## High Dimensional Inference Course Project

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Indian Statistical Institute

20th April, 2024

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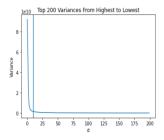


Figure 1: Scree Plot for PCA

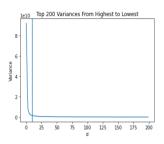


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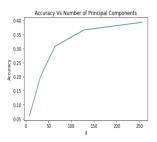


Figure 2: Accuracy of PCA for different intrinsic dimensions using KNN classifier

 PCA: Linear dimensionality reduction by projecting data onto directions of maximum variance

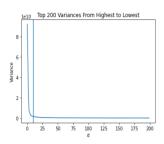


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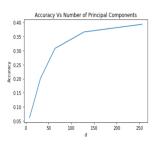


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 Images will be locally similar in many regions and symmetric in few dimensions

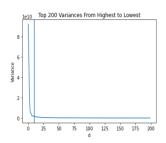


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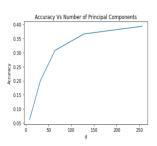
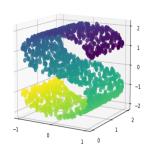


Figure 2: Accuracy of PCA for different intrinsic dimensions using KNN classifier

- Images will be locally similar in many regions and symmetric in few dimensions
- Raises concern over the linear projection of PCA

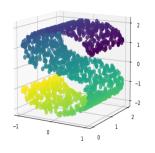


## Why Non-Linear Dimension Reduction



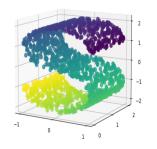
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## Why Non-Linear Dimension Reduction



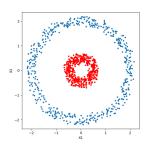
- Direction of maximum variation may not be linear especially in high-dimensional data
- Preserving global/local topology may be of importance

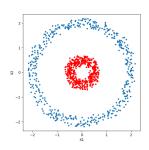
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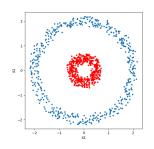
- Direction of maximum variation may not be linear especially in high-dimensional data
- Preserving global/local topology may be of importance
- Captures
   complex non-linear relationships among the variables



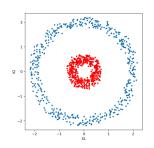




 Apply high dimensional transformation to capture non-linearity



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- Use Kernel trick to compute covariance matrix in transformed space (Gram matrix)



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- Use Kernel trick to compute covariance matrix in transformed space (Gram matrix)
- Apply PCA on the covariance matrix of the transformed data

### Kernel PCA Algorithm (SchSlkopf et al., 1997)

• Consider  $\Phi: \mathbb{R}^p \to \mathcal{H} \; (\dim(\mathcal{H}) > p)$ , assume  $\sum_{i=1}^N \Phi(\mathbf{x}_i) = 0$ 

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- ② For known kernel function  $K(\mathbf{x}, \mathbf{y}) = \Phi(\mathbf{x})^T \Phi(\mathbf{y})$ , define  $K = ((K_{ij}))$ , with  $K_{ij} = \Phi(\mathbf{X}_i)^T \Phi(\mathbf{X}_j)$  ( $\mathbf{X}_1, \dots, \mathbf{X}_N$  are the observations)

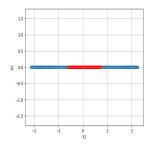
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- 3 Directly compute the projections from a point in the feature space  $\Phi(\mathbf{x})$  onto the *r*-th principal component  $(V^r)$  as:

$$(V^r)^T \Phi(\mathbf{x}) = \left(\sum_{i=1}^N a_i^r \Phi(\mathbf{x_i})\right)^T \Phi(\mathbf{x})$$
 where  $a_i^r$  are obtained by solving

- Eigenvector equation:  $N\lambda a = Ka$
- **2** Normalizing eigenvector equation:  $(V^r)^T V^r = 1$

