COMPSCI361: Machine Learning

Data Preprocessing

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SCIENCE
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Data Preprocessing

This lecture will cover

Data Preprocessing

- Data Reduction
  - Dimensionality Reduction
  - Principal Components Analysis
  - Feature Selection

Data Reduction

Data Reduction

- Data reduction: Obtain a reduced representation of the data set that is much smaller in volume but yet produces the same (or almost the same) analytical results
- Why data reduction? – A database may store terabytes of data, complex data analysis may take a very long time to run on the complete data set
- Data reduction strategies
  - Dimensionality reduction
    - Wavelet transforms
    - Principal Components Analysis (PCA)
    - Feature selection
  - Numerosity reduction
    - Regression and Log-Linear Models
    - Histograms, clustering, sampling
  - Data compression

Dimensionality Reduction

- Curse of dimensionality

x_1	x_2	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	x_n
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	11	12	22	24
0	0	0	0	0	0	0	0	0	0	0	74	38	99	2	4	0	0	0	0	0
0	0	0	0	0	0	0	0	84	69	55	0	0	0	0	0	0	0	0	0	0
0	0	0	0	66	35	14	62	0	0	0	0	0	0	0	0	0	0	0	0	0
32	48	54	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...

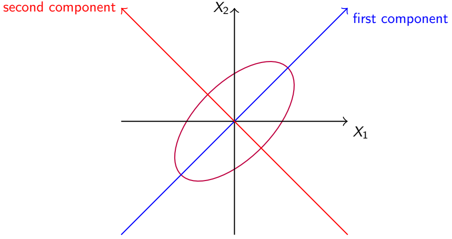
- When dimensionality increases, data becomes increasingly sparse
- Density and distance between points, which is critical to clustering, outlier analysis, classification, regression becomes less meaningful

Dimensionality Reduction

- Why dimensionality reduction?
  - Avoid the curse of dimensionality
  - Help eliminate irrelevant/redundant features and reduce noise
  - Reduce computational resources (memory and time)
  - Allow easier visualization
- Dimensionality reduction techniques
  - Unsupervised linear method: Principal Component Analysis
  - Supervised method: Feature selection

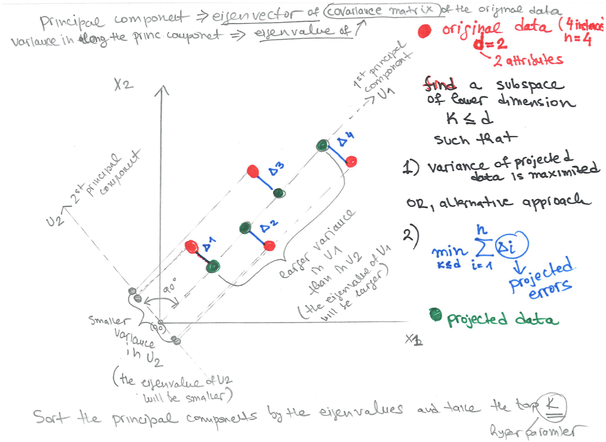
Principal Component Analysis – PCA

- Find a projection that captures the largest amount of variation in data
- The original data are projected onto a much smaller space
- How? – We find the eigenvectors and eigenvalues of the covariance matrix of the input attributes,
  - Eigenvectors: the directions that data variances occur, and they define the new attribute space
  - Eigenvalues: the amount of variance along the corresponding eigenvector



Demo: `https://setosa.io/ev/principal-component-analysis/`

PCA approaches



Detailed theoretical explanation of the two approaches in reference 2

PCA – steps

- Given n data instances (each a vector in d-dimensions), find $k \leq d$ principal components that can be best used to represent the data
  - Normalize input data: Each attribute falls within the same range
  - Compute k orthonormal vectors (i.e. length of 1 and perpendicular to each other), i.e. principal components
  - The input data is a linear combination of the k principal component vectors
  - The principal components are sorted in order of decreasing "significance" or strength (e.g. as measured by the eigenvalue)
  - Since the components are sorted, the size of the data can be reduced by eliminating the $d - k$ weak components, i.e. those with low variance.
- The resulting vectors are orthogonal, are they correlated? No
- Can you use PCA on categorical data? Yes

