DATA MINING 2
Dimensionality Reduction

Riccardo Guidotti

a.a. 2022/2023

UNIVERSITÀ DI PISA

Dimensionality Reduction

- Dimensionality reduction is the process of reducing the number of random variables under consideration by obtaining a set of principal variables.
- Approaches can be divided into **feature selection** and **feature projection**.

X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9	X_{10}
1.1	10	0.3	0.5	A	1	C	15	1.3	a
1.2	12	0.3	0.7	A	0	D	19	1.8	P
…	…	…	…	…	…	…	…	…	…

X_A	X_B
1.8	5.4
1.9	6.3
…	…

Feature Selection

- Select a subset of the features according to different strategies:
  - the **filter** strategy (e.g. information gain),
  - the **wrapper** strategy (e.g. search guided by accuracy),
  - the **embedded** strategy (selected features add or are removed while building the model based on prediction errors).

- Classification and/or regression or can be done in the reduced space more accurately than in the original space.

Feature Selection

- **Variance Threshold.** It removes all features whose variance does not meet some threshold. By default, it removes all zero-variance features, i.e. features that have the same value in all samples.
- **Univariate Feature Selection.** It selects the best features based on univariate statistical tests. For instance, it removes all but the *k* highest scoring features. An example of statistical test is the ANOVA F-value between label/feature.
- F-value = $$\sum_{i=1}^{K} n_i(\bar{Y}_{i\cdot} - \bar{Y})^2/(K-1) / \sum_{i=1}^{K}\sum_{j=1}^{n_i}(Y_{ij} - \bar{Y}_{i\cdot})^2/(N-K)$$
- where Y_i denotes the sample mean in the ith group, n_i is the number of observations in the ith group, denotes the overall mean of the data, Y_{ij} is the jth observation in the ith out of *K* groups, *K* denotes the number of groups, *N* the overall sample size.
- F-value is large if the numerator is large, which is unlikely to happen if the population means of the groups all have the same value.

Recursive Feature Elimination (RFE)

- Given an external estimator that assigns weights to features (e.g., the coefficients of a linear model, or feature importance of decision tree), RFE selects features by recursively considering smaller and smaller sets of features.
- First, the estimator is trained on the initial set of features and the importance of each feature is obtained.
- Then, the least important features are pruned from current set of features.
- That procedure is recursively repeated on the pruned set until the desired number of features to select is eventually reached.

Feature Projection (a.k.a Feature Extraction)

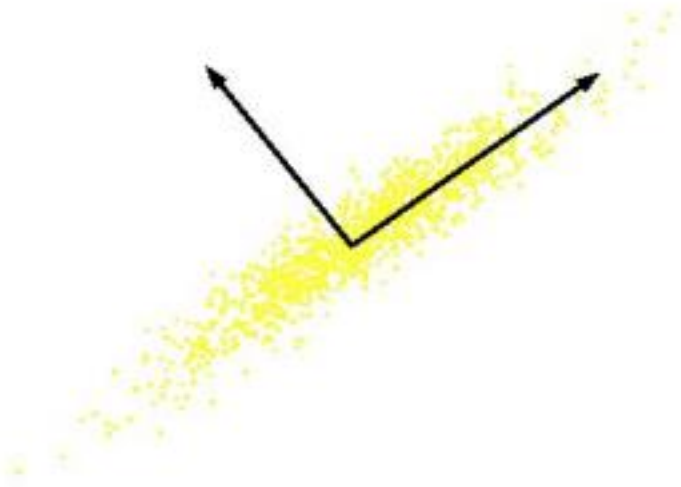
- It transforms the data in the high-dimensional space to a space of fewer dimensions.
- The data transformation may be linear, or nonlinear.
- Approaches:
  - Principal Component Analysis (PCA)
  - Non-negative matrix factorization (NMF)
  - Linear Discriminant Analysis (LDA)
  - Multidimensional Scaling
    - Sammon
    - IsoMap
    - t-SNE
  - Autoencoder

Feature Projection (a.k.a Feature Extraction)

- It transforms the data in the high-dimensional space to a space of fewer dimensions.
- The data transformation may be linear, or nonlinear.
- Approaches:
  - Principal Component Analysis (PCA)
  - Non-negative matrix factorization (NMF)
  - Linear Discriminant Analysis (LDA)
  - Multidimensional Scaling
    - Sammon
    - IsoMap
    - t-SNE
  - Autoencoder

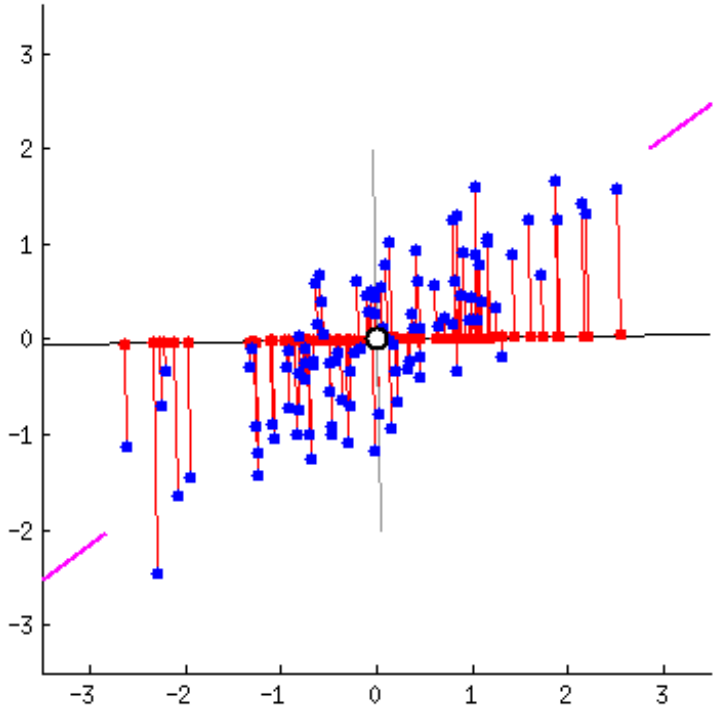
Principal Component Analysis (PCA)

- The goal of PCA is to **find a new set of dimensions** (attributes or features) that better captures the variability of the data.
- The **first dimension** is chosen to capture as **much of the variability as possible**.
- The **second dimension** is orthogonal to the first and, subject to that constraint, captures as much of the **remaining variability** as possible, and so on.
- It is a **linear transformation** that chooses a new coordinate system for the data set



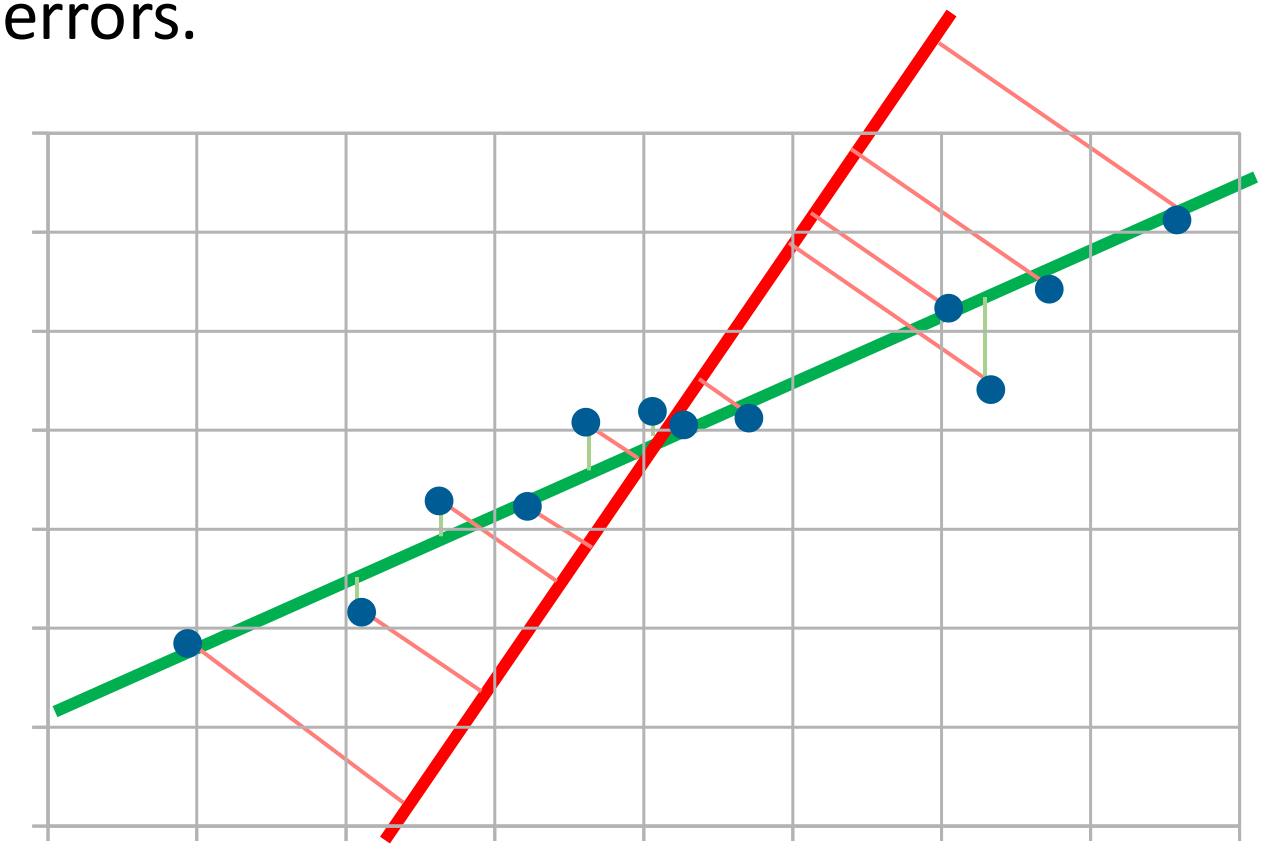
How to construct PC?

