JSC 270 - Lecture 9
Embedding

https://jsc270.github.io/

Dimensionality Reduction

How would you define it?

Dimensionality Reduction

What applications can you think of?

Dimensionality Reduction

Which techniques do you know?

Dimensionality Reduction vs Embedding

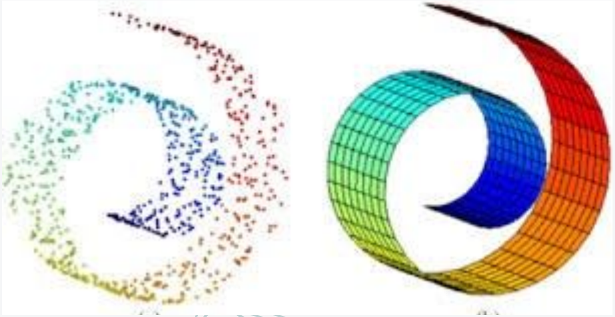
High-dimensional data often lies on or near a much lower dimensional manifold.

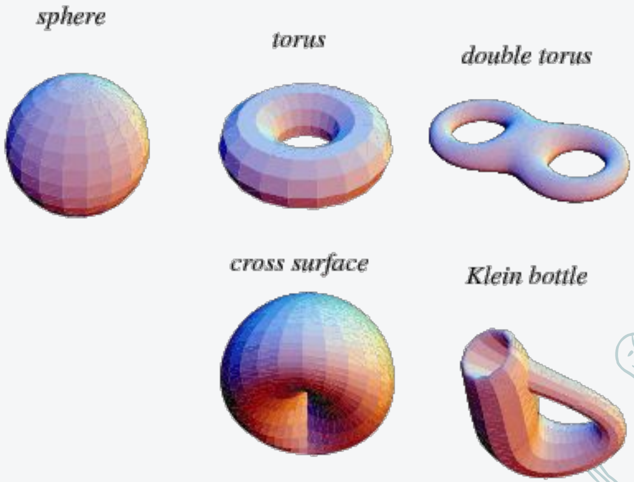
We reduce dimension or *embed* data into the manifold to get the *embedding*, in other words a low dimensional representation

Useful Concepts: Manifold

Manifold - a collection of points forming a certain kind of set, such as those of a topologically closed surface in three or more dimensions (such topological space that locally resembles Euclidean space near each point)

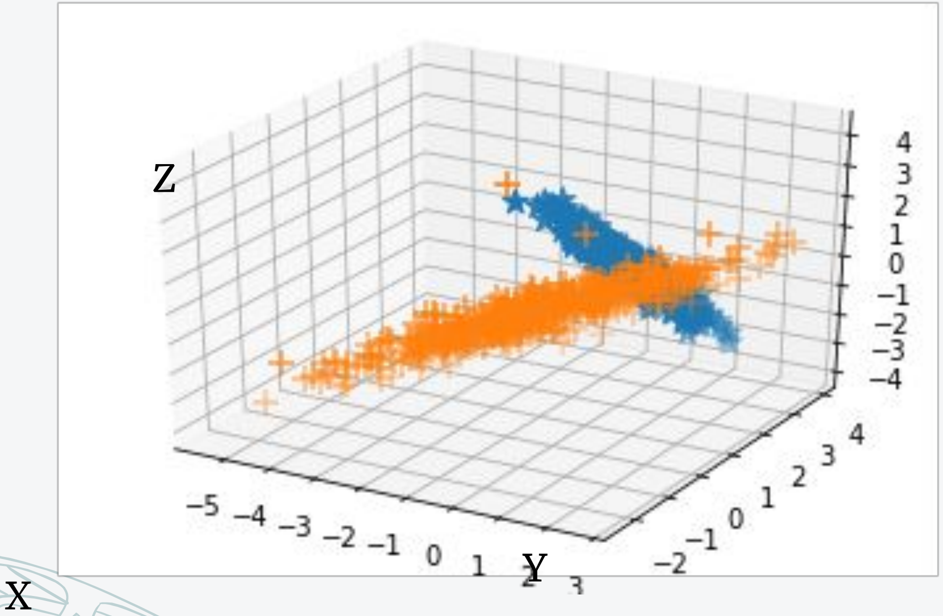
Swiss roll





Data

Number of samples $N = 1000$
Number of features $P = 3$



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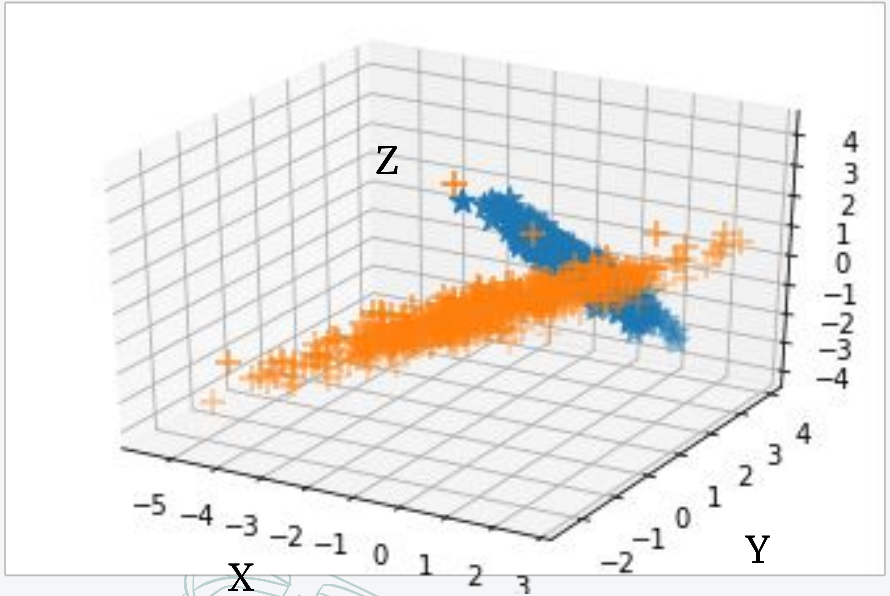
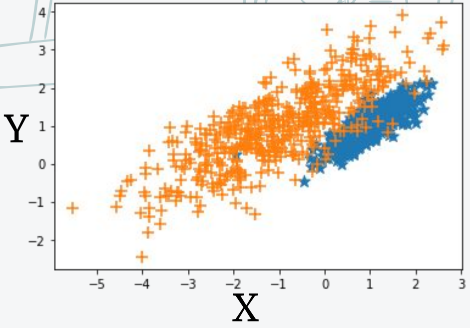
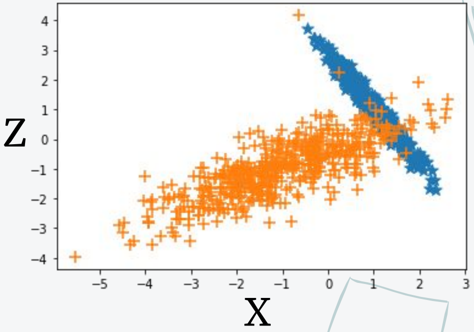
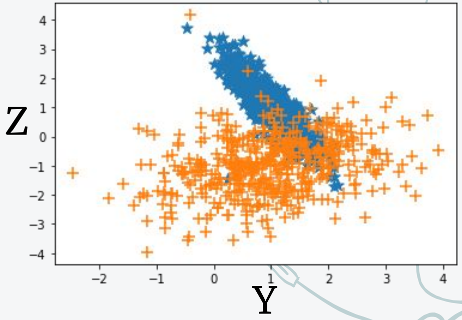








