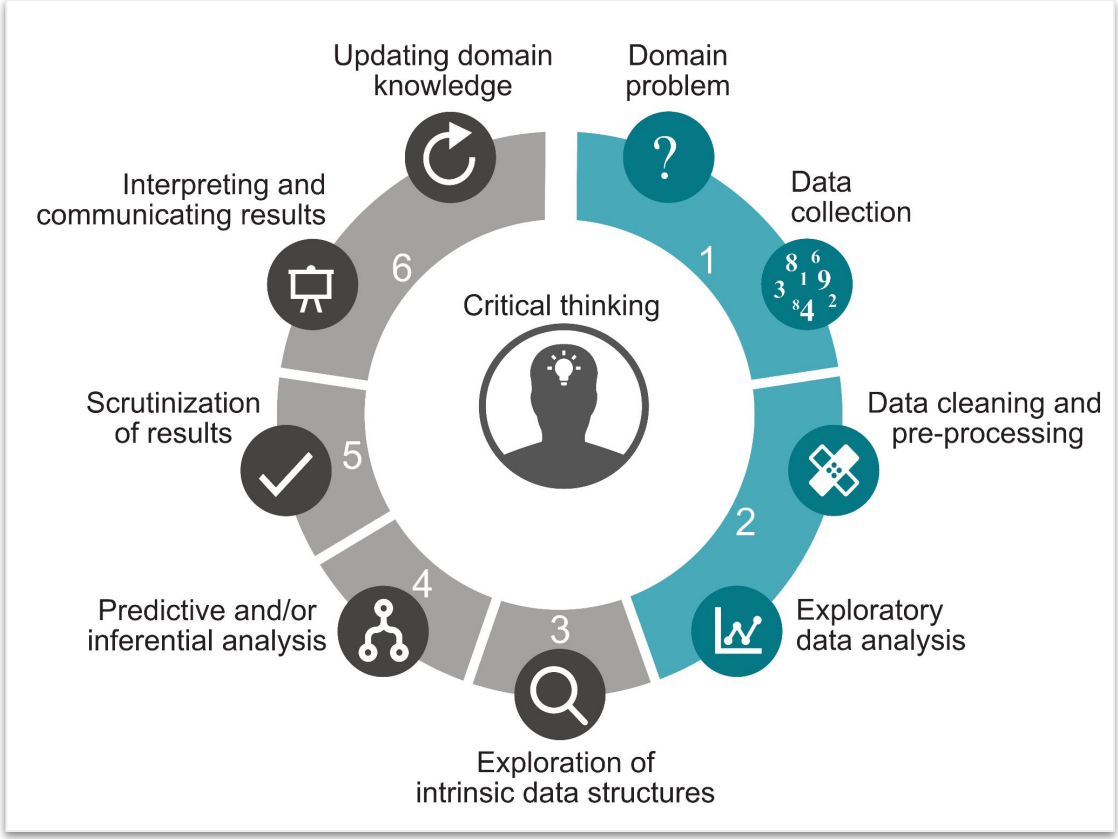
# Introduction to Unsupervised Learning

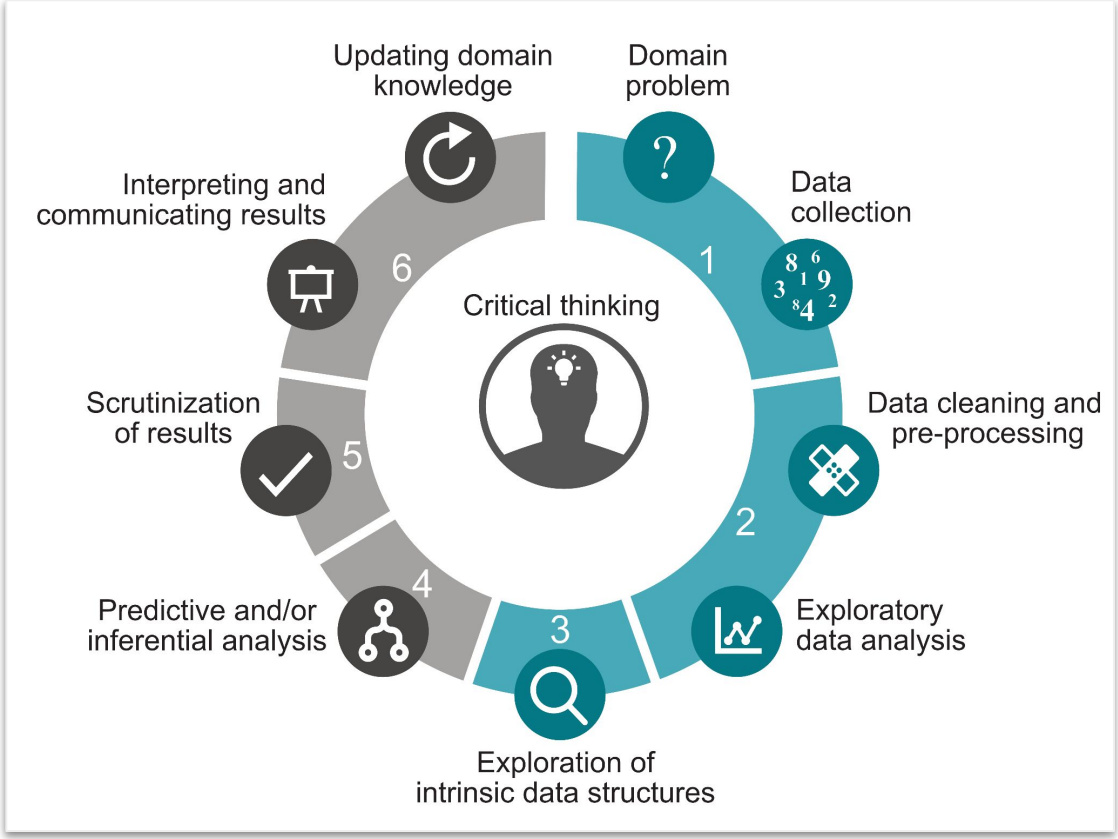
February 10, 2025

# The Big Picture: Data Science Life Cycle




Credits: Veridical Data Science (VDS) Textbook

# The Big Picture: Data Science Life Cycle

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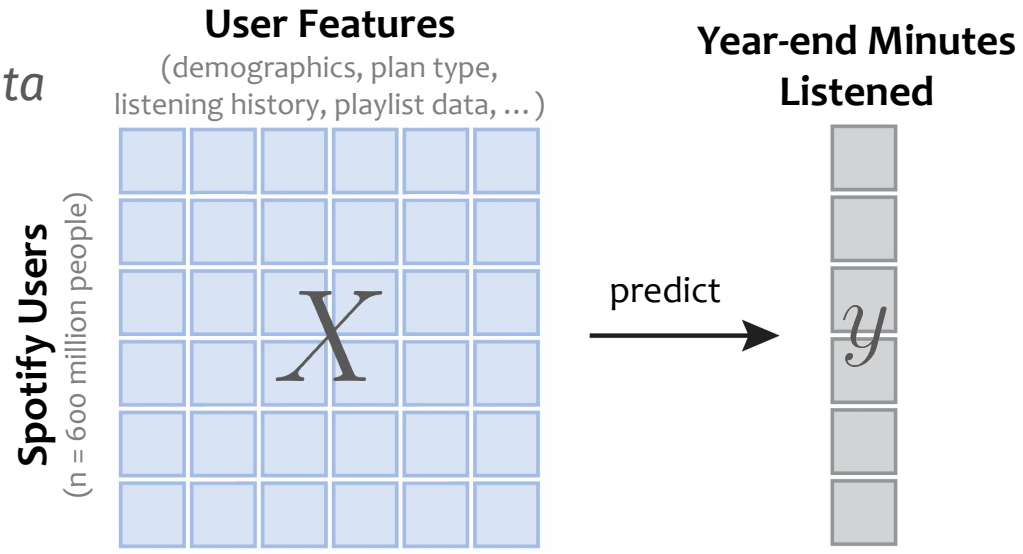
# Today's plan: Introduction to Unsupervised Learning

1. What is **unsupervised learning**?
2. **Applications** of unsupervised learning?
3. Overview of popular **dimension reduction** methods
