Dimension Reduction

Linear Algebra Project Report, Dr.Ramin Javadi

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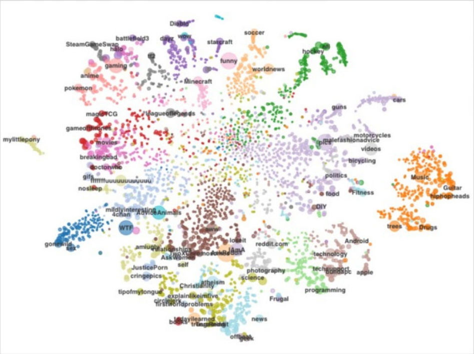
Introduction

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

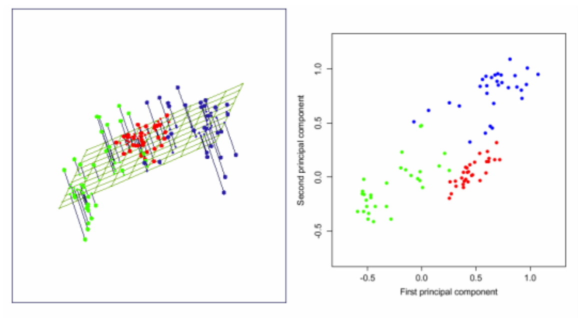
Linear Methods

We discuss and interpret these linear methods:

- PCA
- DUAL PCA
- RANDOM PROJECTION

Principal Component Analysis (PCA)

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



Principal Component Analysis (PCA)

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

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

$$\text{var}(U_1) = \text{var}(\omega^T X) = \omega^T S \omega \tag{2}$$

where S is the n × n sample covariance matrix of X.

$$\max \omega^T \mathrm{S}\, \omega \quad \text{s.t. } \omega^T \omega = 1$$

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

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

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. $$Y = U(:, 1:d)^T X \qquad or \qquad Y = U_d^T X \tag{6}$$
2. Reconstruct the training data:
$$\hat{X} = U_d Y \tag{7}$$
3. For a new test example x we compute $y = U^T x$ 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.

Algorithm:

1. Compute Y:
$$Y = U^T X = \Sigma V^T \tag{9}$$
2. Reconstruct data:
$$\hat{X} = UY = U\Sigma V^T = XV\Sigma^{-1}\Sigma V^T = XVV^T \tag{10}$$
3. Project out of sample point x:
$$y = U^T x = \Sigma^{-1} V^T X^T x \tag{11}$$
4. Finally reconstruct this sample point:
$$\hat{x} = Uy = UU^T x = XV\Sigma^{-2} V^T X^T x \tag{12}$$

Random Projection

- for the cases with large number of samples

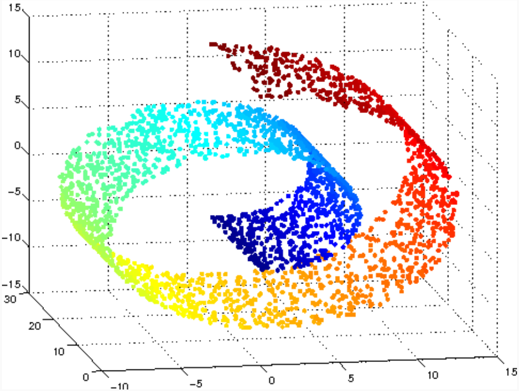
- What does it guarantee?
  after projecting the points from the n-dimensional space to K dimensional space using the randomly drawn matrix W, the distances between the high dimensional points is preserved in the lower dimensional projections up to some approximation factor

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 happen's if we have a manifold ?



