The University of Texas at Austin
Department of Computer Science
College of Natural Sciences

Diffusion Maps

SDS 384 Scientific Machine Learning, Spring 2022

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Talk Points

- Dimensionality Reduction
- Common Reduction Techniques
- Diffusion Maps
  - How do they differ
  - How they work
- Comparing Reduction Algorithms
- Conclusions

Motivation - Need for Dimension Reduction

- Simple problems can easily explode in the number of features -> Curse of dimensionality (Images Case)

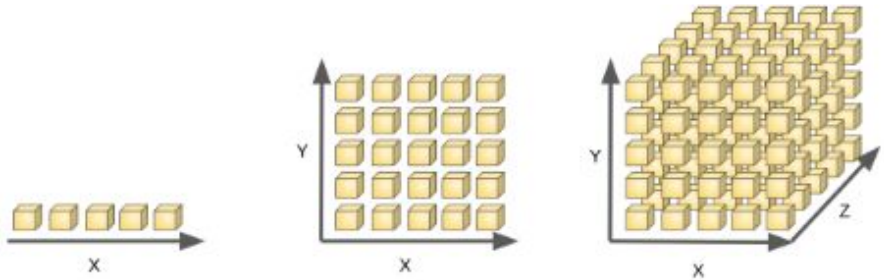
- Extra features obscure or obfuscate the truly informative features

- Local Feature Space -> Global Feature Space

- Goal: Find underlying low dimensional structure, for global similarity

Figure 1: Two images of the same digit at different rotation angles.

https://inside.mines.edu/~whereman/talks/delaPorte-Herbst-Hereman-vanderWalt-DiffusionMaps-PRASA2008.pdf



https://www.i2tutorials.com/what-do-you-mean-by-curse-of-dimensionality-what-are-the-different-ways-to-deal-with-it/

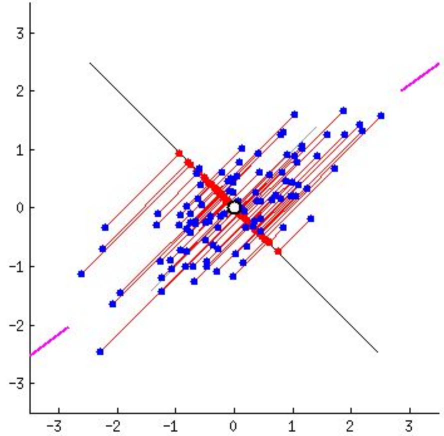
Common Dimensionality Techniques

Principal Component Analysis

- Linear reduction technique
- Principal Components -> Eigenvectors
- Focuses on capturing variability in the data

Draw backs:

- Cannot transform non-linear, real world data very well



https://sagarsaha455.medium.com/pca-for-visualization-and-dimension-reduction-14492e2acf2b

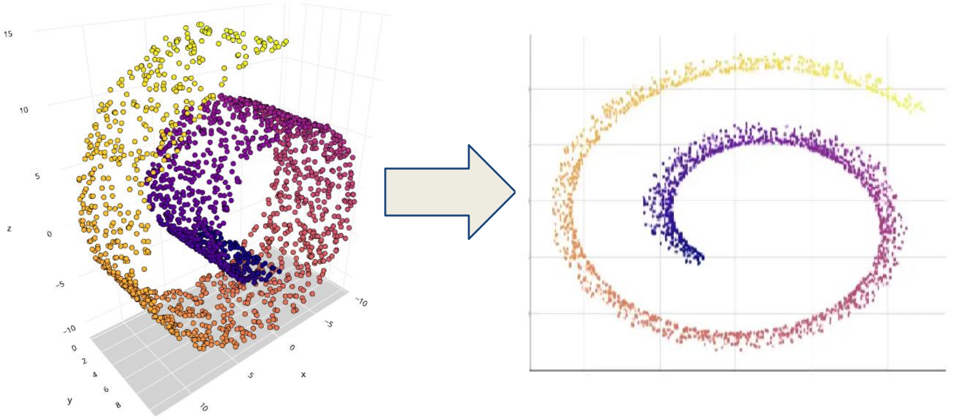
Common Dimensionality Techniques

Multidimensional Scaling (MDS)

