Dimension Reduction

Linear Algebra Project Report, Dr.Ramin Javadi

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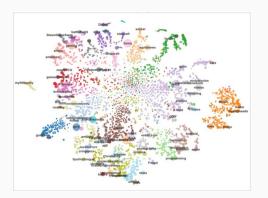
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Introduction

Introduction

Dimensionality reduction: Reducing the number of random variables by obtaining a set of **principal variables**The higher the number of features -> the harder it gets to visualize the training set and then work on it

- · feature selection
- · feature extraction



Linear Methods

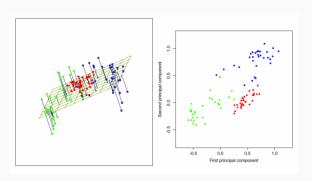
Linear Methods

We discuss and interpret these linear methods:

- · PCA
- · DUAL PCA

PRINCIPAL COMPONENT ANALYSIS (PCA)

- · Very popular technique
- Find a reduced subspace which maintains most of the variability of the data $(n\rightarrow d)$
- d orthogonal vectors that form a new coordinate system which are 'principal components'



PRINCIPAL COMPONENT ANALYSIS (PCA)

Main goal: find maximum variance \rightarrow choose first eigenvector U_1 Given: $n \times t$ matrix X and U_1 is is a combination of X with ω coefficients such that $\omega = [\omega_1 \dots \omega_n]$

$$U_1 = \omega^T X \tag{1}$$

$$var(U_1) = var(\omega^T X) = \omega^T S \omega$$
 (2)

where S is the $n \times n$ sample covariance matrix of X.

$$\max \omega^T S \omega$$
 s.t. $\omega^T \omega = 1$

Using lagrange method and introduce a lagrange multiplier λ we have:

$$L(\omega, \lambda) = \omega^{\mathsf{T}} \mathsf{S}\omega - \lambda(\omega^{\mathsf{T}}\omega - 1) \tag{3}$$

By differentiating L with respect to ω we have:

$$S\omega = \lambda_1 \omega \tag{4}$$

PRINCIPAL COMPONENT ANALYSIS (PCA)

Continuing this method for d eigenvectors of covariance matrix S -> determine the first d principal components Using SVD -> obtain these eigenvectors:

$$X = U\Sigma V^{T} \tag{5}$$

where columns of U are eigenvectors of XX^T (covariance matrix).

Algorithm: We define Y as our projected d-dimensional data (d < n):

1.

$$Y = U(:, 1:d)^{T}X$$
 or $Y = U_{d}^{T}X$ (6)

2. Reconstruct the training data:

$$\hat{X} = U_d Y \tag{7}$$

3. For a new test example x we compute $y = U^Tx$ and then reconstruct it $\hat{x} = Uy$

DUAL PCA

- Very similar to PCA
- Faster in the case that the number of features is bigger than the samples
- Goal: reduce dependence of our algorithm on n (the number of features)
- Decompose X^TX instead of XX^T
- SVD: $X = U\Sigma V^T -> XV = U\Sigma$, where the eigenvectors in U corresponds to nonzero singular values in Σ .

The top d eigenvectors can be derived:

$$U = XV\Sigma^{-1} \tag{8}$$

Replace all uses of U in PCA algorithm.

DUAL PCA

Algorithm:

1. Compute Y:

$$Y = U^{T}X = \Sigma V^{T} \tag{9}$$

2. Reconstruct data:

$$\hat{X} = UY = U\Sigma V^{\mathsf{T}} = XV\Sigma^{-1}\Sigma V^{\mathsf{T}} = XVV^{\mathsf{T}}$$
(10)

3. Project out of sample point x:

$$y = U^{\mathsf{T}} X = \Sigma^{-1} V^{\mathsf{T}} X^{\mathsf{T}} X \tag{11}$$

4. Finally reconstruct this sample point:

$$\hat{\mathbf{x}} = U\mathbf{y} = UU^{\mathsf{T}}\mathbf{x} = XV\mathbf{\Sigma}^{-2}V^{\mathsf{T}}X^{\mathsf{T}}\mathbf{x} \tag{12}$$

Random Projection

for the cases with large number of samples

What does it guarantee?
 after projecting the points from the n-dimensional space to K
 dimensional space using the randomly drawn matrix W, the
 distances between the high dimensional points is preserved in
 the lower dimensional projections up to some approximation
 factor

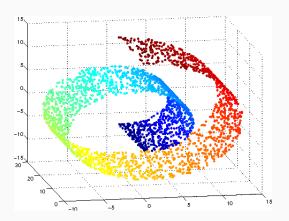
This matrix W is:

$$W[i,j] = \left\{ \begin{array}{ll} +\frac{1}{\sqrt{K}} & \text{with probability 1/2} \\ -\frac{1}{\sqrt{K}} & \text{with probability 1/2} \end{array} \right\}$$

Nonlinear Methods

WHAT'S THE PROBLEM

What happen's if we have a manifold?