Example code step by step PCA calculation in Python in reference 3

Feature or Attribute Selection

Reduce dimensionality by removing set of attributes

- Redundant attributes
  - Duplicate much or all of the information contained in one or more other attributes
    e.g. purchase price of a product and the amount of sales tax paid
- Irrelevant attributes
  - Contain no information that is useful for the data mining task at hand
    e.g. students' ID is often irrelevant to the task of predicting students' GPA

Two types of methods: Filters (fast) and Wrappers (high accuracy, expensive)

- Filters separate feature selection from classifier learning. No bias toward any learning algorithm

Feature Selection using Correlation

- For nominal data, given two attributes A and B with values $a_1, \ldots, a_c$ and $b_1, \ldots, b_r$ the correlation can be calculated using the χ^2 test:

$$\chi^2 = \sum_{i=1}^{c} \sum_{j=1}^{r} \frac{(o_{ij} - e_{ij})^2}{e_{ij}}$$

  - With o_{ij} being the actual frequency of the event (a_i, b_j)
  - And e_{ij} the expected frequency (n is the number of instances)

$$e_{ij} = \frac{count(A = a_i) \times count(B = b_j)}{n}$$

Feature Selection using Correlation

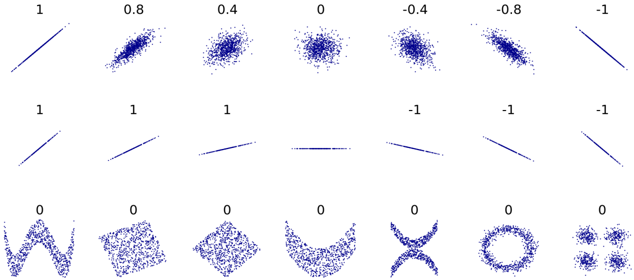
- Numerical data can be compared using Pearson's correlation coefficient

$$\rho_{A,B} = \frac{\sum_{i=1}^{n}(a_i - \bar{A})(b_i - \bar{B})}{n\sigma_A\sigma_B} = \frac{\sum_{i=1}^{n}(a_i b_i) - n\bar{A}\bar{B}}{n\sigma_A\sigma_B}$$

- With means $\bar{A}$ and $\bar{B}$, number of instances n, and standard deviations σ_A and σ_B
- If σ_A and σ_B is zero than the coefficient is undefined.
- Values in the range [-1, 1].

Feature Selection using Correlation

- So what does the correlation measure?



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- How can it be used to remove redundant or unimportant features?

Heuristic Search in Attribute Selection

- There are 2^{d-1} possible attribute combinations of d attributes
  $\rightarrow$ exhaustive search is not feasible (e.g. $d = 300, 2.04x10^{90}$ combinations)
- Typical heuristic attribute selection methods:
  - Best single attribute under the attribute independence assumption
  - Best step-wise feature selection:
    - The best single-attribute is picked first
    - Then next best attribute condition to the first, ...
  - Step-wise attribute elimination:
    - Repeatedly eliminate the worst attribute
  - Best combined attribute selection and elimination
  - Optimal branch and bound:
    - Use attribute elimination and backtracking

Relief - Instance-based heuristic for feature selection

Input: Data set with n_d input attributes and n instances that bellong to one of two classes (i.e.binary classification problem), and number of randomly selected insatnces $n_r \leq n$

First normalize the input attributes

Create a weight vector W with one weight $w_i \in W$ for each attribute

Initialize the weights $W = [w_1, w_2, \ldots, w_n] = 0$

for $j \in 1 \ldots n_r$ **do**

  Randomly select instance $R = [r_1, \ldots, r_n]$

  Choose instance $H = [h_1, \ldots, h_n]$ as the closest neighbour of R in the same class (*nearHit*) w.r.t to some (Euclidian) distance measure

  Choose instance $M = [m_1, \ldots, m_n]$ as the closest neighbour of R in the other class (*nearMiss*) w.r.t to some (Euclidian) distance measure

  for $i \in 1 \ldots n_d$ **do**

    % update the weights $w_i = w_i + distance(R, M; \text{i-th attribute}) - distance(R, H; \text{i-th attribute})$

