STA 437/2005: Methods for Multivariate Data

Week 9: Non-linear Dimension Reduction Techniques

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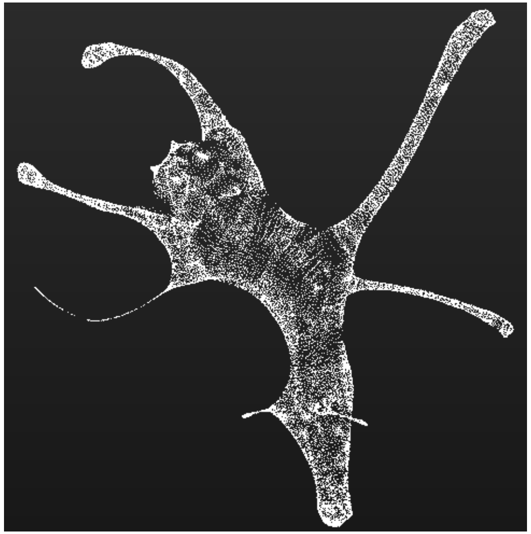
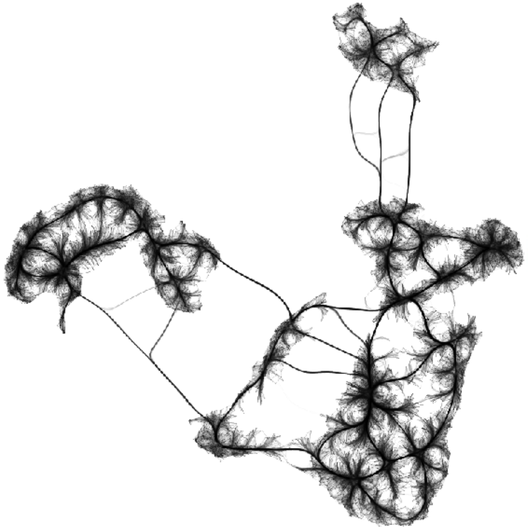
Why Principal Component Analysis may not be enough?

PCA struggles with non-linear relationships.

High-dimensional datasets often lie on low-dimensional manifolds.

Linear projections may destroy these geometric information.





We will now discuss four popular non-linear dimensionality reduction techniques: multi-dimensional scaling, spectral embedding, and UMAP.

Multi-dimensional Scaling (MDS)

- In its classical version this is essentially PCA.
- MDS allows us to introduce some fundamental concepts.

Problem Setup

Consider n objects and a measure $\delta_{ij} \geq 0$ of their dissimilarity (small if similar); $\delta_{ii} = 0$.

Define $\Delta = (\delta_{ij}) \in \mathbb{R}^{n \times n}$: $\delta_{ii} = 0$ for all i, $\delta_{ij} \geq 0$ for all $i \neq j$.

In classical MDS: there exist $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^m$ such that $\delta_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|$.

In general, there need not be a Euclidean distance defining this metric.

Multidimensional Scaling

Find a configuration of points $\mathbf{y}_1, \ldots, \mathbf{y}_n$ in $\mathbb{R}^d$ ($d \ll n$) such that:

$$\|\mathbf{y}_i - \mathbf{y}_j\| \ \approx \ \delta_{ij}.$$

The solution for classical MDS is particularly simple.

Classical MDS: $\delta_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|$

$\|x\| = \sqrt{x^\top x}$ $\quad (XX^\top)_{ij} = x_i^\top x_j$

If $\delta_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|$, we have:

$$\delta_{ij}^2 \;=\; (\mathbf{x}_i - \mathbf{x}_j)^\top(\mathbf{x}_i - \mathbf{x}_j) \;=\; (\mathbf{X}\mathbf{X}^\top)_{i,i} + (\mathbf{X}\mathbf{X}^\top)_{j,j} - 2(\mathbf{X}\mathbf{X}^\top)_{i,j}.$$