Principal Component Analysis

Principle components = axes of greatest variability

When we talk about $X1, X2, \ldots, Xp$ - these features are in cartesian coordinate system

Principle components are a *new* set of p axes in the direction of greatest variability, that are a linear combination of the original

Selecting Principal Components

In one dimension, we would projecting points to a line.

How do we do that?

Selecting Principal Components

In one dimension, we would projecting points to a line.

How do we do that?   Regression (squared loss)

How do we do it in many dimensions?

Linear Algebra (review)

- Eigenvectors for a square m x m matrix **S**

$$\boldsymbol{S}\boldsymbol{v} = \lambda \boldsymbol{v}$$

Eigenvector $\boldsymbol{v} \in \mathbb{R}^m, \boldsymbol{v} \neq \mathbf{0}$

Eigenvalue $\lambda \in \mathbb{R}$

E.g

$$\begin{pmatrix} 6 & -2 \\ 4 & 0 \end{pmatrix} \underbrace{\begin{pmatrix} 1 \\ 2 \end{pmatrix}}_{\text{eigenvector}} = \begin{pmatrix} 2 \\ 4 \end{pmatrix} = \underbrace{2}_{\text{eigenvalue}} \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

Linear Algebra (Review)

How many eigenvalues are there at most?

Linear Algebra (Review)

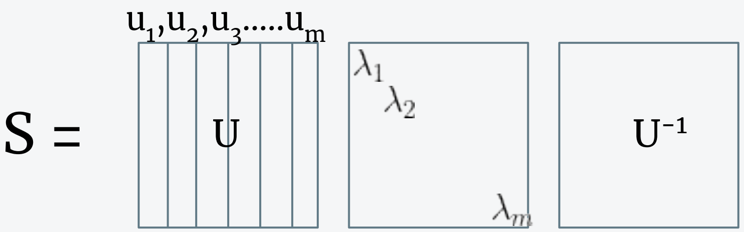
For *symmetric matrices*, eigenvectors for distinct eigenvalues are *orthogonal*

All eigenvalues for a *positive semidefinite matrix* are *non-negative*

Note: S is positive semidefinite if $\forall w \in \mathbb{R}^m, w^T S w \geq 0$

Eigen Decomposition

Eigen decomposition transforms a matrix into its principal vectors of variation



$$S = U \Lambda U^{-1}$$

U are eigenvectors of S, diagonal values of Lambda are eigenvalues.

Eigen Decomposition

Eigen decomposition transforms a matrix into its principal vectors of variation

$u_1,u_2,u_3.....u_m$

$$S = \begin{bmatrix} U \end{bmatrix} \begin{bmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ 0 & & \lambda_m \end{bmatrix} \begin{bmatrix} U^{-1} \end{bmatrix}$$

Decomposition is unique if eigenvalues are unique

$$S = U\Lambda U^{-1}$$

Columns of U are eigenvectors of S

Diagonal values of Lambda are eigenvalues of S

Singular Value Decomposition (SVD)

For an m x n matrix **A** of rank r there exists a factorization (SVD) as follows:

$$\underset{}{A} = \underbrace{U}_{m \times m}\,\underbrace{\Sigma}_{m \times n}\,\underbrace{V^T}_{n \times n}$$

The columns of *U* are orthogonal eigenvectors of $\mathbf{AA}^{T}$

The columns of V are orthogonal eigenvectors of $\mathbf{A}^{T}\mathbf{A}$

Eigenvalues $(\sigma_1, \sigma_2, \ldots, \sigma_r)$ of $\mathbf{AA}^{T}$ are eigenvalues of $\mathbf{A}^{T}\mathbf{A}$

$$\Sigma = \begin{bmatrix} \sigma_1 & & 0 \\ & \sigma_2 & \\ 0 & & \sigma_r \end{bmatrix}$$

Note: rank r means there are max of r linearly independent rows and columns in A

Singular Value Decomposition (SVD)

For an **m x n** matrix **A** of **rank r** there exists a factorization (SVD) as follows:

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$$\Sigma = \begin{bmatrix} \sigma_1 & & 0 \\ & \sigma_2 & \\ 0 & & \sigma_r \end{bmatrix}$$

Singular Values

Note: rank r means there are max of r linearly independent rows and columns in A

Singular Value Decomposition (SVD)

