Non-linear DR Visualization using t-SNE

CK Raju PhD

October 29, 2023

Quotes

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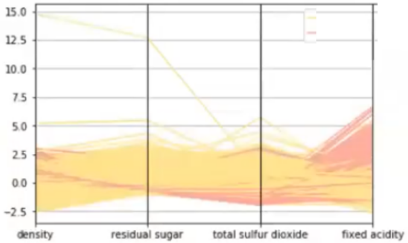
- High-dimensional worlds in visual grace, reborn.

Recap

DR and Visualization

Direct Visualisation

- Parallel Co-ordinates
  - Each vertical line is a dimension
  - A data item is connected by line segments
  - Large number of samples clutters the visualization



Direct Visualisation

- Parallel Co-ordinates
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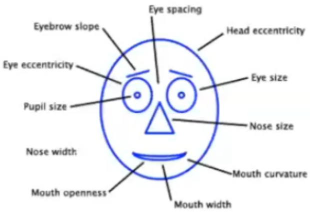
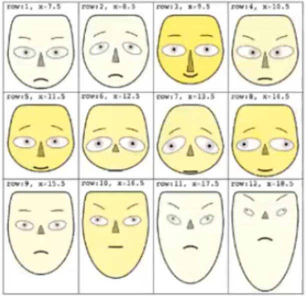
- Chernoff Faces [Herman Chernoff: 1973]





Other Methods for Direct Visualisation

- A few approaches have been proposed to improve upon Chernoff Faces
- Empathic Visualization
  - Improve visual similarity of similar vectors
- Metaphoric 3D glyphs
  - Use metaphors other than faces (say Trees)

Image: The Empathic Visualization Algo: Chernoff Faces Revisited
http://www0.cs.ucl.ac.uk/staff/a.loizides/218.pdf

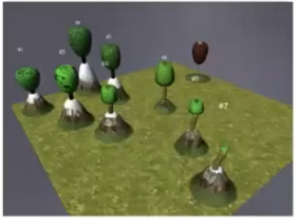
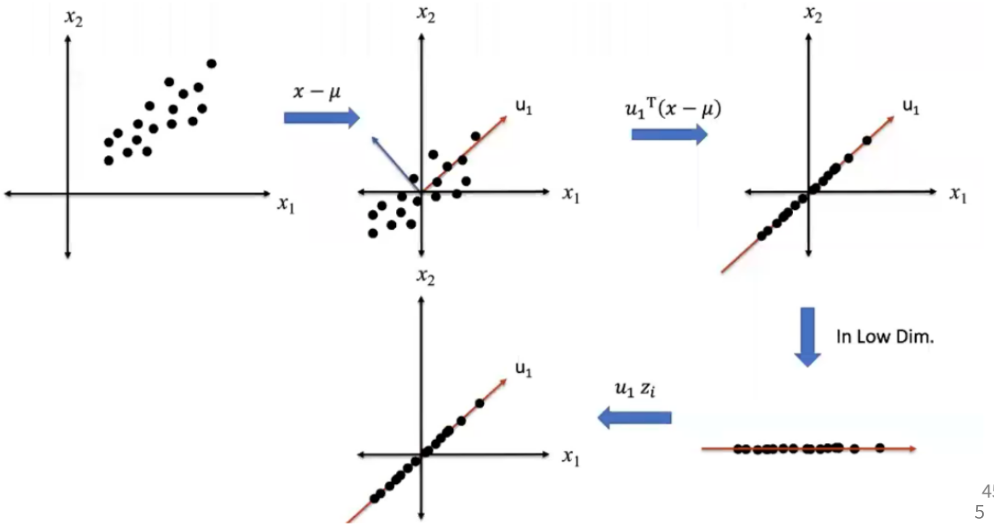
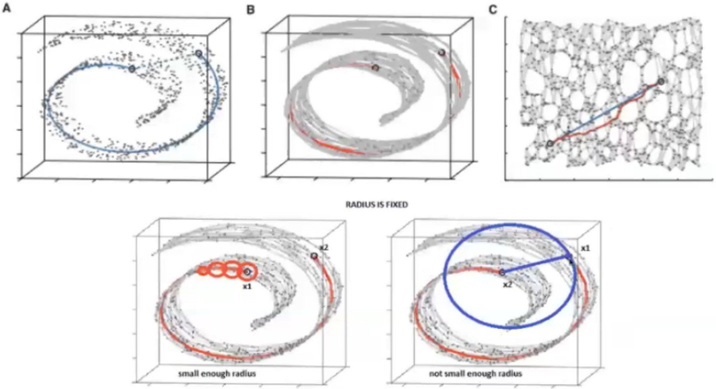