### PCA vs Kernel PCA



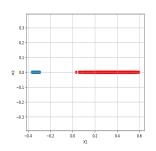


Figure 3: Dimension reduction via PCA Figure 4: Dimension reduction via PCA

• For choice of kernel refer Bernhard et al. (1998)

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- Embed in lower dimensional space preserving pairwise distances

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### MDS Algorithm

- Given a symmetric distance or affinity matrix D, set up the squared proximity matrix  $\mathbf{D}^{(2)} = [d_{ij}^2]$ .
- ② Define  $\mathbf{B} = -\frac{1}{2}\mathbf{H}\mathbf{D}^{(2)}\mathbf{H}$  where  $\mathbf{H} = \mathbf{I} \frac{1}{n}\mathbf{1}_N\mathbf{1}_N^T$
- **3**  $\mathbf{Y} = \mathbf{E}_m \mathbf{\Lambda}_m^{1/2}$  where  $\mathbf{\Lambda}_m$  is the diagonal matrix of m largest eigenvalues of  $\mathbf{B}$  and  $\mathbf{E}_m$  is the matrix of the respective m eigenvectors.

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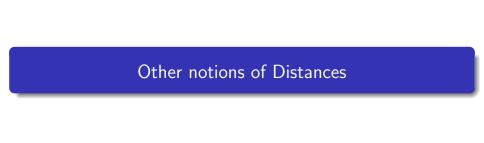
$$\underset{\mathbf{Y}_{1},\cdots,\mathbf{Y}_{N}}{\arg\min} \sum_{i=1}^{N} \sum_{j=1}^{N} (D_{ij} - ||\mathbf{Y}_{i} - \mathbf{Y}_{j}||)^{2}$$

## Connection b/w Kernel PCA & MDS

### Result (Williams, 2002)

Using an Isotropic Kernel function the Kernel PCA can be interpreted as performing a kind of MDS.

Isotropic Kernel: Kernel depending only on the Euclidean distance



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Euclidean distance is "meaningful" for short distances

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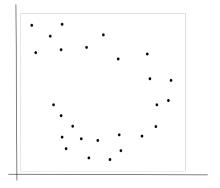


Figure 5: Geodesic Distance

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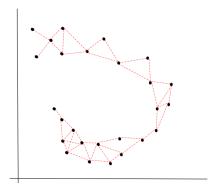


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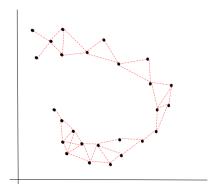


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Geodesic Distance: Shortest distance in this graph

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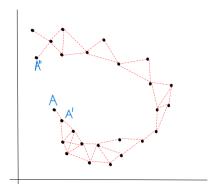


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# Isometric Feature Mapping (ISOMAP)

We have a training set

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### **Application on Swiss Roll**

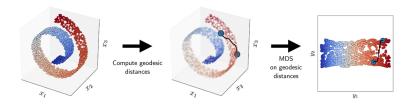


Figure 6: Applying ISOMAP to Swiss Roll data

### ISOMAP Algorithm

- **①** Determine k neighbourhood graph G of the observed data  $\{x_i\}$
- ② Compute shortest paths in the graph for all pairs of data points to form a distance matrix D. Each edge  $x_i$ ,  $x_j$  is weighted by its Euclidean length  $||x_i x_j||$  or by some other useful metric
- $\odot$  Apply MDS to the resulting shortest-path distance matrix D

# Compare PCA with ISOMAP

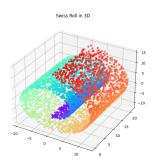


Figure 7: Swiss Roll Data with N = 1000

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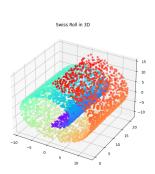


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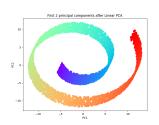


Figure 8: PCA

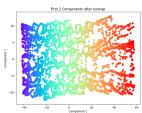


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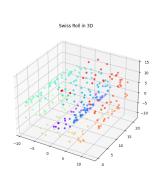