4. Overview of popular **clustering** methods

# Supervised vs Unsupervised Learning

In the **supervised learning** setting, we typically have some *covariate/feature* data matrix $X \in \mathbb{R}^{n \times p}$ and want to predict a *label/response* $y \in \mathbb{R}^n$

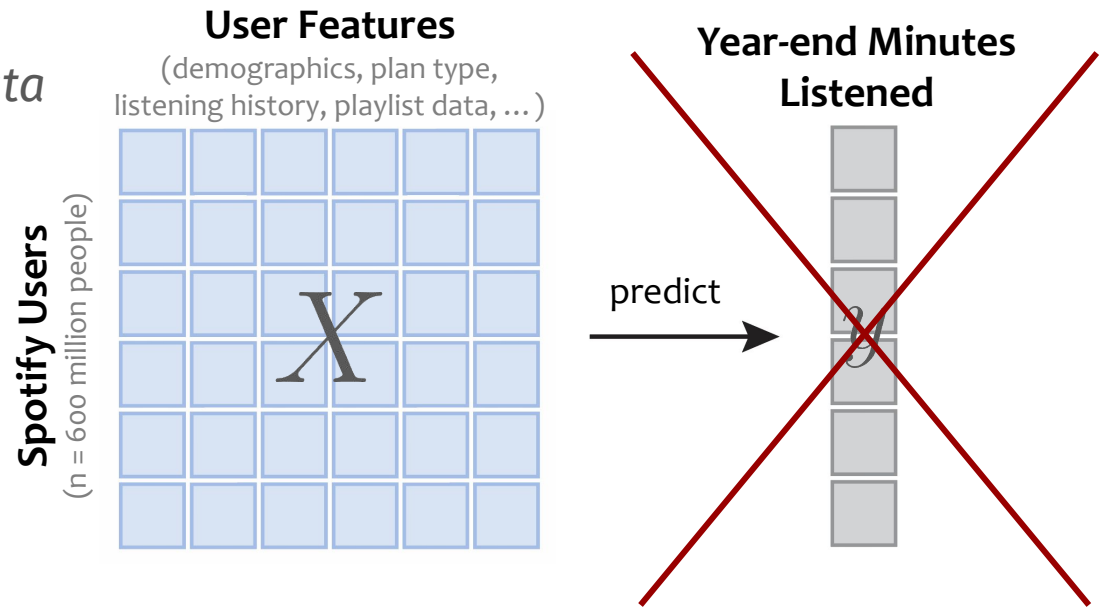
***Example:***
*Spotify data*



# Supervised vs Unsupervised Learning

In the **unsupervised learning** setting, we have some *covariate/feature* data matrix $X \in \mathbb{R}^{n \times p}$ and but **no label/response** $y \in \mathbb{R}^n$

