A Brief Introduction To

# Dimensionality Reduction

Megh Shukla
25th September, 2020

# AGENDA

## 01 *INTRODUCTION*

**Answering the What and the Why**

## 02 CLASSICAL METHODS

PCA, LDA, Laplacian Eigenmaps, Locally Linear Embedding

## 03 MODERN METHODS

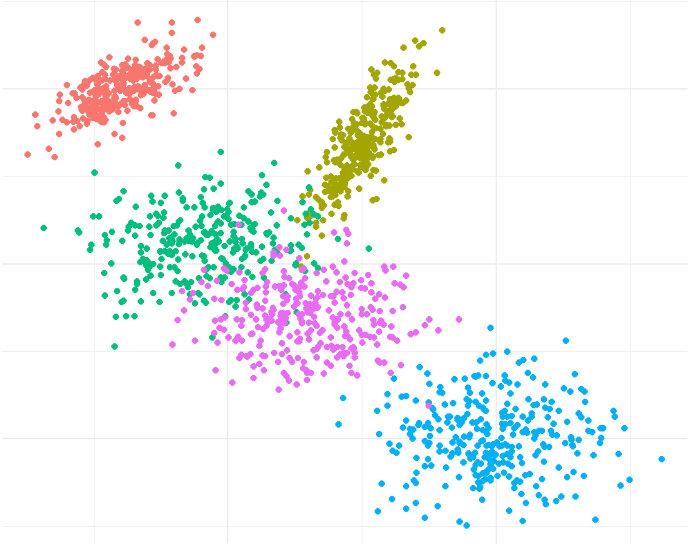
Autoencoders, t-SNE, UMAP

## 04 CONCLUSION

Comparison, Summary and Upcoming Research

# NEED FOR DIMENSIONALITY REDUCTION

## Time and Space Complexity



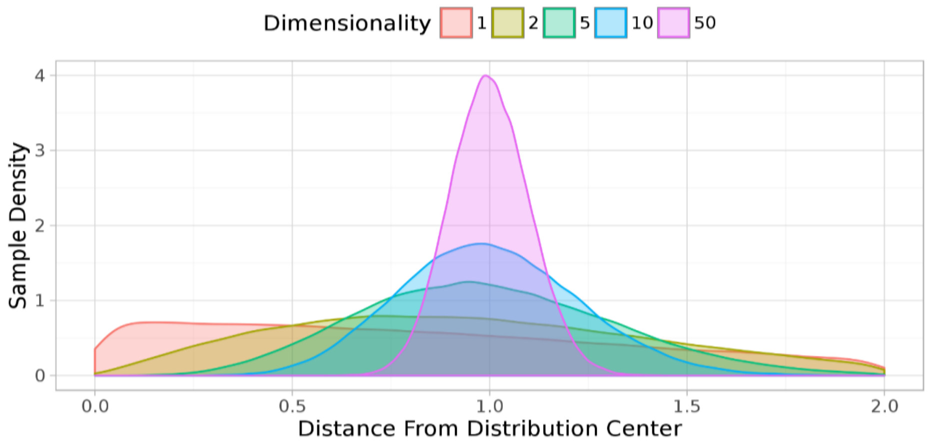
- Time Complexity
- Memory

# NEED FOR DIMENSIONALITY REDUCTION

Visualization

# NEED FOR DIMENSIONALITY REDUCTION

## Curse Of Dimensionality




$$\lim_{d\to\infty} \mathbb{E}\left(\frac{dist_{max}(d) - dist_{min}(d)}{dist_{min}(d)}\right) \to 0$$

### VC Dimension - Overfitting

| | |
|---|---|
| $VC_{dim}(\text{NeuralNet}) = O(WL \log W)$ | $W = \#weights$ $\quad L = \#layers$ |

# AGENDA

## 01 INTRODUCTION

Answering the What and the Why

## 02 *CLASSICAL METHODS*

***PCA, LDA, Laplacian Eigenmaps, Locally Linear Embedding***

## 03 MODERN METHODS

Autoencoders, t-SNE, UMAP

## 04 CONCLUSION

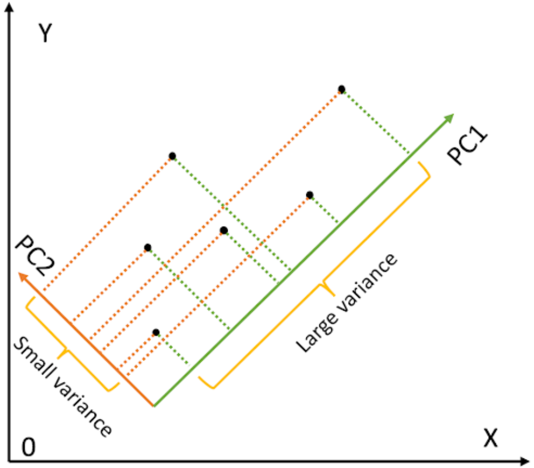
Comparison, Summary and Upcoming Research

