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CSCE 633: Machine Learning

Lecture 10

Overview

- Motivation for dimensionality reduction
- Feature selection
    - Wrappers
    - Filters
    - Embedded methods
- Feature transformation
    - Principal Component Analysis (PCA)
    - Autoencoders
    - Clustering

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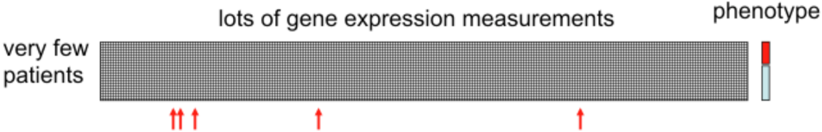
Motivation for dimensionality reduction

Examples of large feature spaces

Predicting recurrence of lung cancer



Only a few genes actually matter!

Need small, interpretable subset to help doctors!

Motivation for dimensionality reduction

Examples of large feature spaces

Text classification


```
<REUTERS TOPICS=''YES'' LEWISSPLIT=''TRAIN''
CGISPLIT=''TRAINING-SET'' OLDID=''12981'' NEWID=''798''>
<DATE> 2-MAR-1987 16:51:43.42</DATE>
<TOPICS><D>livestock</D><D>hog</D></TOPICS>
<TITLE>AMERICAN PORK CONGRESS KICKS OFF TOMORROW</TITLE>
<DATELINE> CHICAGO, March 2 - </DATELINE><BODY>The American Pork
Congress kicks off tomorrow, March 3, in Indianapolis with 160
of the nations pork producers from 44 member states determining
industry positions on a number of issues, according to the
National Pork Producers Council, NPPC.
Delegates to the three day Congress will be considering 26
resolutions concerning various issues, including the future
direction of farm policy and the tax law as it applies to the
agriculture sector. The delegates will also debate whether to
endorse concepts of a national PRV (pseudorabies virus) control
and eradication program, the NPPC said. A large
trade show, in conjunction with the congress, will feature
the latest in technology in all areas of the industry, the NPPC
added. Reuter
\&\#3;</BODY></TEXT></REUTERS>
```

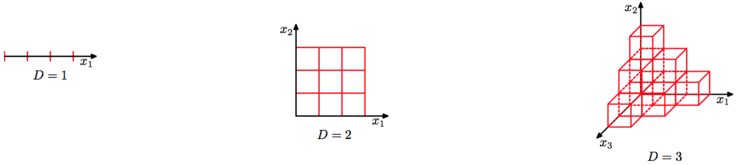

"Bag-of-Words" representation:

$x = \{0, 3, 0, 0, 1, ..., 2, 3, 0, 0, 0, 1\}$ one entry per word!

Easily 50,000 words! Very sparse - easy to overfit!

What is curse of dimensionality

Number of cells grows exponentially as dimensionality increases



\# of cells r^D

r: number of divisions in each dimension

- Large number of cells, even if D is moderately large
- So to cover the whole space reasonably well, you need exponentially number of training data points

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Dimensionality Reduction

Broader question

- How can we detect low dimensional structure in high dimensional data?

Motivations

- Exploratory data analysis & visualization: you can plot data now
- Compact representation: small memory/computational footprint, lossy data compression
- Robust statistical modeling: curse of dimensionality

Dimensionality Reduction

General rules of dimensionality reduction

- Relevant features: the features that we need to perform well
- Irrelevant features: the features that are unnecessary
- Redundant features: the features that that become irrelevant in the presence of others

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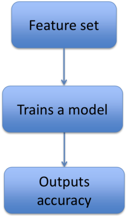
Feature selection

Wrappers

- Rely on a feature search strategy to find an “optimal” subset of features based on the performance of the classifier
- Pros
    - High accuracy
    - Specific to the classifier of interest
- Cons
    - Computationally expensive



Feature selection

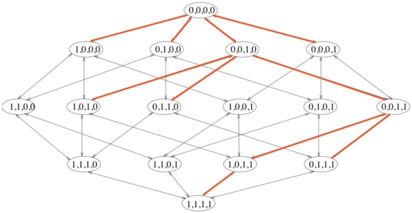
Wrappers - Possible feature search strategies

- Exhaustive search
    - Try all possible feature combinations
    - M features $\rightarrow 2^M$ possible subsets
- Sequential forward selection
    - Greedy incremental selection of best performing features
- Recursive backward elimination
    - Starting from the full feature set, greedy selection of features which hurt performance
- Genetic algorithms
    - Random selection of features
    - Update of feature selection probabilities based on performance metrics

