Feature Learning

Finding the diamonds in the rough

High Dimensionality

Higher Dimensionality

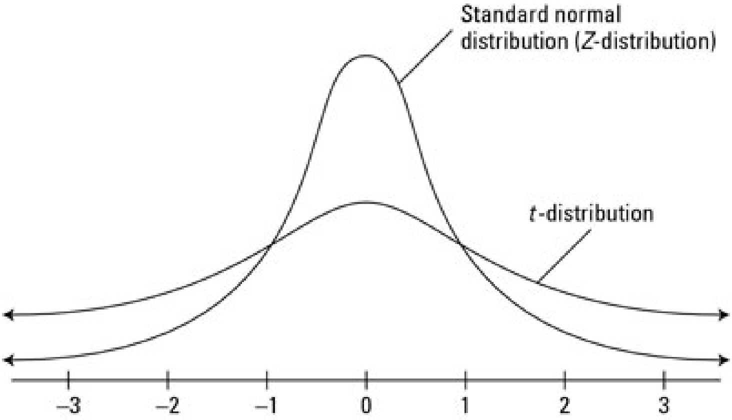
More Data

Feature 1	Feature 2	Feature 3	Feature 4
Value 1, 1	Value 1, 2	Value 1, 3	Value 1, 4
Value 2, 1	Value 2, 2	Value 2, 3	Value 2, 4
Value 3, 1	Value 3, 2	Value 3, 3	Value 3, 4
Value 4, 1	Value 4, 2	Value 4, 3	Value 4, 4
Value 5, 1	Value 5, 2	Value 5, 3	Value 5, 4
Value 6, 1	Value 6, 2	Value 6, 3	Value 6, 4

Feature Extraction

t-distributed Stochastic Neighbor Embeddings

t-SNE - Student-t vs Normal



t-SNE - Conditional Probability

$$p_{j \mid i} = \frac{\exp(-||\mathbf{x}_i - \mathbf{x}_j||_2^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-||\mathbf{x}_i - \mathbf{x}_k||_2^2 / 2\sigma_i^2)},$$

where σ_i^2 is the variance of the Gaussian distribution centered at $\mathbf{x}_i$.

t-SNE - Pairwise Probability

$$p_{ij} = \frac{p_{j \mid i} + p_{i \mid j}}{2n},$$

where n is the total number of samples in the data, $p_{ii} = 0$.

t-SNE - Embedding's Joint Probability

$$q_{ij} = \frac{(1 + ||\mathbf{y}_i - \mathbf{y}_j||_2^2)^{-1}}{\sum_{k \neq i}(1 + ||\mathbf{y}_i - \mathbf{y}_k||_2^2)^{-1}}.$$

t-SNE - Objective

$$\min_{\mathbf{Y}} \sum_{i \neq j} p_{ij} \log \left(\frac{p_{ij}}{q_{ij}} \right).$$

t-SNE - Conditional Probability

$$p_{j \mid i} = \frac{\exp(-||\mathbf{x}_i - \mathbf{x}_j||_2^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-||\mathbf{x}_i - \mathbf{x}_k||_2^2 / 2\sigma_i^2)},$$

where σ_i^2 is the variance of the Gaussian distribution centered at $\mathbf{x}_i$.

t-SNE - Perplexity

$$\text{Perplexity}(P_i) = 2^{\mathcal{H}(P_i)} = 2^{-\sum_j p_{j \mid i} \log p_{j \mid i}}.$$

- Perplexity is used to represent the number of neighbors to consider per point.
- Higher perplexity is a higher weight to the global relationships and a lower perplexity is a higher weight to the local relationships.

t-SNE - Issues

- Hyperparameters in t-SNE are crucial
- Cluster sizes are meaningless
- Distance between clusters can be meaningless
- Random noise may result in some misleading patterns
- Shapes may appear in the output that are misleading
- Testing multiple perplexities may help with understanding the data

Demo

Spectral Embedding

Spectral Embedding - Objective

$$\min_{\mathbf{Y}} \sum_{i=1}^{n} \sum_{j=1}^{n} s_{ij} ||\mathbf{y}_i - \mathbf{y}_j||_2^2,$$
$$s.t.\ \mathbf{Y}^T \mathbf{Y} = \mathbf{I}.$$

Similarity Matrix

$$\mathbf{S} = \begin{bmatrix} s_{11} & s_{12} & s_{13} & \dots & s_{1n} \\ s_{21} & s_{22} & s_{23} & \dots & s_{2n} \\ s_{31} & s_{32} & s_{33} & \dots & s_{3n} \\ \hdotsfor{5} \\ s_{n1} & s_{n2} & s_{n3} & \dots & s_{nn} \end{bmatrix}$$

