Unsupervised machine learning

Statistical Natural Language Processing

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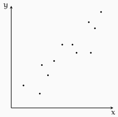
Supervised learning

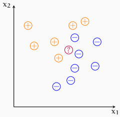
- The methods we studied so far are instances of supervised learning
- In supervised learning, we have a set of predictors $\mathbf{x}$, and want to predict a response or outcome variable y
- During training, we have both input and output variables
- Training consist of estimating parameters $\boldsymbol{w}$ of a model
- During prediction, we are given $\mathbf{x}$ and make predictions based on model we learned

Supervised learning: regression



- The response (outcome) variable (y) is a quantitative variable.
- Given the features ($\mathbf{x}$) we want to predict the value of y

Supervised learning: classification



- The response (outcome) is a label. In the example: positive ⊕ or negative ⊖
- Given the features (x_1 and x_2), we want to predict the label of an unknown instance ?

Supervised learning

how do we learn?

- The aim is to estimate a set of parameters $\boldsymbol{w}$
- We define an *objective function*, and find the parameter values that minimize the objective
- The objective typically involves reducing the training error defined based on the true labels in the training data

Unsupervised learning

- In unsupervised learning, we do not have labels in our training data
- Our aim is to find useful patterns/structure in the data
  - for exploratory study of the data
  - for augmenting / complementing supervised methods
- Close relationships with ‘data mining’, ‘data science / analytics’, ‘knowledge discovery’
- Most unsupervised methods can be cast as graphical models with hidden variables
- Evaluation is difficult: we do not have ‘true’ labels/values

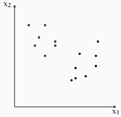
Today’s lecture

- *Clustering*: find related groups of instances
- *Density estimation*: find a probability distribution that explains the data
- *Dimensionality reduction*: find an accurate/useful lower dimensional representation of the data
- Unsupervised learning in ANNs (RBMs, autoencoders)

Clustering: why do we do it?

- The aim is to find groups of instances/items that are similar to each other
- Applications include
  - Clustering languages, dialects for determining their relations
  - Clustering (literary) texts, for e.g., authorship attribution
  - Clustering words for e.g., better parsing
  - Clustering documents, e.g., news into topics
  - ...

Clustering in two dimensional space



- Unlike classification, we do not have labels
- We want to find ‘natural’ groups in the data
- Intuitively, similar or closer data points are grouped together

Similarity and distance

- The notion of distance (similarity) is important in clustering. A distance measure D,
  - is symmetric: $D(a, b) = D(b, a)$
  - non-negative: $D(a, b) \geqslant 0$ for all a, b, and it $D(a, b) = 0$ iff $a = b$
  - obeys triangle inequality: $D(a, b) + D(b, c) \geqslant D(a, c)$
- The choice of distance is application specific
- We will often face with defining distance measures between linguistic units (letters, words, sentences, documents, ...)

Distance measures in Euclidean space

- Euclidean distance:

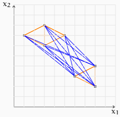
$$\|\mathbf{a} - \mathbf{b}\| = \sqrt{\sum_{j=1}^{k} (a_j - b_j)^2}$$

- Manhattan distance:

$$\|\mathbf{a} - \mathbf{b}\|_1 = \sum_{j=1}^{k} |a_j - b_j|$$

How to do clustering

Most clustering algorithms try to minimize the scatter within each cluster. Which is equivalent to maximizing the scatter between clusters.



$$\sum_{k=1}^{K} \sum_{a \in C_k} \sum_{b \in C_k} d(a, b)$$

$$\sum_{k=1}^{K} \sum_{a \in C_k} \sum_{b \notin C_k} d(a, b)$$

K-means algorithm

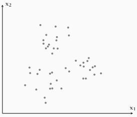
K-means is a popular method for clustering.

1. Randomly choose *centroids*, $m_1, \ldots, m_K$, representing K clusters
2. Repeat until convergence
   - Assign each data point to the cluster of the nearest centroid
   - Re-calculate the centroid locations based on the assignments

Effectively, we are finding a *local minimum* of the sum of squared Euclidean distance within each cluster

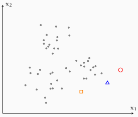
$$\frac{1}{2}\sum_{k=1}^{K}\sum_{a\in C_k}\sum_{b\in C_k}\|a-b\|^2$$

K-means clustering: visualization



- The data
- Set cluster centroids randomly
- Assign data points to the closest centroid
- Recalculate the centroids

K-means clustering: visualization



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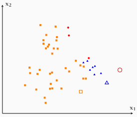
K-means clustering: visualization