For an m x n matrix **A** of rank r there exists a factorization (SVD) as follows:

$$\underset{m \times m}{U}\;\underset{m \times n}{\Sigma}\;\underset{n \times n}{V^T}$$

$$A = U\Sigma V^T$$

m x m m x n n x n

The columns of *U* are orthogonal eigenvectors of $\mathbf{AA}^{\mathrm{T}}$

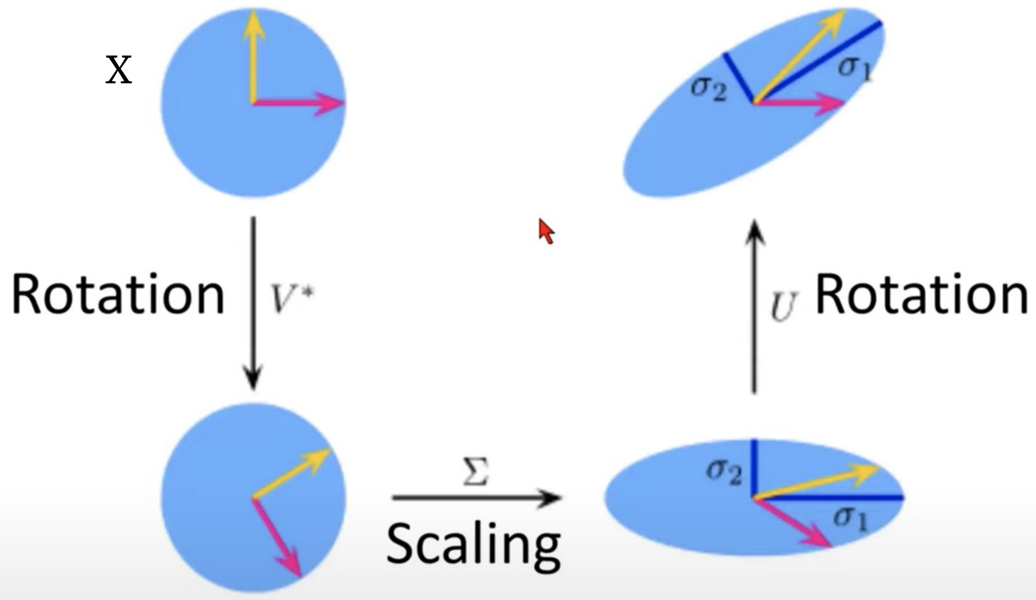
The columns of V are orthogonal eigenvectors of $\mathbf{A}^{\mathrm{T}}\mathbf{A}$

Eigenvalues $(\sigma_1, \sigma_2, \ldots, \sigma_r)$ of $\mathbf{AA}^{\mathrm{T}}$ are eigenvalues of $\mathbf{A}^{\mathrm{T}}\mathbf{A}$

$$\Sigma = \begin{bmatrix} \sigma_1 & & & 0 \\ & \sigma_2 & & \\ & & \ddots & \\ 0 & & & \sigma_r \end{bmatrix} \Leftarrow \boxed{\lambda_i = \sqrt{\sigma_i}}$$

Note: rank r means there are max of r linearly independent rows and columns in A

Geometric interpretation of SVD



$$X = U \cdot \Sigma \cdot V^*$$

Low Rank Approximation

Rank r of matrix A might not be small, but we can find A_k with rank k << r :

$$A_k = \min_{Z:rank(Z)=k} \|A - Z\|_F$$

Frobenius (Euclidean) norm

$$\|X\|_F = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} |X_{ij}|^2}$$

A and Z are both m x n matrices

Low Rank Approximation

Solution via SVD

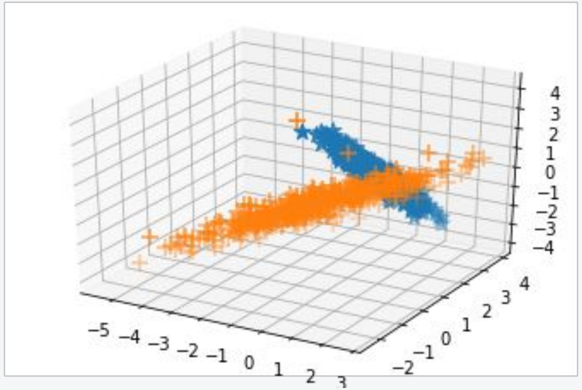
$$A_k = U diag(\sigma_1, \ldots, \sigma_k, \underbrace{0, \ldots, 0}_{\text{Set smallest r-k singular values to 0}})V^T$$

Error: $$\|A - A_k\|_F = \sigma_{k+1}$$

Back to PCA

- Find eigenvectors and eigenvalues using SVD
- Examine how much variance is explained using k components (k is varied)
- For the purposes of explaining (reconstructing the data), pick the number of components based on variance explained
- For plotting purposes can plot the first 2 PCA or all pairs of interest

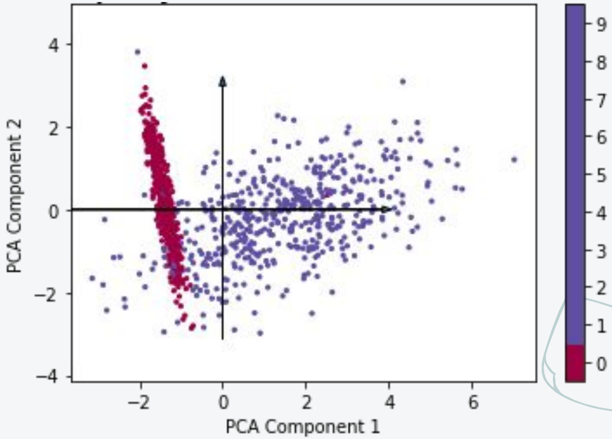
DATA



PCA

Variance explained:

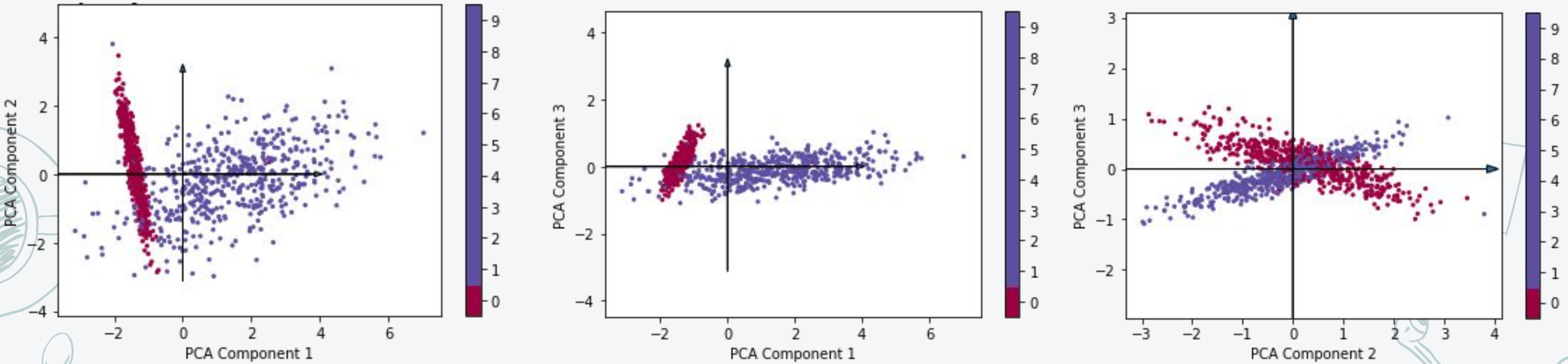
PC1 PC2 PC3
[0.73 0.24 0.03]