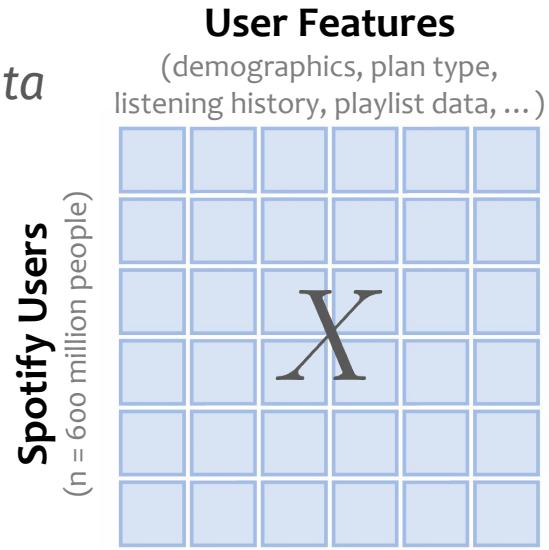
***Example:***
*Spotify data*



# Applications of Unsupervised Learning

In the **unsupervised learning** setting, we have some *covariate/feature* data matrix $X \in \mathbb{R}^{n \times p}$ and but **no label/response** $y \in \mathbb{R}^n$

***Example:***
*Spotify data*




* similar applications in Netflix, Amazon, Youtube, Tiktok, and ad recommendation systems

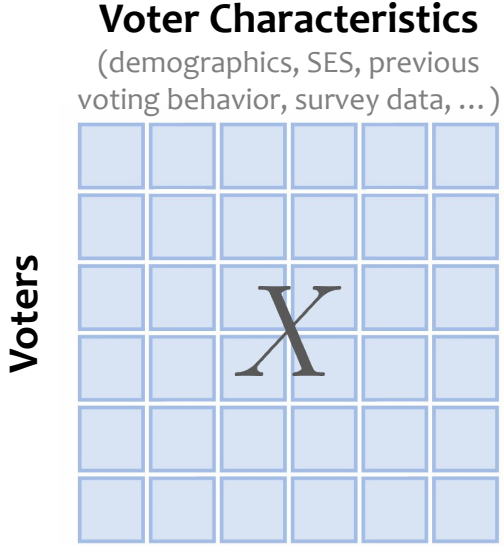
What can we do without labels/responses?

- **Descriptive statistics**
  - Ex. mean age of spotify users
- **Pattern recognition:** discover patterns among observations and/or features
  - Ex. popular song/genre mashups
- **Clustering:** identify groups of similar observations and/or features
  - Ex. groups of people with similar listening histories

# Applications of Unsupervised Learning

In the **unsupervised learning** setting, we have some *covariate/feature* data matrix $X \in \mathbb{R}^{n \times p}$ and but **no label/response** $y \in \mathbb{R}^n$

***Example:***
*Political Behavior*



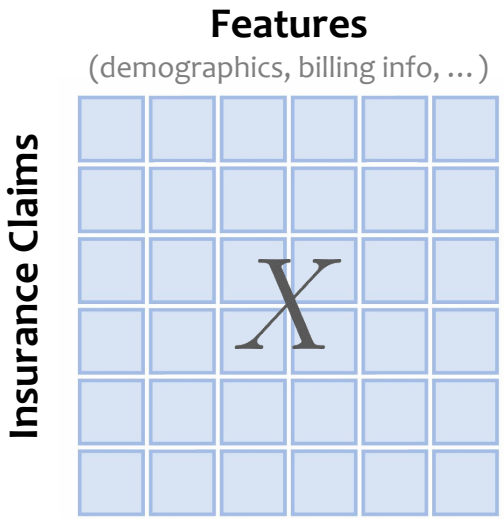

**Clustering/pattern recognition applications:**

- Can we identify groups of similar voters so that we can create targeted messages?
- Who are the swing voters? And what issues are most likely to sway them?

# Applications of Unsupervised Learning

In the **unsupervised learning** setting, we have some *covariate/feature* data matrix $X \in \mathbb{R}^{n \times p}$ and but **no label/response** $y \in \mathbb{R}^n$

***Example:***
*Anomaly/ Fraud Detection*



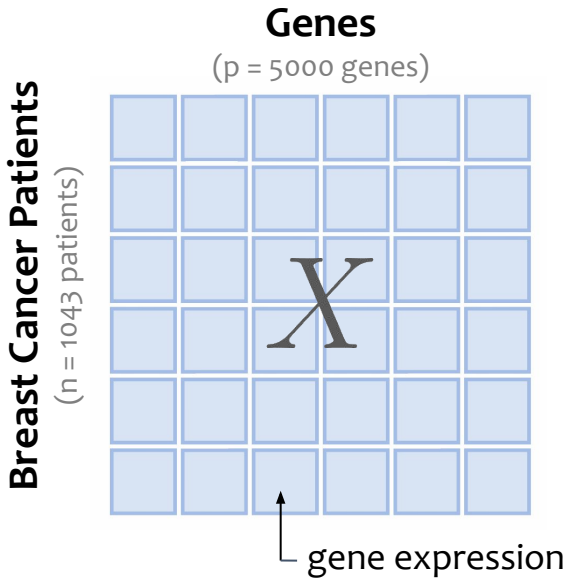

**Clustering/pattern recognition applications:**

- Are there any anomalies in the claims/billing data? Maybe these are fraudulent.
- Can perform clustering to identify similar claims that may be billed incorrectly

# Applications of Unsupervised Learning

In the **unsupervised learning** setting, we have some *covariate/feature* data matrix $X \in \mathbb{R}^{n \times p}$ and but **no label/response** $y \in \mathbb{R}^n$

