CS 60050
Machine Learning

Dimensionality Reduction

Some slides taken from course materials of Jure Leskovec

Dimensionality reduction

- Dimensionality = number of features or attributes in the data set
- Data can have really large number of features
  - E.g., in a corpus of text documents, each distinct word can be a feature (bag of words model)
  - E.g., in an image data set, each of 1024 x 768 pixels can be a feature
- Goal (informal): reduce the number of features, such that information loss is not much

Why dimensionality reduction?

- Some features may be irrelevant
- We want to visualize high dimensional data
- Feature space may be very sparsely populated
  - E.g., in case of a text document corpus, each individual word may be contained in a very small subset of the corpus
  - Some learning algorithms do not perform well on such sparse feature space
  - Curse of dimensionality - the number of training examples required increases exponentially with dimensionality

Intuition behind dimensionality reduction

- Dimensionality reduction = changing the feature space in which the points lie (to a lower dimensional space)
- What should be the desirable properties of the reduced feature set?
- Ultimate goal – good performance in clustering, classification, etc.
  - Identify different groups of similar data points

Intuition behind dimensionality reduction

- If class information is given
  - Identify features that have high influence on the class
  - E.g., for spam email classification: time of day when the email comes vs. number of spam-words
- If class information is not given (unsupervised)
  - Identify (possibly new) features along which the data points vary largely
  - E.g., given marks of school students in 7 subjects (Physics, Chem, Maths, Eng, Hindi, History, Pol. Sc.), maybe variation can be captured considering three (new) dimensions – Science, Social Science, Arts

Ways of dimensionality reduction

- Two broad ways of reducing dimensionality
  - Select a subset of the given features
  - Define a new set of features that is smaller than the given feature set

Ways of dimensionality reduction

- Supervised
  - These methods use both the feature values as well as the class labels of the data points
- Unsupervised
  - These methods use only the feature values, not the class values
- Domain-specific
  - E.g. Text:
    - Remove stop-words (and, a, the, …)
    - Stemming (going → go, Tom's → Tom, …)
    - Select important words based on document frequency

Supervised feature selection

- Score each feature based on some suitable mechanism
- Forward/Backward elimination
  - Choose the feature with the highest/lowest score
  - Re-score other features
  - Repeat
- If you have lots of features (like in text)
  - Just select top K scored features

Supervised feature selection: some ways to score features

- Mutual information between feature & class
  - Mutual info: a measure between two (possibly multi-dimensional) random variables, that quantifies the amount of information obtained about one random variable, through the other random variable.
- χ^2 independence between feature & class
  - Test whether the occurrence of a specific feature value and the occurrence of a specific class are independent
- How classification accuracy varies if a feature is removed (ablation experiments)

See references for some pointers

Unsupervised feature selection

- Differs from supervised feature selection in two ways:
  - Instead of choosing subset of features,
  - Create new features (dimensions) defined as functions over all features
  - Do not consider class labels, just the data points

Unsupervised feature selection

- Idea:
  - Given data points in N-dimensional space,
  - Project into lower dimensional space while preserving as much information as possible
    - E.g., find best planar approximation to 3D data
    - E.g., find best planar approximation to 104D data
  - In particular, choose projection that minimizes the squared error in reconstructing original data – PCA

Principal Component Analysis (PCA)

Background concepts

- Given an N x M data matrix D,
  - whose N rows are data objects, and
  - whose M columns are attributes
- The covariance matrix C of D is a M x M matrix which has entries $c_{ij} = covariance(d_{*i}, d_{*j})$
  - c_{ij} is the covariance of the i-th and j-th attributes (columns) of the data, which measures how strongly the attributes vary together
  - If i=j, then the covariance is the variance of the attribute.

