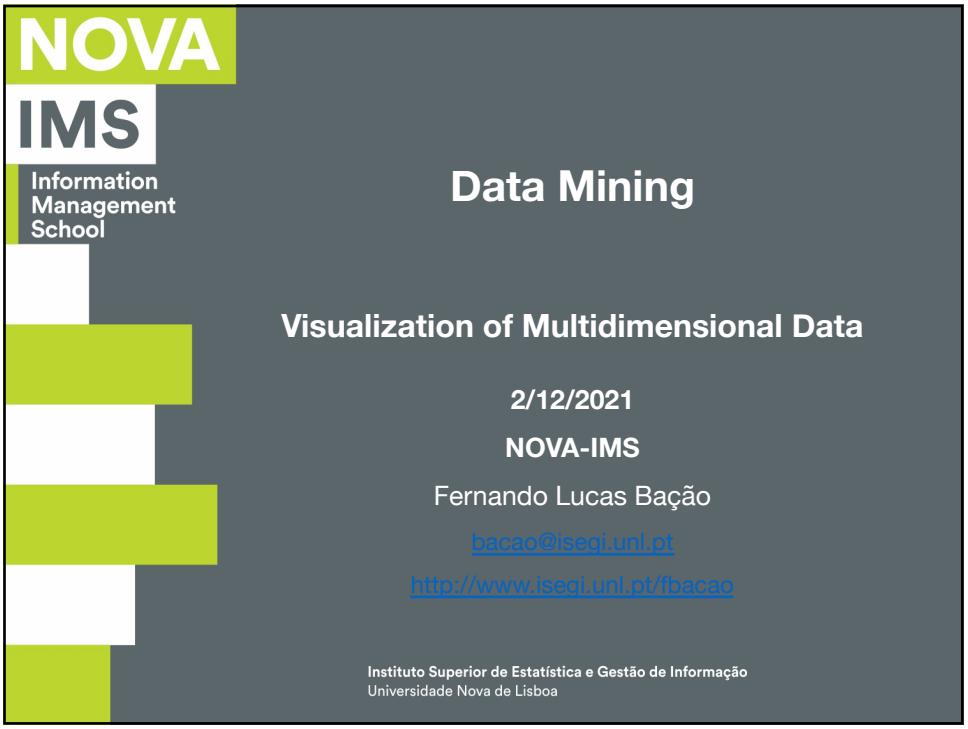
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Visualization of Multidimensional Data
2/12/2021
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Fernando Lucas Bação
bacao@isegi.unl.pt
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Instituto Superior de Estatística e Gestão de Informação
Universidade Nova de Lisboa

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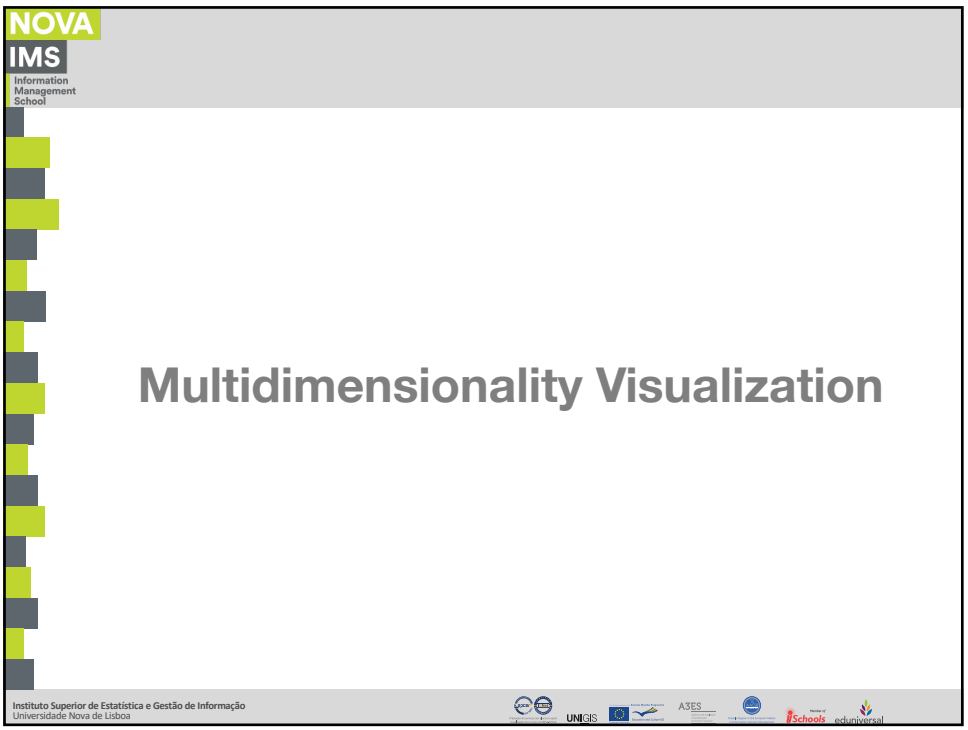
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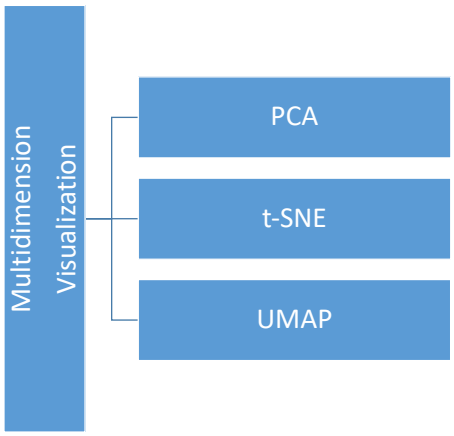
Multidimensionality Visualization