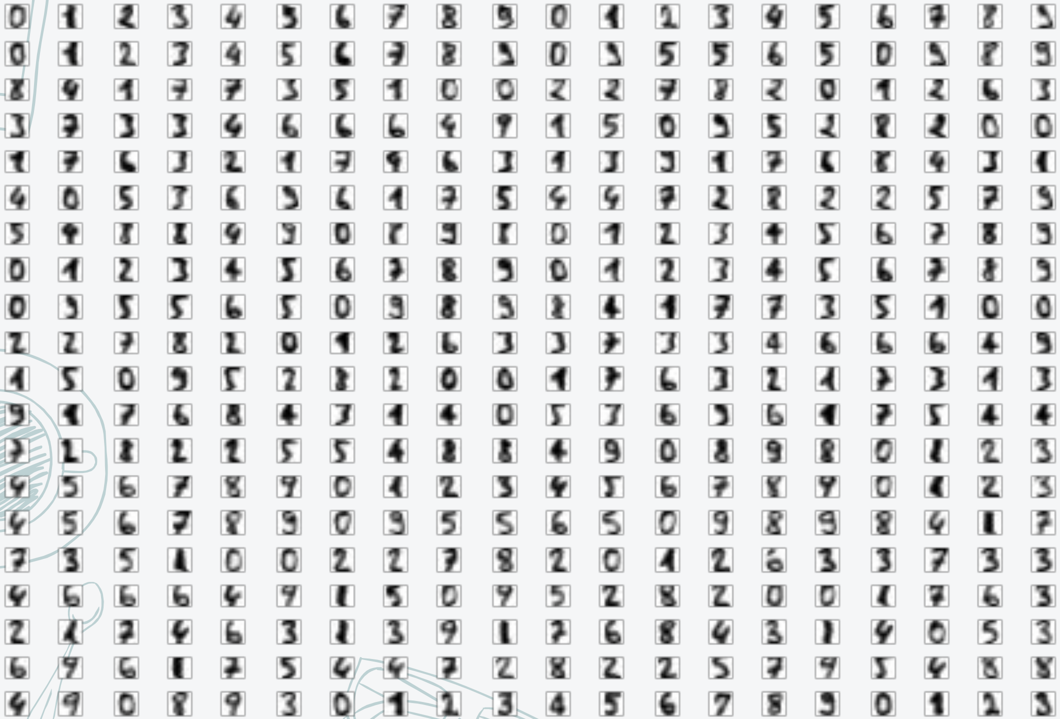
PCA

Variance explained:

PC1	PC2	PC3
[0.73	0.24	0.03]



