DATA SCIENCE

PPGIA/PUCPR

Prof. Jean Paul Barddal

1

REMINDERS

2

Reminders

- Today we will discuss dimensionality reduction
- Next week we will have our test!

3

DIMENSIONALITY REDUCTION

4

Dimensionality reduction

- In opposition to feature selection, dimensionality reduction techniques decrease the dimensionality of a problem by **combining** features
- There are different techniques to achieve this goal
- The most famous is Principal Component Analysis (PCA)

5

PRINCIPAL COMPONENT ANALYSIS

6

Variance and covariance

- Variance and covariance measure how “spread” a set of points are around their mean
- Variance is used for analyzing a single dimension
- Covariance measures how much each of the dimensions vary from the mean with respect to each other
- Covariance is measures between 2 dimensions to see if there is a relationship between them

7

Covariance

- The covariance between 2 variables is computed by:

$$Cov(X,Y) = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{(n-1)}$$

- If you have more than 2 variables, you need to compute a covariance matrix

8

Covariance

- The exact value is not as important as its sign
- A **positive** value indicates both variables increase or decrease together
- A **negative** value indicates that while one variable increases, the other decreases, or vice-versa
- If covariance is **zero**, the two variables are independent from each other

9

But what about correlation?

- Correlation allowed us to infere the same thing
- Why do we need covariance?
- Covariance is used to find relationships between variables in high-dimensional scenarios, where visualization is difficult

10

Principal component analysis (PCA)

- PCA is a technique used to simplify a dataset
- It is a linear transformation that chooses a new coordinate system for the dataset such that:
  - **the greatest variance by any projection lies on the first axis**: the 1st principal component (eigenvector with the largest eigenvalue)
  - **the second greatest variance lies on the y axis (2nd PC), and so forth** (eigenvector with the second largest eigenvalue, etc)
- PCA can be used for reducing dimensionality by eliminating later principal components

11

Steps to use PCA

- Normalize the data
- Calculate the covariance matrix
- Calculate the eigenvalues and eigenvectors
- Choosing principal components
- Forming a feature vector
- Forming principal components

- **All but the first of these steps are covered in scikit-learn's PCA implementation**

12

PCA Limitations

- If the data does not follow a multidimensional normal (gaussian) distribution, the principal components extracted will be distorted

13

Activity

- Let’s run PCA on a dataset representing customers
- Each customer represents either a restaurant, a retail store, etc
- Let’s analyze its principal components

14

T-SNE

15

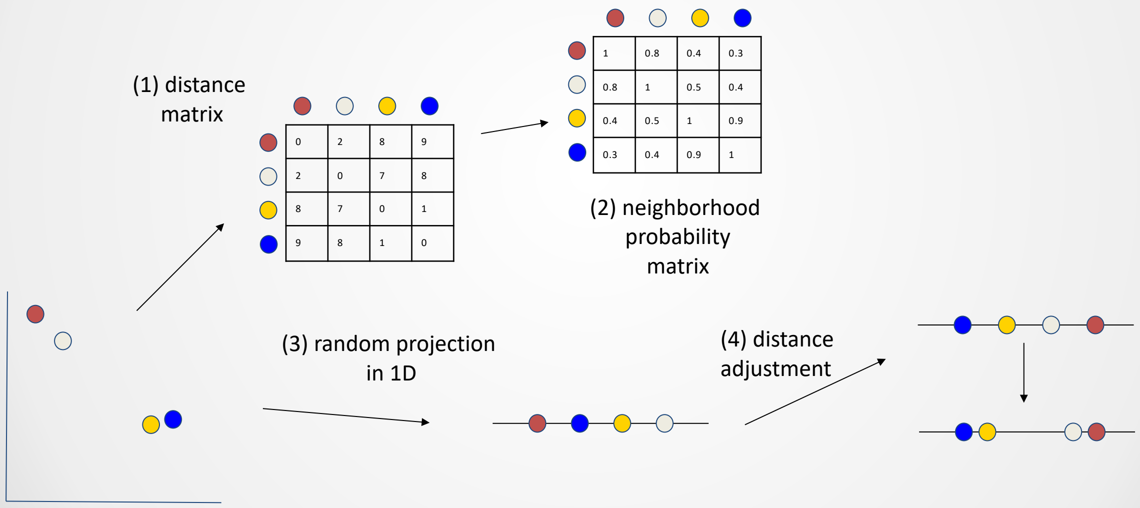
t-Stochastic Neighbor Embedding

- Technique tailored for visualizing high-dimensional datasets
- How do we visualize data in 2D or 3D?
- Two goals:
  - Distance preservation
  - Neighbor preservation
- Unsupervised, but it helps uncovering interesting aspects of the data