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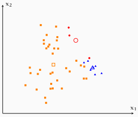

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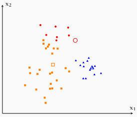

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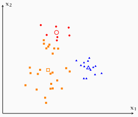
K-means clustering: visualization



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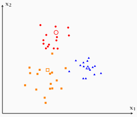
K-means clustering: visualization



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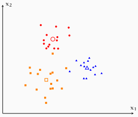
K-means clustering: visualization



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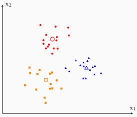
K-means clustering: visualization



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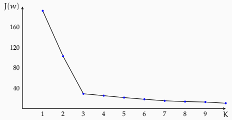
K-means: some issues

- K-means requires the data to be in an Euclidean space
- K-means is sensitive to outliers
- The results are sensitive to initialization
  - There are some smarter ways to select initial points
  - One can do multiple initializations, and pick the best (with lowest within-group squares)
- It works well with approximately equal-size round-shaped clusters
- We need to specify number of clusters in advance

How many clusters?

- The number of clusters is defined for some problems, e.g., classifying news into a fixed set of topics/interests
- For others, there is no clear way to select the best number of clusters
- The error (within cluster scatter) decreases with increasing number of clusters, using a test set or cross validation is not useful either
- A common approach is clustering for multiple K values, and picking where there is an 'elbow' in the graph of the error function

How many clusters?



This plot is sometimes called a *scree plot*.

K-medoids

- K-medoids algorithm is an alternation of K-means
- Instead of calculating centroids, we try to find most typical data point (medoids) at each iteration
- K-medoids can work with distances, does not need feature vectors to be in an Euclidean space
- It is less sensitive to outliers
- It is computationally more expensive than K-means

Hierarchical clustering

- Instead of a flat division to clusters as in K-means, hierarchical clustering builds a hierarchy based on similarity of the data points
- There are two main 'modes of operation':

Bottom-up or *agglomerative* clustering
- starts with individual data points,
- merges the clusters until all data is in a single cluster

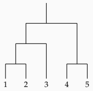
Top-down or *divisive* clustering
- starts with a single cluster,
- and splits until all leaves are single data points

Hierarchical clustering

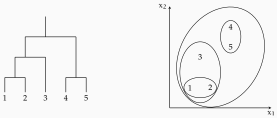
- Hierarchical clustering operates on distances (or similarities)
- The result is a binary tree called *dendrogram*
- Dendrograms are easy to interpret (especially if data is hierarchical)
- The algorithm does not commit to the number of clusters K from the start, the dendrogram can be 'cut' at any height for determining the clusters

Agglomerative clustering

1. Compute the similarity/distance matrix
2. Assign each data point to its own cluster
3. Repeat until no clusters left to merge
   - Pick two clusters that are most similar to each other
   - Merge them into a single cluster

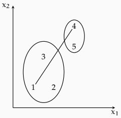


Agglomerative clustering demonstration



How to calculate between cluster distances

Complete maximal inter-cluster distance
Single minimal inter-cluster distance
Average mean inter-cluster distance
Centroid distance between the centroids



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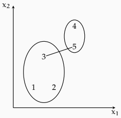

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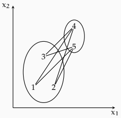

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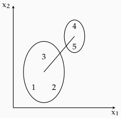


Note: we only need distances, (feature) vectors are not necessary

Clustering evaluation

Evaluating clustering results is often non-trivial

- Internal evaluation is based a metric that aims to indicate 'good clustering': e.g., *Dunn index*, *gap statistic*, *silhouette*
- External metrics can be useful if we have labeled *test* data: e.g., *V-measure*, B^3*ed F-score*
- The results can be tested on the target application: e.g., word-clusters evaluated based on their effect on parsing accuracy
- Human judgments, manual evaluation – 'looks good to me'

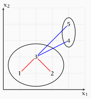
Clustering evaluation

internal metric example: silhouette

$$s_i = \frac{b(i) - a(i)}{\max(a(i), b(i))}$$

where

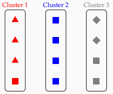
$a(i)$ average distance between object i and and objects in the same cluster
$b(i)$ average distance between object i and and objects in the *closest* cluster



Clustering evaluation

external metrics: general intution

- We want clusters that contain members of a single gold-standard class (homogeniety)
- We want all members of a class to be in a single cluster (completeness)



Note the similarity with precision and recall.

