Statistical Natural Language Processing

Unsupervised machine learning

Çağrı Çöltekin

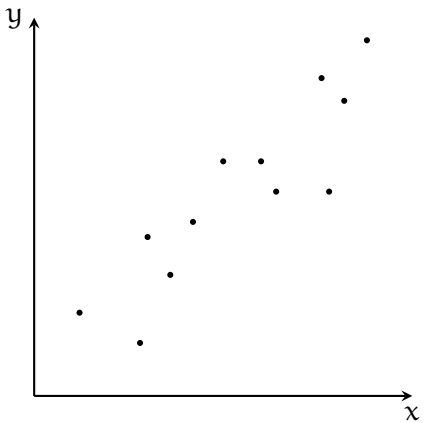
University of Tübingen
Seminar für Sprachwissenschaft

Summer Semester 2019

Supervised learning

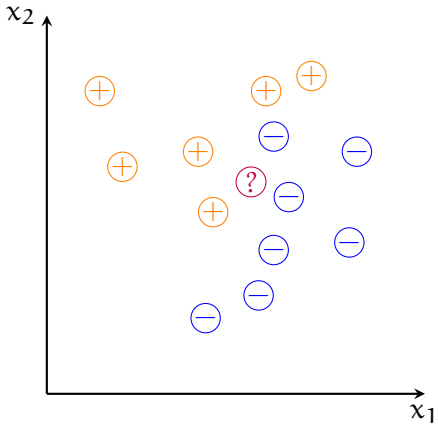
- The methods we studied so far are instances of supervised learning
- In supervised learning, we have a set of predictors $\mathbf{x}$, and want to predict a response or outcome variable $\mathbf{y}$
- During training, we have both input and output variables
- Training consist of estimating parameters $\boldsymbol{w}$ 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 (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 $\boldsymbol{w}$ during training
- We define an *error function*, and find the parameter values that minimize the error
- The error function is 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'
- All unsupervised methods can be cast as graphical models with hidden variables
- Evaluation is difficult: we do not have 'true' labels/values

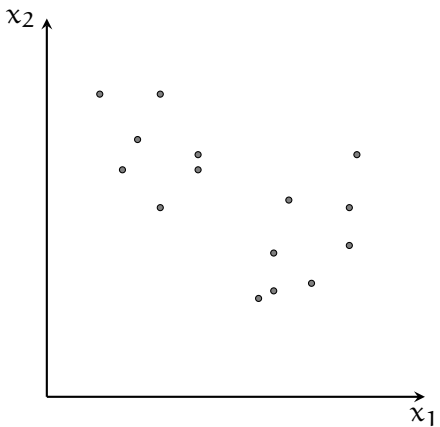
Today's lecture

- *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?

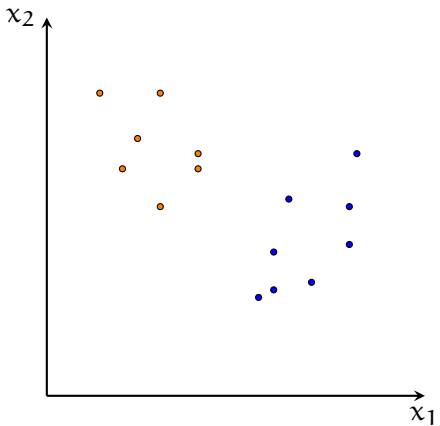
- The aim is to find groups of instances/items that are similar to each other
- Applications include
  - Clustering languages, dialects for determining their relations
  - Clustering (literary) texts, for e.g., authorship attribution
  - Clustering words for e.g., better parsing
  - Clustering documents,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

Clustering in two dimensional space



- Unlike classification, we do not have labels

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:

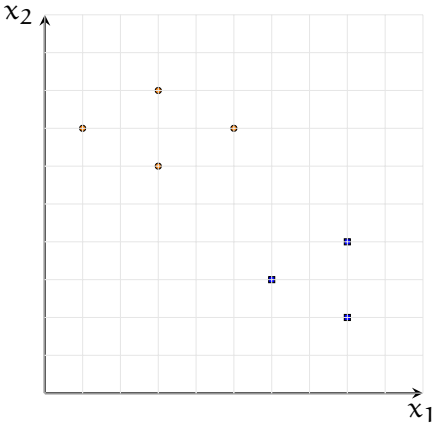
$$\|\mathbf{a} - \mathbf{b}\| = \sqrt{\sum_{j=1}^{k} (a_j - b_j)^2}$$