Covariance matrix

$$\begin{bmatrix} V_a & C_{a,b} & C_{a,c} & C_{a,d} & C_{a,e} \\ C_{a,b} & V_b & C_{b,c} & C_{b,d} & C_{b,e} \\ C_{a,c} & C_{b,c} & V_c & C_{c,d} & C_{c,e} \\ C_{a,d} & C_{b,d} & C_{c,d} & V_d & C_{d,e} \\ C_{a,e} & C_{b,e} & C_{c,e} & C_{d,e} & V_e \end{bmatrix}$$

Covariance matrix: another representation

$$\Sigma = \begin{bmatrix} \mathrm{E}[(X_1 - \mu_1)(X_1 - \mu_1)] & \mathrm{E}[(X_1 - \mu_1)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_1 - \mu_1)(X_n - \mu_n)] \\ \mathrm{E}[(X_2 - \mu_2)(X_1 - \mu_1)] & \mathrm{E}[(X_2 - \mu_2)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_2 - \mu_2)(X_n - \mu_n)] \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{E}[(X_n - \mu_n)(X_1 - \mu_1)] & \mathrm{E}[(X_n - \mu_n)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_n - \mu_n)(X_n - \mu_n)] \end{bmatrix}.$$

Background concepts

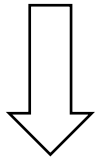
- If the data matrix D is preprocessed so that the mean of each attribute is zero, then $C = D^T D$
- Covariance matrices are examples of positive semidefinite matrices, which have non-negative eigenvalues
  - Eigenvalues of C can be ordered in decreasing order of magnitude
  - Eigenvectors of C can be ordered so that the i-th eigenvector corresponds to i-th largest eigenvalue

PCA: overview

- Say we have a N-dimensional feature space
- We wish to reduce to K dimensions, K << N
- Dimensionality reduction implies information loss; PCA preserves as much information as possible by minimizing the reconstruction error:

$$||x - \hat{x}||$$

$$x = a_1 v_1 + a_2 v_2 + \cdots + a_N v_N$$



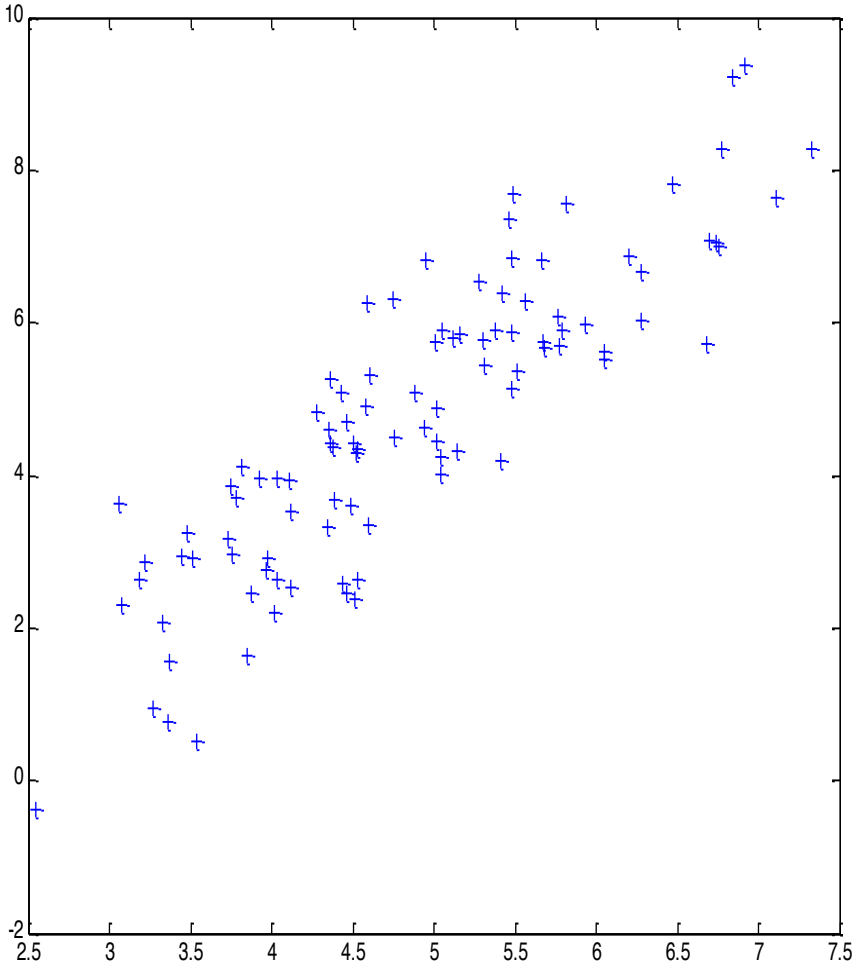
$$\hat{x} = b_1 u_1 + b_2 u_2 + \cdots + b_K u_K$$