    $w_i = w_i + (r_i - m_i)^2 - (r_i - h_i)^2$ % Euclidian distance

  end

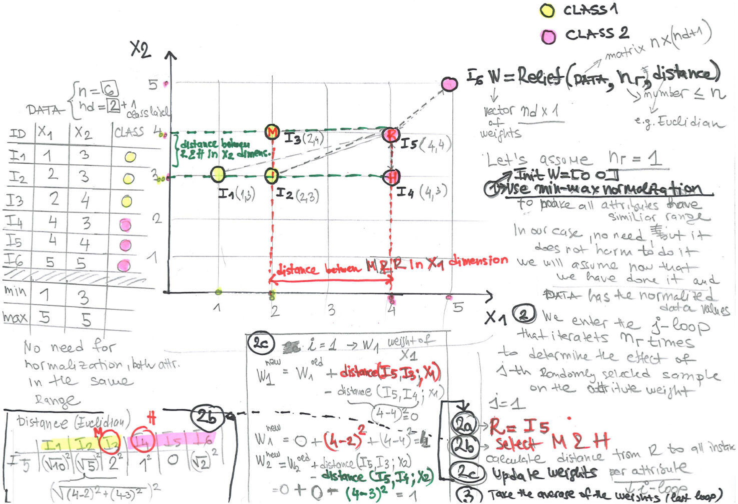
end

for $i \in 1 \ldots n_d$ **do**

  return $w_i = \dfrac{w_i}{n_r}$

end

Relief Example



Relief Example (cont.)

In our case $n_r = 1$, so no more iterations in the j-loop

We go to the last step ③

$$W = \begin{array}{cc} x_1 & x_2 \\ [4 & 1] \end{array}$$ before step ③

$$W = \left[\frac{4}{\underbrace{1}_{=n_r}} \quad \frac{1}{\underbrace{1}_{=n_r}}\right]$$ after step ③ → no change as only one random sample was selected

You can use these weights to rank the attributes

Larger weight more important

In our case $\boxed{X_1 \text{ is the more important}}$

Easy to verify: from the plot we can see that we can use only X_1 to create decision boundary that will separate the ○ samples from the ○ samples

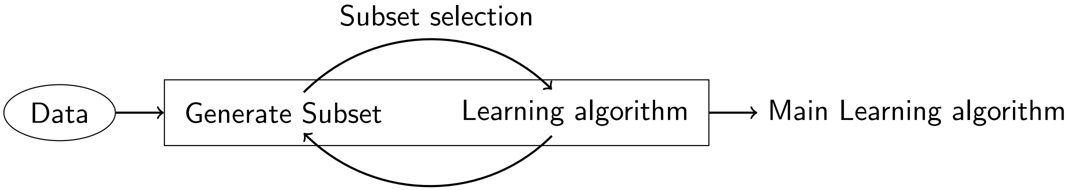
Also note that the variance in the data is larger in the X_1 dimension (link to PCA 2 projections approach)

Relief summary

- Relief takes into account **all** attributes
- Result is a weight vector that represents the importance of each feature
- Features are then selected based on a threshold τ or ranked
- The algorithm above is the basic version of Relief, there are various extensions (ReliefF, RReliefF,...)

Wrappers

- The correlation method and Relief are filters
- Main idea of wrappers:
  - Generate a subset of the features and evaluate the performance of the classifier on the subset
  - Add or remove attributes from the subset and see if the performance of the classifier improves
  - Risk of overfitting, especially if choosing the same classifier as for the main learning task



Preprocessing

- So, to summarize...
  - When are preprocessing approaches useful?
  - When should you avoid them?
  - How about specific cases
    - Many correlated features?
    - Many independent features?
    - Which algorithms you know already would need preprocessing?
    - How about Decision trees? Why?
    - How about Regression? Why?
  - Are we cheating in preprocessing: for example by creating new examples?

Conclusion

- Preprocessing is an important part in machine learning and data analysis
- Missing values can be caused by various reasons depending on what the reasons are, they must be addressed differently
- Various imputation approaches exist, they use the information of other instances and values to impute the missing values
- Noisy data can be addressed for example by binning, clustering, or regression
- Feature selection can be used to reduce the number of redundant and unimportant features
- Imbalanced data sets can be a problem for evaluation and classifiers
- Sampling can be used to overcome class imbalance problems

Literature & other resources

1. Material in Chapter 3 in Han's *Data Mining*
2. Detailed math and application of PCA: Chapter 12.1 and Appendix C Bishop's *Pattern Recognition and Machine Learning*
3. Step by step code on PCA calculation (Python notebook on Canvas)
4. Example code on using sckit-learn PCA implementation `https://colab.research.google.com/github/cpearce/PythonDataScienceHandbook/blob/master/notebooks/05.09-Principal-Component-Analysis.ipynb`

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Thank you for your attention!

`https://ml.acukland.ac.nz`