- Manhattan distance:

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

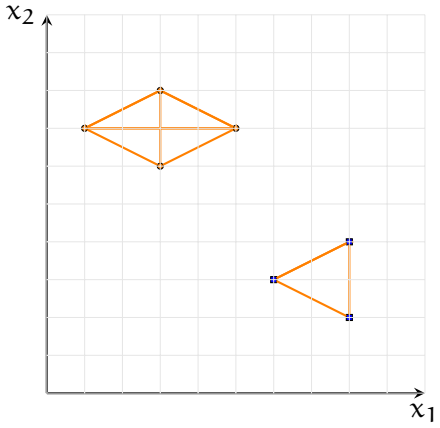
How to do clustering

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



How to do clustering

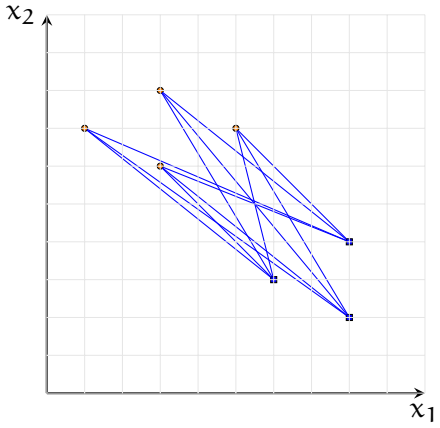
Most clustering algorithms try to minimize the scatter within each cluster. Which is equivalent to maximizing the scatter between clusters.



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

How to do clustering

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

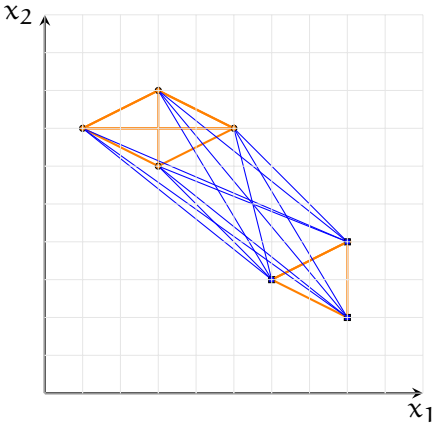


$$\sum_{k=1}^{K} \sum_{a \in C_k} \sum_{b \in C_k} d(a, b)$$

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

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

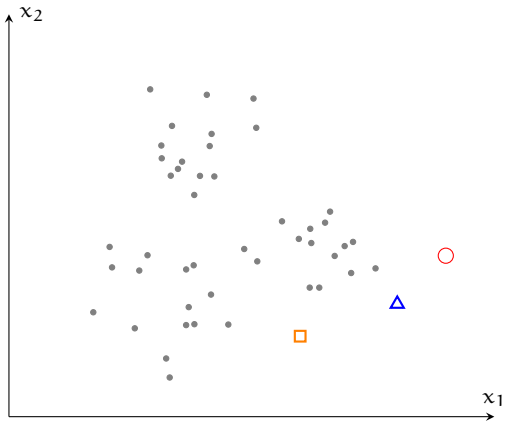
Effectively, we are finding a *local minimum* of the sum of squared Euclidean distance within each cluster

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

K-means clustering: visualization

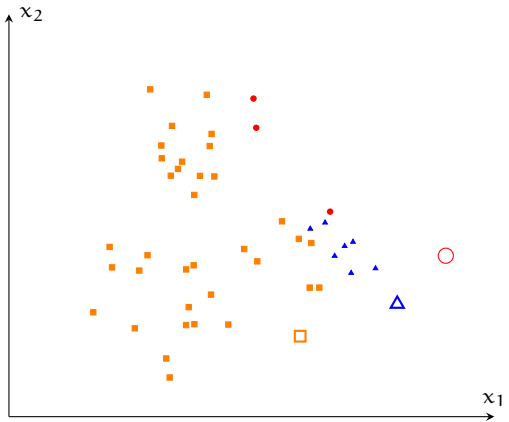
- The data
- Set cluster centroids randomly
- Assign data points to the closest centroid
- Recalculate the centroids