- Linear Reduction Technique
- Focuses on preserving pairwise euclidean distances while minimizing strain cost function

Draw backs:

- Dependent on what distance metric you use
- Breaks down with sparse, separated data

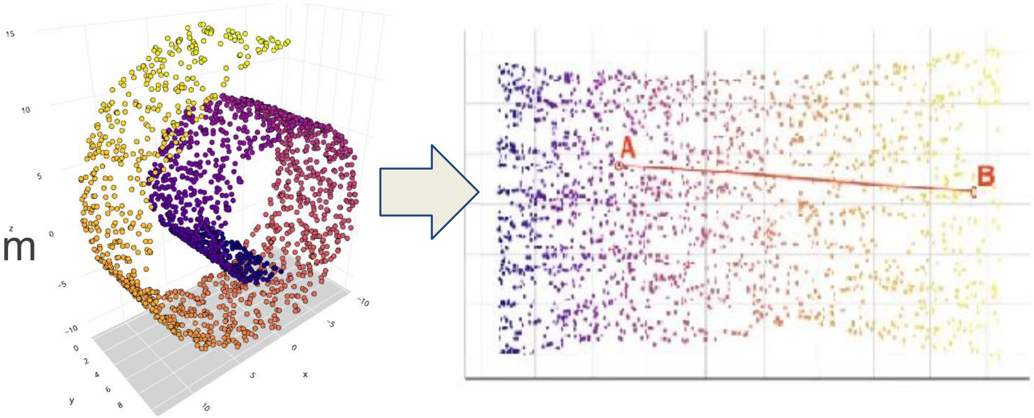


https://towardsdatascience.com/mds-multidimensional-scaling-smart-way-to-reduce-dimensionality-in-python-7c126984e60b

Common Dimensionality Techniques

Isometric Feature Mapping (Isomaps)

- Non-linear reduction technique
- Builds on MDS but focuses on geodesic distance
- Geodesic distance approximated from euclidean using neighborhoods



Draw backs:

- Susceptible to noise in the data
- Need prior knowledge of how to represent the geodesic distance.

https://towardsdatascience.com/isomap-embedding-an-awesome-approach-to-non-linear-dimensionality-reduction-fc7efbca47a0

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Diffusion Maps

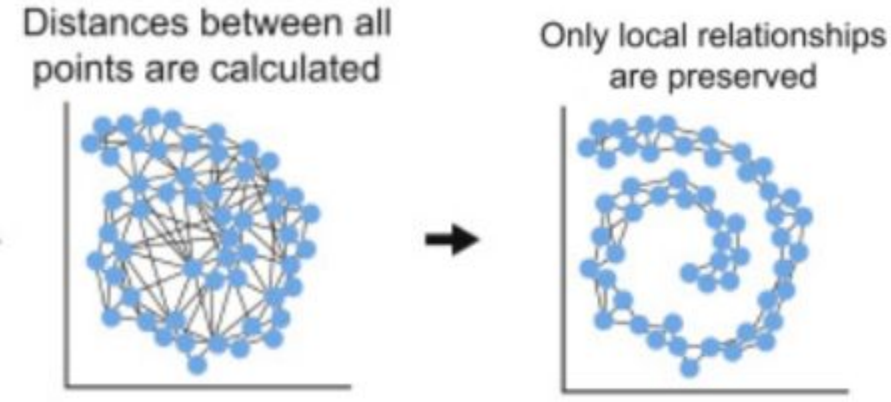
Diffusion Maps

How do they work?

- Consist of 3 parts:
  1) Connectivity

  2) Diffusion

  3) Mapping



Diffusion Maps

Connectivity

- Define a connective measure (i.e. Euclidean distance) between points **if known**

OR

- Define a kernel to help define local measures of similarity

$$k(x, y) = \exp\left(-\frac{|x-y|^2}{\alpha}\right)$$

Create a connectivity matrix P

$$P_{n\times n} = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1n} \\ p_{21} & p_{22} & \cdots & p_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ p_{n1} & p_{n2} & \cdots & p_{nn} \end{bmatrix}$$

