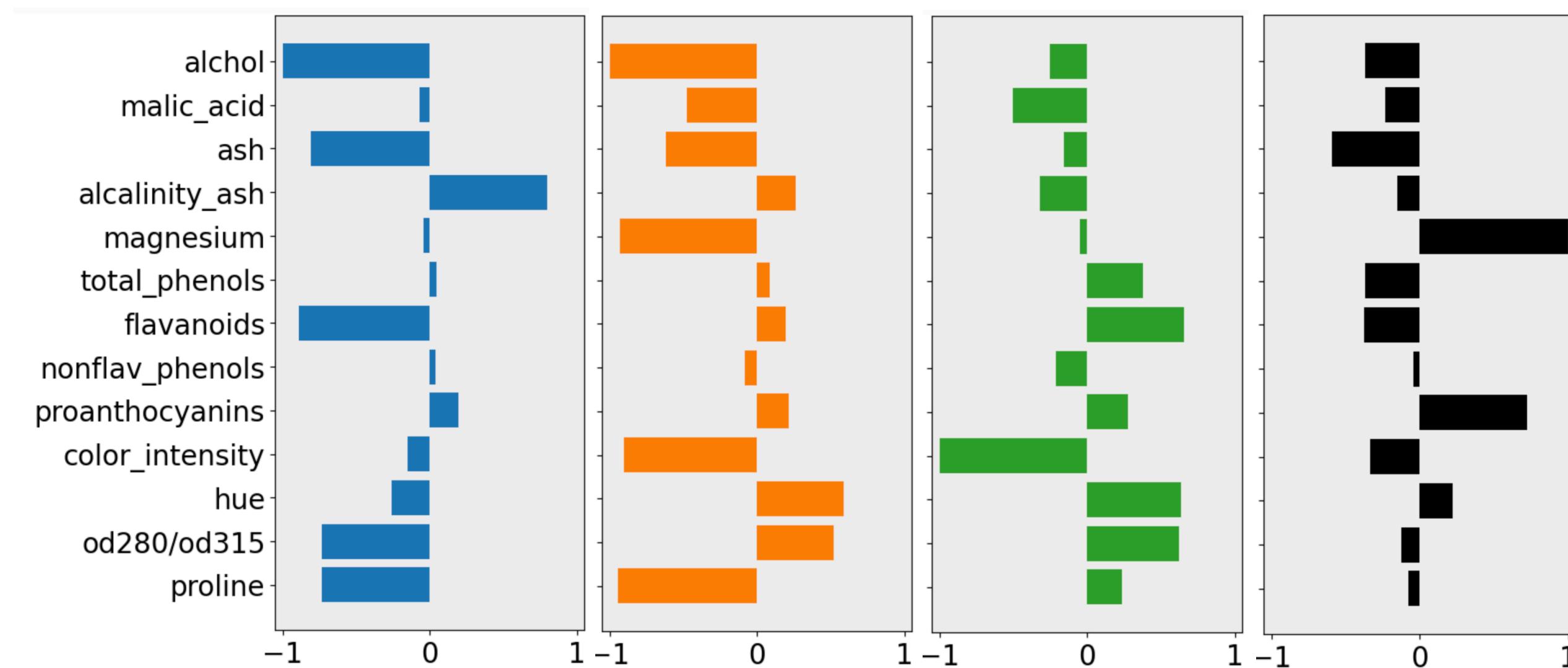
PCA



LDA



ccPCA



Coding exercise (20 minutes)

- Colab notebook link: <http://bit.ly/3ZFOoqv>
- 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



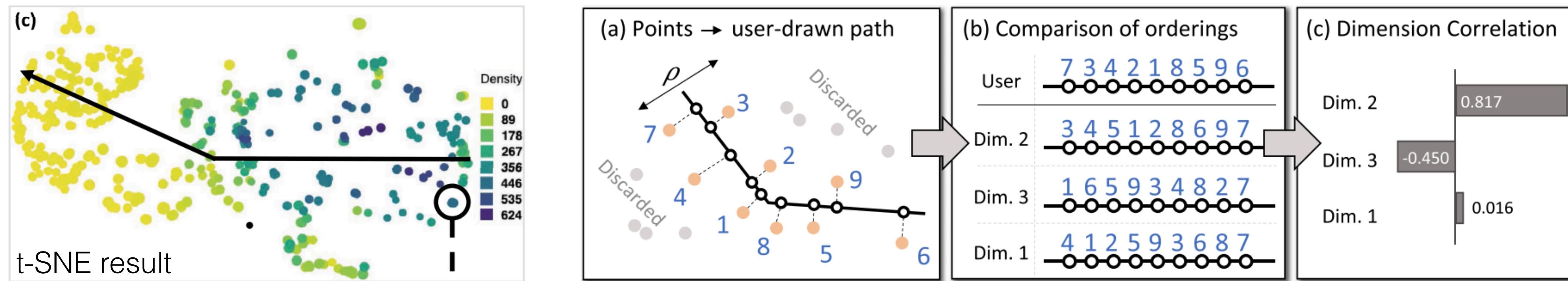
More flexible comparison

- 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.