Feature selection

Wrappers: Sequential Feature Selection

- Cost is $M + (M-1) + \ldots + 1 = \frac{M(M+1)}{2}$, instead of 2^M



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Feature selection

Filters

- We only pick the most informative features for the outcome
- We do not run a machine learning model
- We rank features according to their information and choose a cut-off point
- Pros
  - Computationally cheap
- Cons
  - No feature interaction is taken into account
  - Machine learning model is not taken into account

k	$J(X_k)$
35	0.846
42	0.811
10	0.810
654	0.611
22	0.443
59	0.388
...	...
212	0.09
39	0.05

Feature selection

Filters - Possible feature evaluation metrics

- Correlation of feature x_k with target variable y

$$\rho(x_k, y) = \frac{Cov(x_k, y)}{Var(x_k)Var(y)}$$

  Measures linear dependencies

- Mutual information of feature x_k with target variable y

$$I(x_k, y) = \sum_i \sum_j P(x_k = i, y = j) \frac{P(x_k = i, y = j)}{P(x_k = i)P(y = j)}$$

  where P is the probability estimate from the data
  Assumes known probability distribution of the data.

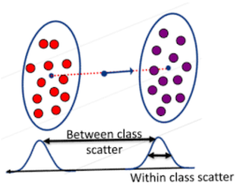
Feature selection

Filters - Possible feature evaluation metrics

- Fisher's criterion of feature d of sample $\mathbf{x_n}$ from class k

$$F(d) = \frac{\sum_k \sum_{\mathbf{x_n} \in C_k} (x_{nd} - \mu_{kd})^2}{\sum_k (\mu_d - \mu_{kd})^2}$$

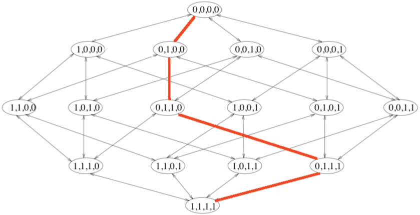
where μ_{kd} is the mean of feature d from class k, and μ_d is the mean of feature d from all samples
Measures within-class scatter in relation to between-class scatter



Feature selection

Filters

- A lot less expensive



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Feature selection

Embedded methods

- The classifier performs feature selection as part of the learning procedure
- Regularization is a great example

$$J(\mathbf{w}) = EC(\mathbf{w}) + \lambda \sum_{d=1}^{D} w_d^2 = EC(\mathbf{w}) + \lambda \|\mathbf{w}\|_2^2$$

- Pros
  - Feature selection is part of learning the procedure
- Cons
  - Computationally demanding

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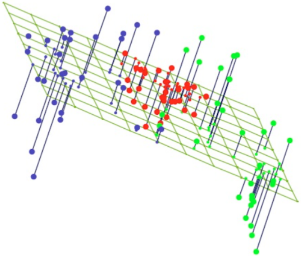
Feature transformation

Linear feature transformation

- $\mathbf{x} \in \mathbb{R}^D \rightarrow \mathbf{y} \in \mathbb{R}^M$, $D \gg M$
- linear transformation of original space: $\mathbf{y} = \mathbf{U}^T \mathbf{x}$, $\mathbf{U} \in \mathbb{R}^{D \times M}$



Feature transformation

Linear feature transformation: Example

Assuming an input vector $\mathbf{x} = [x_1, x_2] \in \mathbb{R}^2$ and a transformation $\mathbf{U}\mathbf{x}$, what transformation do each of the following matrices perform?

If $\mathbf{U}\mathbf{x} = \begin{bmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{bmatrix}$, then $\mathbf{U}\mathbf{x} = \begin{bmatrix} u_{11}x_1 + u_{12}x_2 \\ u_{21}x_1 + u_{22}x_2 \end{bmatrix}$.

If $\mathbf{U}\mathbf{x} = \begin{bmatrix} u_{11} & u_{12} \end{bmatrix}$, then $\mathbf{U}\mathbf{x} = \begin{bmatrix} u_{11}x_1 + u_{12}x_2 \end{bmatrix}$.

1. $\mathbf{U} = [1, 0; 0, 1]$
2. $\mathbf{U} = [1.5, 0; 0, 1.5]$
3. $\mathbf{U} = [0, 1; 1, 0]$
4. $\mathbf{U} = [1, 0]$
5. $\mathbf{U} = [1, 1]$
6. $\mathbf{U} = [1, 1; 0, 1]$

Feature transformation

Linear feature transformation: Example

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If $\mathbf{Ux} = \begin{bmatrix} u_{11} & u_{12} \end{bmatrix}$, then $\mathbf{Ux} = \begin{bmatrix} u_{11}x_1 + u_{12}x_2 \end{bmatrix}$.