3

Principal Component Analysis

PCA

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Principal Component Analysis

- **Size Reduction of the Input Space:**
  - Principal Component Analysis
    - A procedure that uses an **orthogonal transformation** to convert a set of observations of possibly correlated variables into a set of values of **linearly uncorrelated variables called principal components**.
    - The number of principal components is **equal to the number of original variables**.
    - This transformation is defined in such a way that the first principal component has the **largest possible variance** (that is, accounts for as much of the variability in the data as possible), and each succeeding component in turn has the highest variance.

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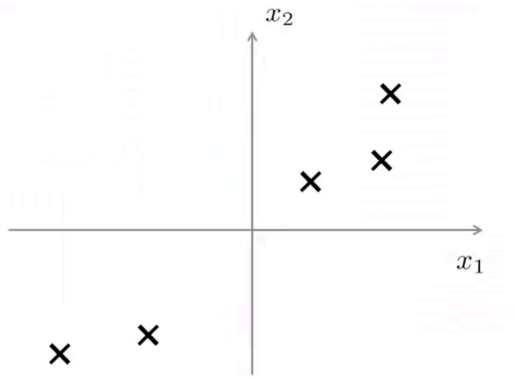
Principal Component Analysis

- **Size Reduction of the Input Space:**
  - Principal Component Analysis



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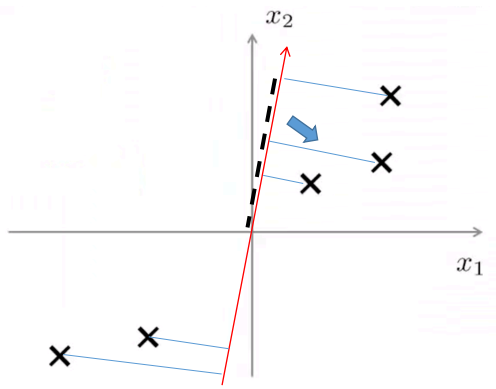
Principal Component Analysis

- **Size Reduction of the Input Space:**
  - Principal Component Analysis (SVD)



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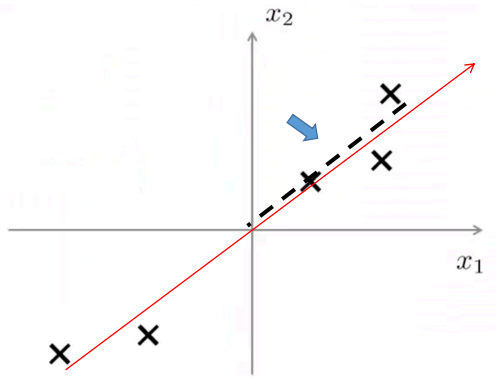
Principal Component Analysis

- **Size Reduction of the Input Space:**
  - Principal Component Analysis (SVD)



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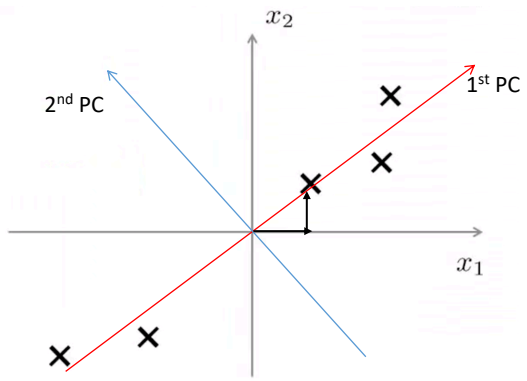
Principal Component Analysis