***Example:***
*Cancer genomics*




**Clustering/pattern recognition applications:**

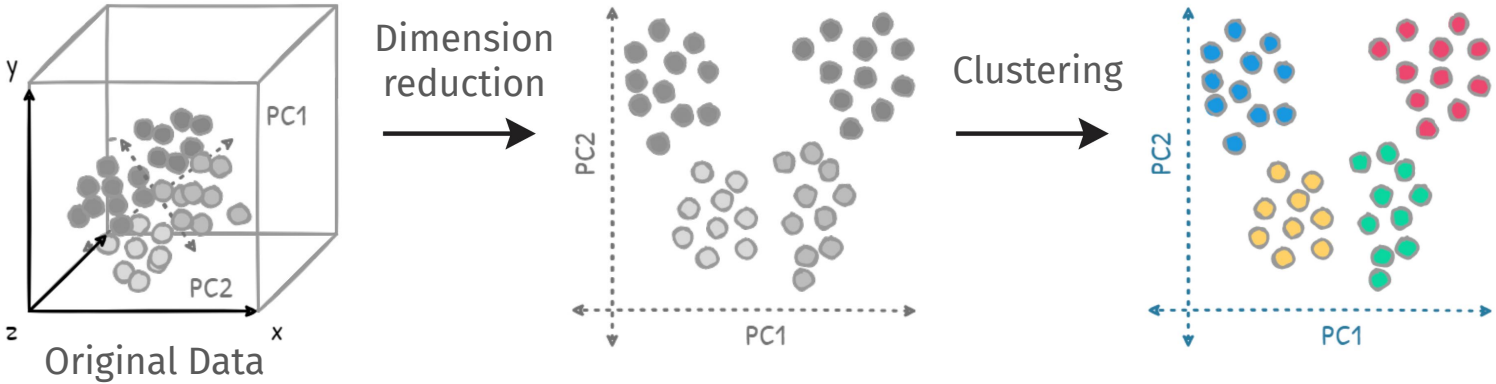
- Are there **subtypes** of patients who have similar tumors? Moreover, are there particular genes that drive these subtypes?
  - Hope is that these groups can be treated similarly and in a more personalized way than what's done for the whole group → *"personalized medicine"*

# How do we "learn" from unsupervised data?

Two common unsupervised learning tools

1. **Dimension Reduction**
   - For pattern recognition, visualizing your data, data compression
2. **Clustering**
   - For identifying groups or clusters in your data

A common dimension reduction + clustering pipeline:



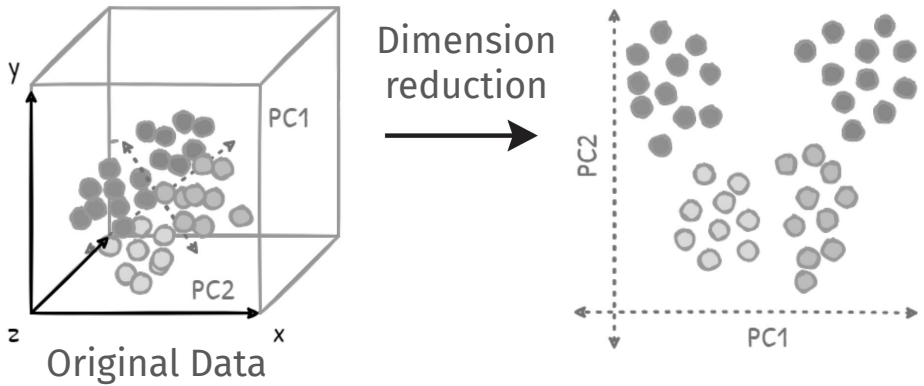
# Dimension Reduction

# Dimension Reduction

In reality, data is often **"high-dimensional"** (i.e., has many covariates/features)

How do we visualize data with > 3 features?

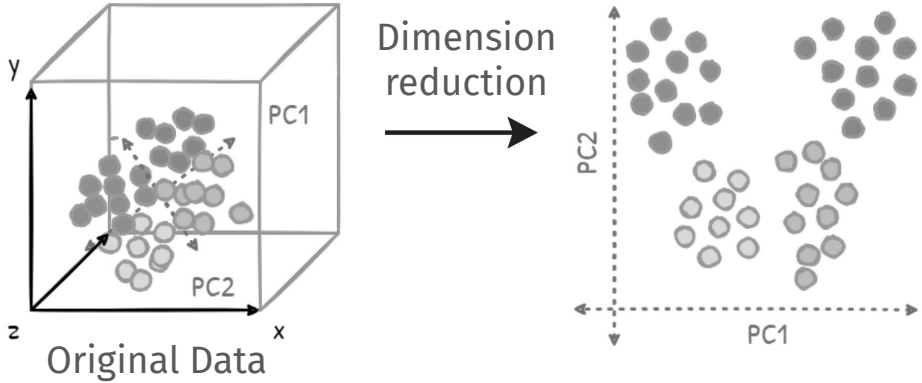
**Dimension Reduction:** aims to find a lower-dimensional representation of the data which preserves as much of the original information as possible