Figure 10: Swiss Roll Data with N = 300

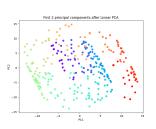


Figure 11: PCA

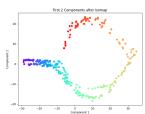


Figure 12: ISOMAP

## Theorem (de Silva and Tenenbaum, 2002)

Let Y be sampled from a bounded convex region in  $\mathbb{R}^p$ , with respect to a density function  $\alpha=\alpha(y)$ . Let f be a  $C^2$ -smooth isometric embedding of that region in  $\mathbb{R}^d$ . Given  $\lambda,\mu>0$ , for a suitable choice of neighborhood size parameter k, we have

$$1 - \lambda \leq \frac{\text{recovered distance}}{\text{original distance}} \leq 1 + \lambda$$

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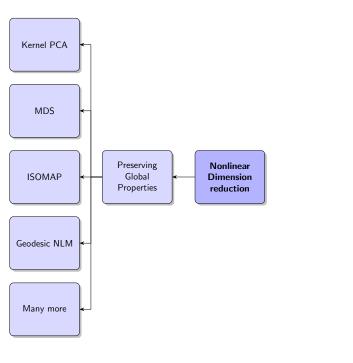
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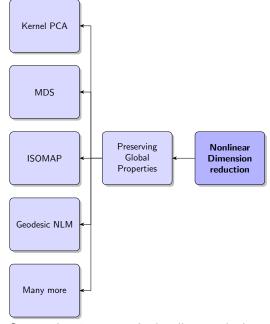
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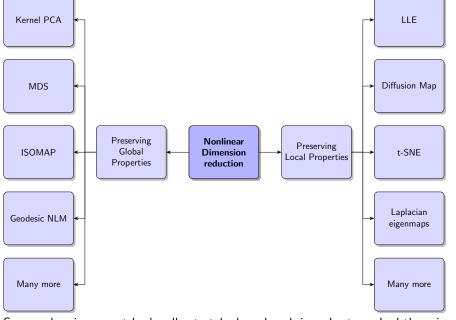
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- MDS is isometric  $C^2$ -smooth embedding
- ISOMAP preserves distance (globally)





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## LLE Algorithm (Ghojogh et al., 2020)

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For each point, identify the weighted sum of the neighbors that predicts the location of the point

$$\hat{\mathbf{X}}_i = \sum_{\mathbf{X}_j \in \mathcal{N}_i} w_{ij} \mathbf{X}_j$$
 s.t.  $\sum_{\mathbf{X}_j \in \mathcal{N}_i} w_{ij} = 1$ 

To calculate weights we minimise:  $\sum_{i=1}^{N} ||\mathbf{X}_i - \hat{\mathbf{X}}_i||^2$ 

# LLE Algorithm (Ghojogh et al., 2020)

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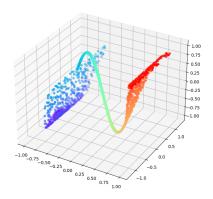
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 subject to  $\frac{1}{N}\mathbf{Y}^T\mathbf{Y}=I$ 

3 Solving Lagrangian we can get,

**Y** is the *eigenvectors* of 
$$(I - \mathbf{W})^T (I - \mathbf{W})$$



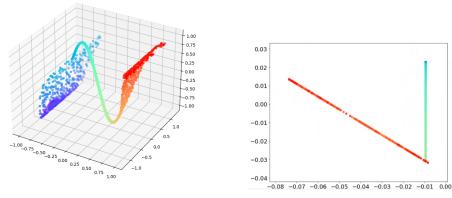


Figure 13: Applying LLE to a synthetic data

# Diffusion Map

**Idea:** If we take random walk on the data then walking at nearby point is more likely.

## Diffusion Map Algorithm

- **1** Similarity Matrix L :  $L_{i,j} = k(x_i, x_j)$
- ② Normalize the matrix according to parameter  $\alpha: L^{(\alpha)} = D^{-\alpha}LD^{-\alpha}$  where  $D_{i,i} = \sum_i L_{i,j}$
- **3** Form the normalized matrix  $M = (D^{(\alpha)})^{-1} L^{(\alpha)}$  where  $D^{(\alpha)}$  is a diagonal matrix and  $D_{i,i}^{(\alpha)} = \sum_{j} L_{i,j}^{(\alpha)}$ .