- **Size Reduction of the Input Space:**
  - Principal Component Analysis (SVD)



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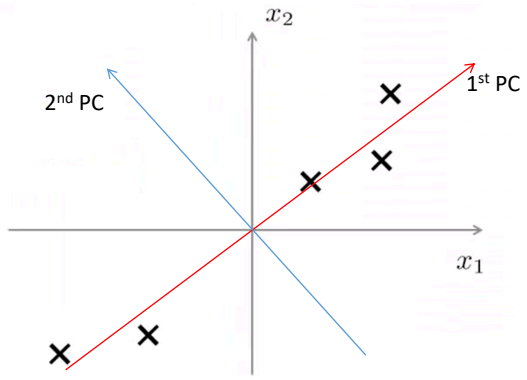
Principal Component Analysis

- **Size Reduction of the Input Space:**
  - Principal Component Analysis (SVD)



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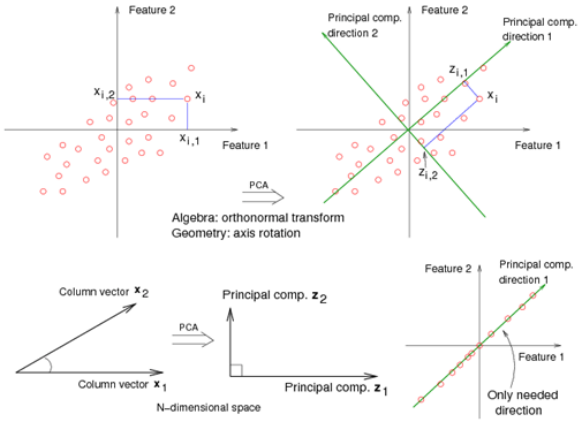
Principal Component Analysis

- **Size Reduction of the Input Space:**
  - Principal Component Analysis



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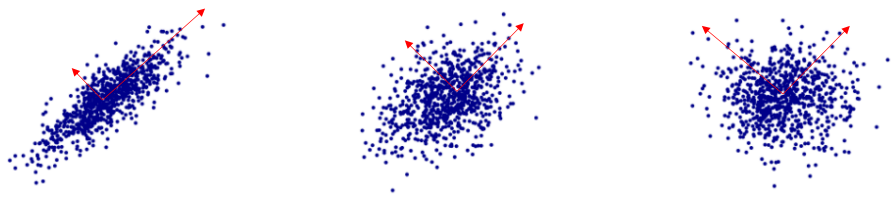
Principal Component Analysis

- **Size Reduction of the Input Space:**
  - Principal Component Analysis



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t-distributed Stochastic Neighbor Embedding

t-SNE

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- **t-SNE:**
  - t-distributed stochastic neighbor embedding (t-SNE) is a statistical method for visualizing high-dimensional data by **giving each datapoint a location in a two or three-dimensional map**.
  - It is a **nonlinear dimensionality reduction technique** well-suited for embedding high-dimensional data for visualization in a low-dimensional space of two or three dimensions.
  - Specifically, it **models each high-dimensional object** by a two- or three-dimensional point in such a way that **similar objects are modeled by nearby points** and dissimilar objects are modeled by distant points with high probability.

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t-SNE

- **t-SNE:**
  - The t-SNE algorithm comprises two stages:
    - First, t-SNE **constructs a probability distribution over pairs of high-dimensional objects** in such a way that similar objects are assigned a higher probability while dissimilar points are assigned a lower probability.
    - Second, t-SNE defines a **similar probability distribution over the points in the low-dimensional map**, and it minimizes the Kullback–Leibler divergence (KL divergence) between the two distributions with respect to the locations of the points in the map.
  - While the original algorithm uses the Euclidean distance between objects as the base of its similarity metric, this can be changed as appropriate.