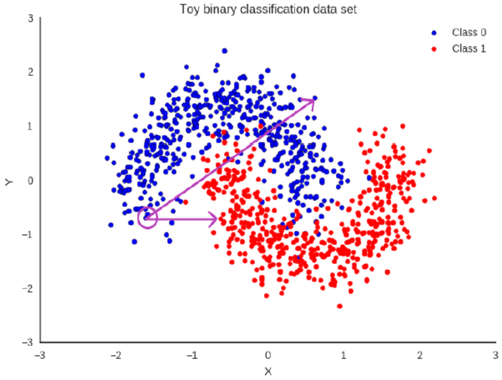
# CLASSICAL METHODS

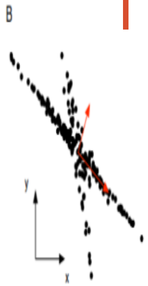
# LINEAR METHODS

## Principal Component Analysis

- Explain the variance in the data!
- Similarity to Linear Regression?




$\mathbb{X}: Samples \in \mathbb{R}^{N \times d}$
$v$ : Projection Vector

**Linear**

$$PC_1 = \mathbb{X}v$$

**Objective**

$$\arg\min_{v} ||\mathbb{X} - \mathbb{X}VV^T||$$

**Constraint**

$$V^T V = I$$

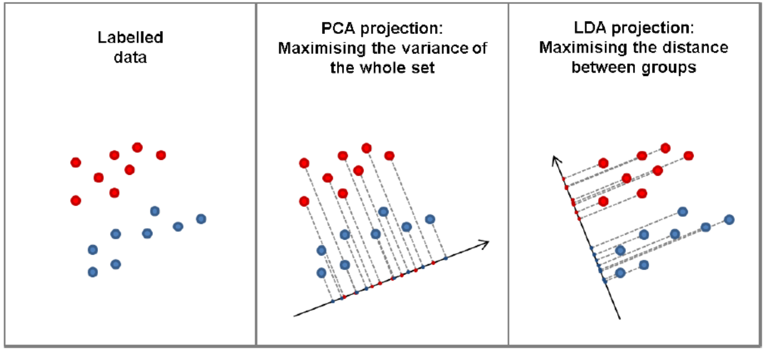
**Solution**

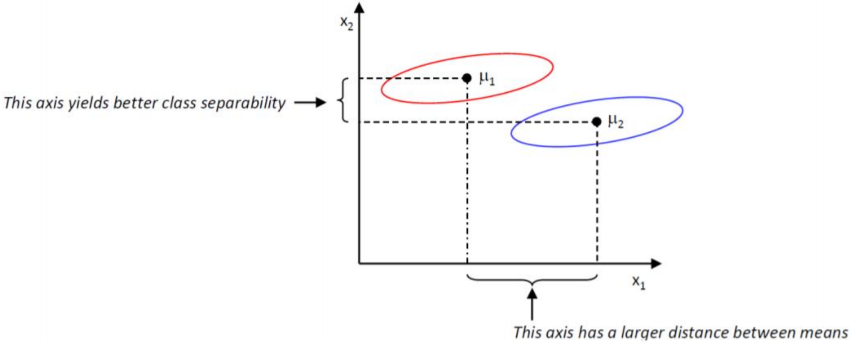
$$\mathbb{X}^T \mathbb{X} V = \lambda V$$

# LINEAR METHODS

## Linear Discriminant Analysis

- Use class information!
- Sometimes, no labels better than having labels!



# LINEAR METHODS

## Linear Discriminant Analysis

Use class information!

Sometimes, no labels better than having labels!

$$\mathbb{Y} = w^T \mathbb{X}$$

The embeddings are linearly dependent on the input

$$\mathcal{J}(w) = \frac{|\tilde{\mu}_1 - \tilde{\mu}_2|^2}{\tilde{s}_1{}^2 + \tilde{s}_2{}^2}$$