The Hadamard product $\Delta \odot \Delta = [\delta_{ij}^2]$ can be written as:

$$\Delta \odot \Delta = \mathrm{diag}(\mathbf{X}\mathbf{X}^\top)\mathbf{1}\mathbf{1}^\top + \mathbf{1}\mathbf{1}^\top\mathrm{diag}(\mathbf{X}\mathbf{X}^\top) - 2\mathbf{X}\mathbf{X}^\top$$

exercise

$\delta_{ij}^2 = (\Delta\odot\Delta)_{ij} = e_i^\top(\Delta\odot\Delta)e_j$

Reintroducing the centering matrix $H = I_n - \frac{1}{n}\mathbf{1}\mathbf{1}^\top$, we obtain

$H\mathbb{1} = \underline{0}$ $\quad \mathbb{1}^\top H = \underline{0}$

$$B \;:=\; -\frac{1}{2}H(\Delta \odot \Delta)H \;=\; H\mathbf{X}(H\mathbf{X})^\top \;=\; \tilde{\mathbf{X}}\tilde{\mathbf{X}}^\top.$$

$\to -2HXX^\top H$

This matrix contains all inner products $\tilde{\mathbf{x}}_i^\top\tilde{\mathbf{x}}_j$ for $1 \le i, j \le n$.

Classical MDS (2)

Recall: $\|\tilde{x}_i - \tilde{x}_j\|^2 \approx \|y_i - y_j\|^2 = y_i^T y_i + y_j^T y_j - 2 y_i^T y_j$

$= \tilde{x}_i^T \tilde{x}_i + \tilde{x}_j^T \tilde{x}_j - 2 \tilde{x}_i^T \tilde{x}_j$

Let $\mathbf{Y} \in \mathbb{R}^{n \times d}$ be the matrix with projected data $\mathbf{y}_1, \ldots, \mathbf{y}_n \in \mathbb{R}^d$.

We want to make sure $B = \tilde{\mathbf{X}}\tilde{\mathbf{X}}^\top \approx \mathbf{Y}\mathbf{Y}^\top =: M$

$M = YY^T$ wrt $Y \in \mathbb{R}^{n \times d}$

- In this way $\|\mathbf{y}_i - \mathbf{y}_j\| \approx \|\mathbf{x}_i - \mathbf{x}_j\|$ as desired.
- One way to assure this is to minimize $\sum_{i,j} (\tilde{\mathbf{x}}_i^\top \tilde{\mathbf{x}}_j - \mathbf{y}_i^\top \mathbf{y}_j)^2 = \|B - M\|_F^2$.
- The Frobenius norm $\|A\|_F = \sqrt{\sum_{i,j} A_{ij}^2}$.

Note that $\operatorname{rank}(M) \leq d$ but otherwise $M \in \mathbb{R}^{n \times n}$ is arbitrary.

Optimization problem: Minimize $\|B - M\|_F^2$ subject to $\operatorname{rank}(M) \leq d$.

Classical MDS (3)

Optimization problem: Minimize $\|B - M\|_F^2$ subject to $\operatorname{rank}(M) \leq d$.

Let $B = V \Lambda V^\top$ be the spectral decomposition with $\operatorname{diag}(\Lambda)$ non-increasing.

Eckart-Young Theorem

The optimal M satisfies $\widehat{M} = V_d \Lambda_d V_d^\top$, where

- $\Lambda_d = \operatorname{diag}(\lambda_1, \ldots, \lambda_d)$ has d largest eigenvalues of B.
- $V_d \in \mathbb{R}^{n \times d}$ contains the first d columns of V.

We then take $\mathbf{Y} = V_d \Lambda_d^{1/2}$, which gives us our low-dimensional embedding.

We next show that this is the same answer we would get using PCA!

Duality Between MDS and PCA

Both methods rely on the singular value decomposition (SVD) of $\tilde{\mathbf{X}} = H\mathbf{X} = VDU^\top$.