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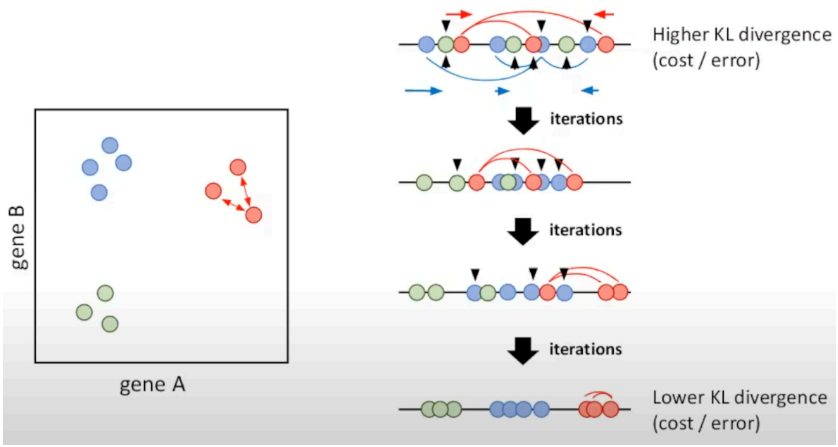
t-SNE

- **t-SNE:**



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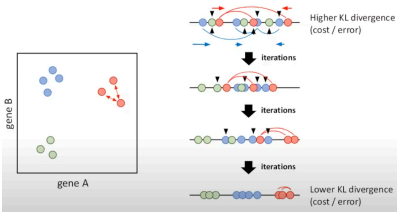
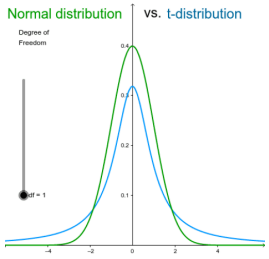
t-SNE

- **t-SNE:**
  - Optimizing the KL divergence is a measure of how one probability distribution is different from a second, reference probability distribution





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t-SNE

- **t-SNE:**
  - t-SNE has been used for **visualization in a wide range of applications**, including genomics, computer security research, natural language processing, music analysis, cancer research, bioinformatics, etc
  - While t-SNE plots often seem to display clusters, **the visual clusters can be influenced strongly by the chosen parameterization** and therefore a good understanding of the parameters for t-SNE is necessary.
  - Interactive exploration may thus be necessary to choose parameters and validate results.

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t-SNE

- **t-SNE:**
  - Perplexity is the main t-SNE parameter, "perplexity,"
    - Basically defines how to balance attention between local and global aspects of your data.
    - Perplexity is a measure for information that is defined as 2 to the power of the Shannon entropy.
    - In t-SNE, the perplexity may be viewed as a knob that sets the number of effective nearest neighbors.
    - It is comparable with the number of nearest neighbors k that is employed in many manifold learners.
    - The original paper says, "The performance of SNE is fairly robust to changes in the perplexity, and typical values are between 5 and 50."

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t-SNE

- **t-SNE:**
  - Perplexity is the main t-SNE parameter, "perplexity,"

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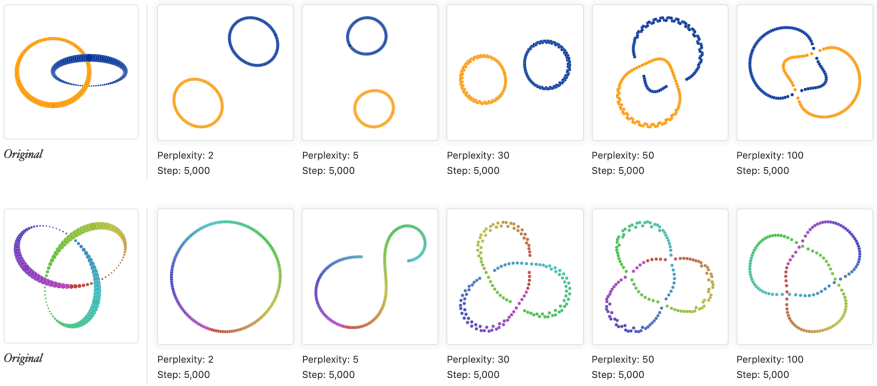
t-SNE

- **t-SNE:**
  - Perplexity is the main t-SNE parameter, "perplexity,"



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Uniform Manifold Approximation and Projection

UMAP

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UMAP

- **UMAP:**
  - Uniform Manifold Approximation and Projection (UMAP) is a dimension reduction technique that can be used for visualisation similarly to t-SNE.
  - The algorithm is founded on three assumptions about the data
    - The data is uniformly distributed on Riemannian manifold (a topological space that locally resembles Euclidean space near each point);
    - The manifold is locally connected.
    - From these assumptions it is possible to model the manifold with a fuzzy topological structure. The embedding is found by searching for a low dimensional projection of the data that has the closest possible equivalent fuzzy topological structure.
    - For a more detailed explanation see https://youtu.be/nq6iPZVUxZU