PCA: overview

- PCA: a mathematical procedure that transforms a number of (possibly) correlated variables into a (smaller) number of uncorrelated variables called principal components

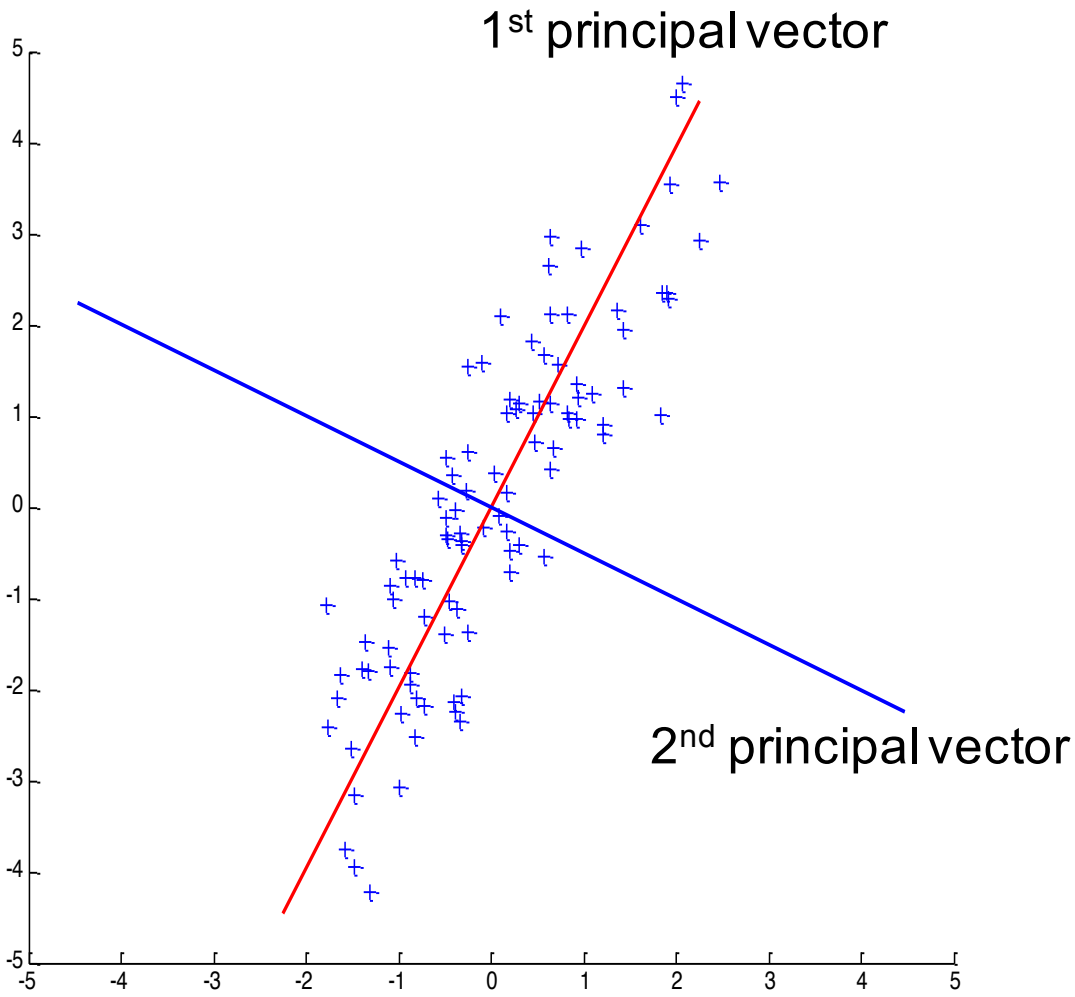
- The first principal component accounts for as much of the variability in the data as possible, and each succeeding component accounts for as much of the remaining variability as possible