16

t-SNE overall idea

- Let's say we have a 2D problem we wish to visualize in 1D



0	2	8	9
2	0	7	8
8	7	0	1
9	8	1	0

1	0.8	0.4	0.3
0.8	1	0.5	0.4
0.4	0.5	1	0.9
0.3	0.4	0.9	1

17

t-SNE

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

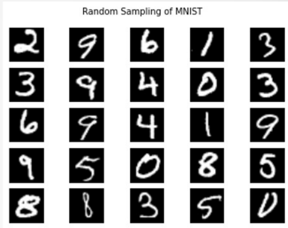
Data: data set $\mathcal{X} = \{x_1, x_2, \ldots, x_n\}$,
cost function parameters: perplexity *Perp*,
optimization parameters: number of iterations T, learning rate η, momentum $\alpha(t)$.
Result: low-dimensional data representation $\mathcal{Y}^{(T)} = \{y_1, y_2, \ldots, y_n\}$.
begin
  compute pairwise 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

18

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

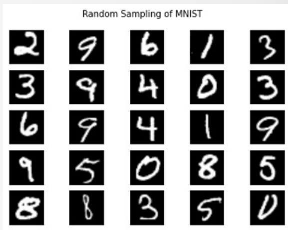


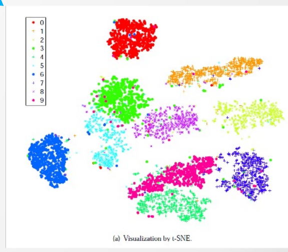
19

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





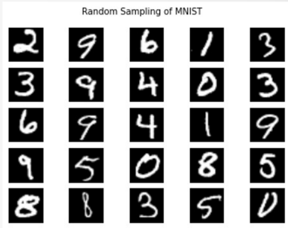
(a) Visualization by t-SNE.

20

t-SNE

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

Data: data set $X = \{x_1, x_2, \ldots, x_n\}$,
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

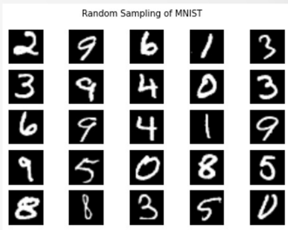


21

t-SNE

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

Data: data set $X = \{x_1, x_2, \ldots, x_n\}$,
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



Perplexity is the number of instances that we want to present the distances

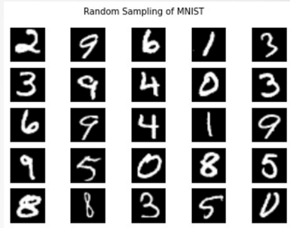
Compute probabilities ***P*** that ***xi*** and ***xj*** are neighbors (based on Euclidian distance in **high-d** space)

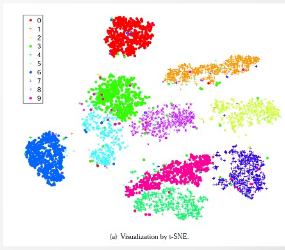
22

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




(a) Visualization by t-SNE.

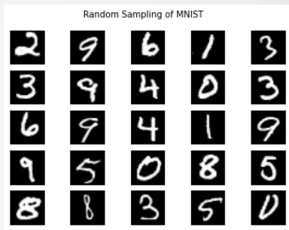
Compute probabilities ***Q*** that ***yi*** and ***yj*** are neighbors (corresponding to *xi, xj*)
(based on Euclidian distance in **low-d** space)

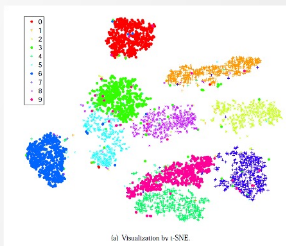
23

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 $\boxed{p_{j|i}}$ 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 $\boxed{q_{ij}}$ (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.

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

24

t-SNE

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

Data: data set $X = \{x_1, x_2, \ldots, x_n\}$,
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**)

25

t-SNE

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

Data: data set $X = \{x_1, x_2, \ldots, x_n\}$,
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**

26

t-SNE details

- Details on t-SNE can be found at the original paper
- https://jmlr.org/papers/volume9/vandermaaten08a/vandermaaten08a.pdf

Journal of Machine Learning Research 9 (2008) 2579-2605 Submitted 5/08; Revised 9/08; Published 11/08

Visualizing Data using t-SNE

Laurens van der Maaten LVDMAATEN@GMAIL.COM
TiCC
Tilburg University
P.O. Box 90153, 5000 LE Tilburg, The Netherlands

Geoffrey Hinton HINTON@CS.TORONTO.EDU
Department of Computer Science
University of Toronto
6 King's College Road, M5S 3G4 Toronto, ON, Canada

Editor: Yoshua Bengio

27

t-SNE

- In opposition to PCA, t-SNE is **not** parametric
- This means that we cannot learn a manifold representation from a dataset and apply it to another dataset
  - Therefore, this cannot be used as a dimensionality reduction technique between training and test data
- There is, however, a parametric version available at:

Learning a Parametric Embedding by Preserving Local Structure

Laurens van der Maaten
TiCC, Tilburg University
P.O. Box 90153, 5000 LE Tilburg, The Netherlands
lvdmaaten@gmail.com

28