- The first principal component accounts for the **largest possible variance** in the data set.
- I want to fix the black line such that the spread on them of the red points, i.e., the original points projected on the black line, is maximised.
- The second principal component is calculated in the same way, with the condition that **it is uncorrelated with the first principal component** and that it accounts for the **next highest variance.**



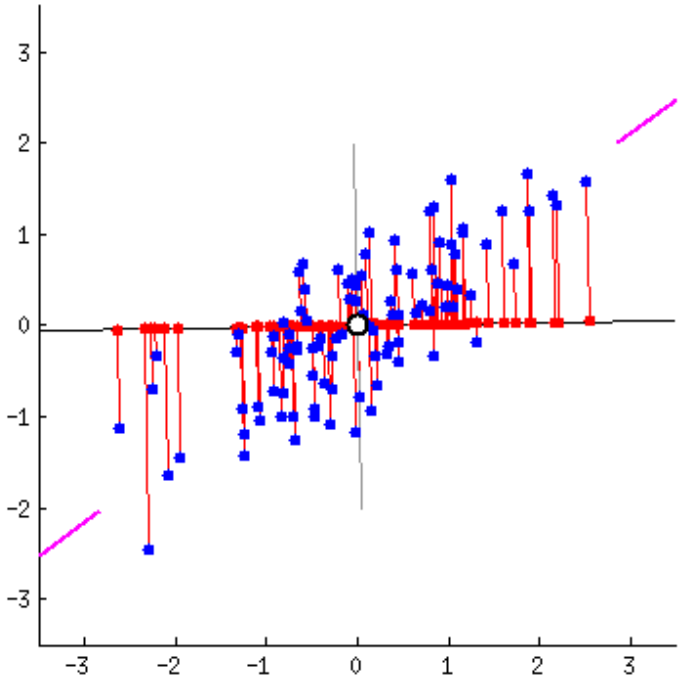
PCA – Conceptual Algorithm

- Find a line such that, when the data is projected onto that line, it has the maximum variance; minimize the sum-of-squares of the projection errors.



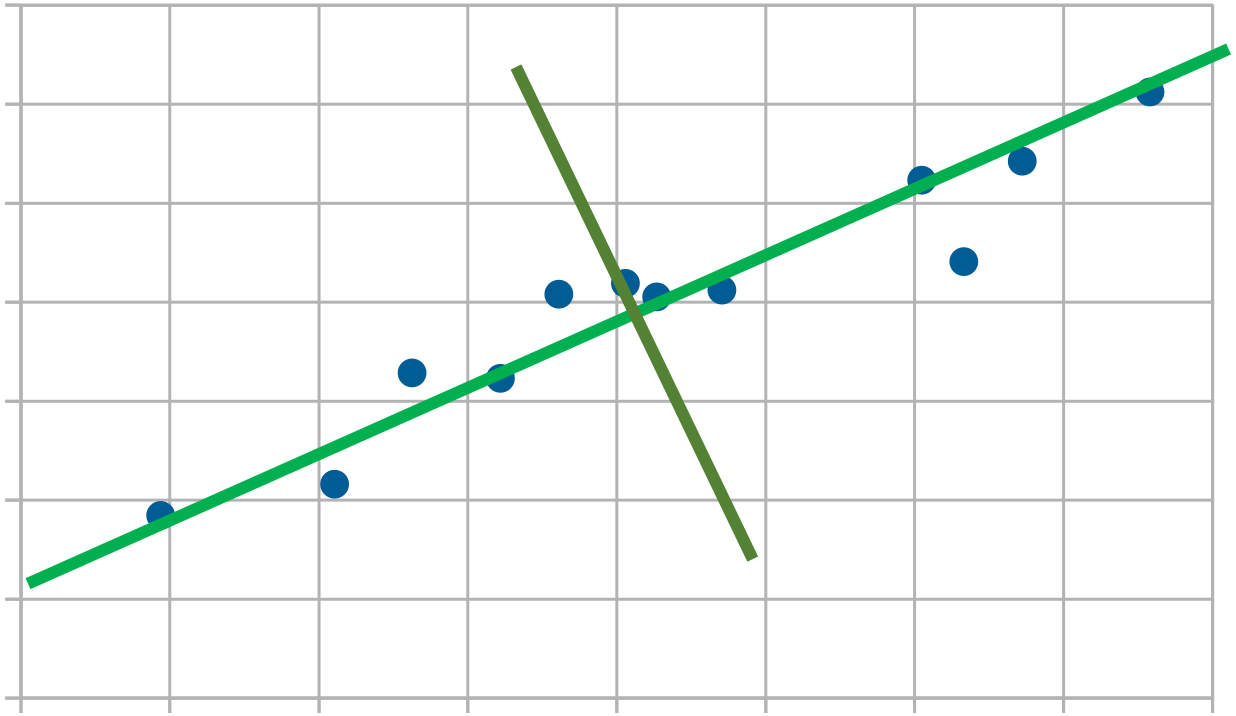
PCA – Conceptual Algorithm

- Find a line such that, when the data is projected onto that line, it has the maximum variance; minimize the sum-of-squares of the projection errors.



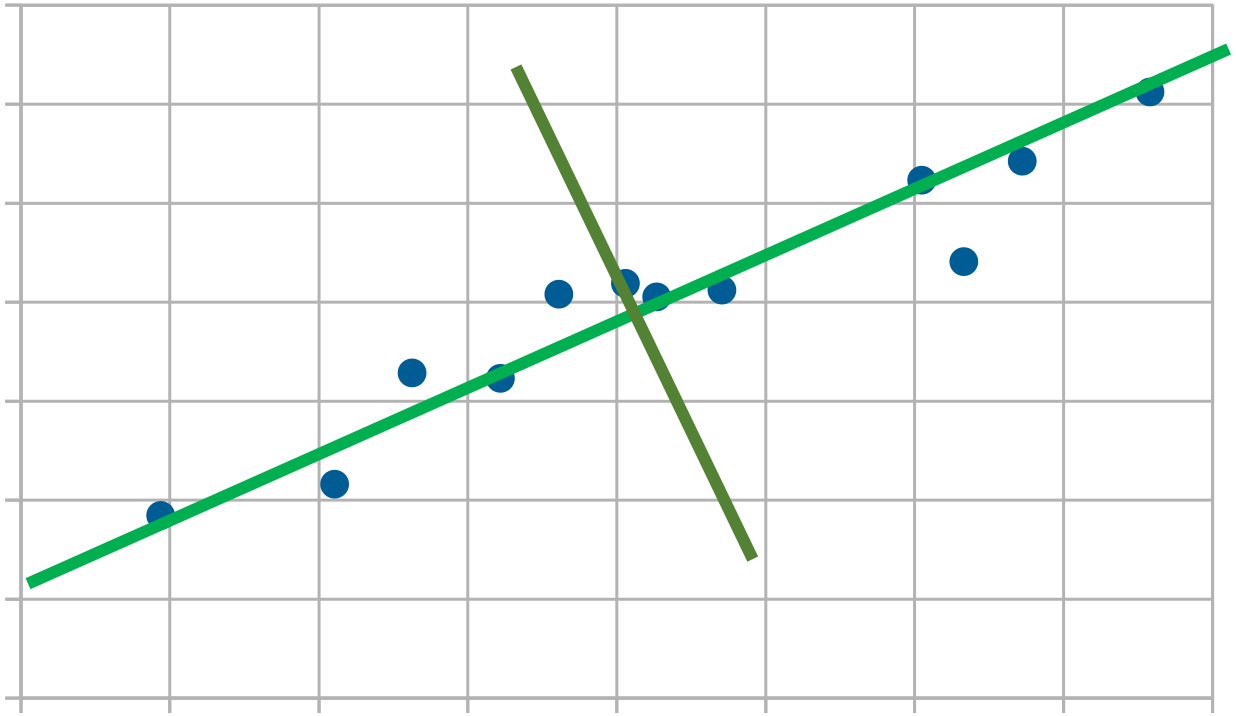
PCA – Conceptual Algorithm

- Find a second line, orthogonal to the first, that has maximum projected variance.



PCA – Conceptual Algorithm

- Repeat until have *k* orthogonal lines.
- The projected position of a point on these lines gives the coordinates in the k-dimensional reduced space.



Background: Covariance, Eigenvalue and Eigenvectors

- The covariance of two attributes is a measure of how strongly the attributes vary together.

$$\text{covariance}(\mathbf{x}, \mathbf{y}) = s_{xy} = \frac{1}{n-1}\sum_{k=1}^{n}(x_k - \overline{x})(y_k - \overline{y})$$

- Eigenvector of matrix *X*: a vector *v* such that Xv=λv
- λ: eigenvalue of eigenvector v
- A square symmetric matrix *X* of rank *r*, has *r* orthonormal eigenvectors v_1, v_2,…, v_r with eigenvalues λ_1, λ_2, …, λ_r.
- Eigenvectors define an orthonormal basis for the column space of *X*

Background: Covariance key factor in PCA

- Variance and Covariance are a measure of the "**spread**" of a set of points around their **center of mass** (mean)
- **Variance** – measure of the deviation from the mean for points in one dimension e.g. heights
- **Covariance** as a measure of how much each of the dimensions vary from the mean with respect to each other.
- Covariance is measured between 2 dimensions to see if there is a relationship between the 2 dimensions
  - e.g. number of hours studied & marks obtained.
- The covariance between one dimension and itself is the variance

Steps in PCA

- **Step 1:** Standardize the dataset.
- **Step 2:** Calculate the mean value of the data of every dimension
- **Step 3:** Calculate the covariance matrix of all pairs of attributes
  - Given matrix of data *X*, remove the mean of each column from the column vectors to get the centered matrix *C*
  - The matrix $\Sigma = C^T C$ is the covariance matrix of the row vectors of *X*.
- **Step 4:** Calculate eigenvalues and eigenvectors of Σ and pick the *k* with largest eigenvalues
  - Methods: power iteration method, Singular Value Decomposition
  - Eigenvector with largest eigenvalue λ_1 is the 1st PC
  - Eigenvector with k^{th} largest eigenvalue λ_k is the k^{th} PC
  - $\lambda_k / \Sigma_i \lambda_i$ is the proportion of variance captured by the k^{th} PC
- **Step 5:** Transform the original dataset X

Compute Covariance Matrix

- The covariance of two attributes is a measure of how strongly the attributes vary together.

$$\text{covariance}(\mathbf{x}, \mathbf{y}) = s_{xy} = \frac{1}{n-1}\sum_{k=1}^{n}(x_k - \overline{x})(y_k - \overline{y})$$

- PCA calculates the covariance matrix of all pairs of attributes
- Given matrix *X* of data
  - remove the mean of each column from the column vectors to get the centered matrix C (standardization).
  - Compute the matrix $V = C^T C$, i.e., the covariance matrix of the row vectors of C.