Here is the key insight:

- **PCA**: Finds principal components from the eigenvectors of $\tilde{\mathbf{X}}^\top\tilde{\mathbf{X}} = U(D^\top D)U^\top$.
- **MDS**: Finds embeddings from the eigenvectors of $\tilde{\mathbf{X}}\tilde{\mathbf{X}}^\top = V(DD^\top)V^\top$.

The columns of U are the principal directions and the scores $\mathbf{y}_1, \ldots, \mathbf{y}_n$ are taken as the first d columns of $\tilde{\mathbf{X}}U = VD$.

As a result, $\mathbf{y}_1, \ldots, \mathbf{y}_n$ are precisely the points obtained by classical MDS.

Spectral Embedding (aka Laplacian Eigenmaps)

Main ideas

Data: $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^m$. Find low dimensional representation $\mathbf{y}_1, \ldots, \mathbf{y}_n \in \mathbb{R}^d$.

Links to manifold learning

We look for a truly nonlinear method that is able to learn the underlying manifold.

The main idea is to keep track of local geometry:

- The embedding of $\mathbf{x}_i$ should depend mostly on points close to $\mathbf{x}_i$.

How to keep track of the local geometry in the data?

Construct a weighted graph $G = (V, E, W)$:

- Vertices $V = \{1, 2, \ldots, n\}$ (data points).
- Edges E based on proximity (e.g., k-nearest neighbors or ϵ-neighborhood).
- Weights W_{ij} measure similarity, e.g. $W_{ij} = 1$ or $W_{ij} = \exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/2\sigma^2)$.

If $ij \notin E$ we always set $W_{ij} = 0$, also $W_{ii} = 0$ for all $i = 1, \ldots, n$.

Graph Laplacian

Graph Laplacian is the main object encoding the "geometry of the data".

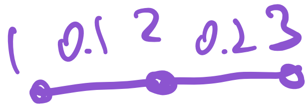
The Laplacian matrix $L \in \mathbb{S}^n$ encodes the structure of the graph:

- Degree matrix D (diagonal): $D_{ii} = \sum_j W_{ij}$, $i = 1, \dots, n$.
- Graph Laplacian: $L = D - W$, where W is the weight matrix $W = (W_{ij})$.
- Normalized Laplacian: $L_{\mathrm{N}} = D^{-1/2} L D^{-1/2}$.

Important exercise: Show $\mathbf{x}^\top L \mathbf{x} = \frac{1}{2}\sum_{i,j} W_{ij}(x_i - x_j)^2$ for all $\mathbf{x} \in \mathbb{R}^n$.

Properties of L:

- L is positive semi-definite.
- $L\mathbf{1} = \mathbf{0}$, that is, smallest eigenvalue is zero with eigenvector $\mathbf{1}$.
- If G is connected $\mathrm{rank}(L) = n - 1$.



$n = 3$

$W_{12} = W_{21} = 0.1$

$W_{23} = W_{32} = 0.2$

$W_{13} = W_{31} = 0$

$$L = \begin{pmatrix} 0.1 & -0.1 & 0 \\ -0.1 & 0.3 & -0.2 \\ 0 & -0.2 & 0.2 \end{pmatrix}$$

$L = D - W$

$$L \cdot \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

The key idea behind spectral embedding

Fix d. The embedding $\mathbf{y}_1, \ldots, \mathbf{y}_n \in \mathbb{R}^d$ is obtained by minimizing:

$$\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} W_{ij} \|\mathbf{y}_i - \mathbf{y}_j\|^2$$

Key insight

High W_{ij} enforces small $\|\mathbf{y}_i - \mathbf{y}_j\|$.

Note: This is still not well defined because $\mathbf{y}_1 = \ldots = \mathbf{y}_n = \mathbf{0}$ is a solution so we need to refine this idea a bit.