# Principal Components Analysis (PCA)

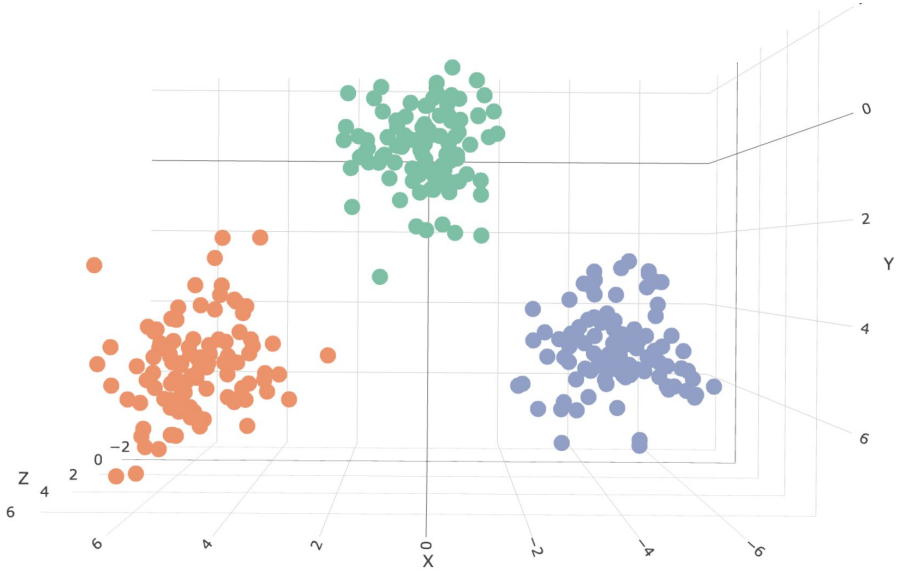
**Principal Components Analysis (PCA):** finds a lower-dimensional representation of the data which preserves as much of the **variance** in the data as possible

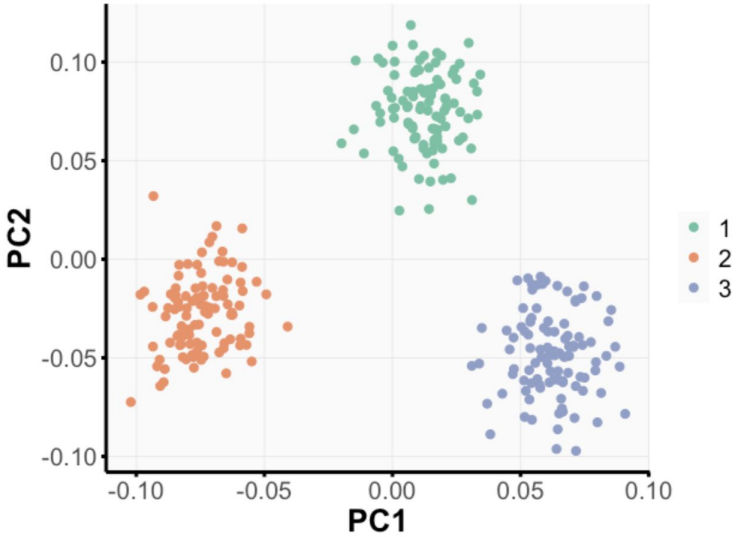
- More specifically, PCA finds a lower-dimensional hyperplane (or orthogonal directions) such that when the data is projected onto the hyperplane, the variance of the data is maximized
- PCA is a **linear projection**



# When does PCA "work" and when does PCA "not work"?

*Scenario:* (High-dimensional) Gaussian data



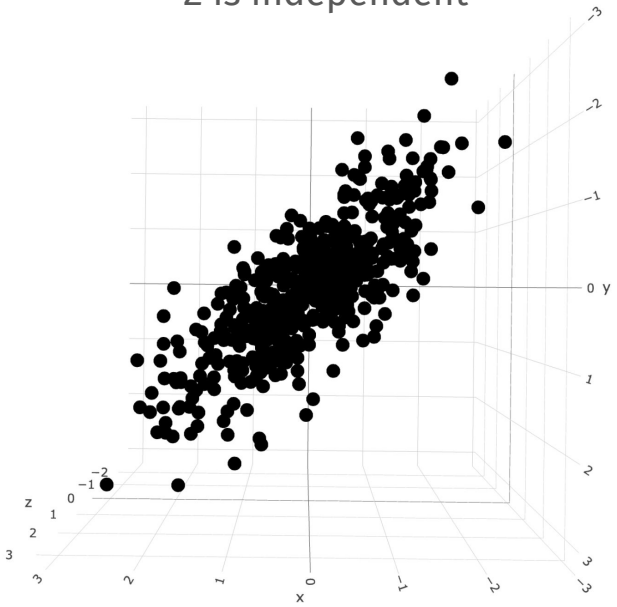




✔ This is the ideal scenario for PCA

# When does PCA "work" and when does PCA "not work"?

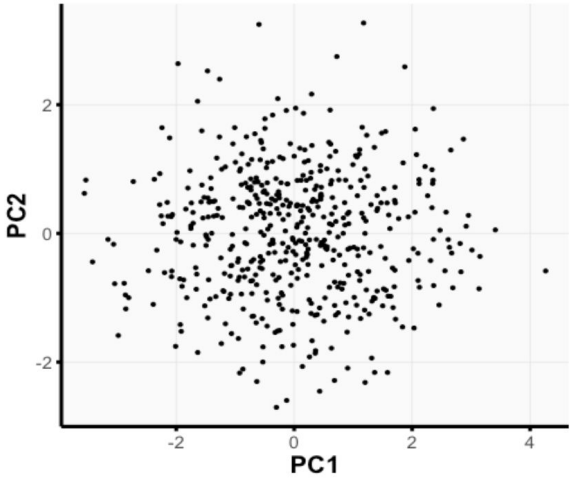
*Scenario:* Correlated Variables

X and Y are highly correlated;
Z is independent




**PC Loadings:**

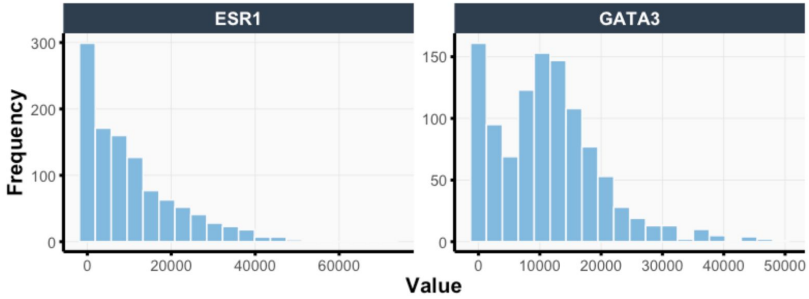
```
PC1 =  0.7X + 0.7Y + 0.1Z
PC2 = -0.1X - 0.1Y + 1.0Z
```