Covariance Matrix

- Diagonal is the variances of x, y and z
- cov(x,y) = cov(y,x) hence matrix is symmetrical about the diagonal

    - Suppose we have 3 attributes. The covariance matrix $V = C^T C$ is as follows:

$$\begin{bmatrix} Cov(x,x) & Cov(x,y) & Cov(x,z) \\ Cov(y,x) & Cov(y,y) & Cov(y,z) \\ Cov(z,x) & Cov(z,y) & Cov(z,z) \end{bmatrix}$$

Meaning of Covariance

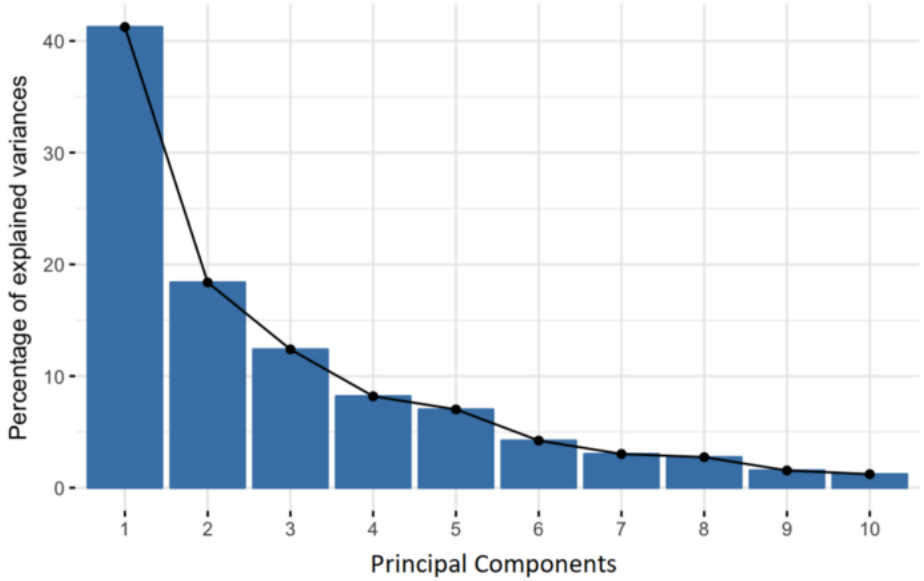
- Exact value is not as important as it's sign.
- A positive value of covariance indicates both dimensions increase or decrease together
  - e.g. as the number of hours studied increases, the marks in that subject increase.
- A negative value indicates while one increases the other decreases, or vice-versa
- If covariance is zero: the two dimensions are independent of each other
  - e.g. heights of students vs the marks obtained in a subject

Identify the Principal Components

- Identify the PC of data by computing the eigenvectors and eigenvalues from the covariance matrix.
- What are Principal Components?
  - New variables that are constructed as linear combinations of the initial variables
  - These new variable are uncorrelated
  - Most of the information within the initial variables is squeezed or compressed into the first components
  - PCA tries to put maximum possible information in the first component, then maximum remaining information in the second and so on

Identify the Principal Components

Given 10-dimensional data you get 10 principal components but only the first PCs capture most of the variability of the data



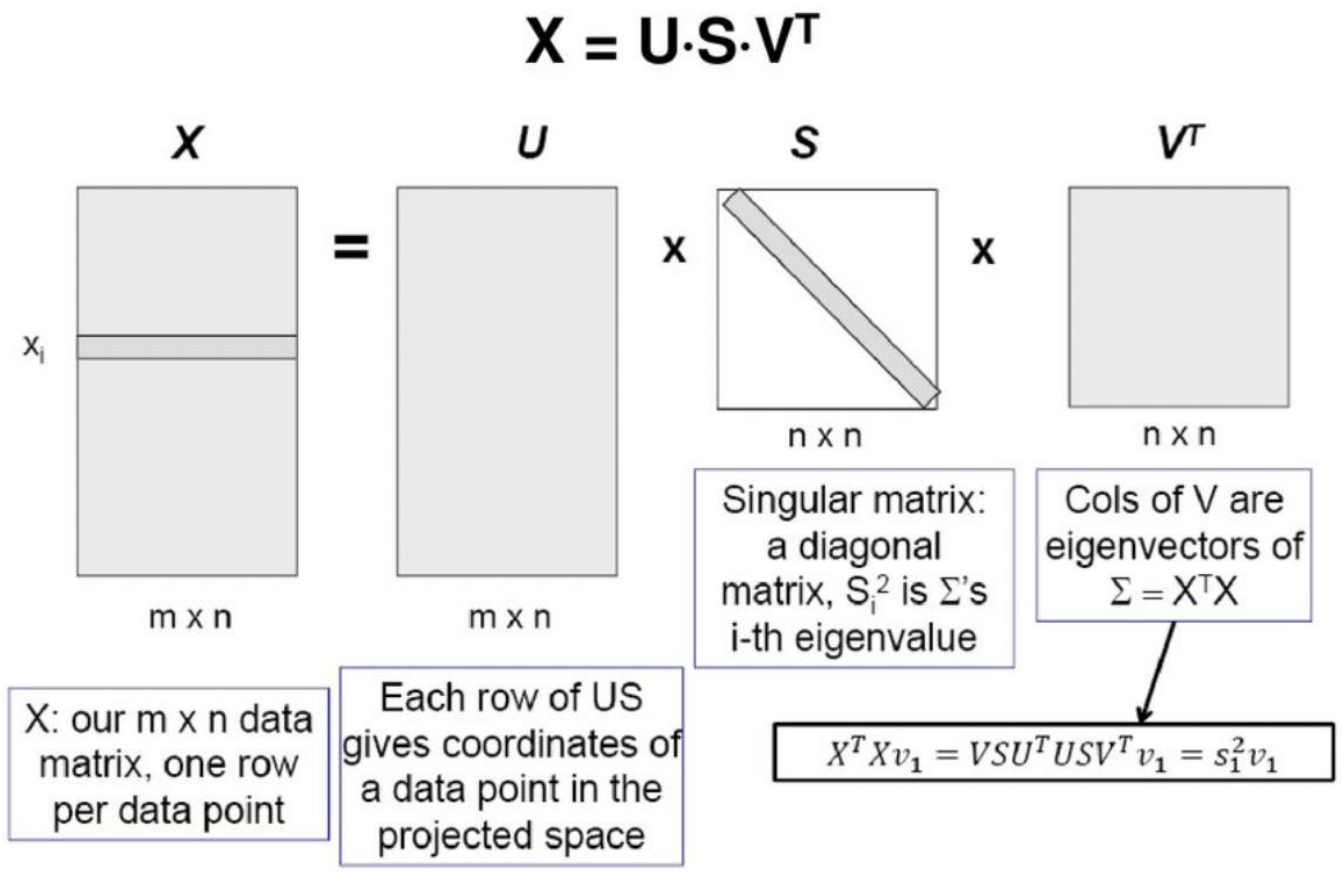
Discarding the components with low information and considering the remaining components as your new variables.

PCA via SVD

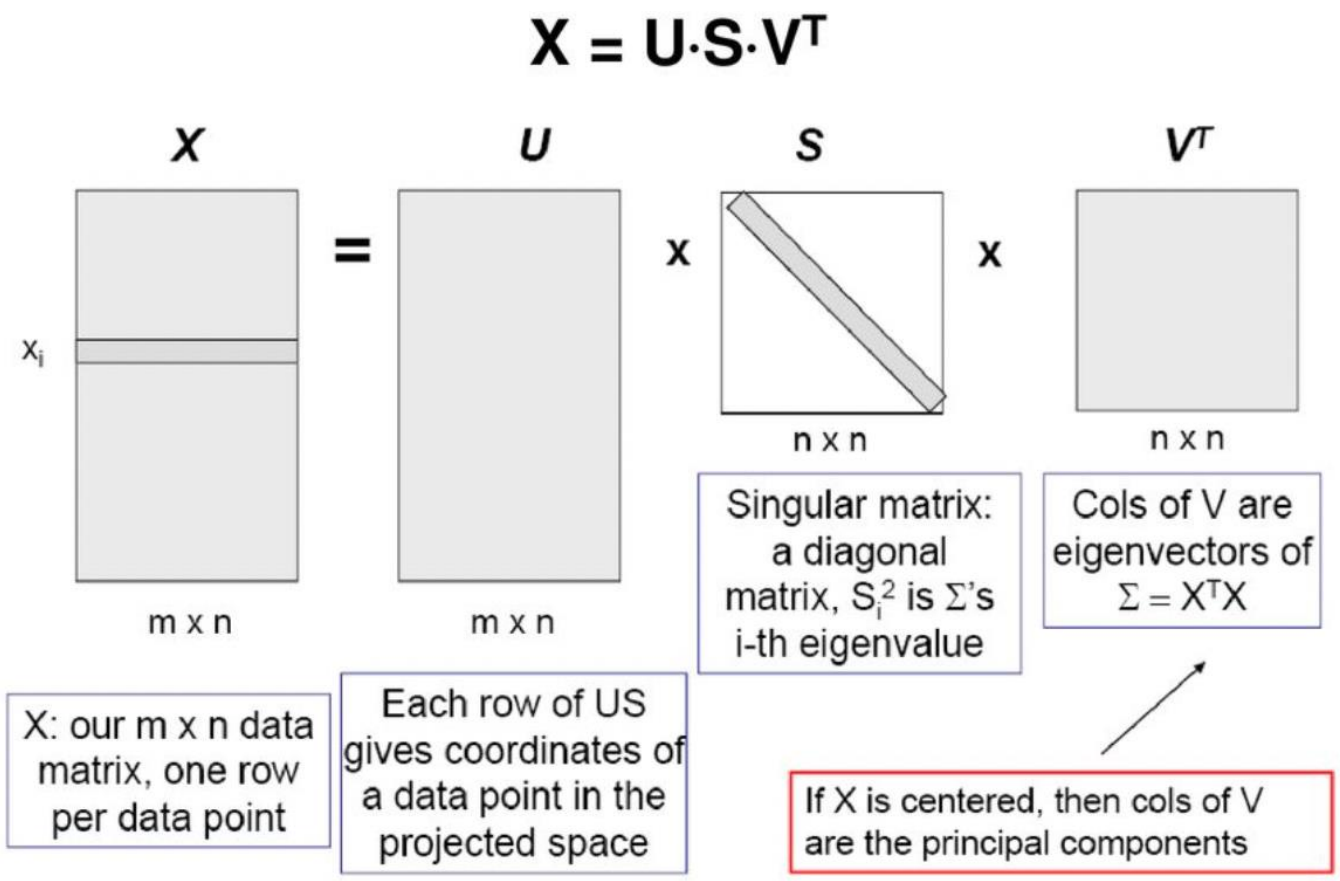
- Create mean-centered data matrix X
- Solve SVD: $X = USV^T$
- Columns of V are the eigenvectors of Σ sorted from largest to smallest eigenvalues.