Problem reformulation

Let $\mathbf{Y} \in \mathbb{R}^{n\times d}$ be the embedded data matrix. Recall $L = D - W$ and $L\mathbf{1} = \mathbf{0}$.

Proposition

We have: $\frac{1}{2}\sum_{i,j} W_{ij}\|\mathbf{y}_i - \mathbf{y}_j\|^2 = \mathrm{tr}(\mathbf{Y}^\top L\mathbf{Y}) = \mathrm{tr}(\mathbf{Y}^\top D\mathbf{Y}) - \mathrm{tr}(\mathbf{Y}^\top W\mathbf{Y})$

Proof: As for MDS we can show that the matrix $E = [\|\mathbf{y}_i - \mathbf{y}_j\|^2]_{i,j}$ takes the form

$$E = \mathrm{diag}(\mathbf{Y}\mathbf{Y}^\top)\mathbf{1}\mathbf{1}^\top + \mathbf{1}\mathbf{1}^\top\mathrm{diag}(\mathbf{Y}\mathbf{Y}^\top) - 2\mathbf{Y}\mathbf{Y}^\top$$

and so $\frac{1}{2}\sum_{i,j} W_{ij}\|\mathbf{y}_i - \mathbf{y}_j\|^2 = \frac{1}{2}\mathrm{trace}(WE)$. → $\mathrm{tr}(WE) = \sum_{i,j} W_{ij} E_{ij}$

D is diagonal and E has zeros on the diagonal and so $\frac{1}{2}\mathrm{trace}(WE) = -\frac{1}{2}\mathrm{trace}(LE)$.

Since $L\mathbf{1} = \mathbf{0}$ we get also that $-\frac{1}{2}\mathrm{trace}(LE) = \mathrm{trace}(L\mathbf{Y}\mathbf{Y}^\top)$.

$\mathrm{tr}(DE) = \sum_{i,j} D_{ij} E_{ij} = 0$

Introducing constraints to the optimization problem

$L_N = D^{-1/2} L D^{-1/2}$

PCA: $u^T \Sigma u \to \max$, $\|u\| = 1$

Constraint 1 (Fixing scale)

To avoid trivial solutions it is convenient to assume $\mathbf{Y}^\top D \mathbf{Y} = I_d$.

Defining $\tilde{\mathbf{Y}} = D^{1/2}\mathbf{Y}$ we get $\tilde{\mathbf{Y}}^\top \tilde{\mathbf{Y}} = I_d$ (orthonormal columns $\tilde{\mathbf{y}}_1, \ldots, \tilde{\mathbf{y}}_d$).

MIN

Now $\mathrm{trace}(\mathbf{Y}^\top L \mathbf{Y}) = \mathrm{trace}(\tilde{\mathbf{Y}}^\top L_{\mathrm{N}} \tilde{\mathbf{Y}}) = \sum_{i=1}^d \tilde{\mathbf{y}}_i^\top L_{\mathrm{N}} \tilde{\mathbf{y}}_i$. $= (\tilde{Y}^T L_N \tilde{Y})_{ii}$

From PCA: the optimum given by eigenvectors of L_{N} for smallest eigenvalues.

Note that $L_{\mathrm{N}} D^{1/2}\mathbf{1} = D^{-1/2} L \mathbf{1} = \mathbf{0}$ so $\tilde{\mathbf{y}}_0 := D^{1/2}\mathbf{1}$ is a zero-eigenvector.