Where P[i, j] refer to connectivity of X_i and X_j

Diffusion Maps

Diffusion

Define a matrix D^t where t is the time step

$$D^t_{n\times n} = \begin{bmatrix} d^t_{11} & d^t_{12} & \cdots & d^t_{1n} \\ d^t_{21} & d^t_{22} & \cdots & d^t_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ d^t_{n1} & d^t_{n2} & \cdots & d^t_{nn} \end{bmatrix}$$

Where $d^t_{i,j}$ is: $\sum_{u\in X} |p_t(X_i,u) - p_t(u,X_j)|^2$

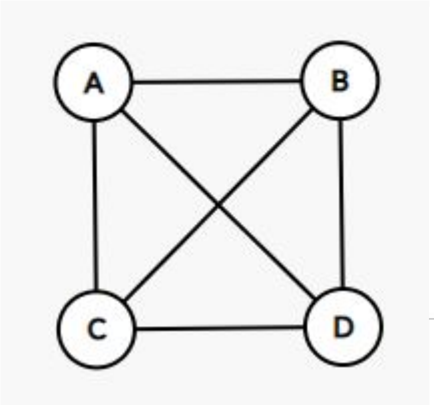
Advantages:

- Helps avoid noise in the data
- With higher values of t, you conform to the geometry of the data.

Diffusion Maps

Example Problem - Probabilistic Jumping

Connectivity



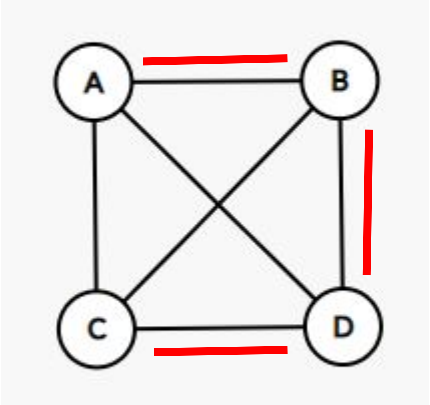
$$P = \begin{array}{cc} & \begin{array}{cccc} A & B & C & D \end{array} \\ \begin{array}{c} A \\ B \\ C \\ D \end{array} & \begin{bmatrix} 0.00 & 0.10 & \underline{0.70} & 0.10 \\ \underline{0.70} & 0.00 & 0.10 & 0.20 \\ 0.20 & 0.20 & 0.00 & \underline{0.70} \\ 0.10 & \underline{0.70} & 0.20 & 0.00 \end{bmatrix} \end{array}$$

$$P^3 = \begin{array}{cc} & \begin{array}{cccc} A & B & C & D \end{array} \\ \begin{array}{c} A \\ B \\ C \\ D \end{array} & \begin{bmatrix} 0.17 & 0.17 & 0.22 & 0.17 \\ 0.54 & 0.20 & 0.14 & 0.54 \\ 0.17 & 0.17 & 0.16 & 0.17 \\ 0.12 & 0.46 & 0.48 & 0.12 \end{bmatrix} \end{array}$$

Diffusion Maps

Example Problem - Probabilistic Jumping

Diffusion



$$P^3 = \begin{array}{c} \\ A \\ B \\ C \\ D \end{array} \begin{array}{cccc} A & B & C & D \\ \end{array}$$

$$P^3 = \begin{array}{c|cccc} & A & B & C & D \\ \hline A & 0.17 & 0.17 & 0.22 & 0.17 \\ B & 0.54 & 0.20 & 0.14 & 0.54 \\ C & 0.17 & 0.17 & 0.16 & 0.17 \\ D & 0.12 & 0.46 & 0.48 & 0.12 \end{array}$$

$$D_3 = \begin{array}{c|cccc} & A & B & C & D \\ \hline A & 0.14 & 0.08 & 0.10 & 0.14 \\ B & \underline{0.43} & 0.14 & 0.11 & \underline{0.43} \\ C & 0.14 & 0.09 & 0.10 & 0.14 \\ D & 0.11 & \underline{0.29} & \underline{0.35} & 0.11 \end{array}$$

$$\sum_{u \in X} |p_t(X_i, u) - p_t(u, X_j)|^2$$

Diffusion Maps

Mapping

- Where the actual reduction occurs

- Creates the following relation:

  Diffusion Distance in Original Space

  Euclidean Distance in the Mapped Space

And Establish them into a mapping matrix:

$$Y_i := \begin{bmatrix} p_t(X_i, X_1) \\ p_t(X_i, X_2) \\ \vdots \\ p_t(X_i, X_N) \end{bmatrix} = P_{i*}^T.$$

Extract the *m* dominant eigenvalues and vectors from the equation:

$$Y_i' = \begin{bmatrix} \lambda_1^t \psi_1(i) \\ \lambda_2^t \psi_2(i) \\ \vdots \\ \lambda_n^t \psi_n(i) \end{bmatrix}$$

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Side by Side Experiments

Presenting the Data

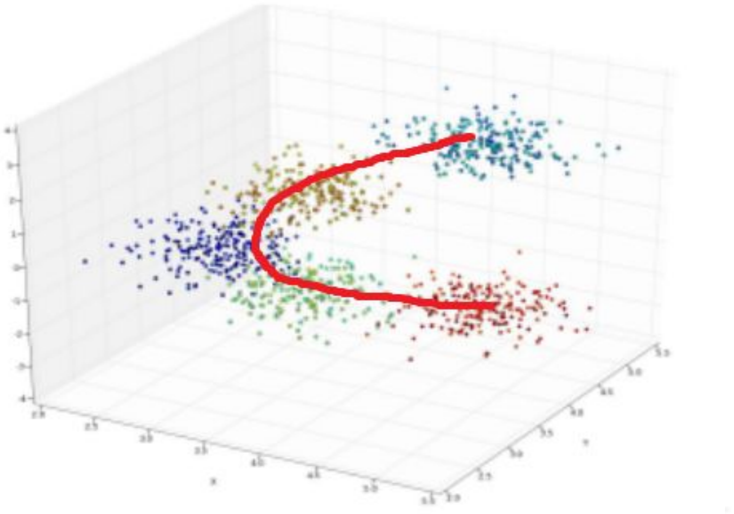
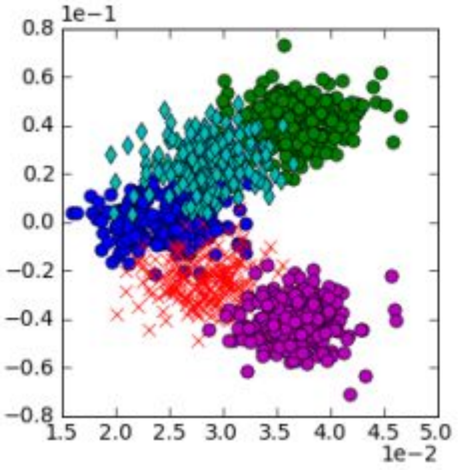