Geometric interpretation on 2d data



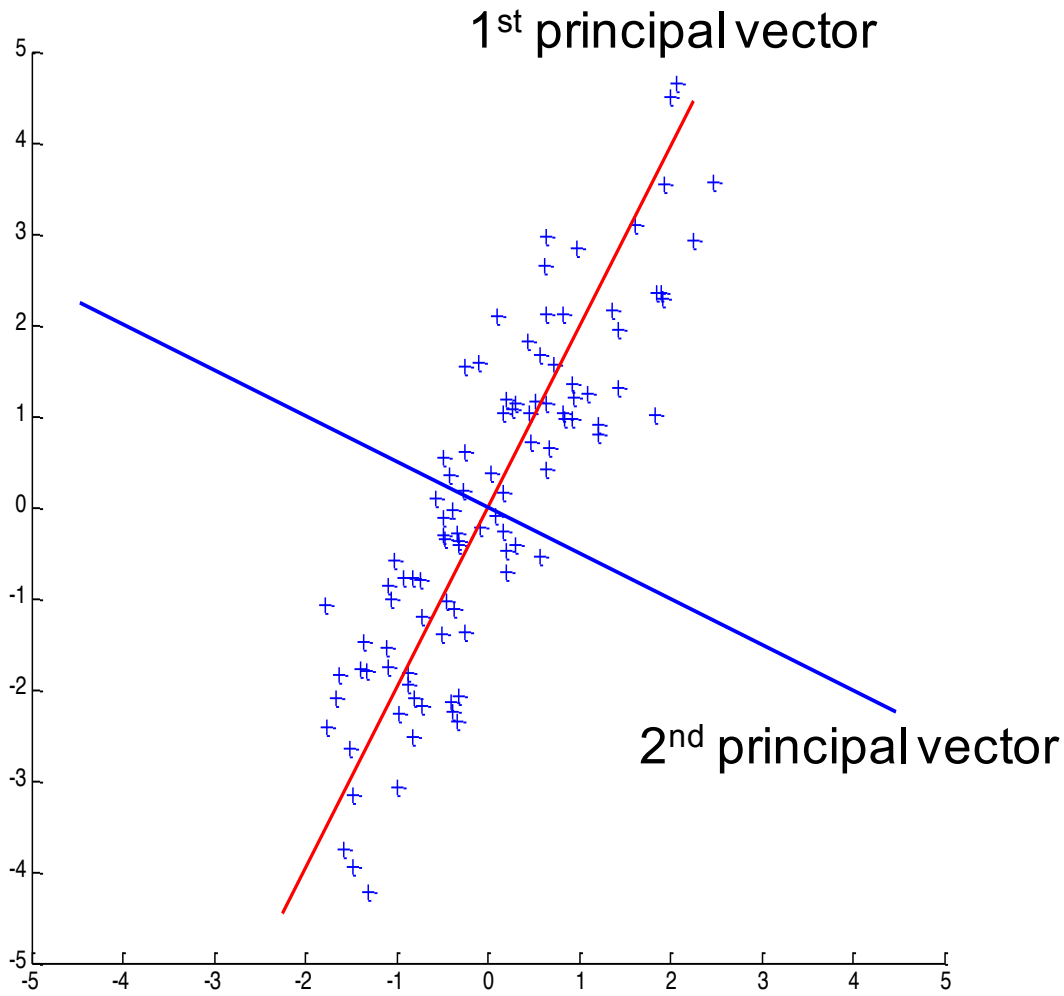
Geometric interpretation on 2d data

- PCA projects the data along the directions where the data varies most
- A rotation of the coordinate system such that the axes show a maximum of variation (covariance) along their directions.
- The directions are orthogonal to each other – these are the new attributes (PCs)



Geometric interpretation on 2d data

- These directions are determined by some of the eigenvectors of the covariance matrix of data
- Specifically, those eigenvectors that correspond to the largest eigenvalues
- Magnitude of the eigenvalues corresponds to the variance of the data along the eigenvector directions
- Each new attribute is a linear combination of the original attributes