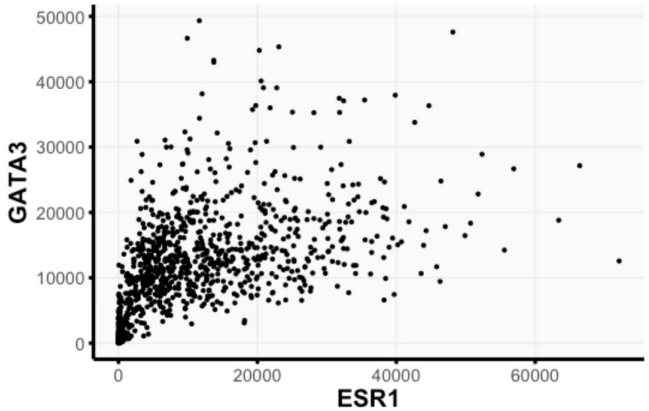



PCs typically group correlated variables together

# When does PCA "work" and when does PCA "not work"?

*Scenario:* Highly skewed data or data with outliers



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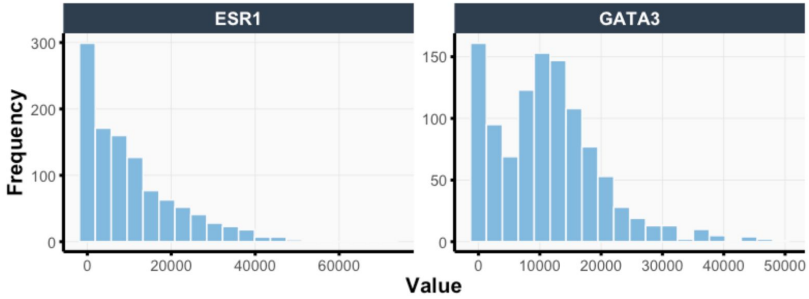
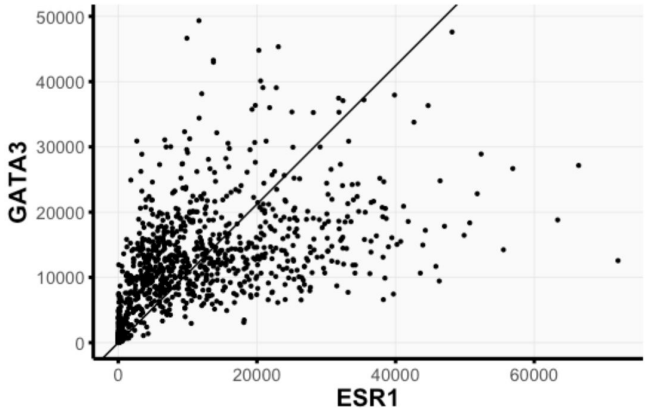
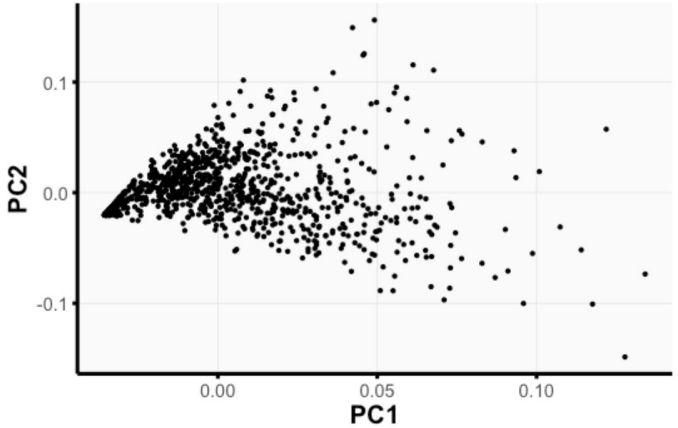