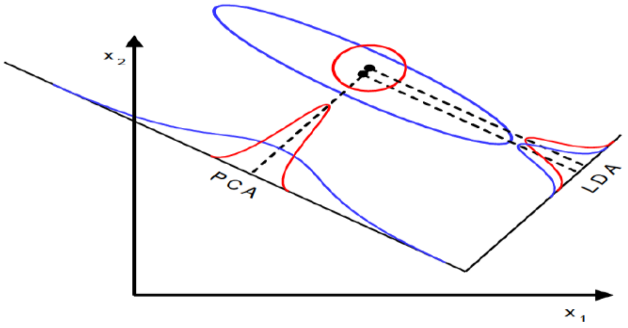
The objective to optimize

$$\mathcal{J}(w) = \frac{w^T S_B w}{w^T S_w w}$$

Optimize with respect to the weights

$$S_w^{-1} S_B w = \mathcal{J} w$$

… Reduced to Eigendecomposition




The solution!

$$w^* = S_w^{-1}(\mu_1 - \mu_2)$$

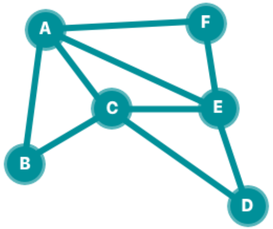
# LINEAR METHODS – Graph Based Algorithms

## Laplacian Eigenmaps

- Construct a Graph with Adjacency Matrix!
- Preserving local structure over global structure

**Graph**

- **Degree** – No of neighbours
- **Adjacency** – Presence of edge
- **Laplacian** – Degree - Adjacency




V: {A,B,C,D,E,F}
E: {AB,AC,AF,BC,CD,CE,DE,EF}

=

| | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| A | 0 | 1 | 1 | 0 | 1 | 1 |
| B | 1 | 0 | 1 | 0 | 0 | 0 |
| C | 1 | 1 | 0 | 1 | 1 | 0 |
| D | 0 | 0 | 1 | 0 | 1 | 0 |
| E | 1 | 0 | 1 | 1 | 0 | 0 |
| F | 1 | 0 | 0 | 0 | 1 | 0 |

# LINEAR METHODS - Graph Based Algorithms

## Laplacian Eigenmaps

- Construct a Graph with Adjacency Matrix!
- Preserving local structure over global structure

$$\mathbb{J}(y) = \sum_{i,j} (y_i - y_j)^2 a_{ij}$$

$$\mathbb{J}(y) = \sum_{i,j} (y_i^2 + y_j^2 - 2y_i y_j) a_{ij}$$

$$\mathbb{J}(y) = \sum_{i} y_i^2 D_i + \sum_{j} y_j^2 D_j - 2 \sum_{i,j} y_i y_j a_{ij}$$

$$\mathbb{J}(y) = 2Y^T L Y$$

Constraint

$$Y^T D Y = 1$$

$$Y^T D \mathbf{1} = 0$$

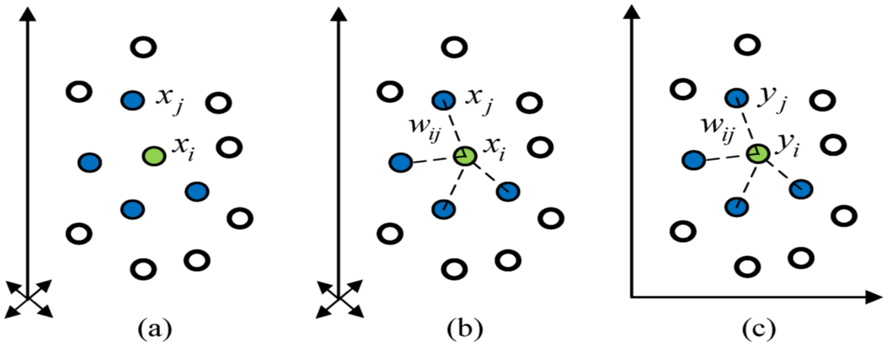
Eigenvalue Eigenvector everywhere!

# LINEAR METHODS

## Locally Linear Embedding

A node is known by the company he keeps!

Locally linear implies dense sampling!




The E-step…?

$$\mathcal{E}(W) = \sum_i |x_i - \sum_j W_{ij} x_j|^2$$

The M-step…?

$$\sum_i |y_i - \sum_j w_{ij} y_j|^2$$

# AGENDA

## 01 INTRODUCTION

Answering the What and the Why

## 02 CLASSICAL METHODS

PCA, LDA, Laplacian Eigenmaps, Locally Linear Embedding

## 03 *MODERN METHODS*

**Autoencoders, t-SNE, UMAP**

## 04 CONCLUSION

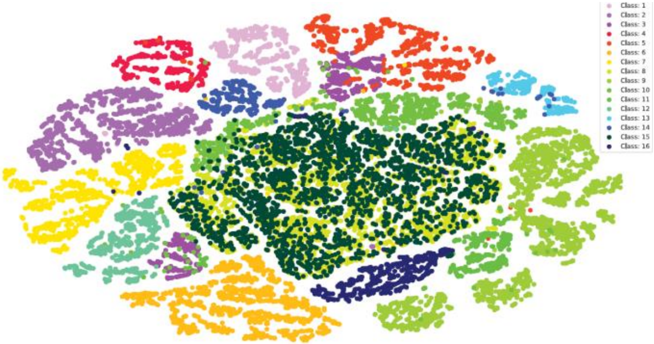
Comparison, Summary and Upcoming Research