- Limits of PCA:
  - Limited to linear projections

Singular Value Decomposition - SVD

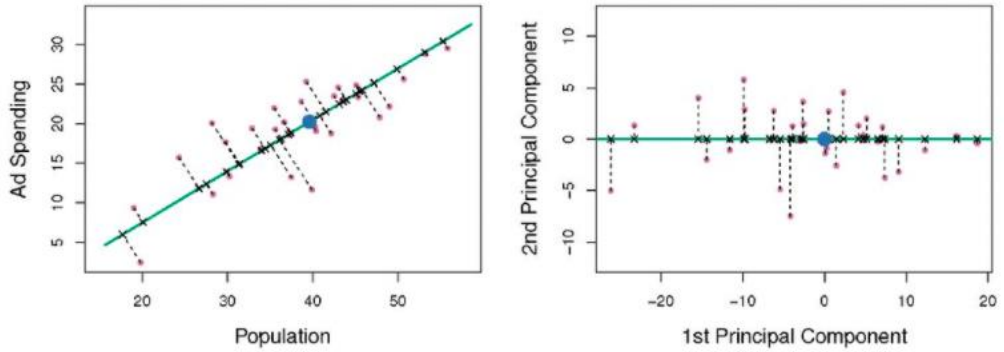


Singular Value Decomposition - SVD



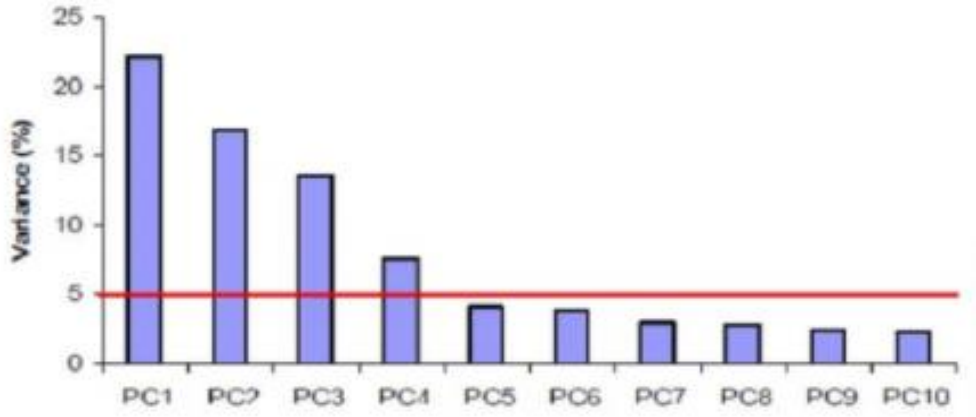
Applying the PCA

- The full set of PCs comprise a new orthogonal basis for feature space, whose axes are aligned with the maximum variances of original data.
- Projection of original data into first *k* PCs gives a reduced dimensionality representation of the data.
- Transforming reduced dimensionality projection back into original space gives a reduced dimensionality reconstruction of the data.
- Reconstruction will have some error.



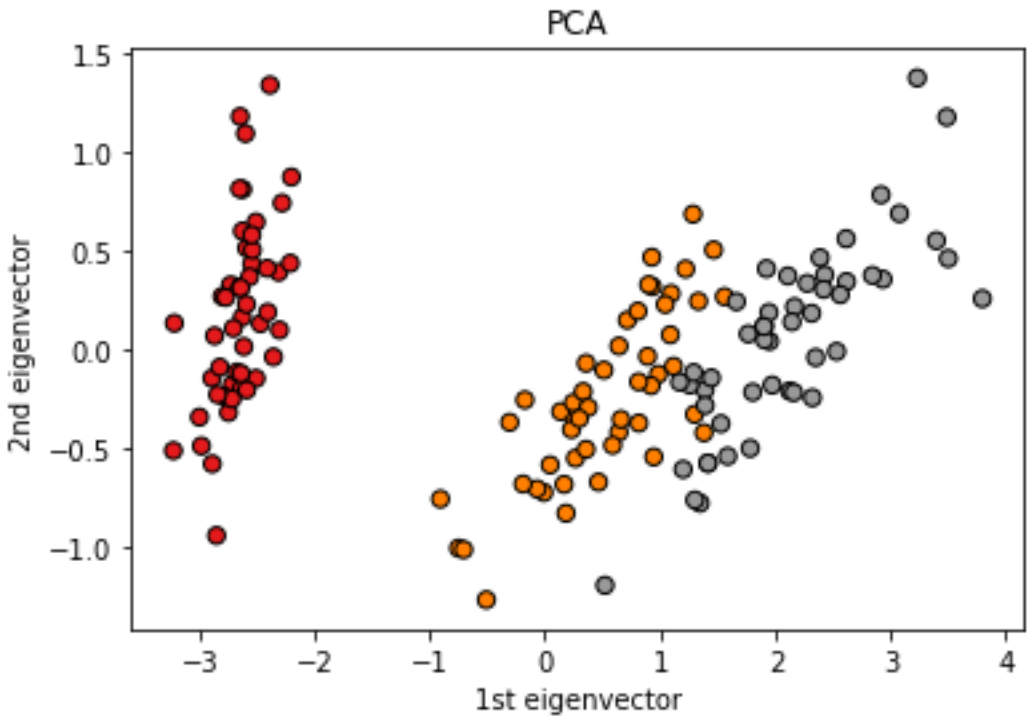
Select the dimension *k*

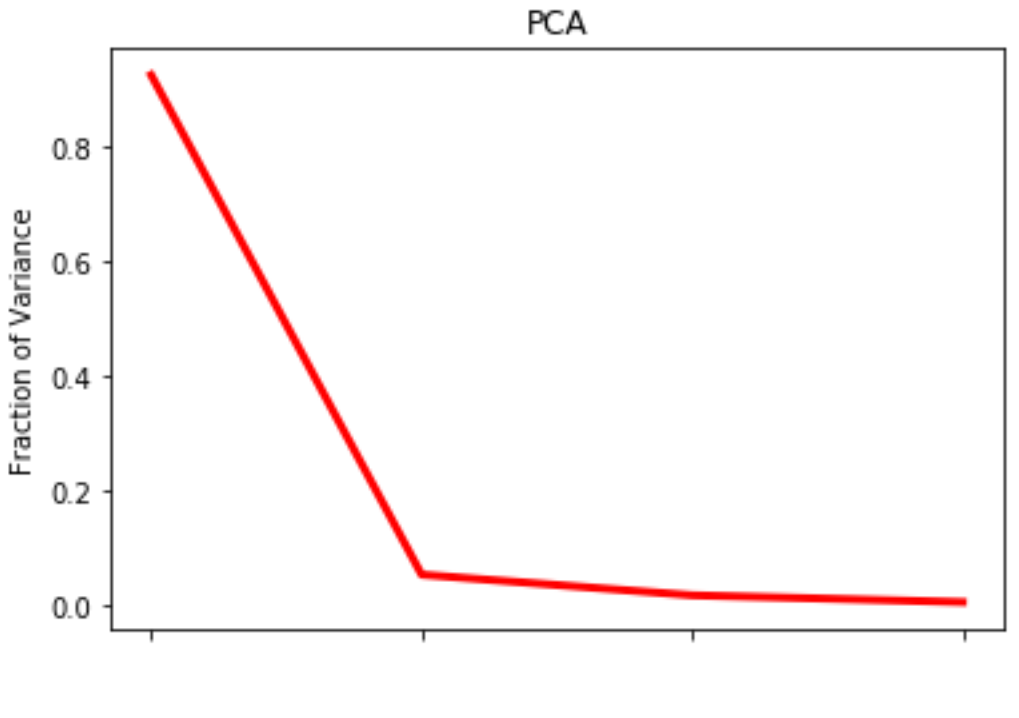
- Rank eigenvalues in decreasing order.
- Select eigenvectors that retain a fixed percentage of variance (e.g., at least a minimum threshold.



Example

- Iris Dataset



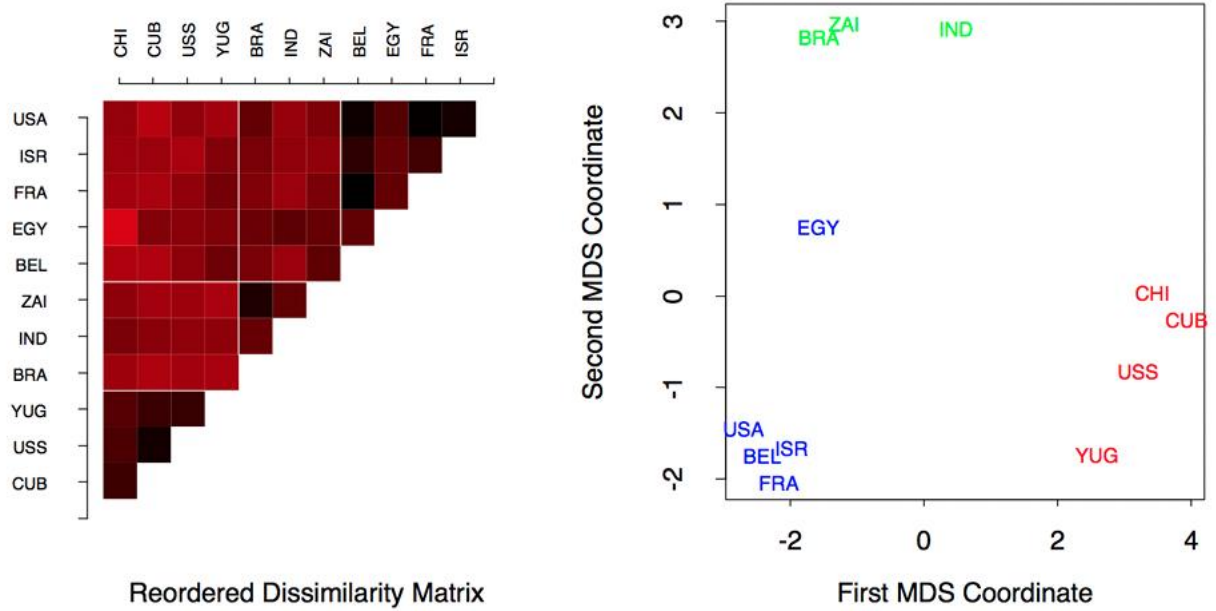


Random Subspace Projection

- High-dimensional data is projected into low-dimensional space using a random matrix whose columns have unit length.
- No attempt to optimize criterion.
- Preserve structure of data (e.g. distances)
- Computationally cheap.