K-means clustering: visualization



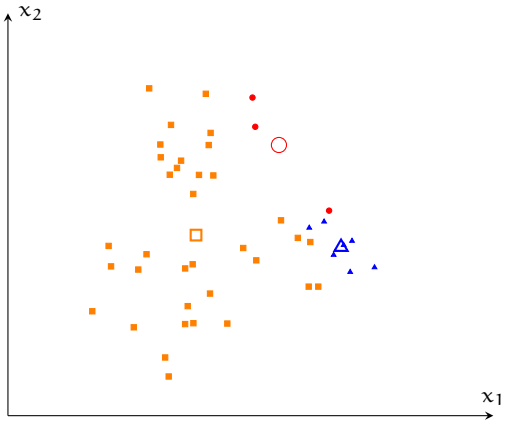
- The data
- Set cluster centroids randomly
- Assign data points to the closest centroid
- Recalculate the centroids

K-means clustering: visualization



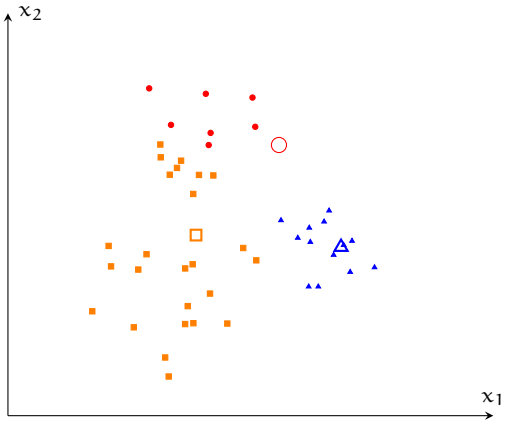
- The data
- Set cluster centroids randomly
- Assign data points to the closest centroid
- Recalculate the centroids

K-means clustering: visualization



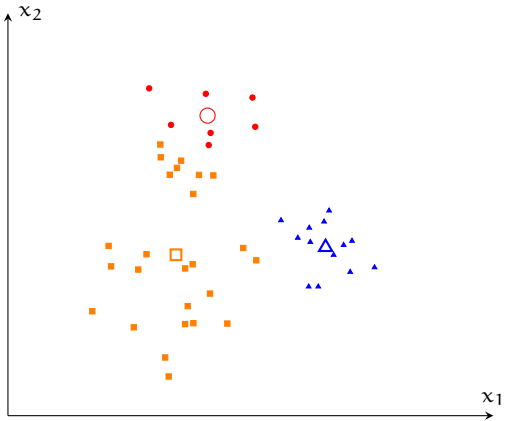
- The data
- Set cluster centroids randomly
- Assign data points to the closest centroid
- Recalculate the centroids

K-means clustering: visualization



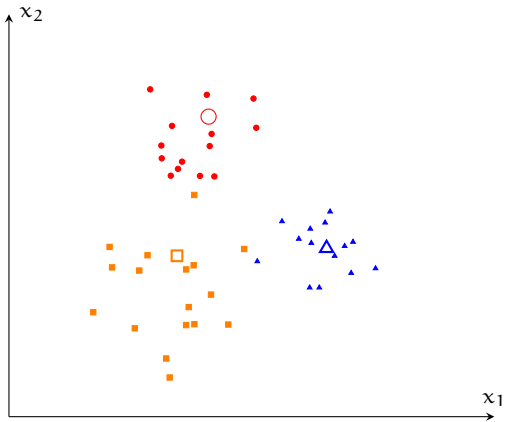
- The data
- Set cluster centroids randomly
- Assign data points to the closest centroid
- Recalculate the centroids

K-means clustering: visualization



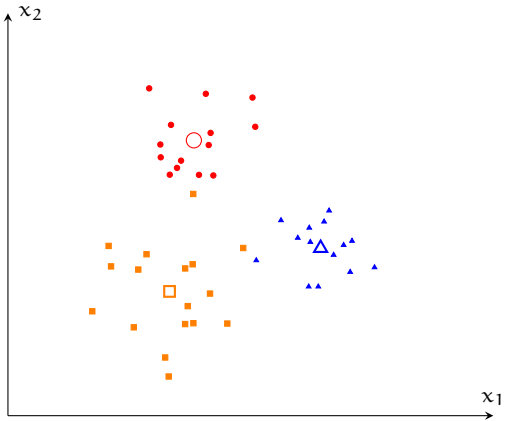
- The data
- Set cluster centroids randomly
- Assign data points to the closest centroid
- Recalculate the centroids