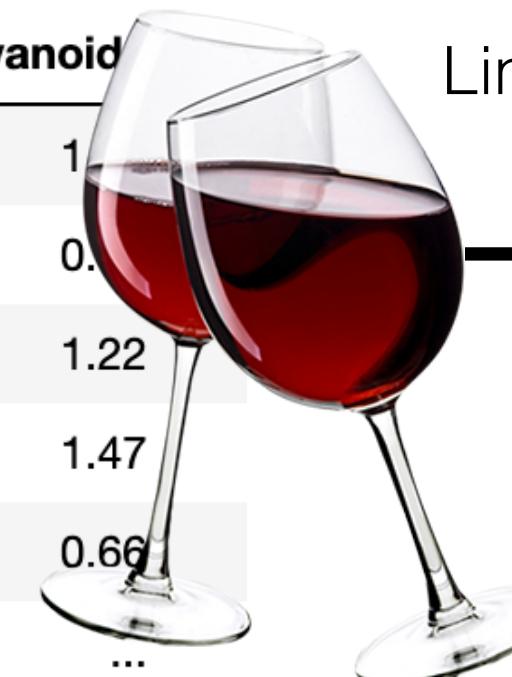


Interpretation of dimensionality reduction results

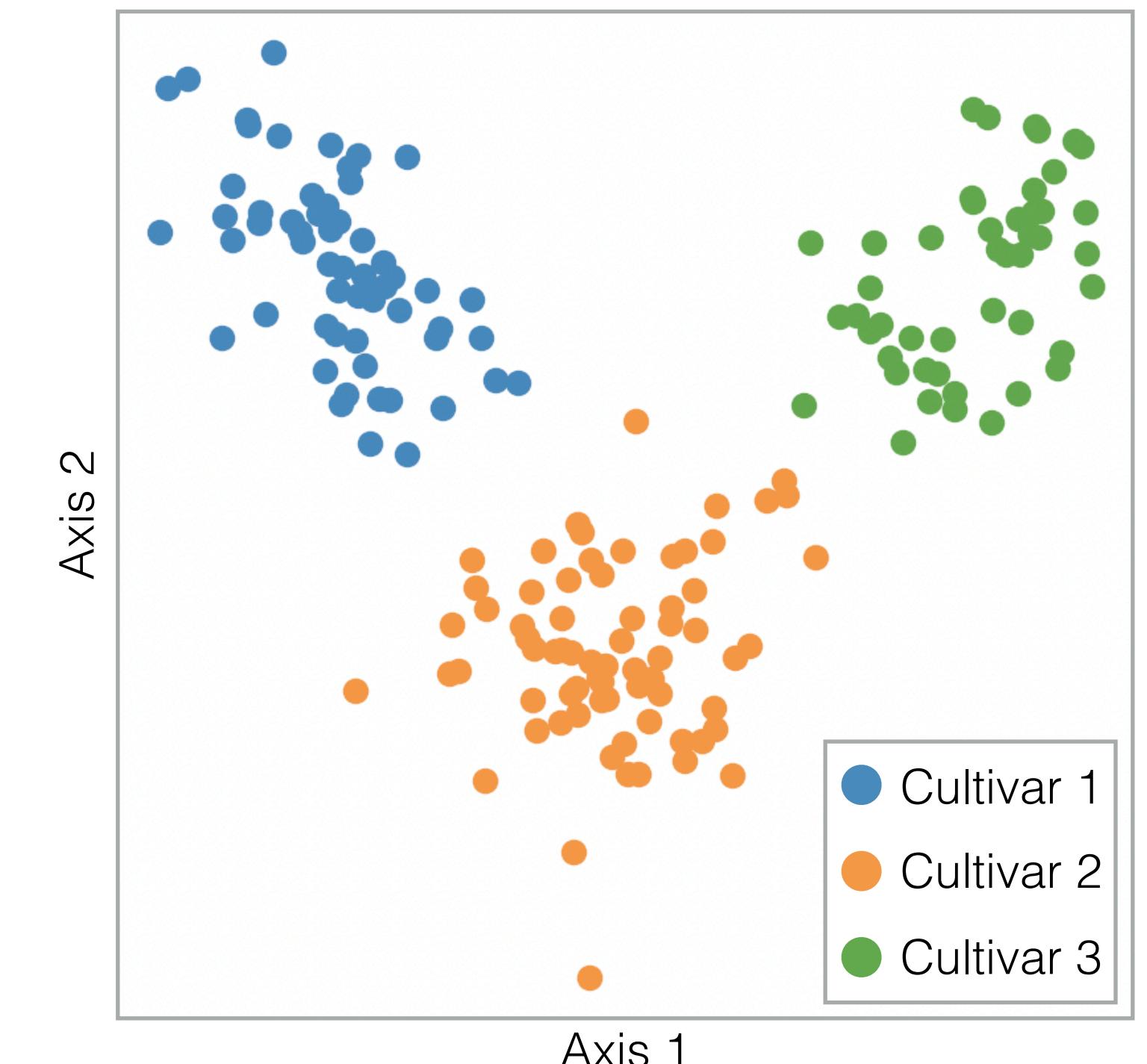
Wine dataset (13D)

	alchol	malic_acid	ash	alcalinity_ash	magnesium	total_phenols	flavanoid
0	1.52	-0.56	0.23	-1.17	1.91	0.81	1.00
1	0.25	-0.50	-0.83	-2.49	0.02	0.57	0.00
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