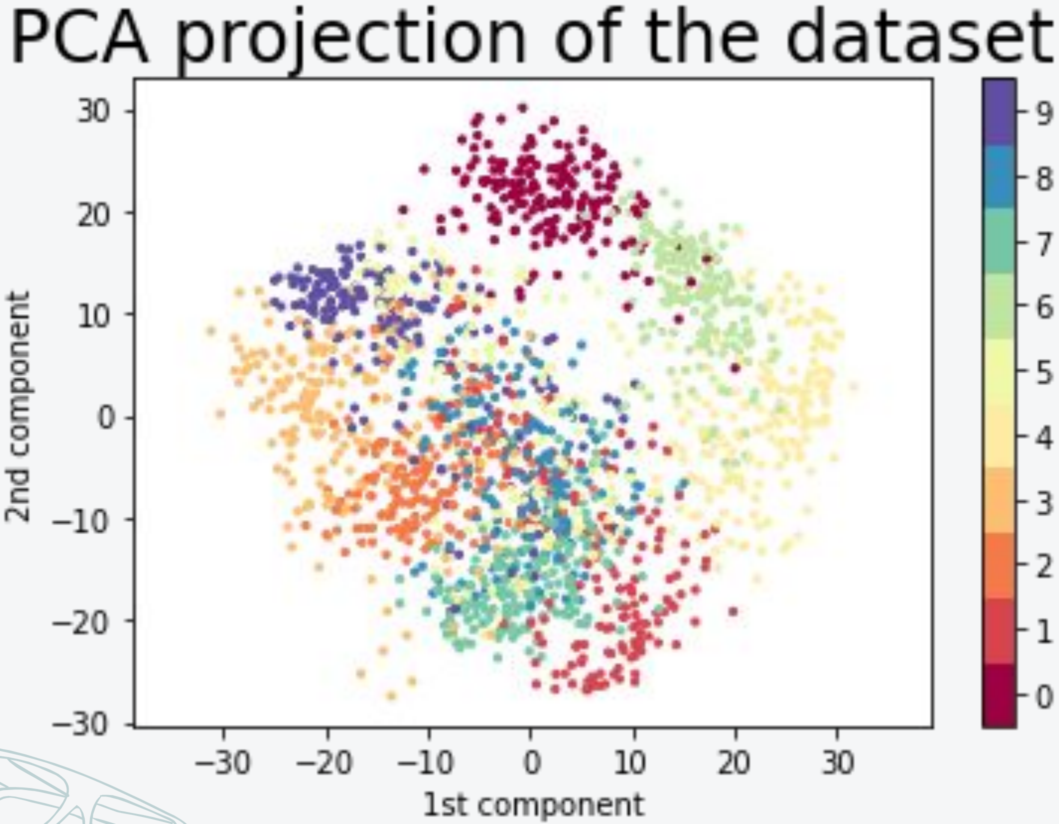
Another dataset: Digits



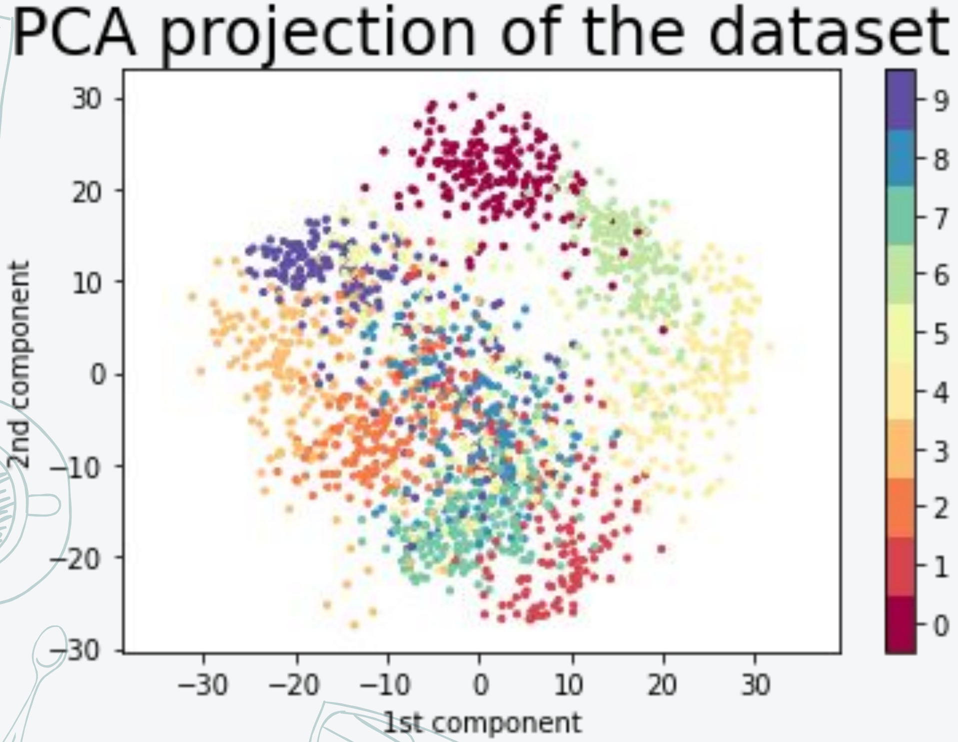
Optical recognition of handwritten digits dataset

Number of Instances: 5620
Number of Attributes: 64
Attribute Information: 8x8 image of integer pixels in the range 0..16
Creator: E. Alpaydin
Date: July, 1998

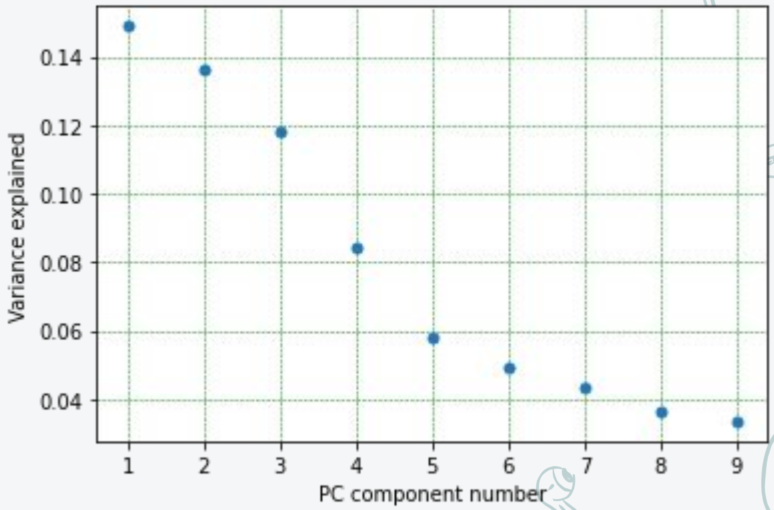
PCA: DIGITS


PCA projection of the dataset
2nd component
1st component
30
20
10
0
−10
−20
−30
0
1
2
3
4
5
6
7
8
9

PCA: DIGITS



Variance explained



PCA

Advantages:

- Relatively Fast
- Gives some sense of intrinsic dimensionality
- Can compute variation explained
- Axes are interpretable

Disadvantages:

- Linear reduction in dimensionality
- Orthogonal components (hard to model non-linear data)

Non-linear Lower Dimensional Embedding

Neighborhood based

- T-SNE
- UMAP
- ISOMAP
- LLE

Autoencoder-based

And many more...

t-SNE : t-distributed Stochastic Network Embedding

- *Distance preservation:* when 2 points are close in high dimensional space, they should be close in 2 dimensional space
- *Neighbor preservation:* neighborhoods of a given point in high-d should be neighborhoods of a given point in low-d

  Note1: effective number of neighbors is a parameter called *perplexity*

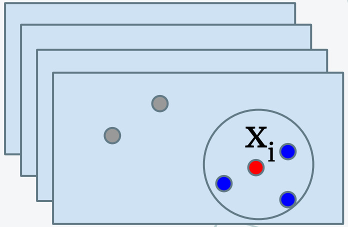
Note2: t-SNE focuses on the order of things, not necessarily on the distance itself

Van der Maaten and Hinton, 2008

T-SNE

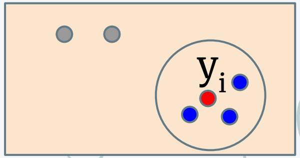
Similarity of data points in High Dimensional space

$$p_{ij} = \frac{exp(-\|x_i - x_j\|^2/2\sigma^2)}{\sum_{k\neq l} exp(-\|x_k - x_l\|^2/2\sigma^2)}$$



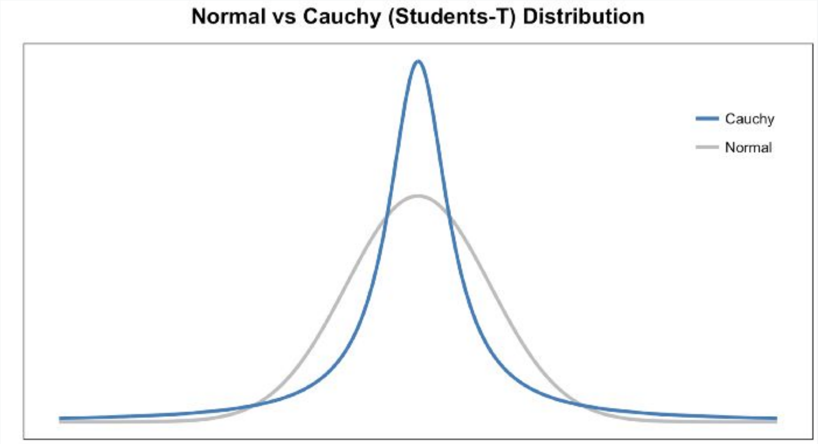
Similarity of points in Low Dimensional space

$$q_{ij} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{k\neq l}(1 + \|y_k - y_l\|^2)^{-1}}$$