Multi-Dimensional Scaling (MDS)

- Given a pairwise dissimilarity matrix (no need to be a metric), the goal of MDS is to learn a mapping of data into a lower dimensionality such that the relative distances are preserved.
- If two points are close in the feature space, it should be close in the latent factor space.



MDS methods

- MDS is a family of different algorithms designed to map data into a very low configuration, e.g., k=2 or k=3.
- MDS methods include
  - Classical MDS
  - Metric MDS
  - Non-metric MDS
- MDS cannot be inverted

Distance, dissimilarity and similarity

- Distance, dissimilarity and similarity (or proximity) are defined for any pair of objects in any space. In mathematics, a distance function (that gives a distance between two objects) is also called *metric*, satisfying:
  - $d(x, y) \geq 0$,
  - $d(x, y) = iff\ x = y$,
  - $d(x, y) = d(y, x)$
  - $d(x, z) \leq d(x, y) + d(y, z)$
- If the last condition does not hold, than *d* is a distance function but it is not a metric.

MDS – Conceptual Algorithm

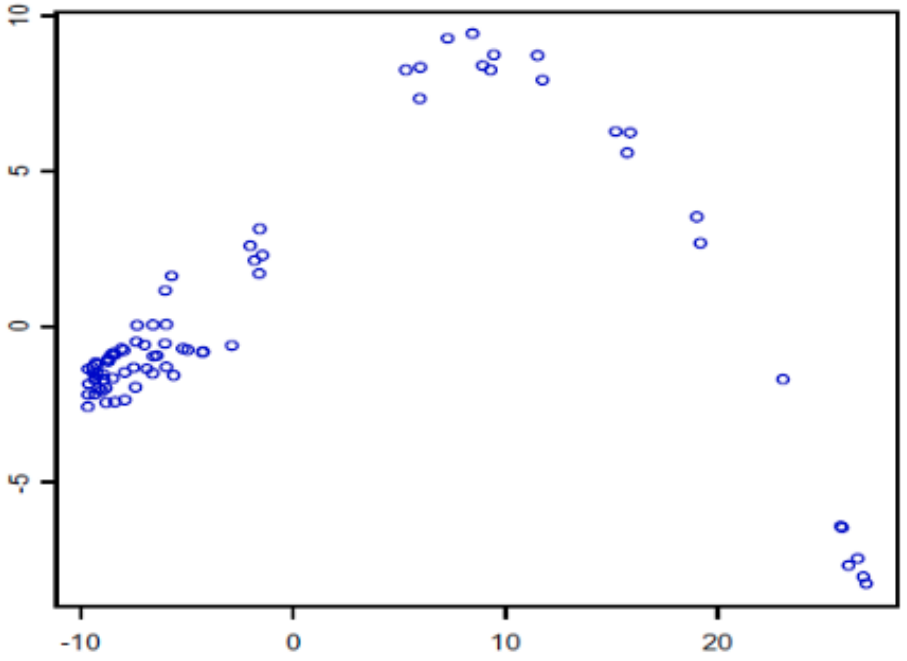
- Given a pairwise dissimilarity matrix *D* and the dimensionality *k,* find a mapping such that $d_{ij} = ||x_i - x_j||$ for all points in *D*.
- Usually, a *gradient descent* approach is adopted to solve an optimization problem that aims at minimizing the function
- $J(x) = \sum_i^n \sum_j^n d_1(d_{ij}, d_2(x_i, x_j))$
- Depending on the distances adopted to calculate *D* and the distance function used for d_1 and d_2 the approach returns a different result.
- The Classic MDS adopts the Euclidean distance for every calculus.
- Metric-MDM adopts metrics as distances
- Non metric-MDS deals with ranks of distances instead of their values

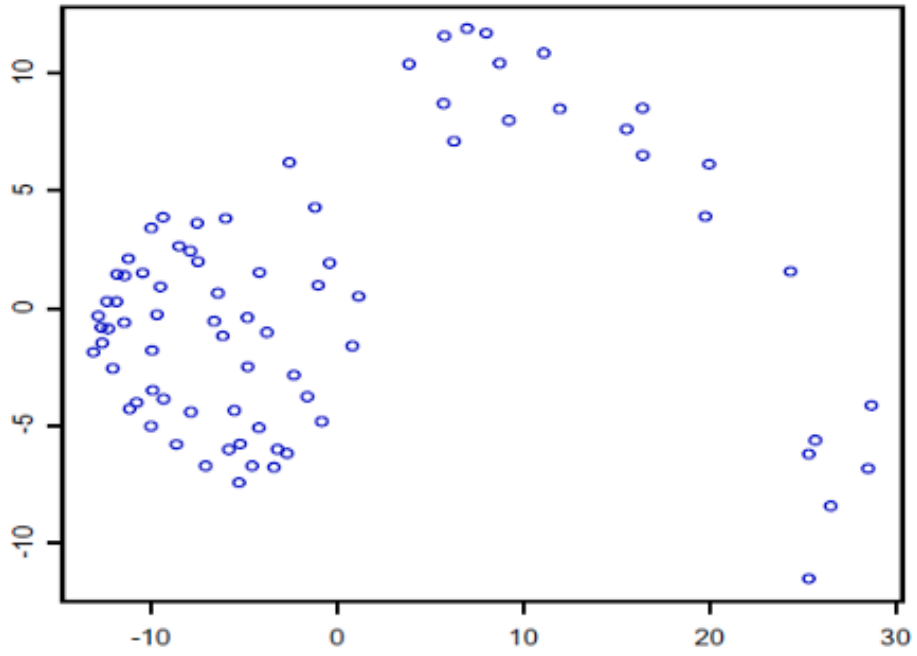
Sammon Mapping

- Sammon mapping is a generalization of the usual metric MDS.
- It introduces a weighting system that normalizes the squared-errors in pairwise distances by using the distance in the original space.
- $J(x) = \sum_i^n \sum_j^n d_1(d_{ij}, d_2(x_i, x_j))/d_{ij}$
- As a result, Sammon mapping preserves the small d_{ij}, giving them a greater degree of importance in the fitting procedure than for larger values of d_{ij}

Classic-MDS vs Sammon Mapping

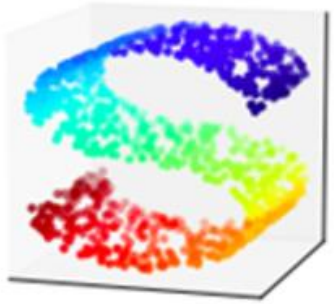
- Sammon mapping better preserves inter-distances for smaller dissimilarities, while proportionally squeezes the inter-distances for larger dissimilarities.

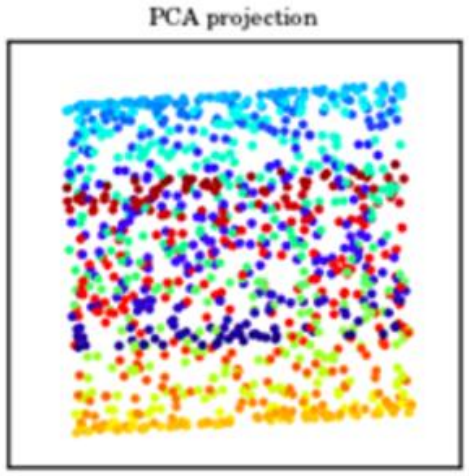


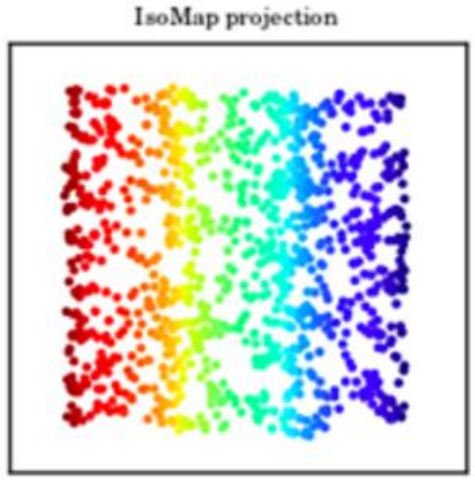


Isometric Feature Mapping (IsoMap)

- Preserves the intrinsic geometry of the data
- Uses the geodesic manifold distances between all pairs.
- It is a MDS method.
- IsoMap Handles non-linear manifold