K-means clustering: visualization



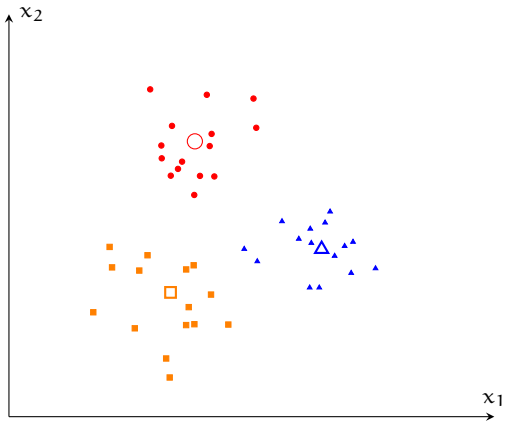
- The data
- Set cluster centroids randomly
- Assign data points to the closest centroid
- Recalculate the centroids

K-means clustering: visualization



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

K-means clustering: visualization



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

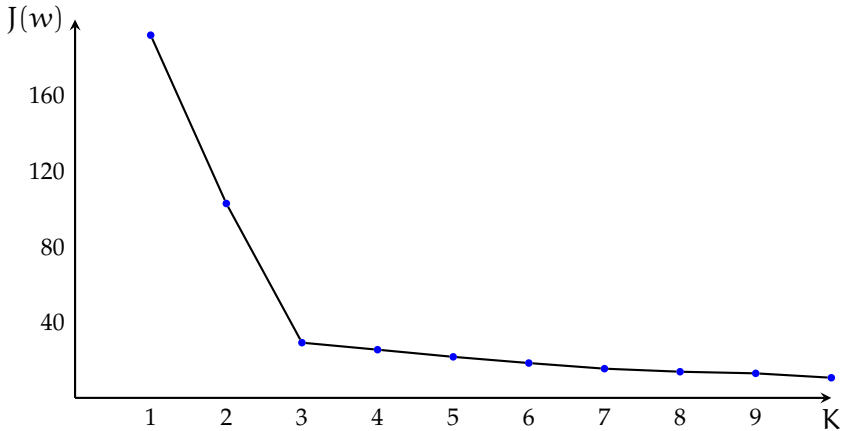
K-means: some issues

- 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) always 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 against 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

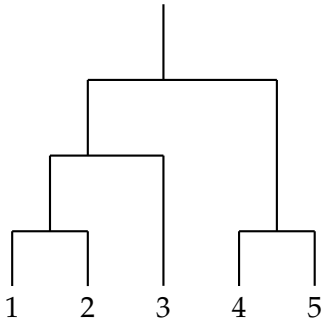
Top-down or *divisive* clustering
- starts with a single cluster,
- and splits until all leaves are single data points

Hierarchical clustering

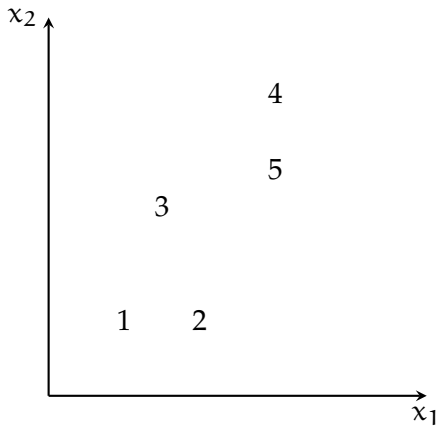
- Hierarchical clustering operates on differences (or similarities)
- The result is a binary tree called *dendrogram*
- Dendrograms are easy to interpret (especially if data is hierarchical)
- The algorithm does not commit to the number of clusters K from the start, the dendrogram can be 'cut' at any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

Agglomerative clustering

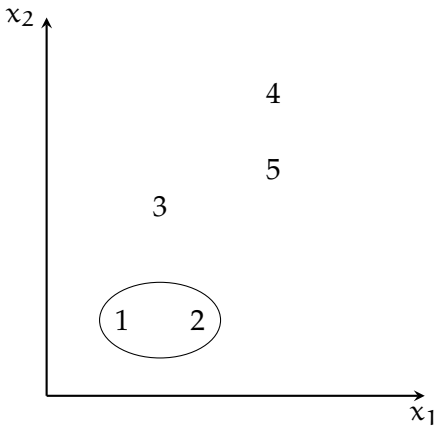
1. Compute the similarity/distance matrix
2. Assign each data point to its own cluster
3. Repeat until no clusters left to merge
   - Pick two clusters that are most similar to each other
   - Merge them into a single cluster