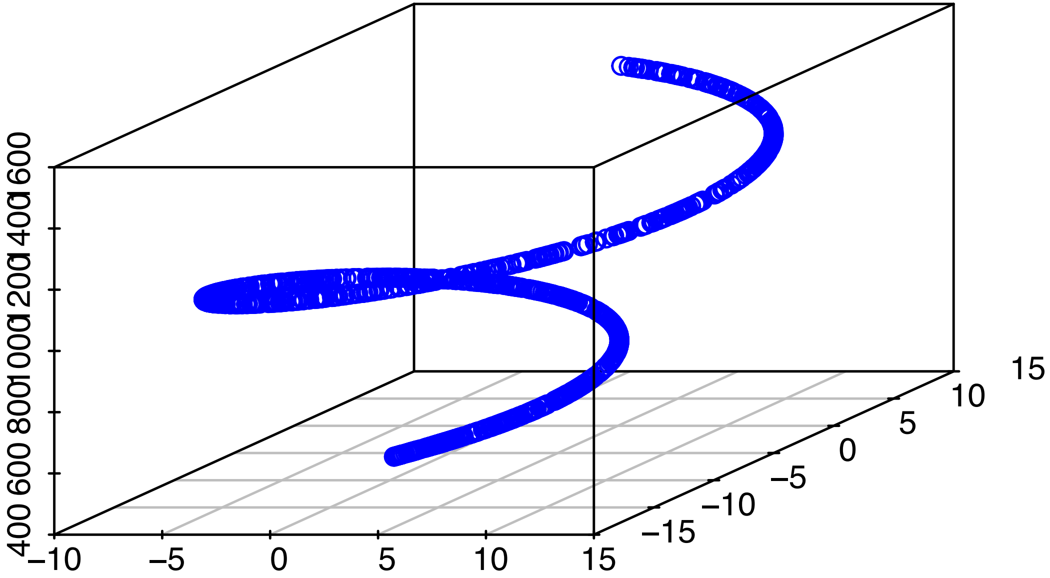
Constraint 2: $\tilde{\mathbf{y}}_0 \perp \tilde{\mathbf{y}}_i$ for $i = 1, \ldots, n$

In addition we assume $\tilde{\mathbf{Y}}^\top D^{1/2}\mathbf{1} = \mathbf{Y}^\top D \mathbf{1} = \mathbf{0}$.

Spectral embedding: minimize $\mathrm{trace}(\mathbf{Y}^\top L \mathbf{Y})$ subject to $\mathbf{Y}^\top D \mathbf{Y} = I_d$ and $\mathbf{Y}^\top D \mathbf{1} = \mathbf{0}$