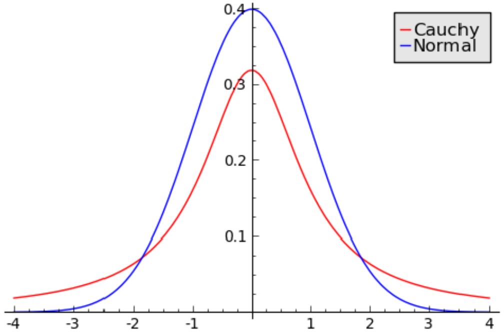
# MODERN METHODS

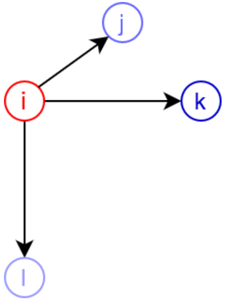
# MODERN APPROACHES

## t-Distributed Stochastic Neighbour Embedding

- Use class information!
- Sometimes, no labels better than having labels!




$$p_{j|i} = \frac{exp(-\| x_i - x_j \|^2 / 2\sigma_i^2)}{\sum_{k \neq i} exp(-\| x_i - x_k \|^2 / 2\sigma_i^2)}$$

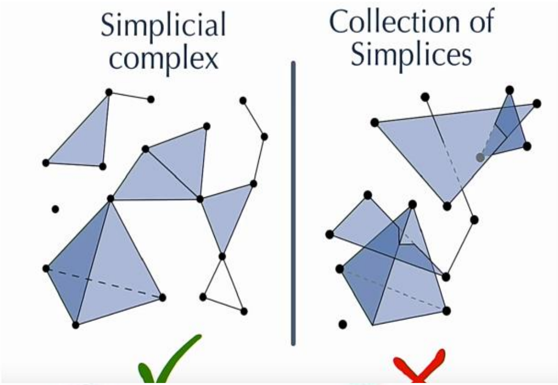
$$q_{j|i} = \frac{exp(-\| y_i - y_j \|^2)}{\sum_{k \neq i} exp(-\| y_i - y_k \|^2)}$$

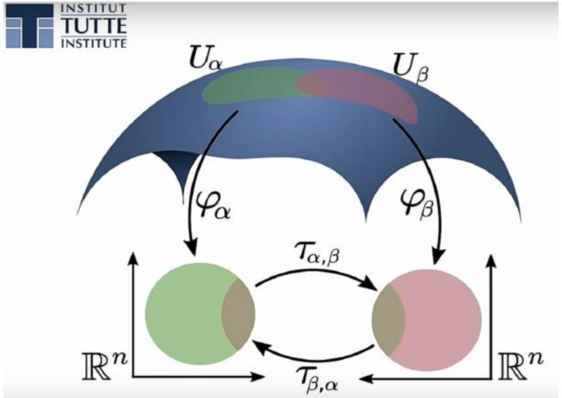
**KL Divergence!**

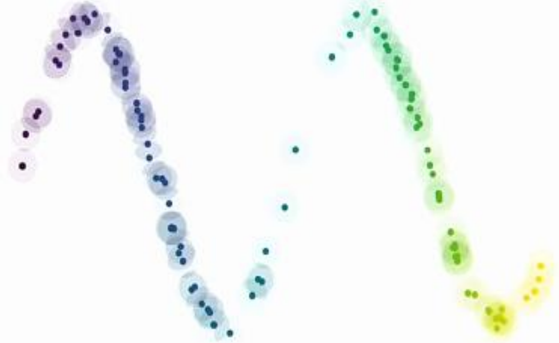
# MODERN APPROACHES

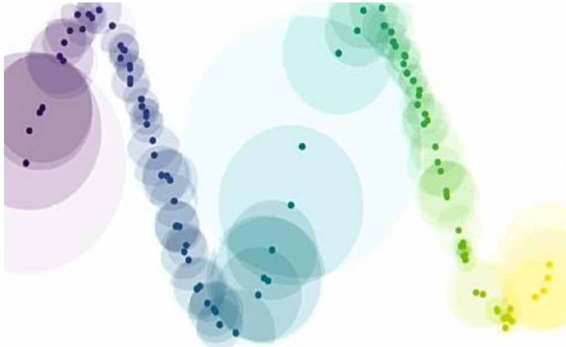
## Uniform Manifold Approximation and Projection

- Projection on a Reimannian Manifold
- Interpretability…?