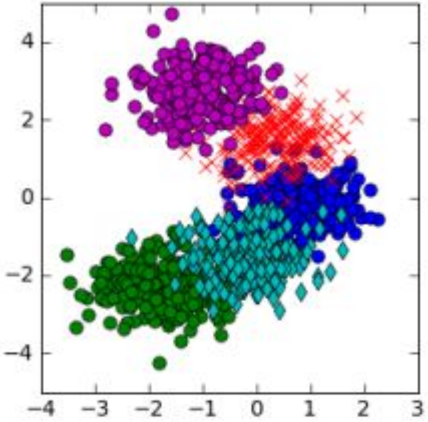
Figure 5: Original Data

PCA, MDS, Isomap Results

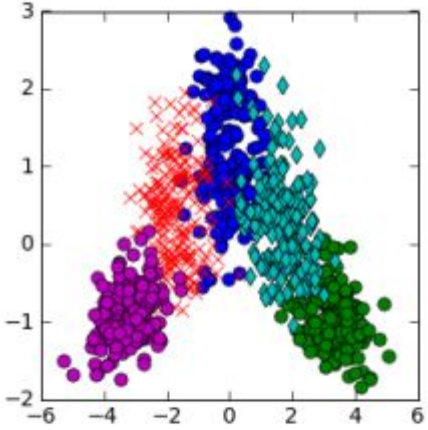
2 Dimensions PCA



2 Dimensions MDS

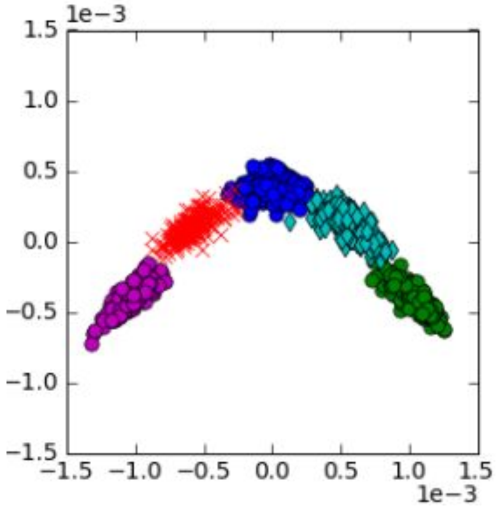


2 Dimensions Isomap

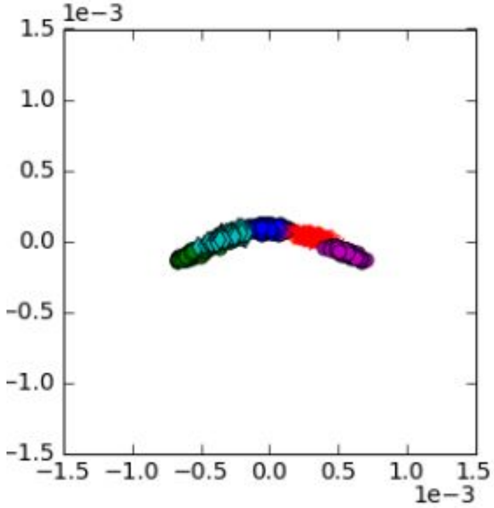


Diffusion Map Results

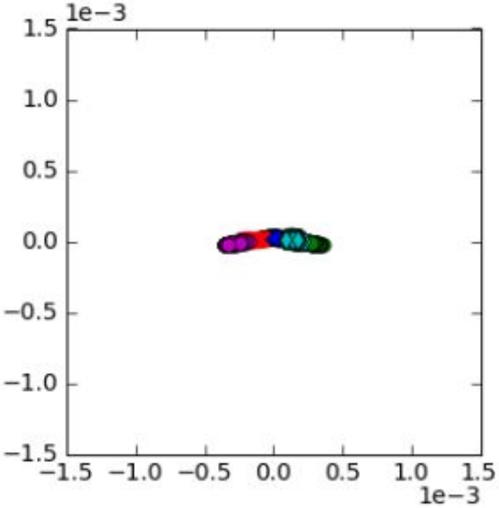
Diffusion t = 1



Diffusion t = 2

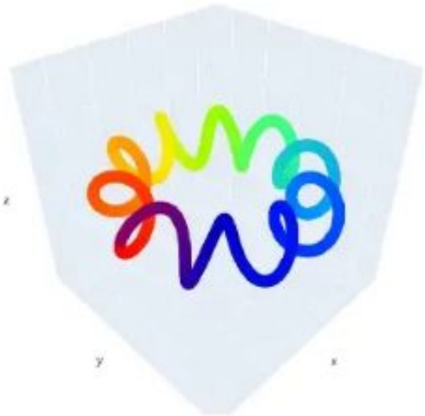


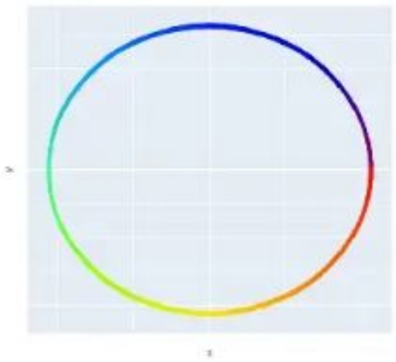
Diffusion t = 3



Takeaways

- Helps to expose the underlying Geometric Structure of the data through time steps
- Diffusion Translation allows for Euclidean measures to not be distorted
- Extremely expensive for the best results





https://towardsdatascience.com/unwrapping-the-swiss-roll-9249301bd6b7

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Contributions

- Chris Lawson - 65%
- Slides Presented:
  - 9-17

- Jeffrey Gordon - 35%
- Slides Presented:
  - 1-8, 18