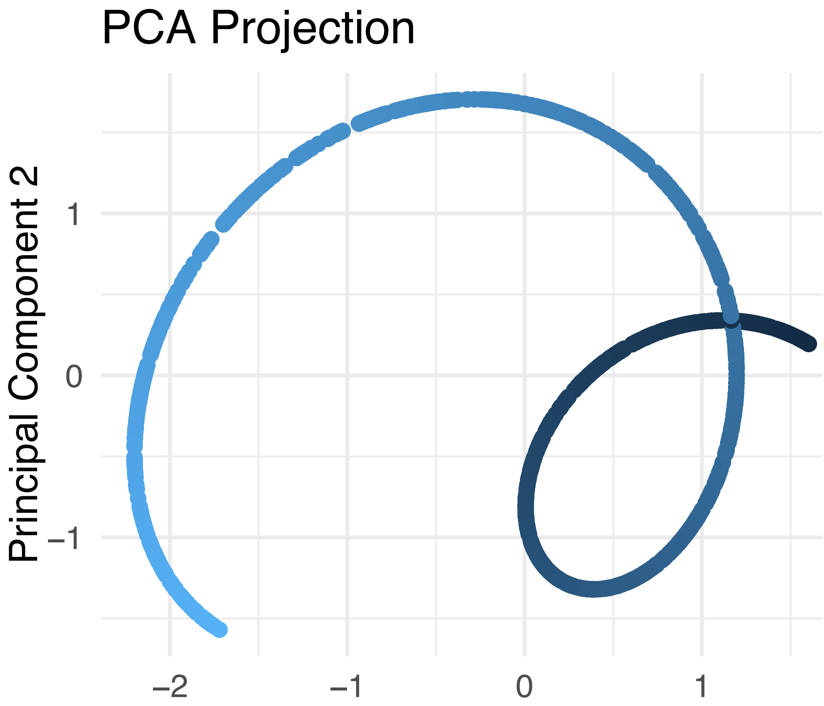
Example: Twisted curve

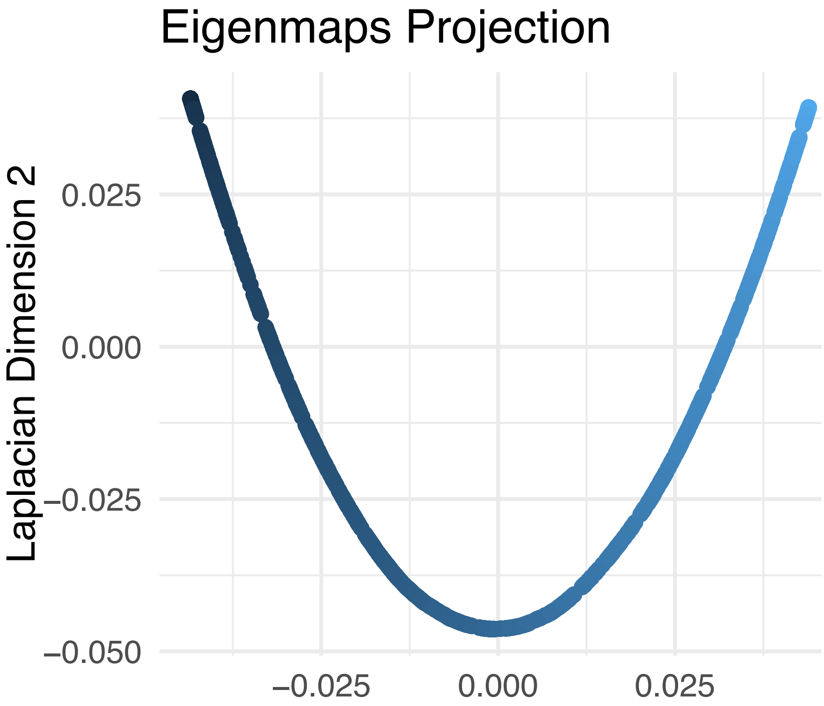
Consider datapoints lying on the twisted curve as on the picture below:



We now represent these data in 2D comparing PCA and Laplacian Eigenmaps.

- **PCA**: Projects data linearly, collapsing structure.
- **Laplacian Eigenmaps**: Preserves local geometry, unfolding the manifold.





Note that PCA joins points that are far from each other in the original dataset.

Uniform Manifold Approximation and Projection (UMAP)

- This is a popular, state-of-the-art method.
- It relies on various choices that are not fully theoretically justified.
- We provide a high level overview.

Introduction to UMAP

UMAP is a nonlinear dimensionality reduction technique that improves on eigenmaps.

Advantages over PCA, MDS, and Eigenmaps:

- Has manifold learning abilities.
- Balances local and global structure.
- Scales efficiently to large datasets.
- More robust to parameter choices.

UMAP is a state-of-the-art data visualization and pattern discovery tool.

UMAP Algorithm Overview

The key idea is similar to the spectral embedding.

1. **Construct k-Nearest Neighbor (kNN) Graph**.
2. **Initialize Embedding** using Laplacian Eigenmaps.
3. **Optimize** embedding via stochastic gradient descent (SGD).

UMAP uses a different loss function than Laplacian Eigenmaps, which makes it, in principle, more robust to parameter choices.

Step 1: Data Graph in the Input Space

Construct k-Nearest Neighbors (kNN) graph; e.g. with $k = 15$.

Define "probabilities" of i, j being connected based on neighbor distances:

$$p_{j|i} = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\| - \rho_i}{\sigma_i}\right),$$

where $\rho_i = \min_{k \neq i} \|\mathbf{x}_i - \mathbf{x}_k\|$ and σ_i is a scaling factor.