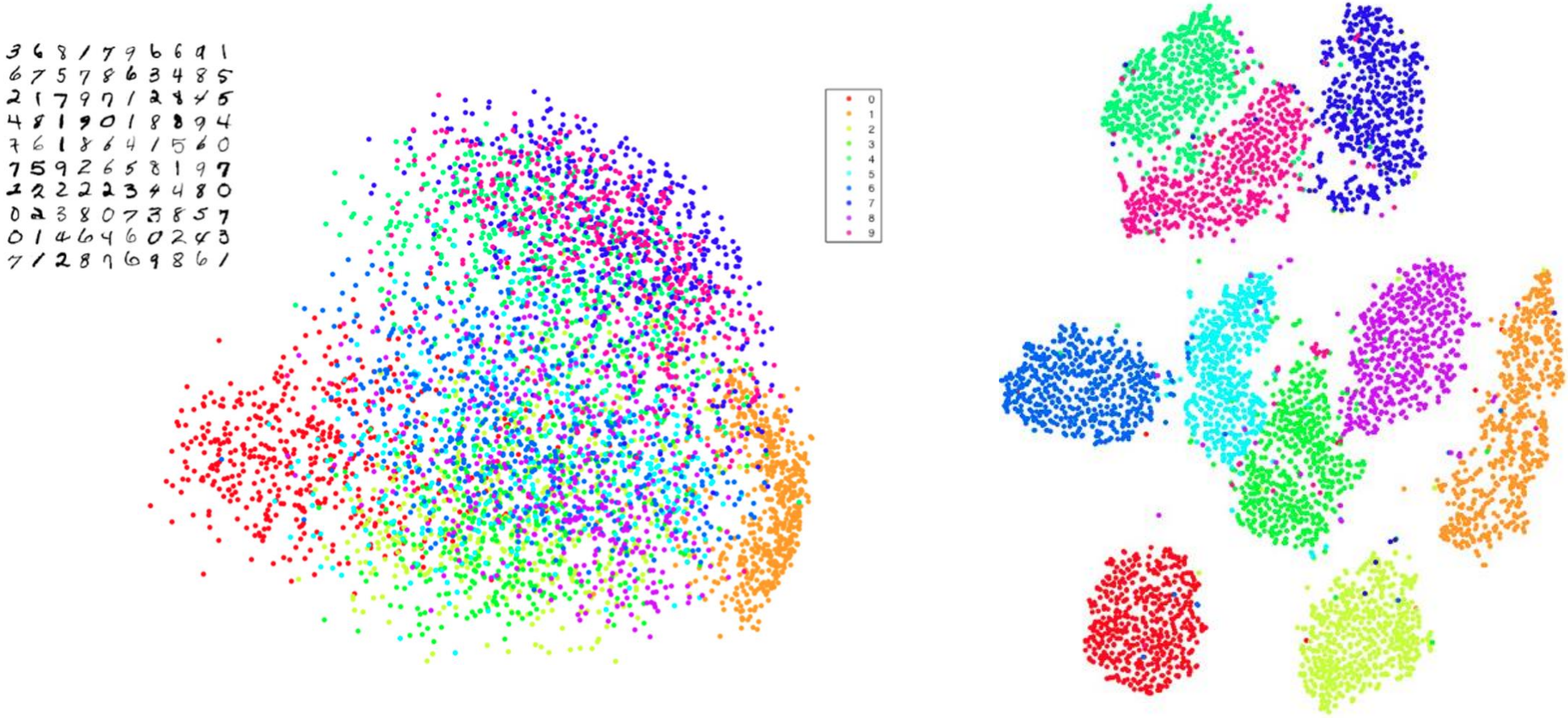
IsoMap Algorithm

- Step 1
  - Determine neighboring points within a fixed radius based on the input space distance (Euclidean)
  - These neighborhood relations are represented as weighted graph *G* over the data points.
- Step 2
  - Estimate the geodesic distance between all pairs of points on the manifold by computing their shortest path distances on the graph *G*
- Step 3
  - Construct an embedding of the data in a *k* dimensional Euclidean space that best preserves the manifold geometry

t-Distributed Stochastic Neighbor Embedding (t-SNE)

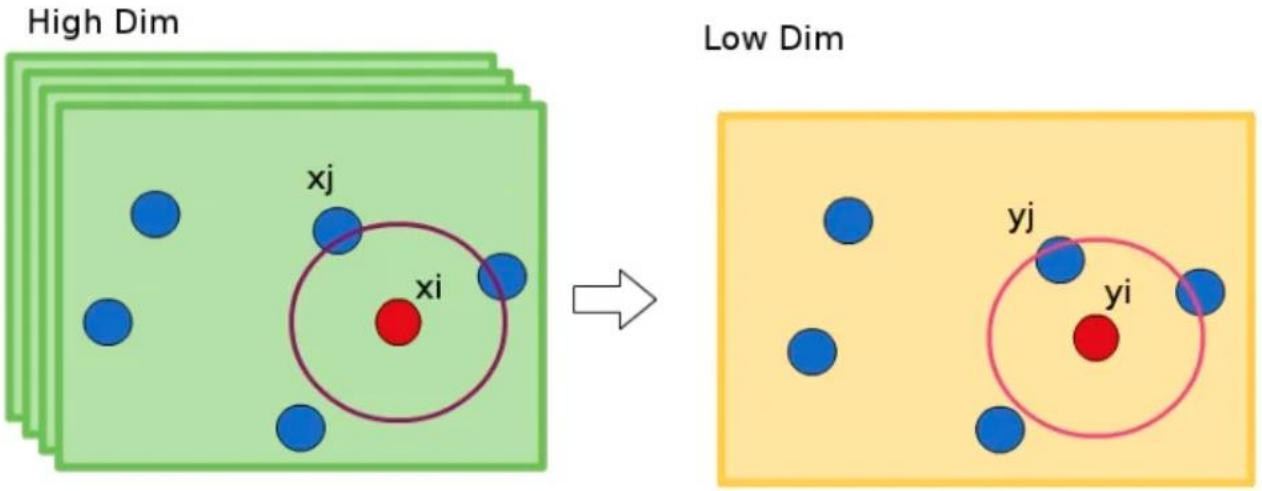
- PCA tries to find a global structure
  - Low dimensional subspace
  - Can lead to local inconsistencies
    - Far away points can become neighbors
- t-SNE tries to preserve local structure
  - Local dimensional neighborhood should be the same as original neighborhood
  - Distance Preservation
  - Neighbor Preservation
- Unlike PCA almost only used for visualization

PCA vs t-SNE



SNE Intuition

- Measure pairwise similarities between high-dimensional and low-dimensional objects.



Stochastic Neighbor Embedding (SNE)

- Encode high dimensional neighborhood information as a distribution
- Intuition: Random walk between data points.
  - High probability to jump to a close point
- Find low dimensional points such that their neighborhood distribution is similar.
- How do you measure distance between distributions?
  - Most common measure: KL divergence

Neighborhood Distributions

- Consider the neighborhood around an input data point x_i
- Imagine that we have a Gaussian distribution centered around x_i
- Then the probability that x_i chooses some other datapoint x_j as its neighbor is in proportion with the density under this Gaussian
- A point closer to x_i will be more likely than one further away

Probabilities

- This $p_{j|i}$ probability is the probability that point x_i chooses x_j as its neighbor

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

- The parameter sigma sets the size of the neighborhood
  - Very low sigma -> all the probability is in the newest neighbor
  - Very high sima -> uniform weights
- We set sigma differently for each data point
- Results depend heavily on sigma as it defines the neighborhood we are trying to preserve
- The final distribution over pairs is symmetrized $p_{ij} = 1/2N(p_{i|j} + p_{j|i})$

Perplexity

- For each distribution $p_{j|i}$ depends on sigma we define the perplexity
  - $perp(p_{j|i}) = 2^{H(pj|i)}$ where $H(p) = - \Sigma\ p\ log(p)$ is the entropy
- If p is uniform over k elements perplexity is k
  - Smooth version of k in kNN
  - Low perplexity equals to small sigma
  - High perplexity equals to large sigma
  - Typically values of sigma between 5-50 work well
- Important parameter that can capture different scales in the data

SNE objective

- Given $x_1, \ldots, x_n \in R^m$ define the distribution p_{ij}
- Goal: find good embedding $y_1, .., y_n \in R^k$ *for* $k < m$
- How do we measure embedding quality?
- For points $y_1, .., y_n$ we can define distribution q similarly to the same (but not sigma and not symmetric)

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

- The idea is to optimize q to be close to p by minimizing the KL-divergence
- The embeddings $y_1, .., y_n$ are the parameters we are optimizing

KL-divergence

- Measures distance between two distributions, P and Q

$$C = \sum_i KL(P_i||Q_i) = \sum_i \sum_j p_{j|i} log \frac{p_{j|i}}{q_{j|i}}$$

- It is not a metric function as is not symmetric
- Based on the information theory intuition: if we are transmitting information distributed according to *p* then the optimal lossless compression will need to send on average *H(p)* bits
- Thus, *K(P||Q)* is the penalty for using a wrong distribution

Distances to Conditional Probabilities

- Converting the high-dimensional Euclidean distances into conditional probabilities that represent similarities
- Similarities of datapoints in High Dimension

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

- Similarity of datapoints in Low Dimension

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

- Cost function

$$C = \sum_i KL(P_i||Q_i) = \sum_i \sum_j p_{j|i} log \frac{p_{j|i}}{q_{j|i}}$$

- Minimize *C* using gradient descent

$$\frac{\partial C}{\partial y_i} = \sum_{j \neq i} (p_{j|i} - q_{j|i} + p_{i|j} - q_{i|j})(y_i - y_j)$$

SNE problems

- Not a convex problem! No guarantees, can use multiple restarts.
- Crowding problem
  - In high dim we have a lot of different neighbors
  - In 2 dimensions we have few neighbors at the same distance and far from each other
  - Thus, we do not have space to accommodate all neighbors

- t-SNE solution: change the Gaussian in Q to a heavy tailed distribution

$$q_{ij} = \frac{(1 + ||y_i - y_j||^2)^{-1}}{\sum_{k \neq l}(1 + ||y_k - y_l||^2)^{-1}}$$

Student-t Probability Density

Algorithm 1: Simple version of t-Distributed Stochastic Neighbor Embedding.