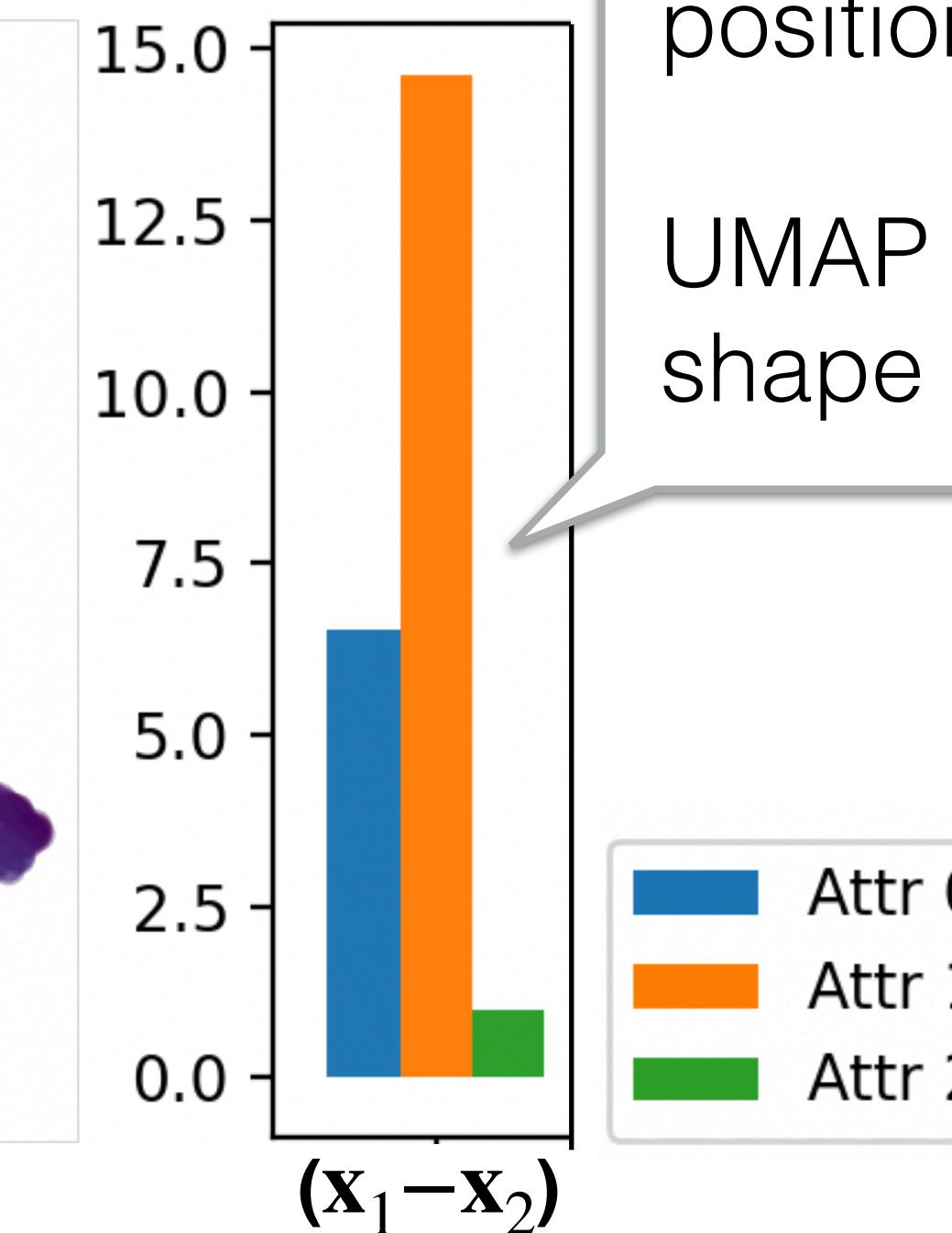
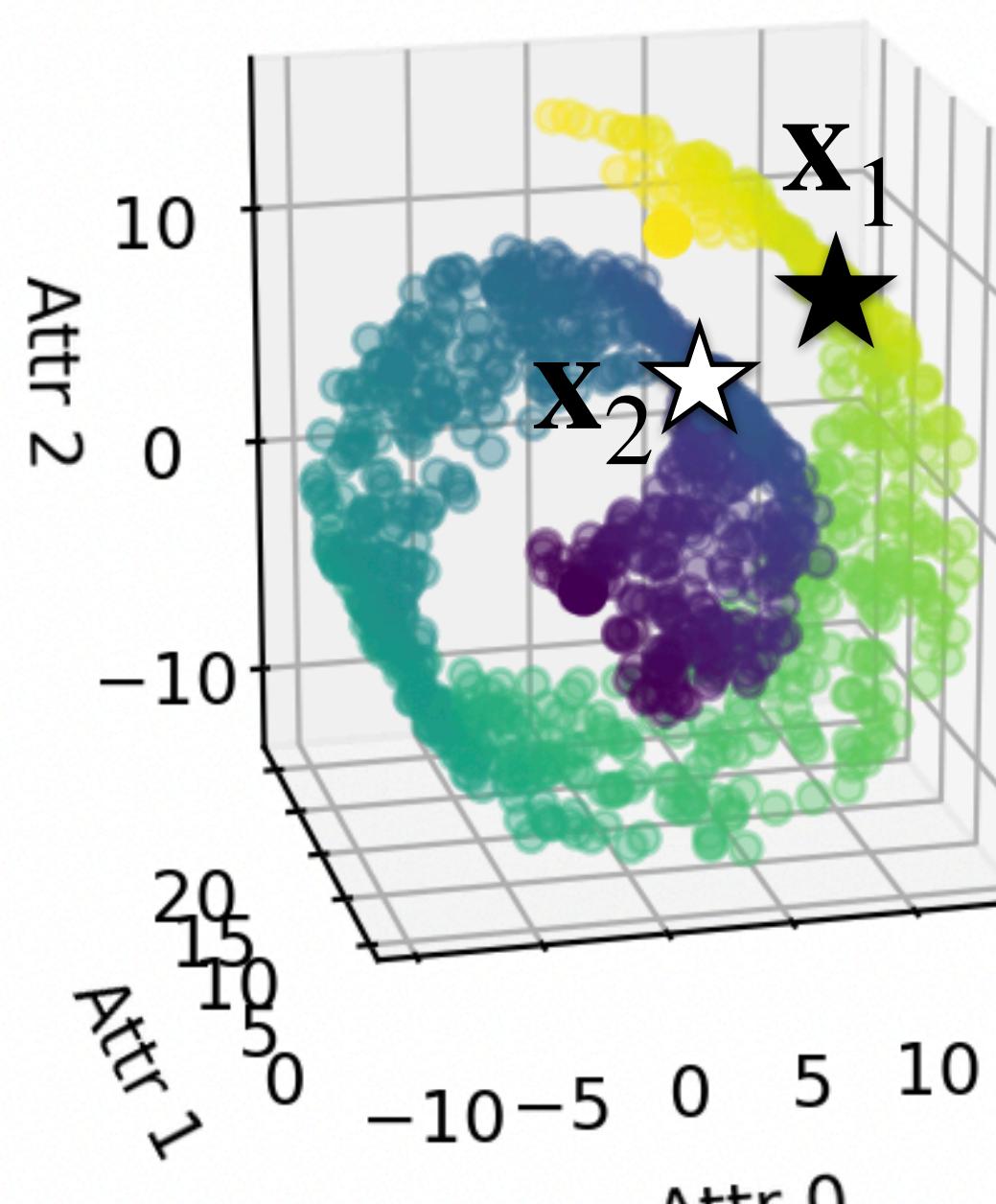
Linear discriminant analysis
LDA



- 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**

Critical problem of observed-level interpretations

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



Attr1 strongly contributes to the positional difference in the DR result?
UMAP seems to capture the spiral shape related to Attr 0 and Attr 2.

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.