Image: "Beyond Chernoff faces: Multivariate visualization with metaphoric 3D glyphs", Marco Lardelli

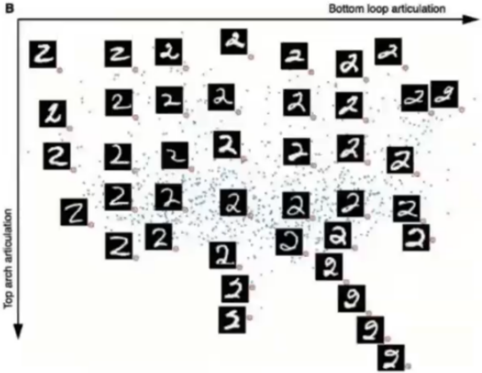
Dimensionality Reduction and Inverse Mapping



ISOMAP - Effect of Radius in Computation



Example - Handwritten Letters



Neighborhood Embedding

Prioritizing the Near and Dear

Neighborhood Embedding

- **Neighborhood**: A collection of samples that are close to a given sample. Defined by:
  - A radius
  - Number of samples

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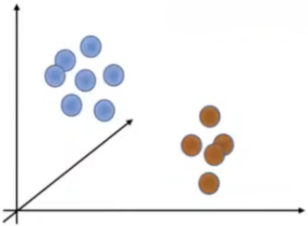

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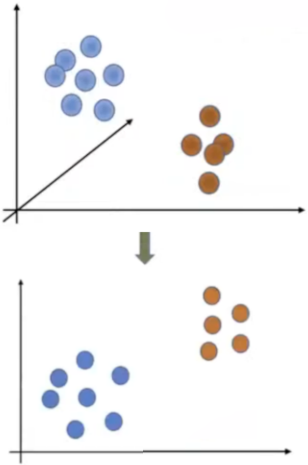

Neighborhood Embedding

- **Neighborhood**: A collection of samples that are close to a given sample. Defined by:
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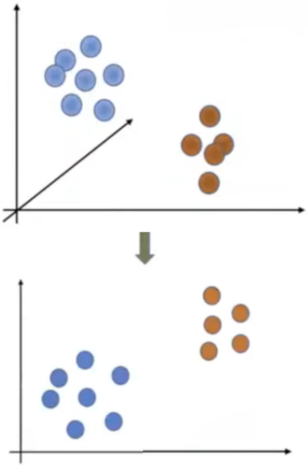
- **Embedding**: Representation of samples in a low-dimensional subspace
- **Goal**: Preserve the structure of local neighborhood



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  1. Randomly Initialize X_i'.
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Optimization

What Metric to Minimize

- Distance between points in a neighborhood

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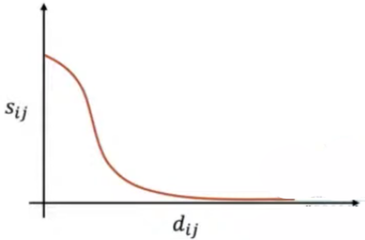

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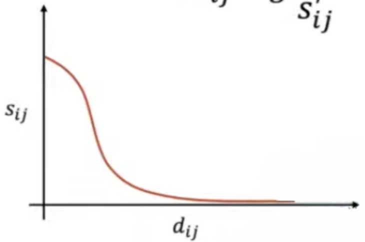

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SNE

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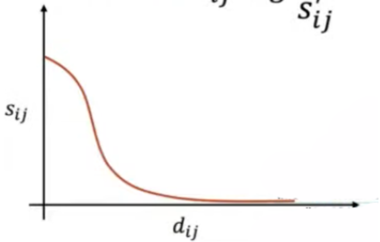


PCA vs SNE

PCA on MNIST *(0-9)*

SNE on MNIST *(0-5)*

..in short

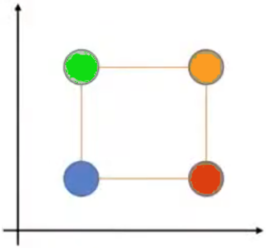
- preserve similarity in lower dimensional representation
- known as stochastic neighborhood embedding
- unsupervised technique, improvement over PCA