Data: data set $\mathcal{X} = \{x_1, x_2, \ldots, x_n\}$,
cost function parameters: perplexity *Perp*,
optimization parameters: number of iterations T, learning rate η, momentum $\alpha(t)$.
Result: low-dimensional data representation $\mathcal{Y}^{(T)} = \{y_1, y_2, \ldots, y_n\}$.
begin
  compute pairwise affinities $p_{j|i}$ with perplexity *Perp* (using Equation 1)
  set $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$
  sample initial solution $\mathcal{Y}^{(0)} = \{y_1, y_2, \ldots, y_n\}$ from $\mathcal{N}(0, 10^{-4}I)$
  for t=1 **to** T **do**
    compute low-dimensional affinities q_{ij} (using Equation 4)
    compute gradient $\frac{\delta C}{\delta \mathcal{Y}}$ (using Equation 5)
    set $\mathcal{Y}^{(t)} = \mathcal{Y}^{(t-1)} + \eta \frac{\delta C}{\delta \mathcal{Y}} + \alpha(t)\left(\mathcal{Y}^{(t-1)} - \mathcal{Y}^{(t-2)}\right)$
  end
end

The basic algorithm …

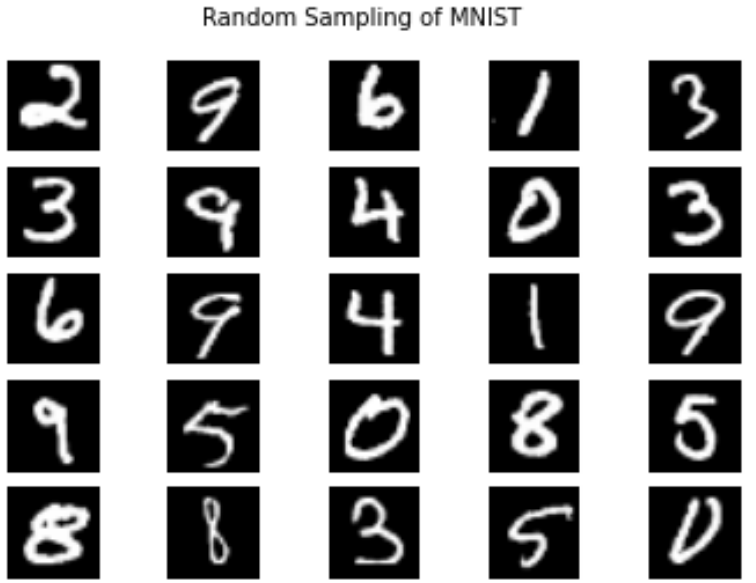
Complete slides available here: https://kawahara.ca/visualizing-data-using-t-sne-slides/

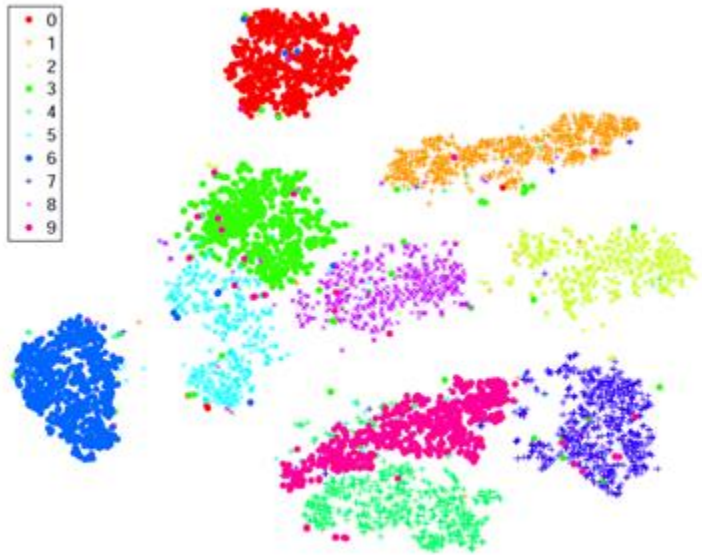
Algorithm 1: Simple version of t-Distributed Stochastic Neighbor Embedding.

Data: data set $\mathcal{X} = \{x_1, x_2, \ldots, x_n\}$,
cost function parameters: perplexity *Perp*,
optimization parameters: number of iterations T, learning rate η, momentum $\alpha(t)$.
Result: low-dimensional data representation $\mathcal{Y}^{(T)} = \{y_1, y_2, \ldots, y_n\}$.
begin
  compute pairwise affinities $p_{j|i}$ with perplexity *Perp* (using Equation 1)
  set $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$
  sample initial solution $\mathcal{Y}^{(0)} = \{y_1, y_2, \ldots, y_n\}$ from $\mathcal{N}(0, 10^{-4}I)$
  for t=1 **to** T **do**
    compute low-dimensional affinities q_{ij} (using Equation 4)
    compute gradient $\frac{\delta C}{\delta \mathcal{Y}}$ (using Equation 5)
    set $\mathcal{Y}^{(t)} = \mathcal{Y}^{(t-1)} + \eta \frac{\delta C}{\delta \mathcal{Y}} + \alpha(t)\left(\mathcal{Y}^{(t-1)} - \mathcal{Y}^{(t-2)}\right)$
  end
end

Algorithm 1: Simple version of t-Distributed Stochastic Neighbor Embedding.

Data: data set $\mathcal{X} = \{x_1, x_2, \ldots, x_n\}$,
cost function parameters: perplexity *Perp*,
optimization parameters: number of iterations T, learning rate η, momentum $\alpha(t)$.
Result: low-dimensional data representation $\mathcal{Y}^{(T)} = \{y_1, y_2, \ldots, y_n\}$.
begin
  compute pairwise affinities $p_{j|i}$ with perplexity *Perp* (using Equation 1)
  set $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$
  sample initial solution $\mathcal{Y}^{(0)} = \{y_1, y_2, \ldots, y_n\}$ from $\mathcal{N}(0, 10^{-4}I)$
  for t=1 **to** T **do**
    compute low-dimensional affinities q_{ij} (using Equation 4)
    compute gradient $\frac{\delta C}{\delta \mathcal{Y}}$ (using Equation 5)
    set $\mathcal{Y}^{(t)} = \mathcal{Y}^{(t-1)} + \eta \frac{\delta C}{\delta \mathcal{Y}} + \alpha(t)\left(\mathcal{Y}^{(t-1)} - \mathcal{Y}^{(t-2)}\right)$
  end
end



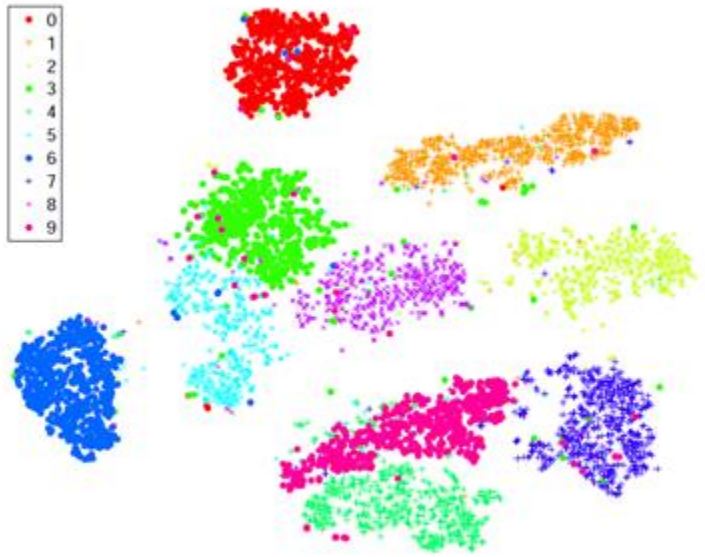


(a) Visualization by t-SNE.

Algorithm 1: Simple version of t-Distributed Stochastic Neighbor Embedding.

Data: data set $\mathcal{X} = \{x_1, x_2, \ldots, x_n\}$,
cost function parameters: perplexity *Perp*,
optimization parameters: number of iterations T, learning rate η, momentum $\alpha(t)$.
Result: low-dimensional data representation $\mathcal{Y}^{(T)} = \{y_1, y_2, \ldots, y_n\}$.
begin
  compute pairwise affinities $p_{j|i}$ with perplexity *Perp* (using Equation 1)
  set $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$
  sample initial solution $\mathcal{Y}^{(0)} = \{y_1, y_2, \ldots, y_n\}$ from $\mathcal{N}(0, 10^{-4}I)$
  for t=1 **to** T **do**
    compute low-dimensional affinities q_{ij} (using Equation 4)
    compute gradient $\frac{\delta C}{\delta \mathcal{Y}}$ (using Equation 5)
    set $\mathcal{Y}^{(t)} = \mathcal{Y}^{(t-1)} + \eta \frac{\delta C}{\delta \mathcal{Y}} + \alpha(t)\left(\mathcal{Y}^{(t-1)} - \mathcal{Y}^{(t-2)}\right)$
  end
end

Compute probabilities ***P*** that ***xi*** and ***xj*** are neighbors (based on Euclidian distance in **high-d** space)

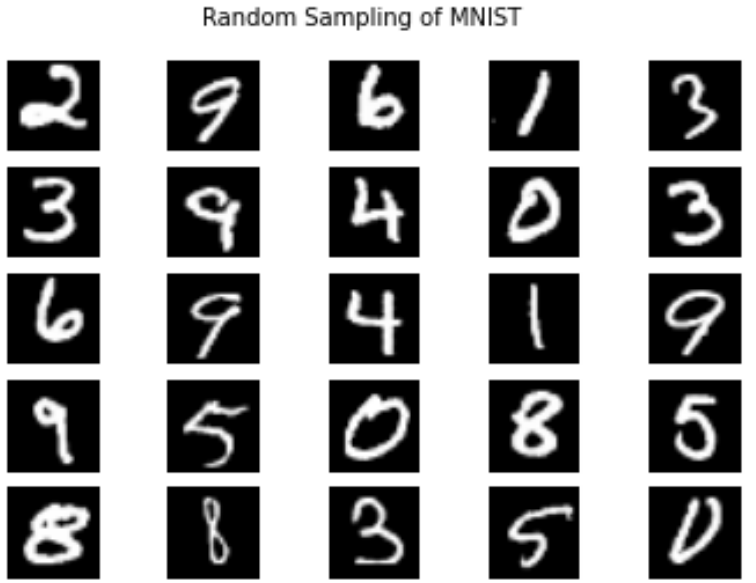


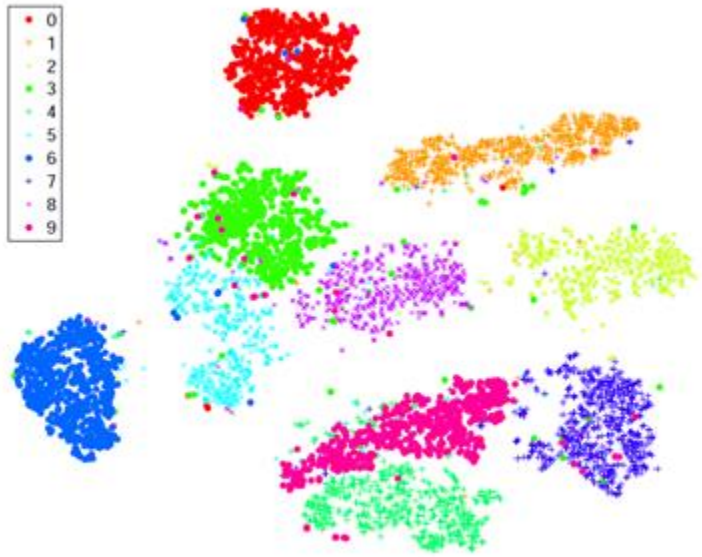
(a) Visualization by t-SNE.