Clustering: some closing notes

- We do not have proper evaluation procedures for clustering results (for unsupervised learning in general)
- Some clustering methods are unstable, slight changes in the data or parameter choices may change the results drastically
- Approaches against instability include some validation methods, or producing 'probabilistic' dendrograms by running clustering with different options

Density estimation

- K-means treats all data points in a cluster equally
- A 'soft' version of K-means is density estimation for Gaussian mixtures, where
  - We assume the data comes from a mixture of K Gaussian distributions
  - We try to find the parameters of each distribution (instead of centroids) that maximizes the likelihood of the data
- Unlike K-means, mixture of Gaussians assigns probabilities for each data point belonging to one of the clusters
- It is typically estimated using the expectation-maximization (EM) algorithm

Density estimation using the EM algorithm

- The EM algorithm (or its variations) is used in learning models with latent/hidden variables
- It is closely related to the K-means algorithm

1. Initialize the parameters (e.g., randomly) of K multivariate normal distributions $(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
2. Iterate until convergence:

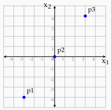
E-step Given the parameters, compute the membership 'weights', the probability of each data point belonging to each distribution

M-step Re-estimate the mixture density parameters using the calculated membership weights in the E-step

Principal component Analysis

- Principal component analysis (PCA) is a method of *dimensionality reduction*
- PCA maps the original data into a lower dimensional space by a linear transformation (rotation)
- The transformed lower-dimensional variables retain most of the variation (=information) in the input
- PCA can be used for
  - visualization
  - data compression
  - reducing dimensionality of features for other machine learning methods
  - eliminating noise

PCA: a toy example



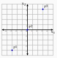
Questions:

- How many dimensions do we have?
- How many dimensions do we need?
- Short divergence: calculate the covariance matrix

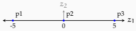
$$\Sigma = \begin{bmatrix} \frac{18}{3} & 8 \\ 8 & \frac{32}{3} \end{bmatrix}$$

  - What is the correlation between x_1 and x_2?

PCA: A toy example (2)



What if we reduce the data to:



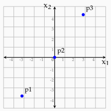
Going back to the original coordinates is easy, rotate using:

$$A = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} = \begin{bmatrix} \frac{3}{5} & -\frac{4}{5} \\ \frac{4}{5} & \frac{3}{5} \end{bmatrix}$$

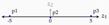
$$p1 = A \times \begin{bmatrix} -5 \\ 0 \end{bmatrix} = \begin{bmatrix} -3 \\ -4 \end{bmatrix} \quad p2 = A \times \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} p3 = A \times \begin{bmatrix} 5 \\ 0 \end{bmatrix} = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$$

We can recover the original points perfectly. In this example the inherent dimensionality of the data is only 1.

PCA: A toy example (3)



- What if the variables were not perfectly but strongly correlated?
- We could still do a similar transformation:



- Discarding z_2 results in a small reconstruction error:

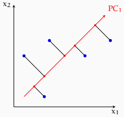
$$p1 = A \times \begin{bmatrix} -5 \\ 0 \end{bmatrix} = \begin{bmatrix} -3 \\ -4 \end{bmatrix}$$

- Note: z_1 (also z_2) is a linear combination of original variables

Why do we want to reduce the dimensionality

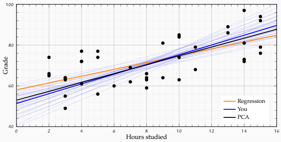
- Visualizing high-dimensional data becomes possible
- If we use the data for other ML methods,
  - we reduce the computation time
  - we may avoid 'the curse of dimensionality'
- Decorrelation is useful in some applications
- We compress the data (in a lossy way)
- We eliminate noise (assuming a high signal to noise ratio)

Different views on PCA



- Find the direction of the largest variance
- Find the projection with the least reconstruction error
- Find a lower dimensional latent Gaussian variable such that the observed variable is a mapping of the latent variable to a higher dimensional space (with added noise)

Aside: your regression estimates and PCA



How to find PCs

- When viewed as *maximizing variance* or *reducing the reconstruction error*, we can write the appropriate objective function and find the vectors that minimize it
- In latent variable interpretation, we can use EM as in estimating mixtures of Gaussians
- The principal components are the eigenvectors of the correlation matrix, where large eigenvalues correspond to components with large variation
- A numerically stable way to obtain principal components is doing *singular value decomposition* (SVD) on the input data

PCA as matrix factorization (eigenvalue decomposition)

- One can compute PCA by decomposing the covariance matrix as (note $\mathbf{\Sigma} = \mathbf{X}^T\mathbf{X}$)

$$\mathbf{\Sigma} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$$

  - the columns of $\mathbf{U}$ are the principal components (eigenvectors)
  - $\mathbf{\Lambda}$ is a diagonal matrix of eigenvalues
- Another option is SVD, which factorizes the input vector (k variables × n data points) as

$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^*$$

  - $\mathbf{U}$ ($k \times k$) contains the eigenvectors as before,
  - $\mathbf{D}$ ($k \times n$) diagonal matrix $\mathbf{D}^2 = \mathbf{\Lambda}$
  - $\mathbf{V}^*$ is a $n \times n$ unitary matrix

* The above is correct for centered variables, otherwise the formulas get slightly more complicated.