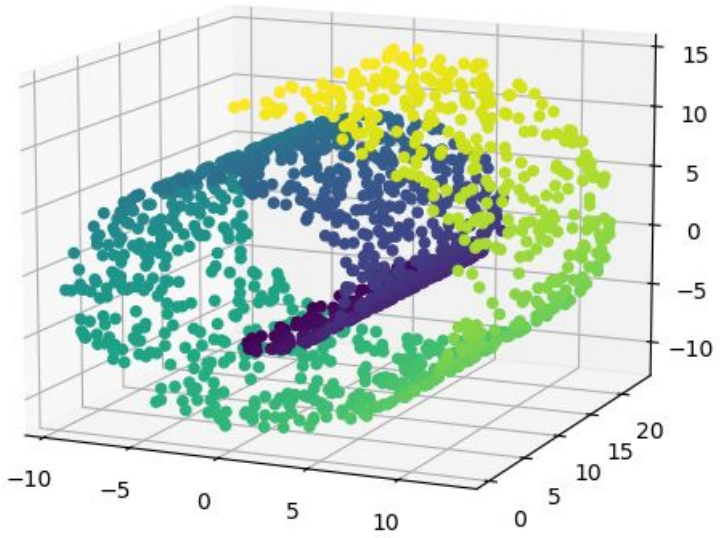



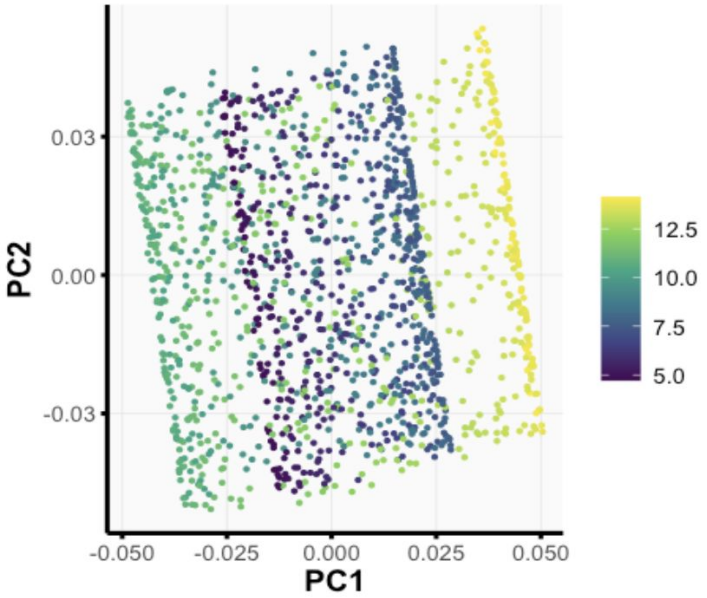




✔ **if** variance is still a meaningful measure of information

# When does PCA "work" and when does PCA "not work"?

*Scenario:* Swiss roll




✘ not great for nonlinear manifolds

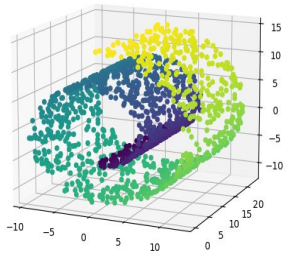
# **Nonlinear** Dimension Reduction Methods

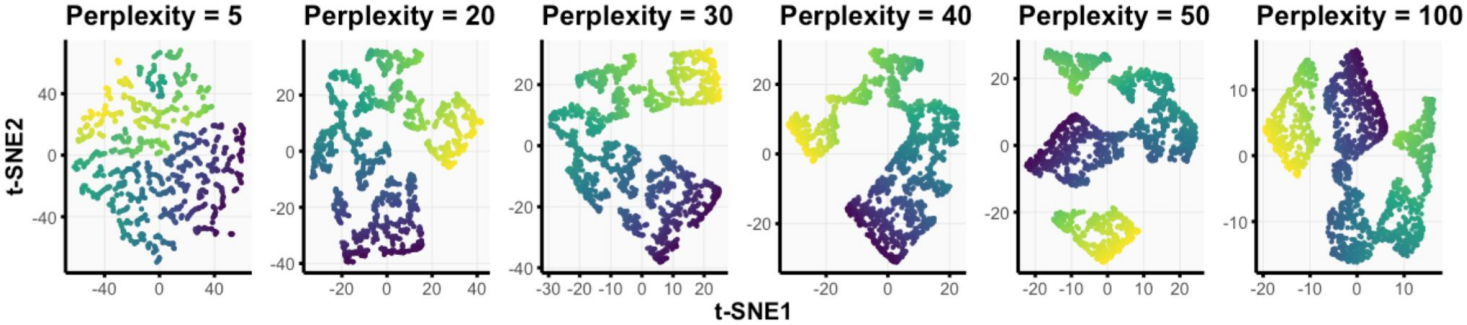
## tSNE

1. Compute Euclidean distance between every pair of points in X
2. Translate these pairwise distances into probability of being neighbors
   + Large pairwise distance → low probability of being neighbors
3. Find lower-dimensional representation such that

Prob(i and j are neighbors) in **original high-dimensional** space ≈ Prob(i and j are neighbors) in **new low-dimensional** space

*Hyperparameter:* perplexity



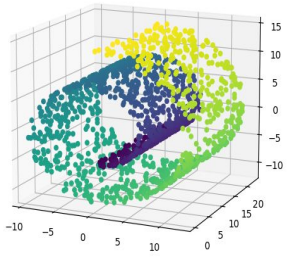


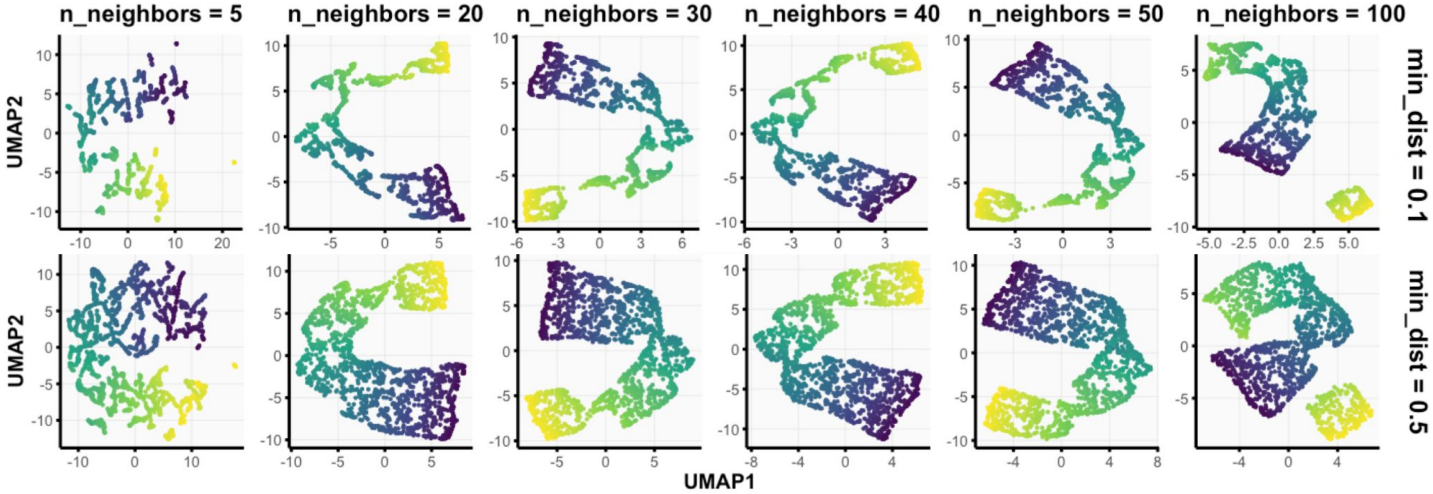
# **Nonlinear** Dimension Reduction Methods