Algorithm 1: Simple version of t-Distributed Stochastic Neighbor Embedding.

Data: data set $\mathcal{X} = \{x_1, x_2, \ldots, x_n\}$,
cost function parameters: perplexity *Perp*,
optimization parameters: number of iterations T, learning rate η, momentum $\alpha(t)$.
Result: low-dimensional data representation $\mathcal{Y}^{(T)} = \{y_1, y_2, \ldots, y_n\}$.
begin
  compute pairwise affinities $p_{j|i}$ with perplexity *Perp* (using Equation 1)
  set $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$
  sample initial solution $\mathcal{Y}^{(0)} = \{y_1, y_2, \ldots, y_n\}$ from $\mathcal{N}(0, 10^{-4}I)$
  for t=1 **to** T **do**
    compute low-dimensional affinities q_{ij} (using Equation 4)
    compute gradient $\frac{\delta C}{\delta \mathcal{Y}}$ (using Equation 5)
    set $\mathcal{Y}^{(t)} = \mathcal{Y}^{(t-1)} + \eta \frac{\delta C}{\delta \mathcal{Y}} + \alpha(t)\left(\mathcal{Y}^{(t-1)} - \mathcal{Y}^{(t-2)}\right)$
  end
end

Key assumption is that the **high-d** *P* and the **low-d** *Q* probability distributions should be the same





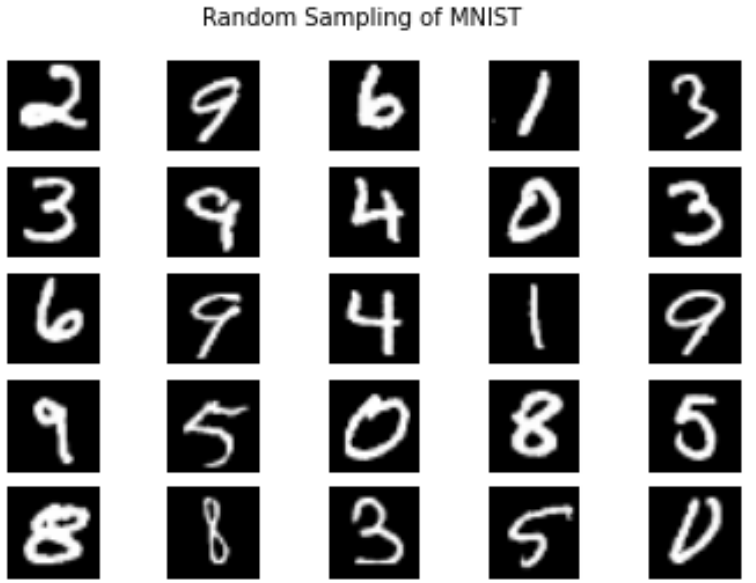
(a) Visualization by t-SNE.

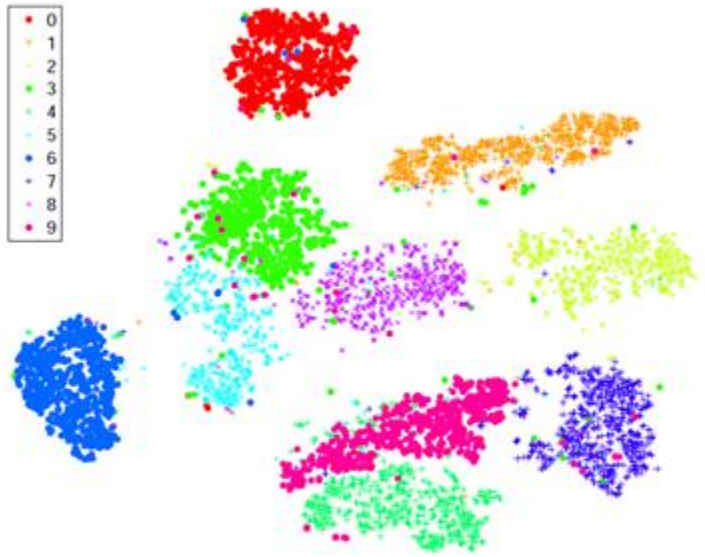
Algorithm 1: Simple version of t-Distributed Stochastic Neighbor Embedding.

Data: data set $\mathcal{X} = \{x_1, x_2, \ldots, x_n\}$,
cost function parameters: perplexity *Perp*,
optimization parameters: number of iterations T, learning rate η, momentum $\alpha(t)$.
Result: low-dimensional data representation $\mathcal{Y}^{(T)} = \{y_1, y_2, \ldots, y_n\}$.
begin
  compute pairwise affinities $p_{j|i}$ with perplexity *Perp* (using Equation 1)
  set $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$
  sample initial solution $\mathcal{Y}^{(0)} = \{y_1, y_2, \ldots, y_n\}$ from $\mathcal{N}(0, 10^{-4}I)$
  for t=1 **to** T **do**
    compute low-dimensional affinities q_{ij} (using Equation 4)
    compute gradient $\frac{\delta C}{\delta \mathcal{Y}}$ (using Equation 5)
    set $\mathcal{Y}^{(t)} = \mathcal{Y}^{(t-1)} + \eta \frac{\delta C}{\delta \mathcal{Y}} + \alpha(t)\left(\mathcal{Y}^{(t-1)} - \mathcal{Y}^{(t-2)}\right)$
  end
end

Find a **low-d** map that minimizes the difference between the ***P*** (high-d) and ***Q*** (low-d) distributions

(if *xi,xj* has high probability of being neighbors in **high-d**, then *yi,yj* should have high probability in **low-d**)



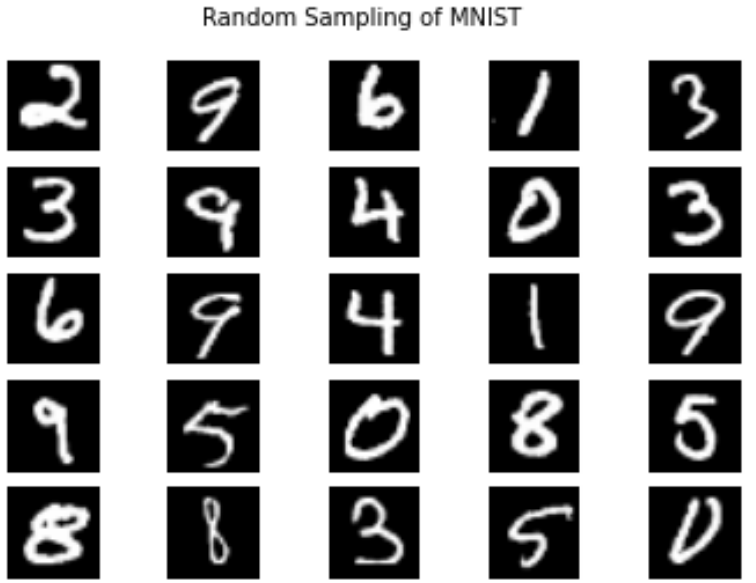


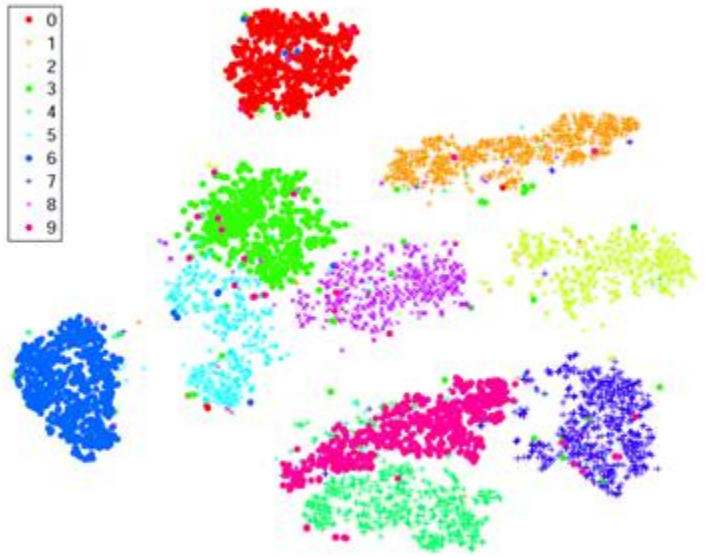
(a) Visualization by t-SNE.

Algorithm 1: Simple version of t-Distributed Stochastic Neighbor Embedding.

Data: data set $\mathcal{X} = \{x_1, x_2, \ldots, x_n\}$,
cost function parameters: perplexity *Perp*,
optimization parameters: number of iterations T, learning rate η, momentum $\alpha(t)$.
Result: low-dimensional data representation $\mathcal{Y}^{(T)} = \{y_1, y_2, \ldots, y_n\}$.
begin
  compute pairwise affinities $p_{j|i}$ with perplexity *Perp* (using Equation 1)
  set $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$
  sample initial solution $\mathcal{Y}^{(0)} = \{y_1, y_2, \ldots, y_n\}$ from $\mathcal{N}(0, 10^{-4}I)$
  for t=1 **to** T **do**
    compute low-dimensional affinities q_{ij} (using Equation 4)
    compute gradient $\frac{\delta C}{\delta \mathcal{Y}}$ (using Equation 5)
    set $\mathcal{Y}^{(t)} = \mathcal{Y}^{(t-1)} + \eta \frac{\delta C}{\delta \mathcal{Y}} + \alpha(t)\left(\mathcal{Y}^{(t-1)} - \mathcal{Y}^{(t-2)}\right)$
  end
end

We will minimize the difference between the **high-d** and **low-d** maps using **gradient descent**





(a) Visualization by t-SNE.

References

- Dimensionality Reduction. Appendix B. Introduction to Data Mining.
- Cox, T.F.; Cox, M.A.A. (2001). Multidimensional Scaling. Chapman and Hall.
- Maaten, L. van der, & Hinton, G. (2008). Visualizing Data using t-SNE. Journal of Machine Learning Research (JMLR), 9, 2579–2605. [pdf]
- J. B. Tenenbaum, V. de Silva, J. C. Langford, A Global Geometric Framework for Nonlinear Dimensionality Reduction, Science 290, (2000), 2319–2323. [pdf]