T-SNE

Reason for t-distribution as opposed to Gaussian as in high d is crowding - need fatter tails to accommodate distant points



T-SNE COST FUNCTION

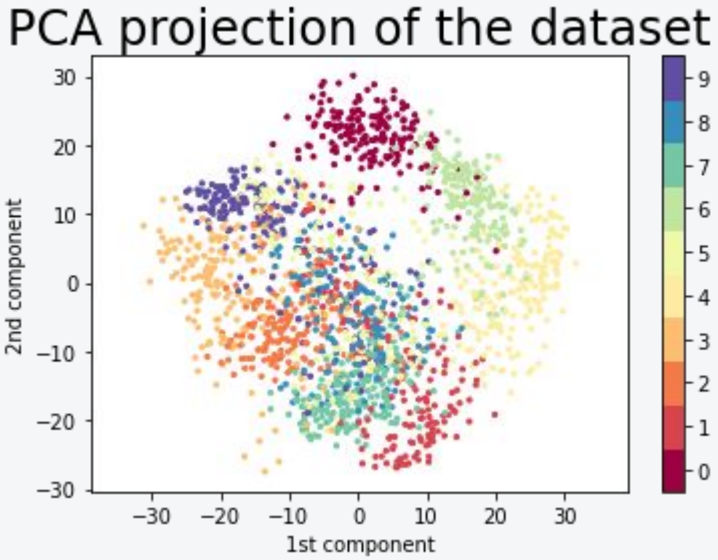
Cost function: Kullback Leibler divergence (relative entropy) - measures distance between two distributions

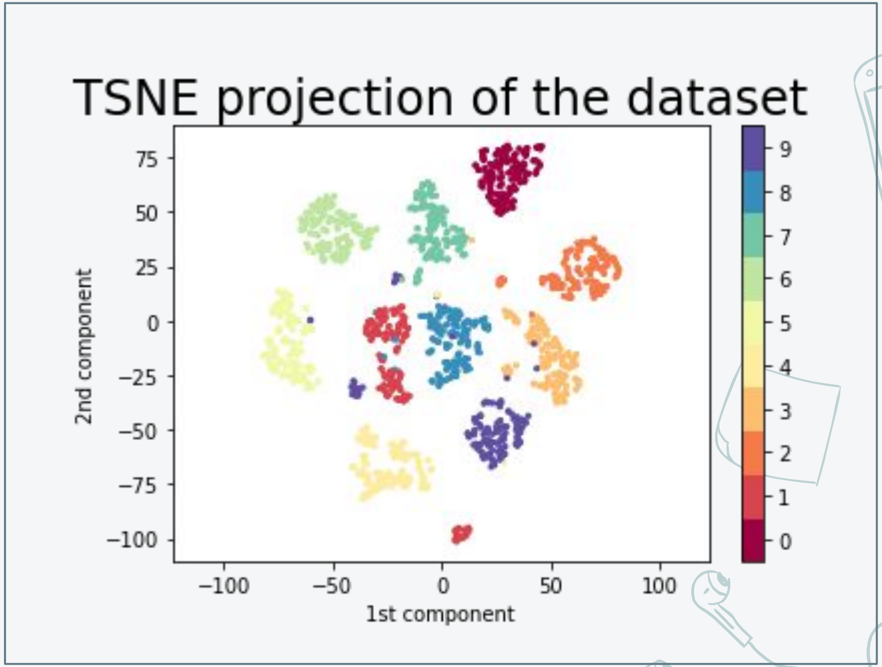
$$C = KL(P||Q) = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

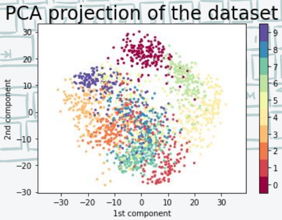
(Kullback and Leibler, 1951)

Properties?