ISOMAP

Distance

- · Euclidean distance
- · Geodesic distance

Algorithm:

- 1. Construct a k-nearest neighbor graph on n data points
- Compute shortest path between all the points (DG) as an estimation of geodesic distance
 - · Dijkstra's algorithm
 - · Floyd-Warshall
- 3. Compute $k = -\frac{1}{2}H(D^G)^2H$. find eigenvectors of k and call it V. then find the top p eigenvalues of k and form $\hat{\Lambda}$. The final solution is $Y = \hat{\Lambda}^{\frac{1}{2}}V^T$.

LAPLACIAN EIGENMAP (SPECTRAL EMBEDDING)

- 1. Using Spectral Clustering
- 2. Affinity Matrix
 - · The neighbourhood graph can be constructed by finding the k nearest neighbours and computing the adjacency matrix
 - · Gaussian Distance

$$W_{ij} = e^{-\frac{||x_i - x_j||^2}{\gamma}} \tag{13}$$

3. Objective Function

$$\min_{Y} \sum_{i=1}^{t} \sum_{j=1}^{t} (y_i - y_j)^2 W_{ij}$$
 (14)

From spectral clustering we know that:

$$\sum_{i,j} (y_i - y_j)^2 W_{ij} = Y^T L Y$$
 (15)

$$\min_{Y} Tr(YLY^{T})$$
s.t. $YY^{T} = I$
(16)

$$YY^T = I$$

Experiment

EXPERIMENT

start by generating three different data to compare the algorithms

- · simple "Hello" in three dimension
- · curved "Hello"
- · S-shape data

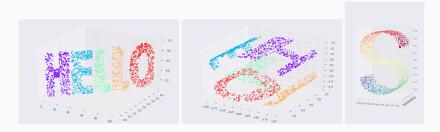
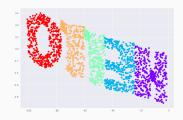


Figure 1: data points that are used

THE RESULT OF ALGORITHMS ON THE FIRST DATA POINT



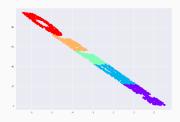
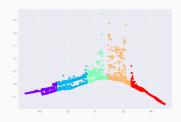


Figure 2: PCA and Random Projection applied to the first data point



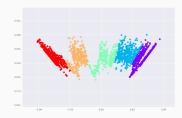
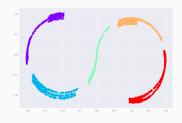


Figure 3: Isomap and Laplacian eigenmap applied to the first data point

THE RESULT OF ALGORITHMS ON THE SECOND DATA POINT



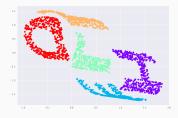
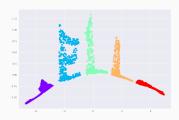


Figure 4: PCA and Random Projection applied to the second data point



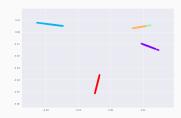
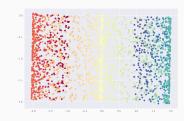


Figure 5: Isomap and Laplacian eigenmap applied to the second data point

The result of algorithms on the third data point



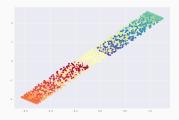
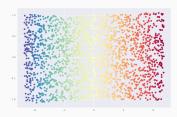


Figure 6: PCA and Random Projection applied to the third data point



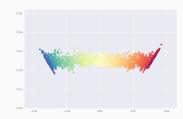


Figure 7: Isomap and Laplacian eigenmap applied to the third data point

SOURCE

Get the source of the project from here:

https://github.com/Linear-Algebra-Course/dimension-reduction



REFERENCES 1

[1] [2] [3]



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Dimensionality Reduction A Short Tutorial.

Science, page 25, 2006.



E Kokiopoulou, J Chen, and Y Saad.

Trace Optimization and eigenproblem in dimension reduction methods.

Numerical Linear Algebra with Applications, pages 1–35, 2011.



Random Projections.

Machine Learning for Data Science (CS 4786) Why Random **Projection Works ?!**

(Cs 4786):1-5.