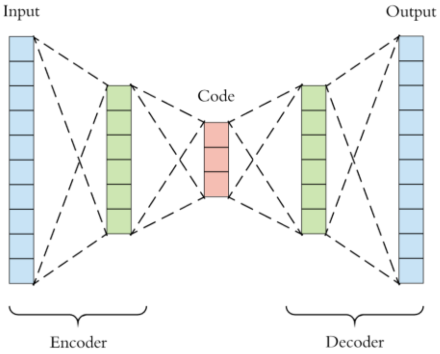





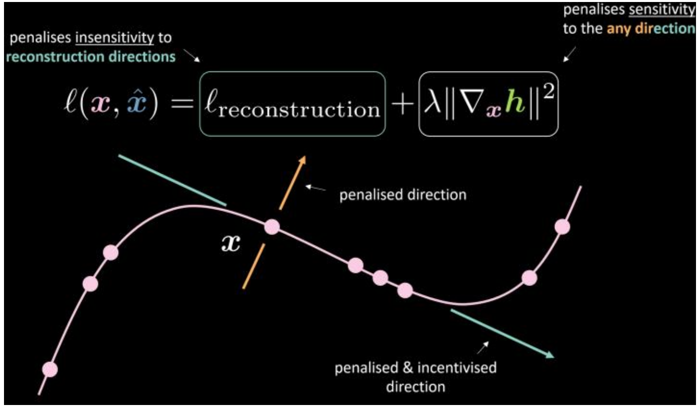
# MODERN APPROACHES

## Autoencoders

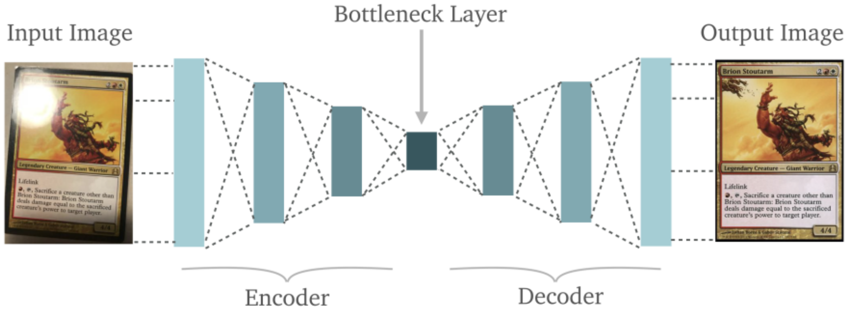
- Deep Learning magic!
- Overfitting … ?




### Contractive Autoencoders




### Denoising Autoencoders



# AGENDA

## 01 INTRODUCTION

Answering the What and the Why

## 02 CLASSICAL METHODS

PCA, LDA, Laplacian Eigenmaps, Locally Linear Embedding

## 03 MODERN METHODS

Autoencoders, t-SNE, UMAP

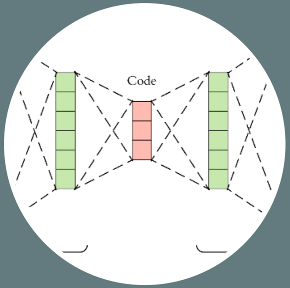
## 04 *CONCLUSION*

**Comparison, Summary and Upcoming Research**

# IS DIMENSIONALITY REDUCTION SOLVED?

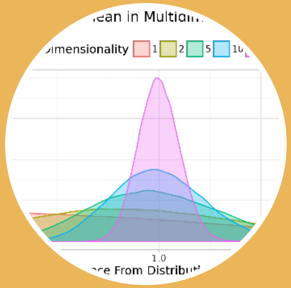
Sure the answer is No. But why?

# SHORTCOMINGS



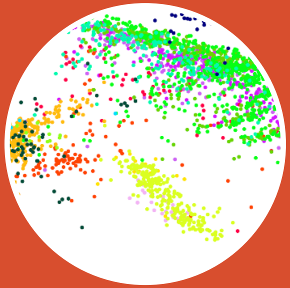

## Parameterization

What if we have new data? Need more dimensions?




## Curse Of Dimensionality

Euclidean distance can sometimes fail in high-dimensions



## Visualization and Clustering

Are they the same problem? Or are they different?

# THANK YOU!