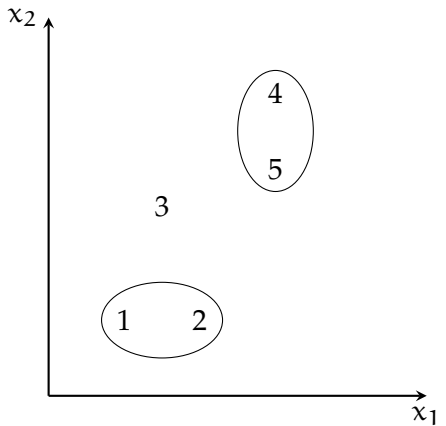
Agglomerative clustering demonstration



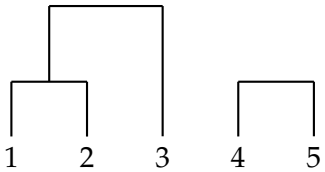
Agglomerative clustering demonstration

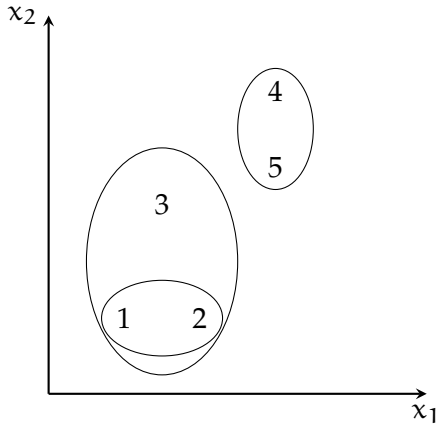


Agglomerative clustering demonstration

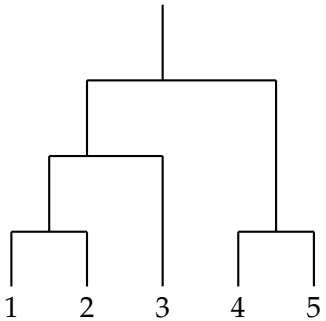


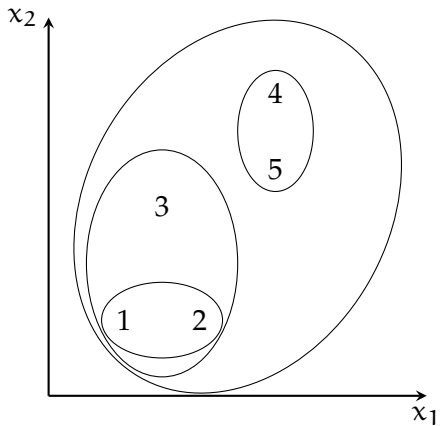
Agglomerative clustering demonstration





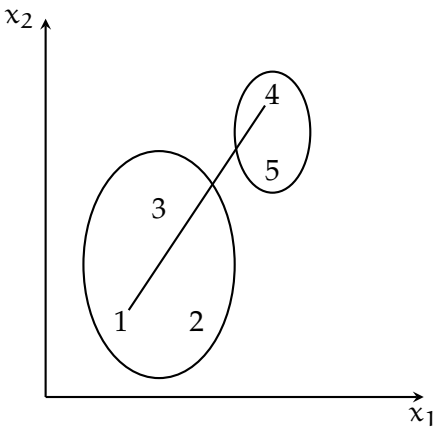
Agglomerative clustering demonstration





How to calculate between cluster distances

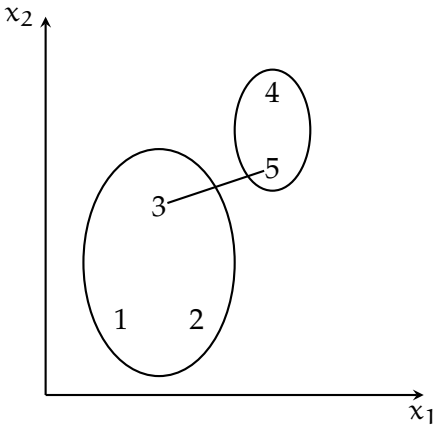
Complete maximal inter-cluster distance



How to calculate between cluster distances

Complete maximal inter-cluster distance

Single minimal inter-cluster distance

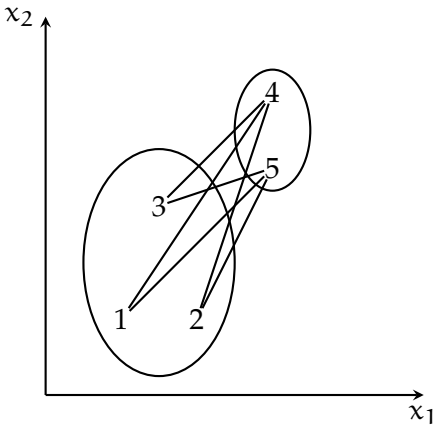


How to calculate between cluster distances

Complete maximal inter-cluster distance

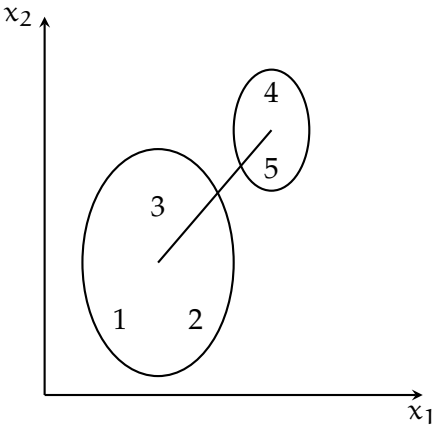
Single minimal inter-cluster distance

Average mean inter-cluster distance



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



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^3ed 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'