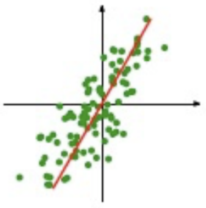
1. $\mathbf{U} = [1, 0; 0, 1]$ Identity
2. $\mathbf{U} = [1.5, 0; 0, 1.5]$ Dilation
3. $\mathbf{U} = [0, 1; 1, 0]$ Flipping of axes
4. $\mathbf{U} = [1, 0]$ Preserving only first dimension
5. $\mathbf{U} = [1, 1]$ Substituting the first dimension by the sum of the two. Removing the second dimension.
6. $\mathbf{U} = [1, 1; 0, 1]$ Substituting the first dimension by the sum of the two. Preserving the second dimension.

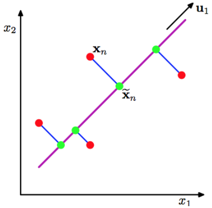
Principal Component Analysis (PCA): Representation

- Input: Data $\mathcal{D} = \{\mathbf{x_1}, \ldots, \mathbf{x_N}\}$, $\mathbf{x_n} \in \mathbb{R}^D$,centered inputs
- Output: Projected data $\{\mathbf{y_1}, \ldots, \mathbf{y_N}\}$, $\mathbf{y_n} \in \mathbb{R}^M$, $D \gg M$
- Projection into subspace: $\mathbf{U} \in \mathbb{R}^{D \times M}$

$$\mathbf{y_n} = \mathbf{U}^T \mathbf{x_n} \ , \quad \mathbf{U}^T \mathbf{U} = \mathbf{I}$$

- Evaluation metric: many possible metrics yielding the same solution
  - Derivation 1: Maximize captured variance
  - Derivation 2: Minimize projection error

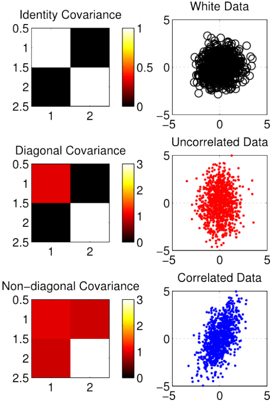




Covariance Matrix

For 2-dimensional samples $\mathbf{x_n} = [x_{n1}, x_{n2}]^T$, we assume means μ_1 and μ_2 for dimensions 1 and 2.

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sum_{n=1}^{N} (x_{n1} - \mu_1)^2 & \sum_{n=1}^{N} (x_{n1} - \mu_1)(x_{n2} - \mu_2) \\ \sum_{n=1}^{N} (x_{n1} - \mu_1)(x_{n2} - \mu_2) & \sum_{n=1}^{N} (x_{n2} - \mu_2)^2 \end{bmatrix}$$



Matrix Diagonalization

- Converting a square matrix into a special type of matrix, i.e. diagonal, which shares the same fundamental properties of the underlying matrix
- Eigen-decomposition theorem: A square matrix $\mathbf{A} \in \mathbb{R}^{D \times D}$ can be decomposed into

$$\mathbf{A} = \mathbf{P}\boldsymbol{\Lambda}\mathbf{P}^{-1}$$

  - $\boldsymbol{\Lambda} = \text{diag}(\lambda_1, \ldots, \lambda_D)$: diagonal constructed from eigenvalues of $\mathbf{A}$
  - $\mathbf{P} = \begin{bmatrix} | & & | \\ \mathbf{e_1} & \ldots & \mathbf{e_D} \\ | & & | \end{bmatrix} \in \mathbb{R}^{M \times M}$: matrix decomposed from the eigenvectors of $\mathbf{A}$

Matrix Diagonalization

- Assuming that we have a matrix equation $\mathbf{AX} = \mathbf{Y}$
- This can be written as $\mathbf{P\Lambda P}^{-1}\mathbf{X} = \mathbf{Y}$
- Multiplying both sides by $\mathbf{P}^{-1}$ we get $\mathbf{\Lambda P}^{-1}\mathbf{X} = \mathbf{P}^{-1}\mathbf{Y}$
- The same linear transformation $\mathbf{P}^{-1}$ is being applied to $\mathbf{X}$ and $\mathbf{Y}$, therefore we can transform the equation into another space $\mathbf{X}' = \mathbf{P}^{-1}\mathbf{X}$ and $\mathbf{Y}' = \mathbf{P}^{-1}\mathbf{Y}$
- Now the new system that we have to solve it $\mathbf{PX}' = \mathbf{Y}'$
- The most important advantage of this transformation is that it decorrelates the matrices (i.e., "canonicalizes" the system), therefore some computations might be easier of less expensive