PCA - Steps

Suppose $x_1, x_2, \ldots, x_M$ are N x 1 vectors

Step 1: $\bar{x} = \frac{1}{M}\sum_{i=1}^{M} x_i$

Step 2: subtract the mean: $\Phi_i = x_i - \bar{x}$ (i.e., center at zero)

Step 3: form the matrix $A = [\Phi_1 \; \Phi_2 \cdots \Phi_M]$ (NxM matrix), then compute:

$$C = \frac{1}{M}\sum_{n=1}^{M} \Phi_n \Phi_n^T = \frac{1}{M} A A^T$$

(sample **covariance** matrix, NxN, characterizes the *scatter* of the data)

Step 4: compute the eigenvalues of C: $\lambda_1 > \lambda_2 > \cdots > \lambda_N$

Step 5: compute the eigenvectors of C: $u_1, u_2, \ldots, u_N$

PCA - Steps

an orthogonal basis

- Since C is symmetric, $u_1, u_2, \ldots, u_N$ form ~~a basis~~, (i.e., any vector x or actually $(x - \bar{x})$, can be written as a linear combination of the eigenvectors):

$$x - \bar{x} = b_1 u_1 + b_2 u_2 + \cdots + b_N u_N = \sum_{i=1}^{N} b_i u_i \qquad \text{where } b_i = \frac{(x - \bar{x}).u_i}{(u_i.u_i)}$$

Step 6: (**dimensionality reduction step**) keep only the terms corresponding to the K largest eigenvalues:

$$\hat{x} - \bar{x} = \sum_{i=1}^{K} b_i u_i \text{ where } K << N$$

- The representation of $\hat{x} - \bar{x}$ into the basis $u_1, u_2, \ldots, u_K$ is thus

$$\begin{bmatrix} b_1 \\ b_2 \\ \ldots \\ b_K \end{bmatrix}$$

How to choose K?

- Choose *K* using the following criterion:

$$\frac{\sum_{i=1}^{K} \lambda_i}{\sum_{i=1}^{N} \lambda_i} > Threshold \quad \text{(e.g., 0.9 or 0.95)}$$

- In this case, we say that we “preserve” 90% or 95% of the information (variance) in the data.

- If K=N, then we “preserve” 100% of the information in the data.

Error due to dimensionality reduction

- The original vector *x* can be reconstructed using its principal components:

$$\hat{x} - \bar{x} = \sum_{i=1}^{K} b_i u_i \text{ or } \hat{x} = \sum_{i=1}^{K} b_i u_i + \bar{x}$$

- PCA minimizes the reconstruction error:

$$e = \|x - \hat{x}\|$$

- It can be shown that the reconstruction error is:

$$e = 1/2 \sum_{i=K+1}^{N} \boldsymbol{\lambda}_i$$

Normalization

- The principal components are dependent on the *units* used to measure the original variables as well as on the *range* of values they assume.
- Data should always be normalized prior to using PCA.
- A common normalization method is to transform all the data to have zero mean and unit standard deviation:

$$\frac{x_i - \mu}{\sigma} \quad (\mu \text{ and } \sigma \text{ are the mean and standard deviation of } x_i\text{'s})$$

Benefits of PCA

- Identify the strongest patterns in the data in an unsupervised way
- Capture most of the variability of the data by a small fraction of the total set of dimensions
- Eliminate much of the noise in the data making it beneficial for classification and other learning algorithms

Problems and limitations

- What if very large dimensional data?
  - e.g., Images ($d \geq 10^4$)
- Problem:
  - Covariance matrix Σ is size (d^2)
  - $d=10^4 \rightarrow |\Sigma| = 10^8$
- Singular Value Decomposition (SVD)
  - efficient algorithms available
  - some implementations find just top N eigenvectors

References

- Mutual information-based feature selection https://thuijskens.github.io/2017/10/07/feature-selection/
- A Gentle Introduction to the Chi-Squared Test for Machine Learning https://machinelearningmastery.com/chi-squared-test-for-machine-learning/
- Feature Selection For Machine Learning in Python https://machinelearningmastery.com/feature-selection-machine-learning-python/