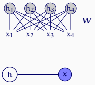
Some practical notes on PCA

- Variables need to be centered
- Scales of the variables matter, standardizing may be a good idea depending on the units/scales of the individual variables
- The sign/direction of the principal component (vector) is not important
- If there are more variables than the data points, we can still calculate the principal components, but there will be at most $n - 1$ PCs
- PCA will be successful if variables are correlated, there are extensions for dealing with nonlinearities (e.g., kernel PCA, ICA, t-SNE)

Unsupervised learning in ANNs

- *Restricted Boltzmann machines* (RBM) similar to the latent variable models (e.g., Gaussian mixtures), consider the representation learned by hidden layers as hidden variables ($\mathbf{h}$), and learn $p(\mathbf{x}, \mathbf{h})$ that maximize the probability of the (unlabeled)data
- *Autoencoders* train a constrained feed-forward network to predict its output

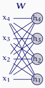
Restricted Boltzmann machines (RBMs)



- RBMs are unsupervised latent variable models, they learn only from unlabeled data
- They are generative models of the joint probability $p(\mathbf{h}, \mathbf{x})$
- They correspond to undirected graphical models
- No links within layers
- The aim is to learn useful features ($\mathbf{h}$)

*Biases are omitted in the diagrams and the formulas for simplicity.

The distribution defined by RBMs



$$p(\mathbf{h}, \mathbf{x}) = \frac{e^{\mathbf{h}^T \mathbf{W} \mathbf{x}}}{Z}$$

This calculation is intractable (Z is difficult to calculate). But conditional distributions are easy to calculate

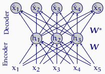
$$p(\mathbf{h}|\mathbf{x}) = \prod_j p(h_j|\mathbf{x}) \quad = \frac{1}{1 + e^{\mathbf{W}_j \mathbf{x}}}$$

$$p(\mathbf{x}|\mathbf{h}) = \prod_k p(x_k|\mathbf{h}) \quad = \frac{1}{1 + e^{\mathbf{W}_k^T \mathbf{h}}}$$

Learning in RBMs

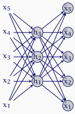
- We want to maximize the probability the model assigns to the input, $p(\mathbf{x})$, or equivalently minimize $-\log p(\mathbf{x})$
- In general, this is computationally expensive
- *Contrastive divergence algorithm* is a well known algorithm that efficiently finds an approximate solution

Autoencoders



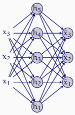
- Autoencoders are standard feed-forward networks
- The main difference is that they are trained to predict their input (they try to learn the identity function)
- The aim is to learn useful representations of input at the hidden layer
- The weights are often shared/tied ($W^* = W^T$)

Under-complete autoencoders



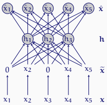
- An autoencoder is said to be *under-complete* if there are fewer hidden units than inputs
- The network is forced to learn a compact representation of the input (compress)
- An autoencoder with a single hidden layer approximates the PCA
- We need multiple layers for learning non-linear features

Over-complete autoencoders



- An autoencoder is said to be *over-complete* if there are more hidden units than inputs
- The network can normally memorize the input perfectly
- This type of networks are useful if trained with a regularization term resulting in sparse hidden units (e.g., L1 regularization)

Denoising autoencoders



- Instead of providing the exact input, we introduce noise by
  - randomly setting some inputs to 0 (dropout)
  - adding random (Gaussian) noise
- Network is still expected to reconstruct the original input (without noise)

Unsupervised pre-training

- A common use case for RBMs and autoencoders are as pre-training methods for supervised networks
- Autoencoders or RBMs are trained using unlabeled data
- The weights learned during the unsupervised learning is used for initializing the weights of a supervised network
- This approach has been one of the reasons for success of deep networks

Summary

- In unsupervised learning, we do not have labels. Our aim is to find/exploit (latent) structure in the data
- Unsupervised methods try to discover 'hidden' structure in the data
  Clustering finds groups in the data
  Density estimation estimates parameters of latent probability distributions
  Dimensionality reduction transforms the data in a low dimensional space while keeping most of the information in the original data

Next:

- Dense vector representations
- Sequence learning