## Diffusion Map

**Idea:** If we take random walk on the data then walking at nearby point is more likely.

## Diffusion Map Algorithm

- Compute the d largest eigenvalues of  $M^t$  and the corresponding eigenvectors.
- Use diffusion map to get the embedding  $\Psi_t$  where  $\Psi_t(x) = (\lambda_1^t \psi_1(x), \lambda_2^t \psi_2(x), \dots, \lambda_d^t \psi_d(x))$
- Thus we get the diffusion map from the original data to a *d*-dimensional space which is embedded in the original space.

Minimize the KL divergence between high and low dimensional affinities  $p_{ij} \ \& \ q_{ij}$ 

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$$\mathcal{L} = \sum_{i,j} p_{ij} \log rac{p_{ij}}{q_{ij}}$$

High penalty for putting close neighbour far away



### t-SNE Algorithm

High-dimensional similarities:

$$p_{j|i} = \frac{\exp\left(-\left\|\mathbf{x}_{i} - \mathbf{x}_{j}\right\|^{2} / 2\sigma_{i}^{2}\right)}{\sum_{k \neq i} \exp\left(-\left\|\mathbf{x}_{i} - \mathbf{x}_{k}\right\|^{2} / 2\sigma_{i}^{2}\right)}$$

- ② Then symmetrize and normalize to sum to one:  $p_{ij} = \frac{p_{i|j} + p_{j|i}}{2n}$
- Substitution of the sub

$$q_{ij} = \frac{w_{ij}}{Z}, \quad w_{ij} = k(\|\mathbf{y}_i - \mathbf{y}_j\|), \quad Z = \sum_{k \neq l} w_{kl}$$

#### t-SNE Algorithm

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**4** SNE:  $k(d) = \exp(-d^2)$  and t-SNE:  $k(d) = 1/(1+d^2)$ 

### t-SNE Algorithm

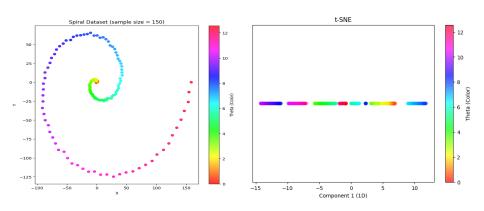
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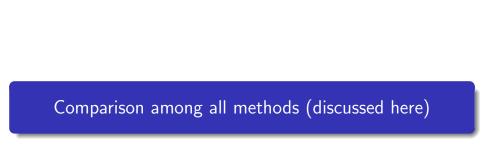
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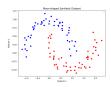
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- $\bullet \mathcal{L} = -\sum_{i,j} p_{ij} \log q_{ij} = -\sum_{i,j} p_{ij} \log w_{ij} + \log \sum_{i,j} w_{ij}$
- Apply gradient descent





# 2-d Data (Half Moons Data)



(a) Actual data

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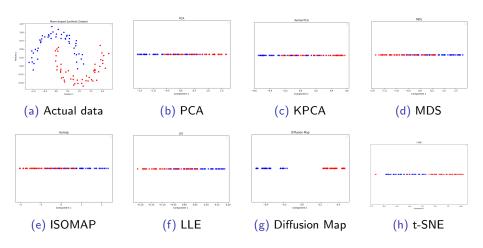
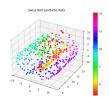


Figure 14: Comparison among six methods for half moon data (N = 100)