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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

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

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

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

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

- 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

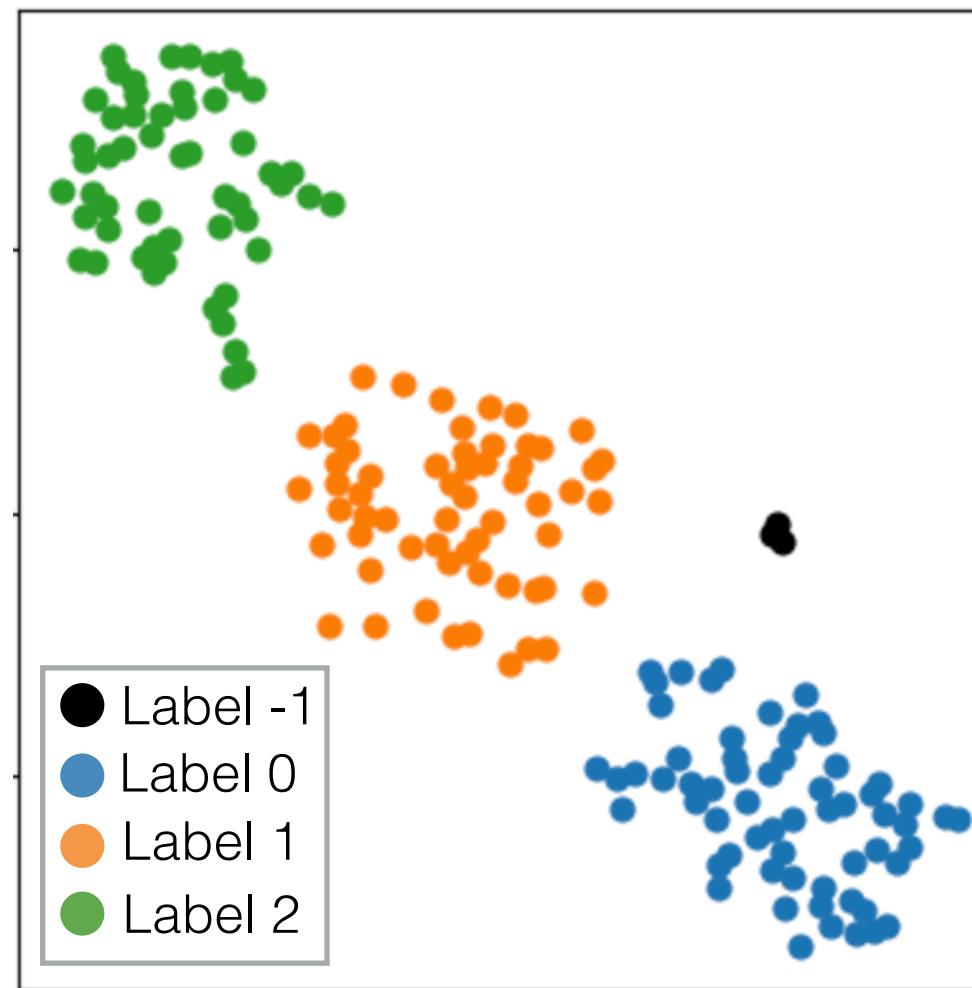
Gould et al., “On differentiating parameterized argmin and argmax problems with application to bi-level optimization.” *arXiv*, 2016.