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UMAP

- **UMAP:**
  - Uniform Manifold Approximation and Projection (UMAP) is a dimension reduction technique that can be used for visualisation similarly to t-SNE.
  - Two phases in the UMAP algorithm
    - The first phase consists of constructing a fuzzy topological representation in the original space;
    - The second phase is simply optimizing (through stochastic gradient descent) the low dimensional representation to have as close a fuzzy topological representation as possible as measured by cross entropy.

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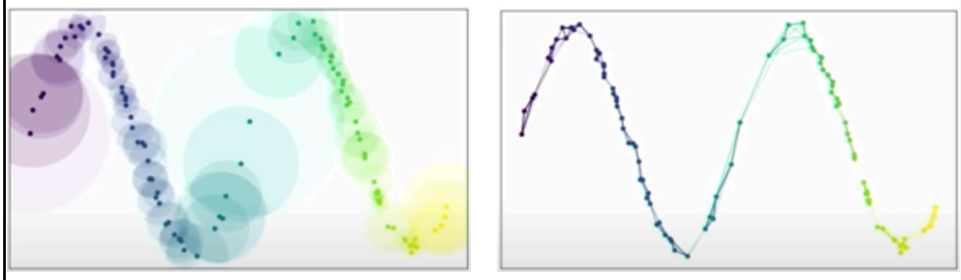
UMAP

- **UMAP:**
  - The first phase consists of constructing a fuzzy topological representation;



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UMAP

- **UMAP:**
  - The second phase is simply optimizing (through stochastic gradient descent) the low dimensional representation to have as close a fuzzy topological representation as possible as measured by cross entropy.

Get the clumps right

$$\sum_{a \in A} \mu(a) \log\left(\frac{\mu(a)}{\nu(a)}\right) + (1-\mu(a)) \log\left(\frac{1-\mu(a)}{1-\nu(a)}\right)$$

Get the gaps right

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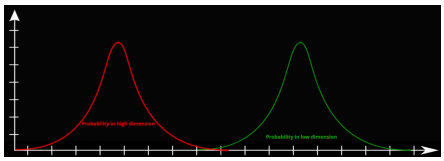
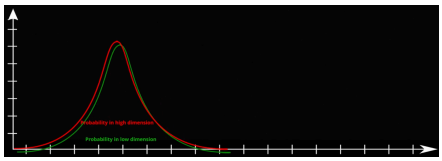
UMAP

- **UMAP:**
  - The second phase is simply optimizing (through stochastic gradient descent) the low dimensional representation to have as close a fuzzy topological representation as possible as measured by cross entropy.





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UMAP

- **UMAP:**
  - Uniform Manifold Approximation and Projection (UMAP) is a dimension reduction technique that can be used for visualisation similarly to t-SNE.
  - Parameters
    - Number of nearest neighbors - controls how UMAP balances local versus global structure in the data;
    - Minimum distance - controls how tightly UMAP is allowed to pack points together. It provides the minimum distance apart that points are allowed to be in the low dimensional representation

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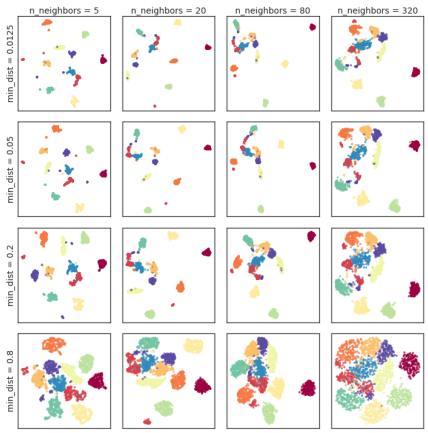
UMAP

- **UMAP:**



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Comparison Between the 3 Methods

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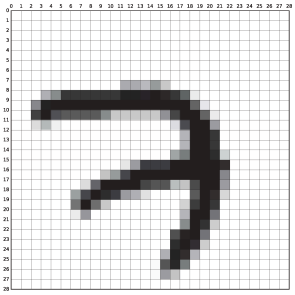
Multidimensionality Visualization

- **Mnist Digits:**
  - 28x28 image (784 dimensions)
  - grayscale images of handwritten single digits
  - 60,000 examples, and a test set of 10,000 examples



(a) MNIST sample belonging to the digit '7'.