Principal Component Analysis (PCA): Optimization

- Compute covariance matrix

$$\mathbf{S} = \frac{1}{N}\mathbf{X}^T\mathbf{X}\,, \quad \mathbf{X} = \begin{bmatrix} - \tilde{\mathbf{x}}_\mathbf{1}^T - \\ \vdots \\ - \tilde{\mathbf{x}}_\mathbf{N}^T - \end{bmatrix}$$

$$\mathbf{U} \in \mathbb{R}^{D \times M}$$

- Diagonalize S, i.e. compute eigenvalues and eigenvectors

$$\mathbf{S} = \mathbf{P}\Lambda\mathbf{P}^{-1}\,, \quad \mathbf{P} = \begin{bmatrix} | & & | \\ \mathbf{u_1} & \dots & \mathbf{u_D} \\ | & & | \end{bmatrix} \in \mathbb{R}^{D \times D}$$

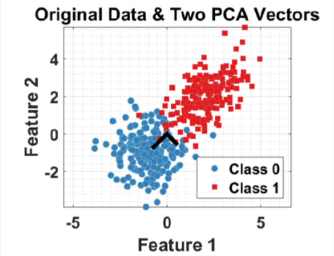
- Use the eigenvectors corresponding to the M largest eigenvalues

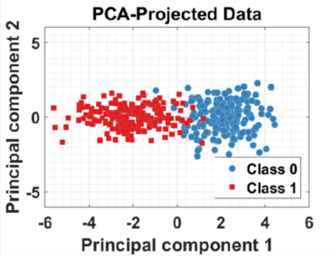
$$\mathbf{U} = \begin{bmatrix} | & & | \\ \mathbf{u_1} & \dots & \mathbf{u_M} \\ | & & | \end{bmatrix} \in \mathbb{R}^{D \times M}$$

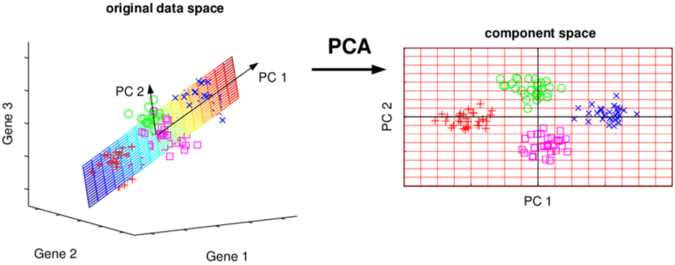
Principal Component Analysis (PCA): Algorithm

- Step 0: Mean normalize input features
- Step 1: Compute covariance matrix $\mathbf{S} = \frac{1}{N}\mathbf{X}^T\mathbf{X} = \frac{1}{N}\sum_n \mathbf{x_n}\mathbf{x_n}^T$
- Step 2: Diagonalize $\mathbf{S}$ and find eigenvector matrix $\mathbf{P}$
- Step 3: Take the first $M \ll D$ eigenvectors or *principal components* (corresponding to the M largest eigenvalues) and form reduced matrix $\mathbf{U}$
- Step 3: Project data into reduced space: $\mathbf{z_n} = \mathbf{U}^T\mathbf{x_n}$

Principal Component Analysis (PCA): Example







Principal Component Analysis (PCA)

Original Images

Eigenvectors

they look like blurred original images

Mean $\quad \lambda_1 = 3.4 \cdot 10^5 \quad \lambda_2 = 2.8 \cdot 10^5 \quad \lambda_3 = 2.4 \cdot 10^5 \quad \lambda_4 = 1.6 \cdot 10^5$

Used to centralize inputs

Principal Component Analysis (PCA)

How to determine the number of principal components M?

Plot eigenspectrum

$$\frac{\sum_{d=1}^{M} \lambda_d}{\sum_{d=1}^{D} \lambda_d} \geq \text{threshold}, \text{ where common choices are } 95\%, 99\%$$

https://www.freecodecamp.org/news/an-overview-of-principal-component-analysis-6340e3bc4073/

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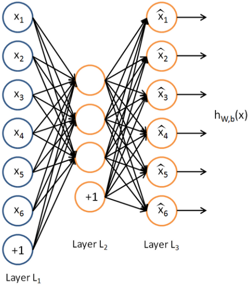
Autoencoders

- Unsupervised algorithm that tries to learn an approximation of the identity function $h_{\mathbf{W},\mathbf{b}}(x) \approx \mathbf{x}$
- The middle layer of the autoencoder can be used as the transformed feature set



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Clustering

- Grouping of "similar" instances in the data sample
- Replacing a high dimensional data entry with a cluster label
- Deterministic clustering (e.g., K-Means) gives only one label per input
- Soft clustering gives probability of a sample belonging to each cluster
- More in the next lecture!

What have a learned so far

- Dimensionality reduction for visualization, compression, avoid curse of dimensionality
- Feature selection to select the most informative features
- Feature transformation to transform the features into a reduced space
- **Readings:** Alpaydin 6.1-6.3