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

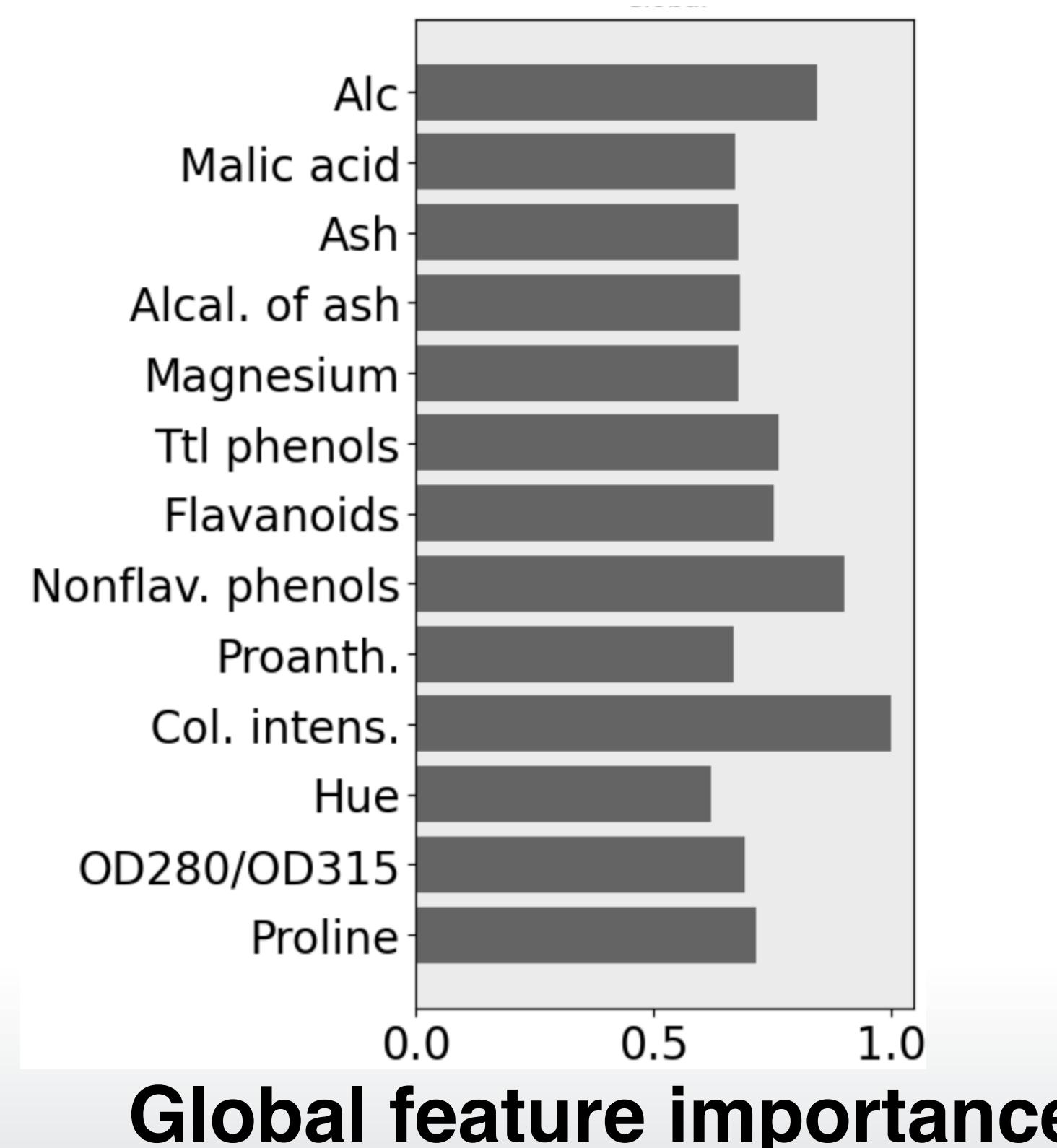
Gradient-based interpretation