# 3-d Data (Swiss Roll)



(a) Actual data

# 3-d Data (Swiss Roll)

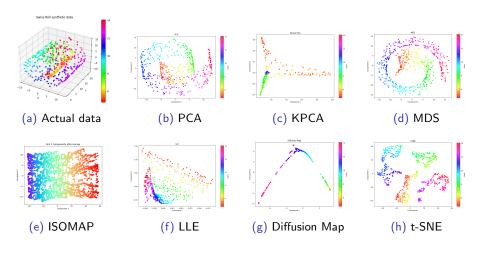
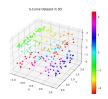


Figure 15: Comparison among six methods for swiss roll data (N = 500)

# 3-d Data (S-Curve Data)



(a) Actual data

# 3-d Data (S-Curve Data)

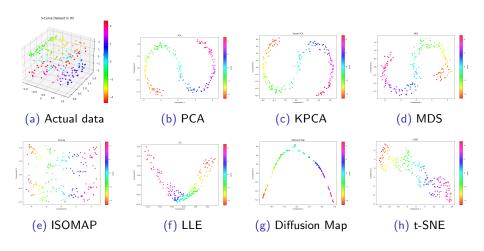


Figure 16: Comparison among six methods for S-curve data (N = 200)



### Where is the problem?

Imagine a library with bookshelves (features) with two scenarios:

- Many shelves with few books (low spread-outness).
- Few shelves with books scattered across (high spread-outness).



Traditional methods (e.g., number of features) can't capture this "spread-outness." **Here's where fractal dimension comes in.** 

### Definition: q-Dimension

- Fractal dimension (DF) refers to dimensions of fractals (capacity, correlation, information). q-dimension unifies these.
- Suppose **y** is a random variable with DF F(.) and pdf f(.)
- For  $\epsilon >$  0, support of F is covered with a grid of cubes with edge length  $\epsilon$
- $N(\epsilon)$  be the number of cubes intersecting the support and  $p_i$  the probability of populated cubes:

$$D_q = \lim_{\epsilon \to 0} \frac{\left(\sum_{i=1}^{N(\epsilon)} p_i^q\right)}{(q-1)\log(\epsilon)}$$

• If the limit exists,  $D_q$  is the q-dimension of F.

# Capacity Dimension

- Setting q = 0 in the q-dimension formula yields the capacity dimension  $(d_{cap})$ .
- Focuses on the number of covering boxes  $(N(\epsilon))$  as cube size  $(\epsilon)$  shrinks.

$$d_{cap} = \lim_{\epsilon o 0} rac{\log(N(\epsilon))}{\log(\epsilon)}$$

Unlike other dimensions, it ignores individual point probabilities.

## Application on a Synthetic Dataset

- Generation n=500 observation from  $N(0, I_p)$  where  $I_p$  is a Identity matrix of order p=1000 and it is normalised.
- Oscillated Box Counting dimension is calculated by the above algorithm

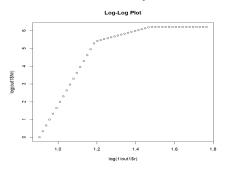


Figure 17: Log-Log Plot

Box Counting Dimension Estimated: 16.77263



### Application on Yale Dataset

Intrinsic dimension was found out to be 12

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Methods	Accuracy(%)
PCA	24.637
Kernel PCA	24.637
MDS	14.285
Isomap	46.376
LLE	42.443
Diffusion maps	27.950
t-SNE	57.142

Table 1: Accuracy of 5-NN classifier for the dimension reduced data



#### Further Exploration

- Computational Complexity
- Estimation of Intrinsic Dimension

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- Use of non-linear modelling architecture after linear dimension reduction over Nonlinear dimension reduction?

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- Computational Complexity
- Estimation of Intrinsic Dimension
- Use of non-linear modelling architecture after linear dimension reduction over Nonlinear dimension reduction?
- Extensions of the NLDR methods to incorporate handling out-of-sample data

#### References

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