Distance

- Euclidean distance
- Geodesic distance

Algorithm:

1. Construct a k-nearest neighbor graph on n data points
2. 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

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

From spectral clustering we know that:

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

$$\min_{Y} Tr(YLY^T) \tag{16}$$

$$\text{s.t. } YY^T = I$$

Experiment

start by generating three different data to compare the algorithms

- simple ”Hello” in three dimension
- curved ”Hello”
- S-shape data

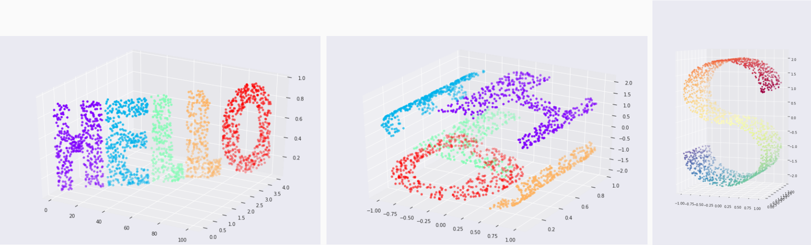


Figure 1: data points that are used

The result of algorithms on the first data point

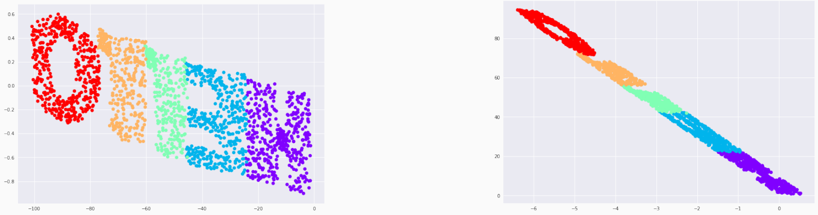


Figure 2: PCA and Random Projection applied to the first data point

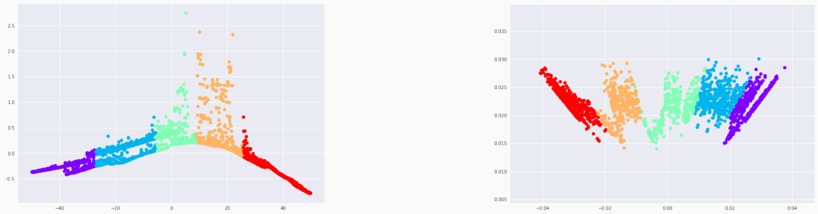


Figure 3: Isomap and Laplacian eigenmap applied to the first data point

The result of algorithms on the second data point

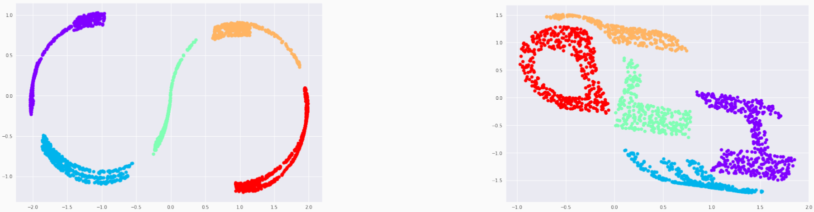


Figure 4: PCA and Random Projection applied to the second data point

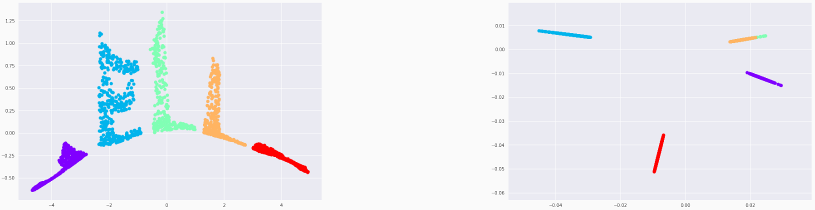


Figure 5: Isomap and Laplacian eigenmap applied to the second data point

The result of algorithms on the third data point

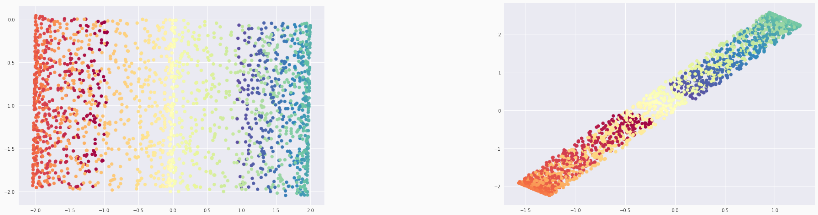


Figure 6: PCA and Random Projection applied to the third data point

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 I

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