(b) 100 samples from the MNIST training set.

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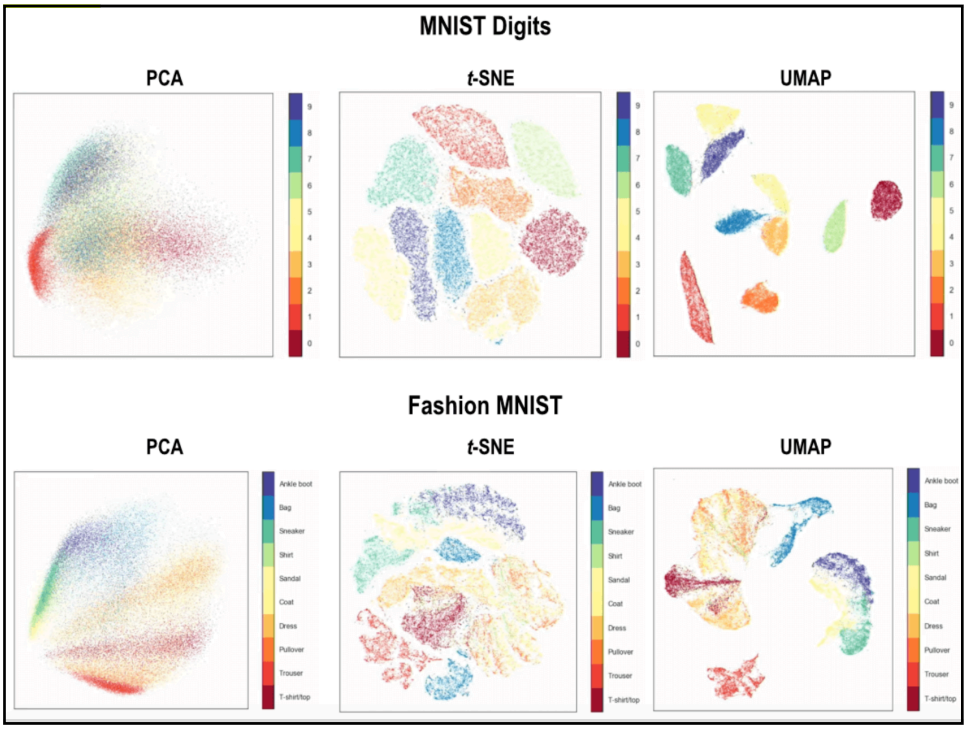
Multidimensionality Visualization

- **Mnist Fashion:**
  - 28x28 image (784 dimensions)
  - grayscale images of handwritten single digits
  - The dataset has 60,000 images



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Multidimensionality Visualization

- **Mnist Digits:**
  - 3D woolly mammoth skeleton
  - https://pair-code.github.io/understanding-umap/

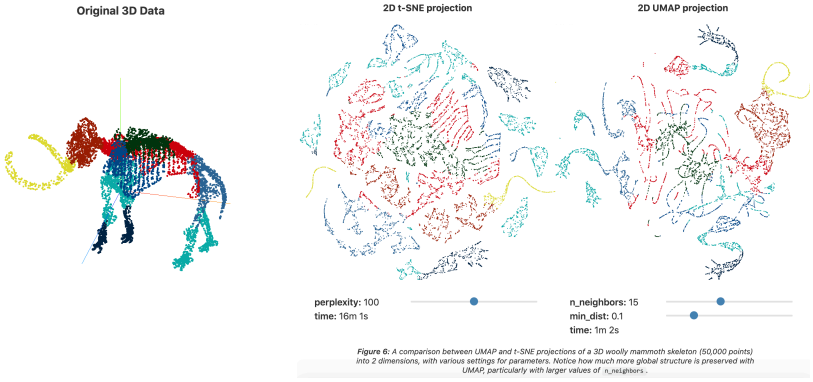

Figure 6: A comparison between UMAP and t-SNE projections of a 3D woolly mammoth skeleton (50,000 points) into 2 dimensions, with various settings for parameters. Notice how much more global structure is preserved with UMAP, particularly with larger values of `n_neighbors`.

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UMAP

- **UMAP:**

	t-SNE	UMAP
COIL20	20 seconds	7 seconds
MNIST	22 minutes	98 seconds
Fashion MNIST	15 minutes	78 seconds
GoogleNews	4.5 hours	14 minutes

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Questions?

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