## UMAP

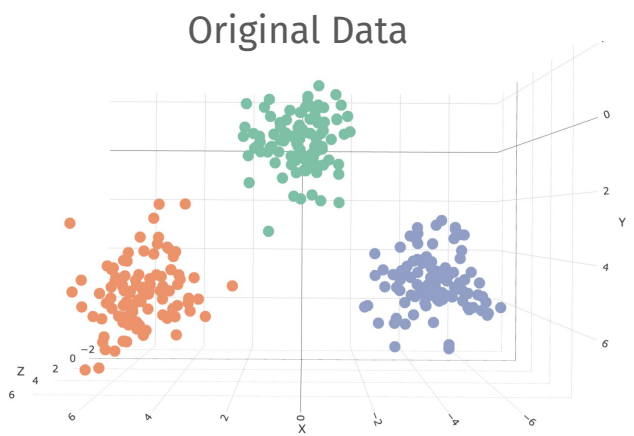
- UMAP often does better than tSNE at preserving the global structure
- Like tSNE, the idea is that pairs of points that are close in the original high-dimensional space should also be close in the new low-dimensional space
- How does UMAP differ from tSNE? Different similarity metrics, loss function, optimization algorithm

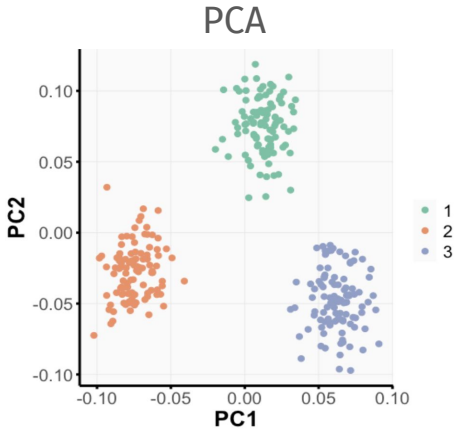
*Hyperparameter:* n_neighbors and min_distance

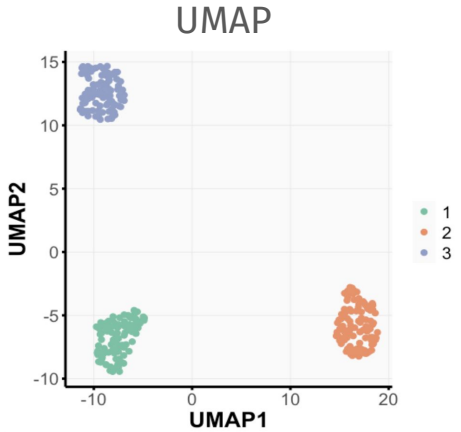


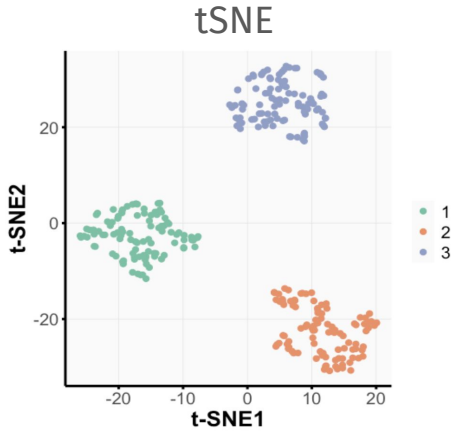


# Word of caution: tSNE and UMAP can exaggerate clusters



# Recap: Dimension Reduction Methods

| | **PCA** | **tSNE** | **UMAP** |
|---|---|---|---|
| *Feature Interpretability* | Yes | No | No |
| *Linear/nonlinear* | Linear | Nonlinear | Nonlinear |
| *Number of components* | Orthogonal, nested;<br>Can compute all *p* components at once | Non-nested and need to re-run for each chosen rank;<br>Typically only 2-3 components | Non-nested and need to re-run for each chosen rank;<br>Typically only 2-3 components |
| *Computation* | Fast | Slower | Slower but faster than tSNE |
| *Unique, global solution* | Yes | Converges to local solution | Converges to local solution |
| *Other considerations?* | No hyperparameters | Results can change drastically depending on hyperparameters;<br>Not good at preserving global structure;<br>"Curse of dimensionality" | Results can change drastically depending on hyperparameters;<br>Better at preserving global structure than tSNE;<br>"Curse of dimensionality" |

Other dimension reduction methods: MDS, NMF, ICA, Isomap, LLE, Autoencoders, …

# Additional Resources

A more detailed review of these unsupervised learning methods + more can be found at https://tiffanymtang.github.io/dsip-s25/#unsupervised-learning

- Also includes R and Python code for implementing these methods

The quarto notebook that generated this walkthrough can be found here:

https://github.com/tiffanymtang/dsip-s25/blob/main/unsupervised_learning/notebooks/unsupervised_learning.qmd

**Additional Resources for Unsupervised Learning Methods**

- Elements of Statistical Learning Textbook Chapter 14