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



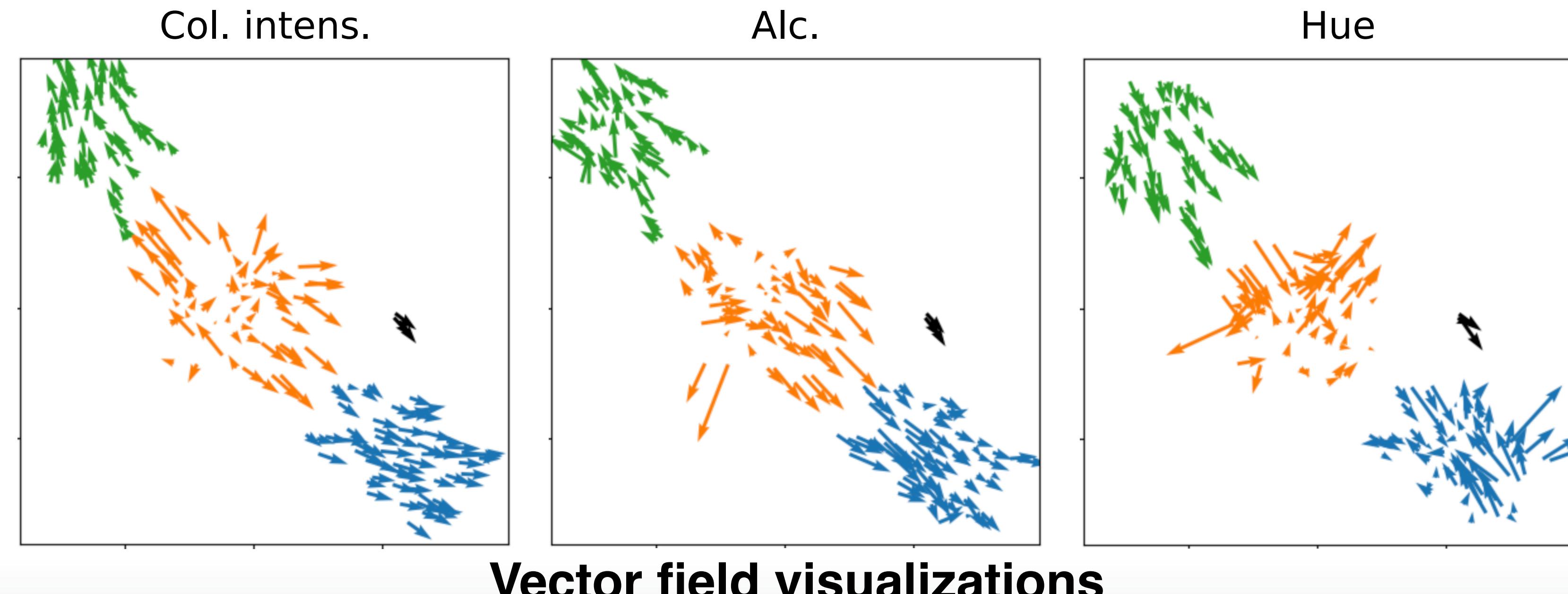
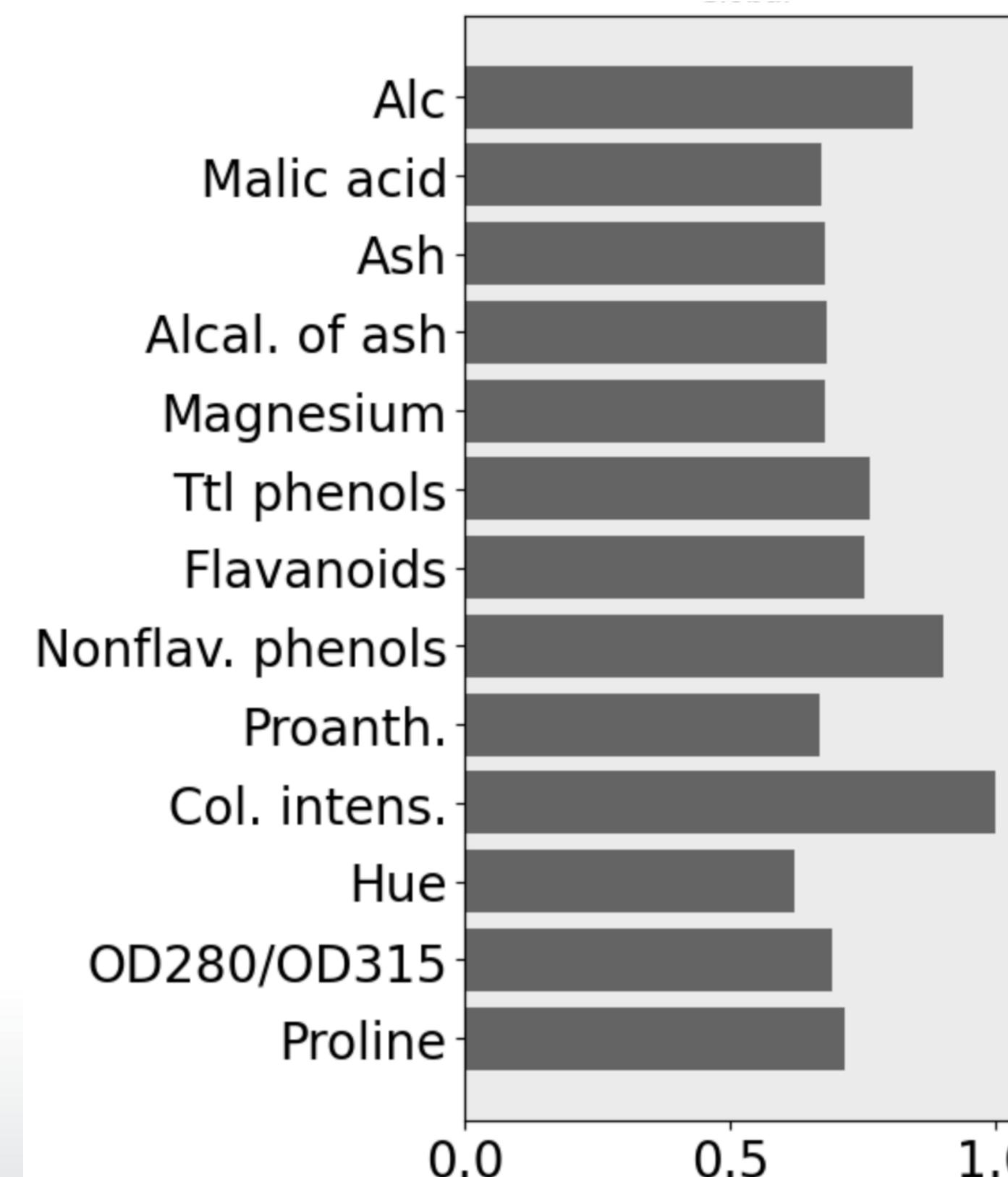
t-SNE result