Symmetrize probabilities:

$$p_{ij} = p_{j|i} + p_{i|j} - p_{j|i} p_{i|j}.$$

Note that the closest neighbor gets always connected with pr. 1.

- This about p_{ij} as edge weights.

j is closest to i
then $p_{j|i} = 1$
$p_{ij} = 1 + p_{i|j} - 1 \cdot p_{i|j}$
$= 1$

Step 2 and 3: Data Graph in the Embedding Space and matching

Compute pairwise similarities in low-dimensional space:

$$q_{ij} = \frac{1}{1 + a\|\mathbf{y}_i - \mathbf{y}_j\|^{2b}}, \quad \in (0,1) \tag{1}$$

where, by default, $a \approx 1.929$, $b \approx 0.7915$.

The matching between the original and the embedded space is probability-inspired.

Cost Function (Fuzzy Cross-Entropy)

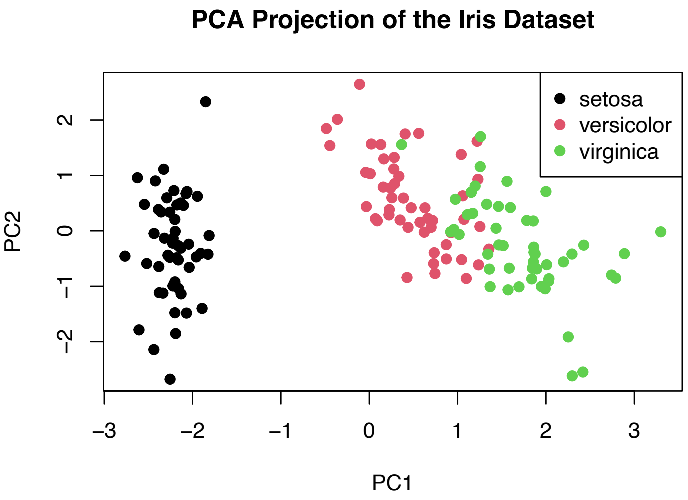
$$c(\mathbf{y}_1, \ldots, \mathbf{y}_n) = \sum_{i \neq j} \left(p_{ij} \log \frac{p_{ij}}{q_{ij}} + (1 - p_{ij}) \log \frac{1 - p_{ij}}{1 - q_{ij}} \right).$$

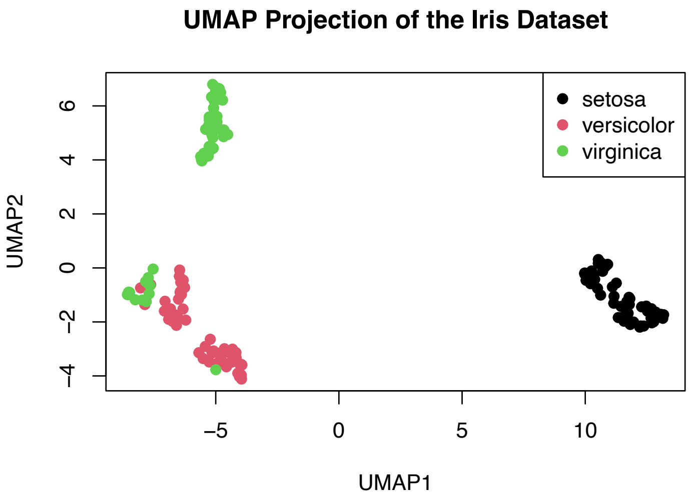
Here c depends on $\mathbf{y}_1, \ldots, \mathbf{y}_n$ through q_{ij}'s defined in (1).

- Attractive and repulsive forces to balance local and global structure.
- Uses block-coordinate descent to minimize cost.

Example: Iris Dataset

- Comparison of PCA and UMAP on Iris dataset.
- PCA struggles to separate classes clearly.
- UMAP better preserves local and global structures.





Note: Given a new data point UMAP has to be recalculated from scratch!