T-SNE on Digits

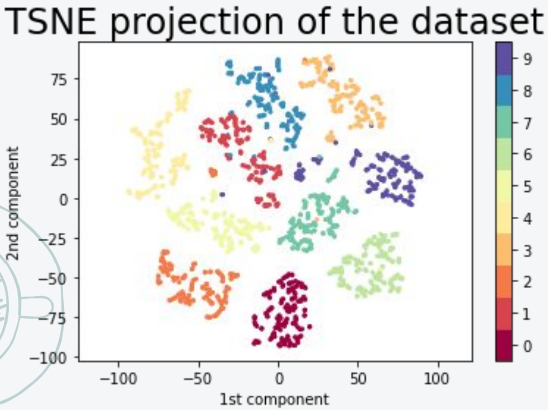




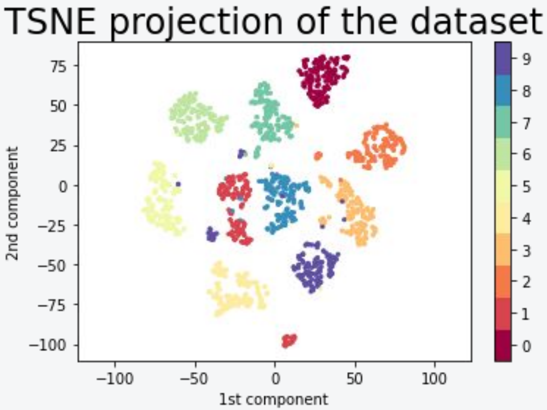


T-SNE sensitivity to parameters: Perplexity

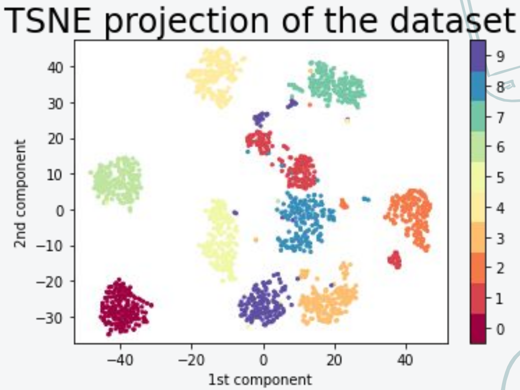
Perplexity = 5



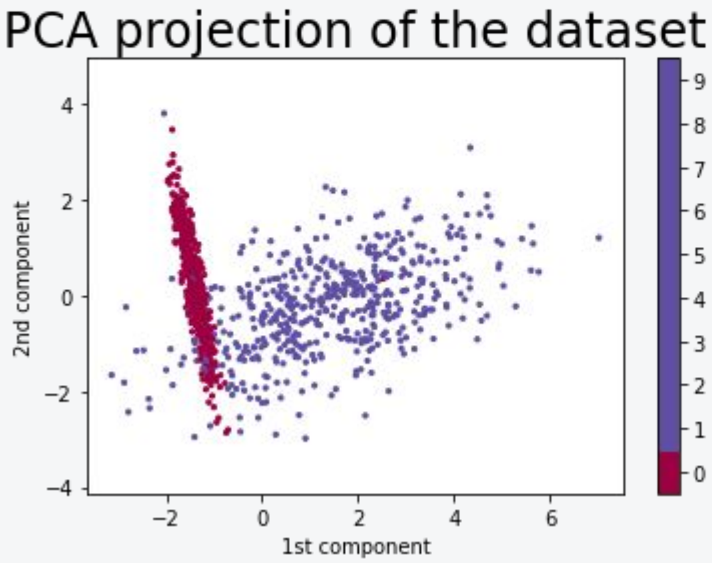
Perplexity = 10

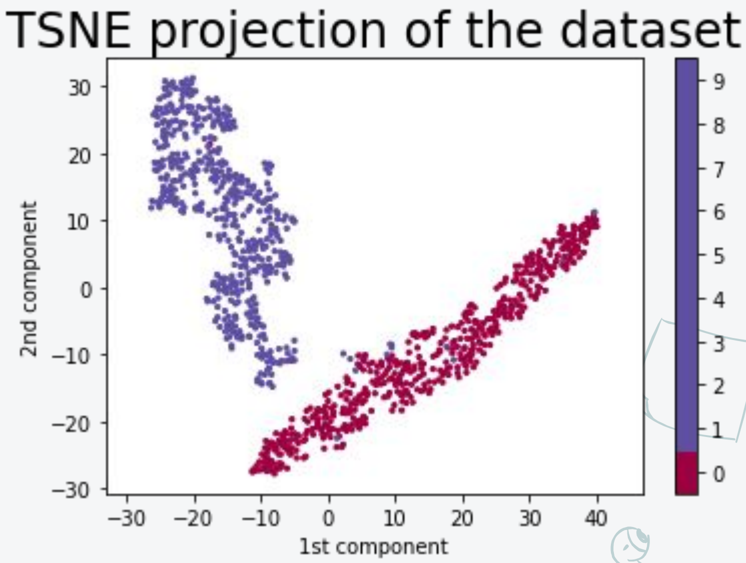


Perplexity = 50



T-SNE ON THE ORIGINAL DATASET





T-SNE

Advantages

- Retains local structure
- Excels at visualizing complex high-d data in 2d

Disadvantages

- Slower
- Doesn't really capture global structure
- Sensitive to params
- Clustering and distance depend on perplexity (shouldn't be interpreted off the plot)
- Stochasticity leads to different results
- Not guaranteed to converge to the global optimum of the cost function

https://distill.pub/2016/misread-tsne/

UMAP: Uniform Manifold Approximation and Projection

UMAP - preserves both local and global structure by

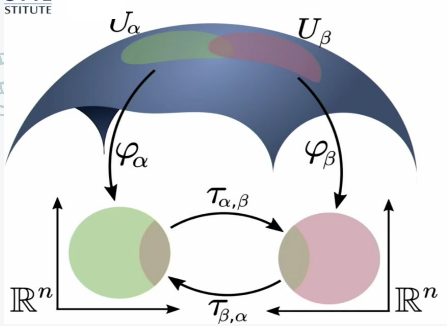
1. :earning the manifold of the data
2. Embedding that manifold into a low dimensional space
   - Builds on neighborhood based approaches but adds mathematical foundations

Key intuition:

While the assumptions may not be true in the original space, they can be true on the manifold

L McInnes, J Healy, J Melville, arXiv, 2018

UMAP



Assumptions:

- The points are covering manifold uniformly
- There is local connectedness between points (confident in the distance to the 1st neighbor)

Using topological theory, construct the neighborhood graph on the low dimensional manifold.

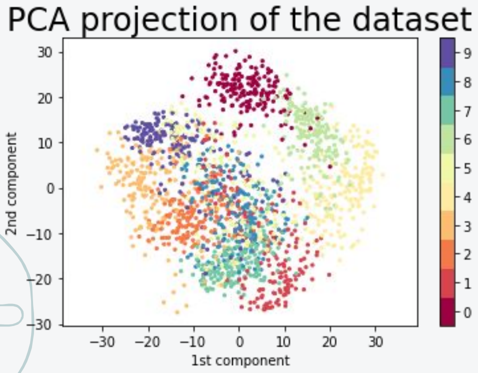
Similar to t-SNE

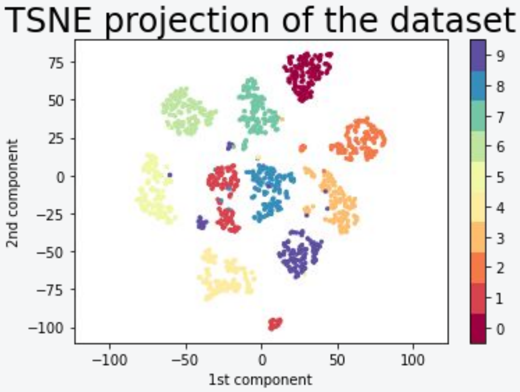
Optimize cross entropy:

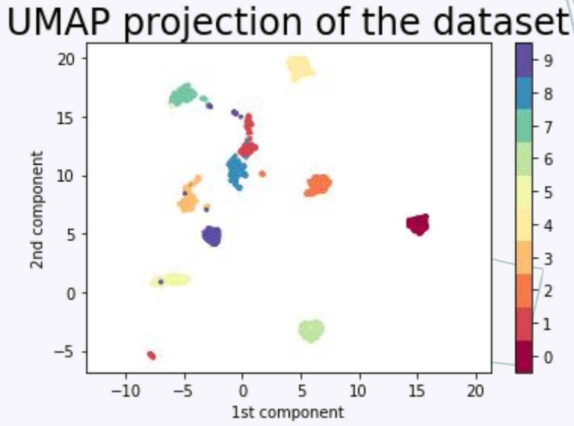
$$\sum_{a\in A} \overbrace{\mu(a)\log\left(\frac{\mu(a)}{\nu(a)}\right)}^{\text{Get the clumps right}} + \underbrace{(1-\mu(a))\log\left(\frac{1-\mu(a)}{1-\nu(a)}\right)}_{\text{Get the gaps right}}$$

L McInnes, J Healy, J Melville, arXiv, 2018

UMAP ON DIGITS



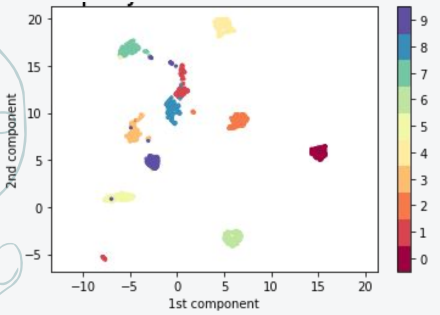




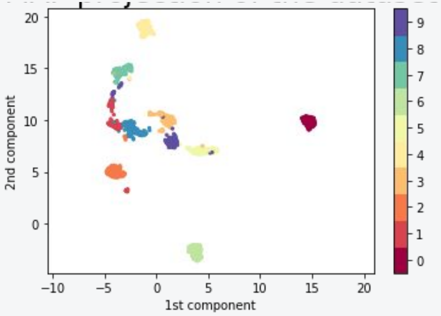
UMAP HYPERPARAMETERS

- Number of neighbors - local vs global structure
- Minimum distance - how tightly points can be packed together
- Number of components (we set 2 for all)
- Distance metric

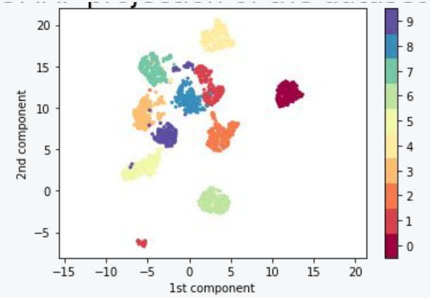
neighbors = 15
metric = euclidian
min_dist = 0.1



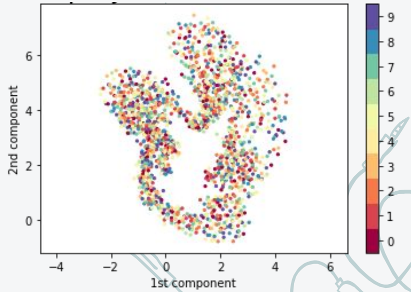
neighbors = 50
metric = euclidian
min_dist =0.1



neighbors = 5
metric = euclidian
min_dist =0.5

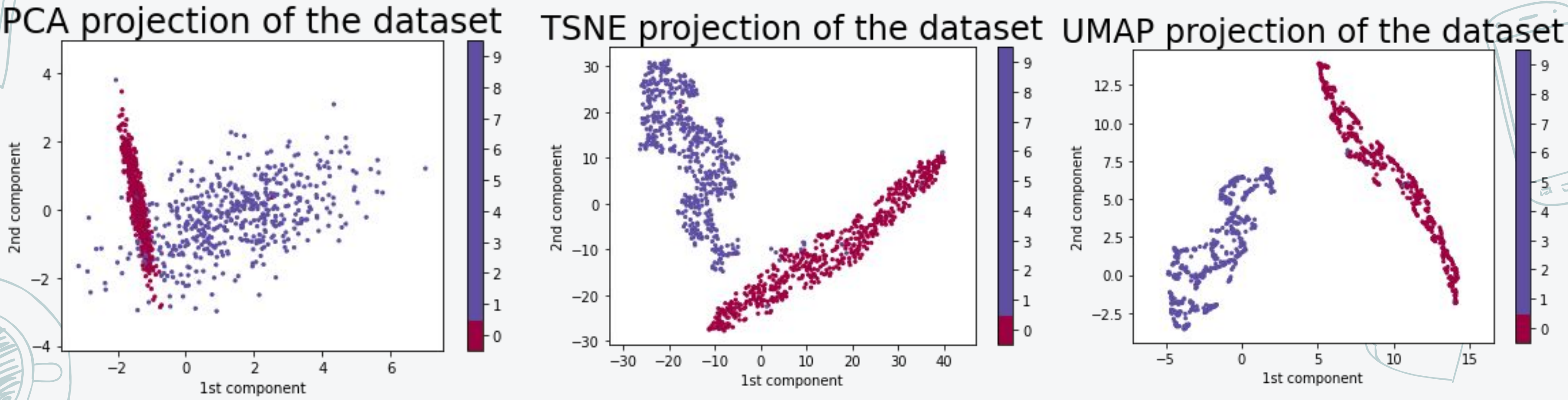


neighbors = 5
metric = mahalanobis
min_dist = 0.1



https://umap-learn.readthedocs.io/en/latest/parameters.html - on all parameters and their effects

UMAP ON THE ORIGINAL DATA



UMAP

Advantages

- Preserves global as well as local structure
- Has mathematical guarantees
- More robust to hyperparameter changes (e.g. number of neighbors)

Disadvantages

- Depends on hyperparameters
- Slow-ish

Reading

PCA

- In depth PCA with examples from the Python handbook: https://jakevdp.github.io/PythonDataScienceHandbook/05.09-principal-component-analysis.html

t-SNE

- Playing with t-sne: https://distill.pub/2016/misread-tsne/
- Intro to t-sne with python: https://towardsdatascience.com/an-introduction-to-t-sne-with-python-example-5a3a293108d1

UMAP

- Talk (26min): https://www.youtube.com/watch?v=nq6iPZVUxZU
- Examples with code in python: https://umap-learn.readthedocs.io/en/latest/basic_usage.html

t-SNE vs UMAP: https://towardsdatascience.com/tsne-vs-umap-global-structure-4d8045acba17