Gradient-based interpretation

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

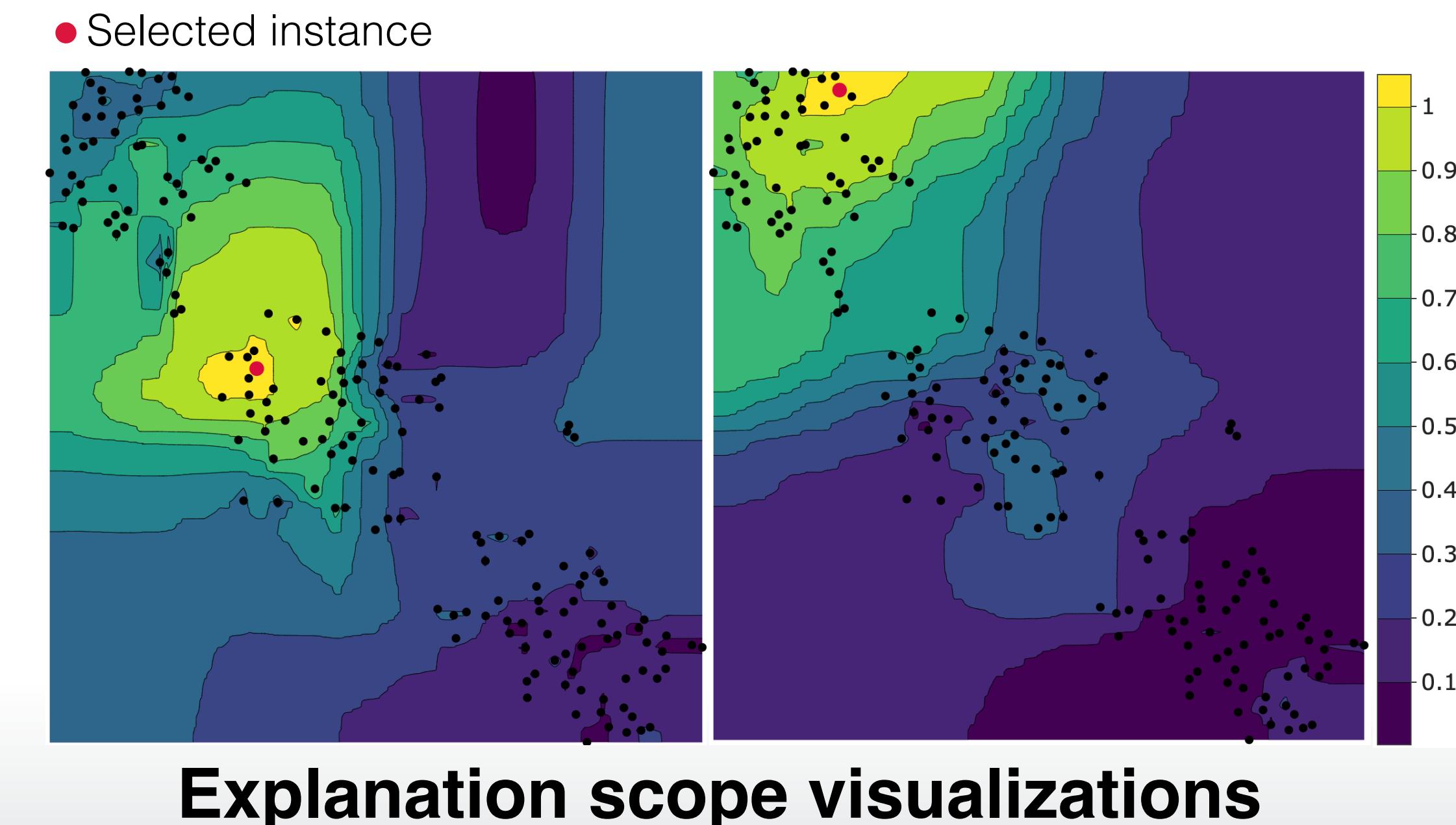
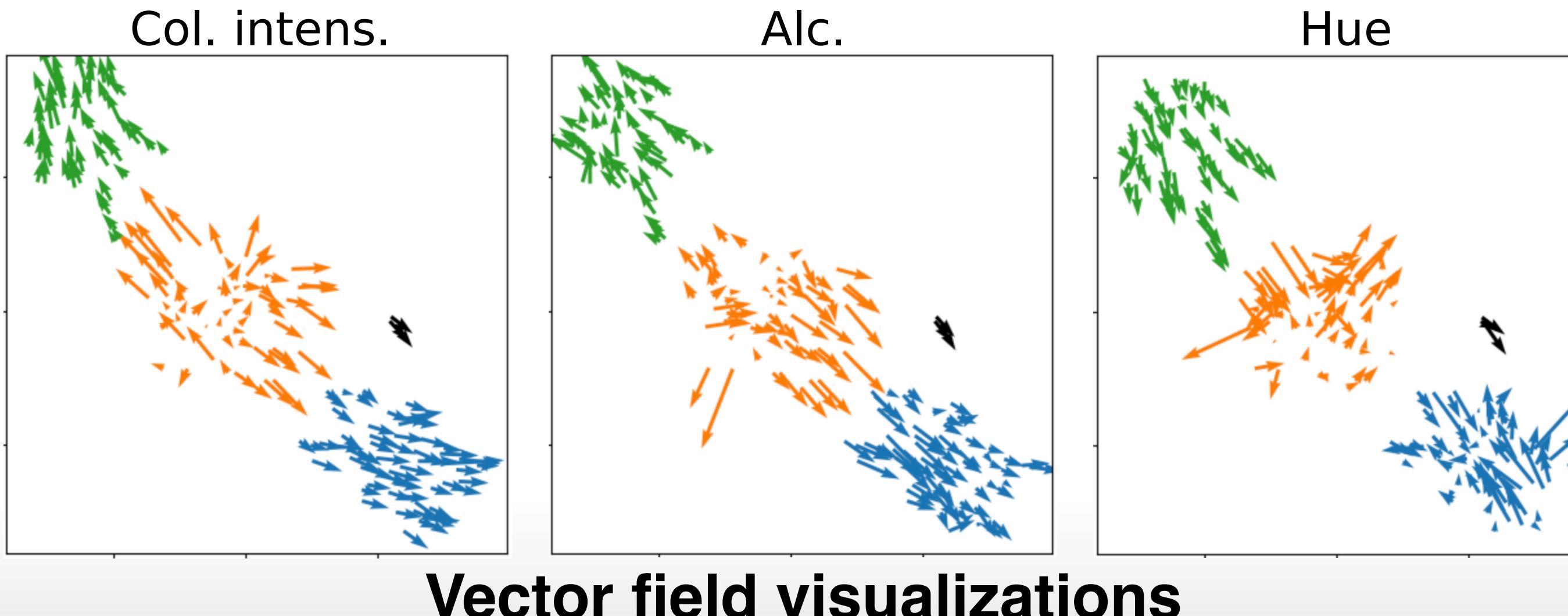
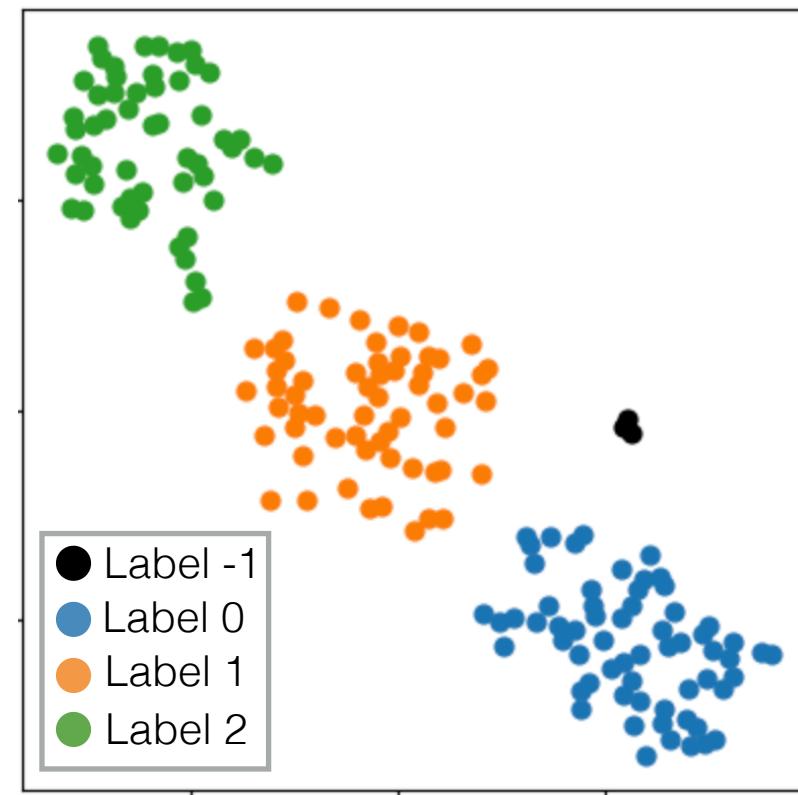
- Complementary tools
 - Global feature importance
 - Vector field visualization for a selected attribute