The t-SNE Algorithm

Computing the Embedding

SNE - Properties/Issues

- Much better embedding than PCA
- Problem of Crowding



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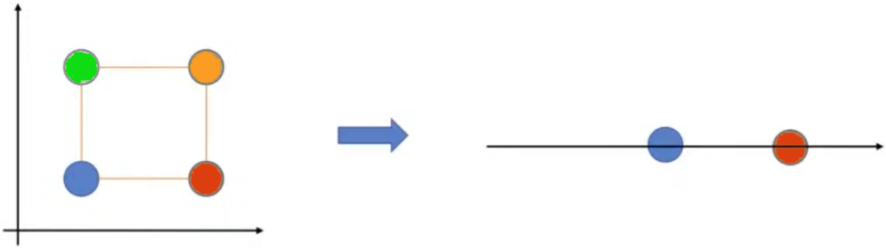

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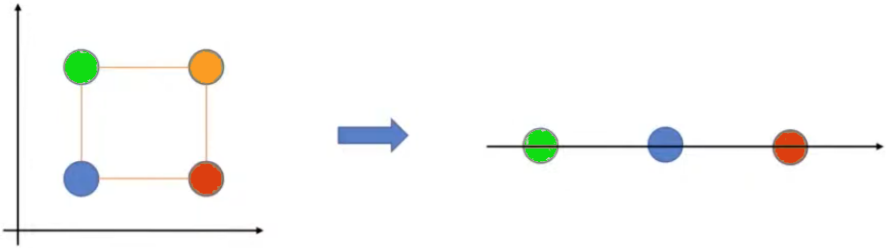

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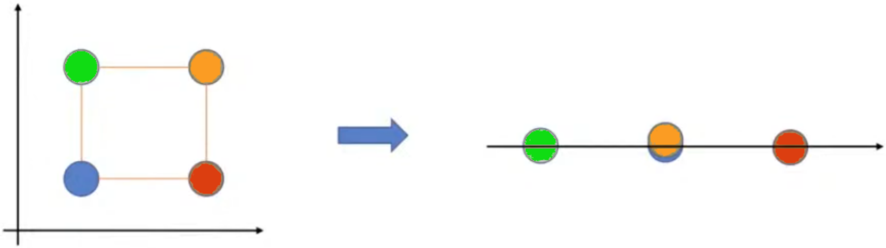
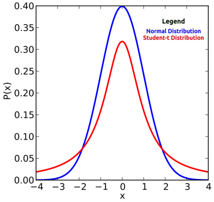


t-SNE

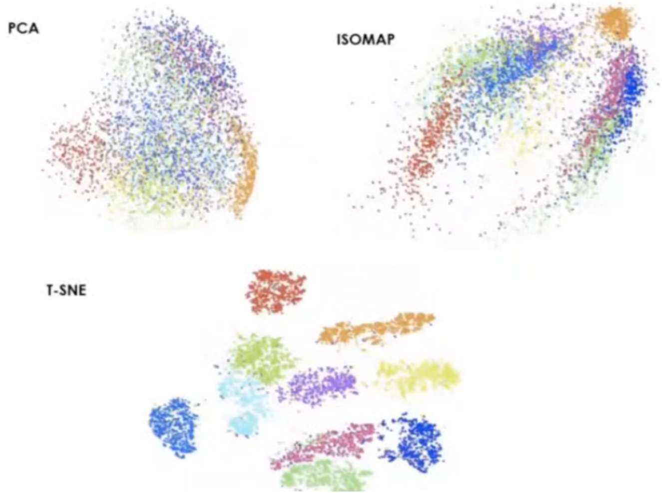
- Solution
  - Distant points drift farther apart
  - More flexibility in point distribution
- How to do this ?
  - Student-t distribution - computes S'_{ij}
  - Rest of the solution is same as SNE



Parameters of t-SNE

- Perplexity
  - Number of effective neighbors to consider
- Iterations
  - Steps after which we stop updating the embedding
- Step-size
  - Size of each update
- Initialization
  - Different initialisations lead to different visualisations

Comparison



Examples of t-SNE

Inferences from t-SNE Visualization

Example - Blog distill.pub

Link to t-SNE Visualization

Using and Reading t-SNE Results

- Running t-SNE

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- Running t-SNE
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  - Do not give importance to distances between points far-away
  - Do not give significance to density of clusters
  - Do not infer anything from a single output