Degree Matrix

$$
\mathbf{D} = \begin{bmatrix}
\sum_{i=1}^{n} s_{1i} & 0 & 0 & \dots & 0 \\
0 & \sum_{i=1}^{n} s_{2i} & 0 & \dots & o \\
0 & 0 & \sum_{i=1}^{n} s_{3i} & \dots & 0 \\
\hdotsfor{5} \\
0 & 0 & 0 & \dots & \sum_{i=1}^{n} s_{ni}
\end{bmatrix}
$$

Laplacian Matrix

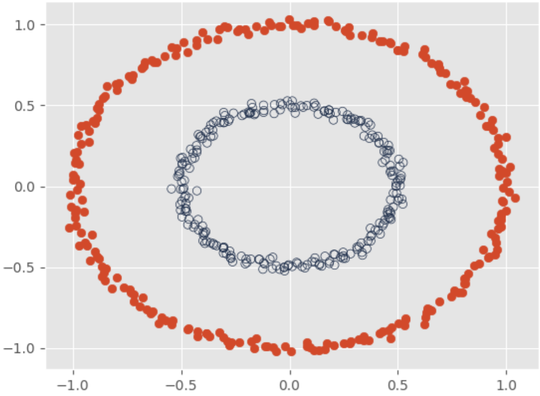
$$
\begin{aligned}
\mathbf{L} &= \mathbf{D} - \mathbf{S} \\
&= \begin{bmatrix}
\left(\sum_{i=2}^{n} s_{1i}\right) & -s_{12} & -s_{13} & \dots & -s_{1n} \\
-s_{21} & \left(\sum_{i=1, i\neq 2}^{n} s_{2i}\right) & -s_{23} & \dots & -s_{2n} \\
-s_{31} & -s_{32} & \left(\sum_{i=1, i\neq 3}^{n} s_{3i}\right) & \dots & -s_{3n} \\
\dots & \dots & \dots & \dots & \dots \\
-s_{n1} & -s_{n2} & -s_{n3} & \dots & \left(\sum_{i=1, i\neq n}^{n} s_{ni}\right)
\end{bmatrix}
\end{aligned}
$$

Spectral Embedding - Solution

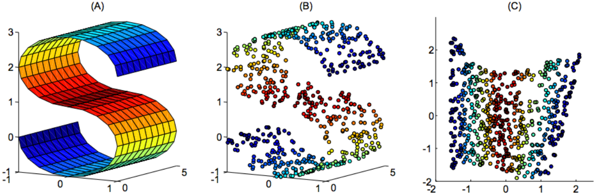
$$\mathbf{Y} = eig(\mathbf{L}, r).$$

The embeddings are the r eigenvectors of the Laplacian matrix corresponding to the smallest r non-zero eigenvalues.

Spectral Clustering



Spectral Clustering



Linear Discriminant Analysis

LDA - Projection

$$\mathbf{y}_i = \mathbf{W}^T \mathbf{x}_i,$$

where **W** is the $r \times d$ projection matrix by which we transform the original data from d dimensions into the new r-dimensional space.

LDA - Class Means

$$\mathbf{m}_k = \frac{1}{n_k} \sum_{i \in \mathcal{C}_k} \mathbf{x}_k,$$

where $\mathcal{C}_k$ is the set of all points belonging to class k.

LDA - Variances

$$\mathbf{S}_B = (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T,$$

$$\mathbf{S}_W = \sum_{i \in \mathcal{C}_1} \left((\mathbf{x}_i - \mathbf{m}_1)(\mathbf{x}_i - \mathbf{m}_1)^T \right) + \sum_{j \in \mathcal{C}_2} \left((\mathbf{x}_j - \mathbf{m}_2)(\mathbf{x}_j - \mathbf{m}_2)^T \right).$$

LDA - Objective

$$\max_{\mathbf{W}} \mathbf{tr}\left(\frac{\mathbf{W}\mathbf{S}_B\mathbf{W}^T}{\mathbf{W}\mathbf{S}_W\mathbf{W}^T}\right).$$

Dimensionality Reduction Methods

- **PCA** - maximize variance per embedding dimension
- **t-SNE** - maximize relative entropy between embedding and original
- **Spectral Embedding** - minimize the distance between embeddings weighted by original point similarities
- **LDA** - maximize class separation (supervised)

Questions