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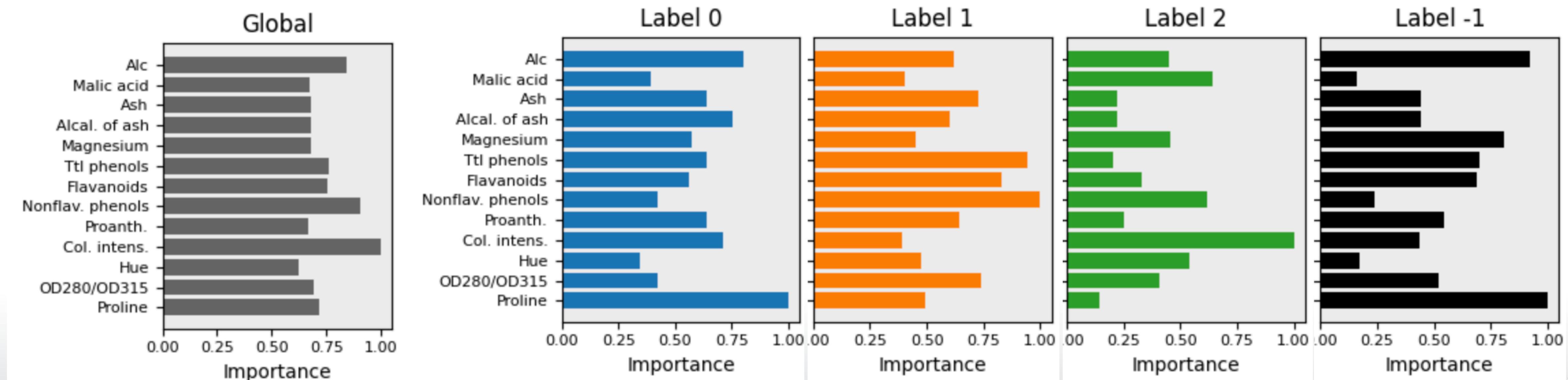
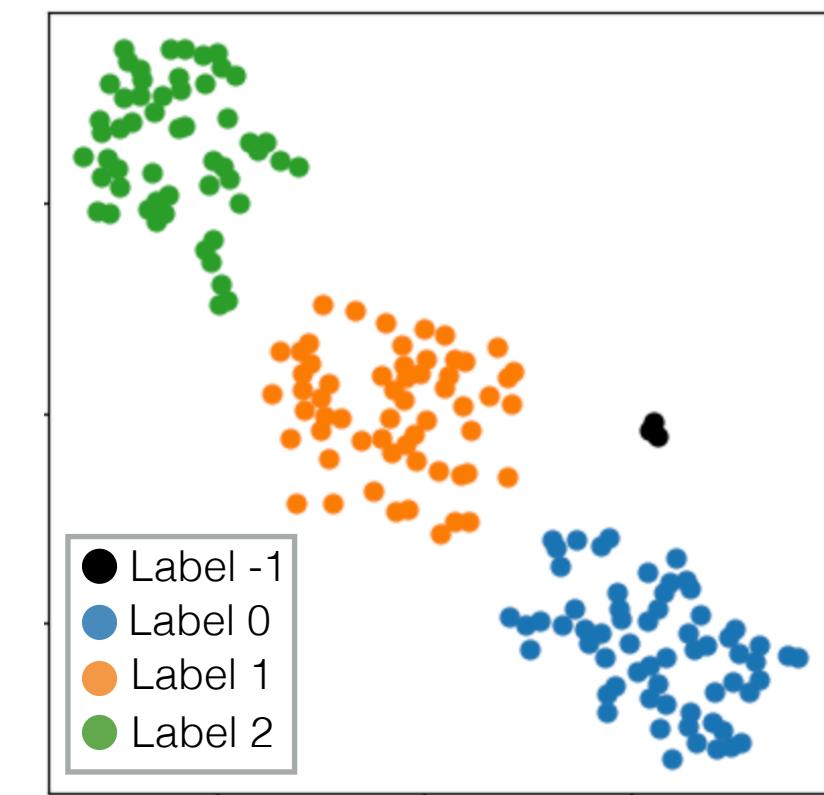
- Complementary tools
 - Global feature importance
 - Vector field visualization for a selected attribute
 - Explanation scope from a selected instance
 - Based on similarities of the gradient vectors



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)



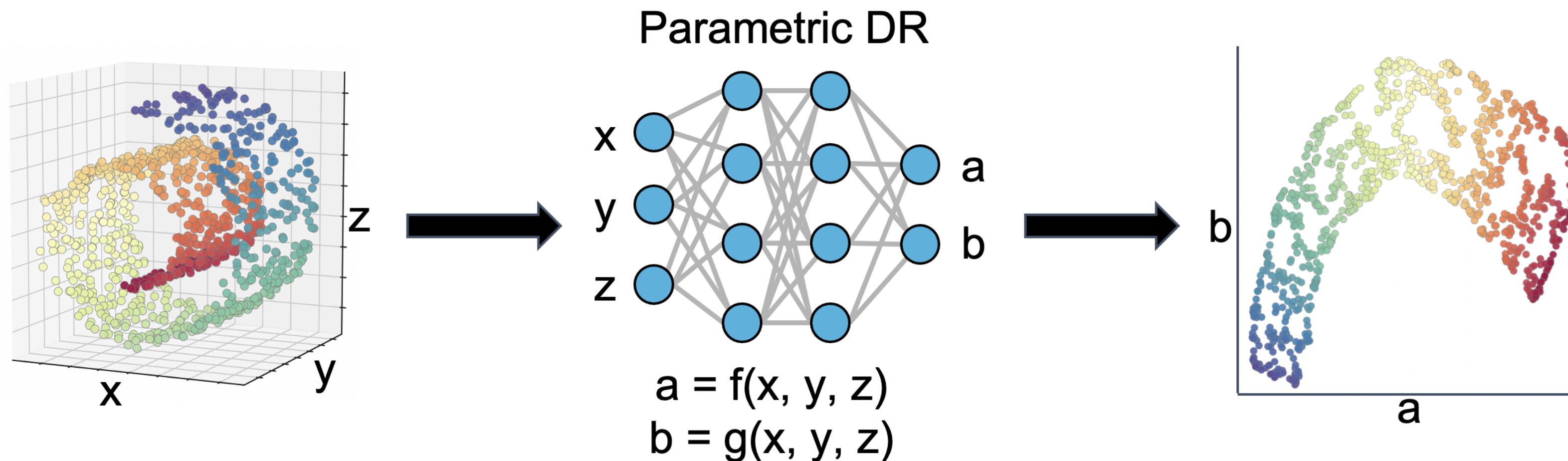
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e.g., Espadoto et al., “UnProjection: Leveraging inverse-projections for visual analytics of high-dimensional data.” *IEEE TVCG*, 2023.

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.
- Chatzimparmpas 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.
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- Marcílio-Jr et al., "Contrastive analysis for scatterplot-based representations of dimensionality reduction." *C&G*, 2021.
- Sainburg et al., "Parametric UMAP embeddings for representation and semisupervised learning." *Neural Computation*, 2021.
- Salmanian et al., "DimVis: Interpreting visual clusters in dimensionality reduction with explainable boosting machine." *MLVis*, 2024.
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- Sundararajan et al., "Axiomatic Attribution for Deep Networks." *arXiv*, 2017.
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- 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