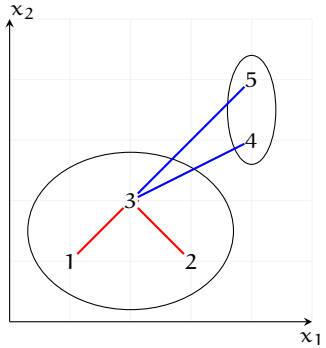
Clustering evaluation

internal metric example: silhouette

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

where

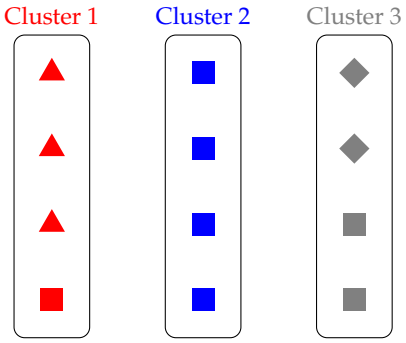
- $a(i)$ average distance between object i and and objects in the same cluster
- $b(i)$ average distance between object i and and objects in the *closest* cluster



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:

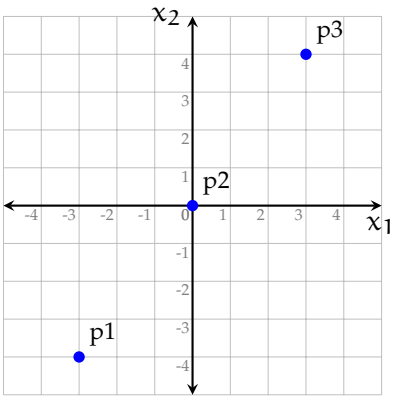
E-step Given the parameters, compute the membership 'weights', the probability of each data point belonging to each distribution

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

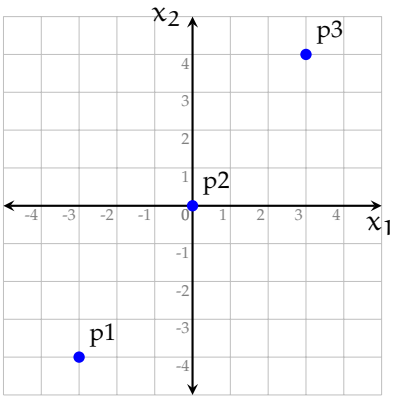
PCA: a toy example



Questions:

- How many dimensions do we have?
- How many dimensions do we need?

PCA: a toy example



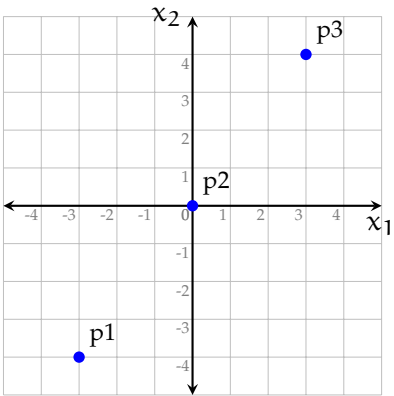
Questions:

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

$$\Sigma = \begin{bmatrix} ? & ? \\ ? & ? \end{bmatrix}$$

  - What is the correlation between x_1 and x_2?

PCA: a toy example



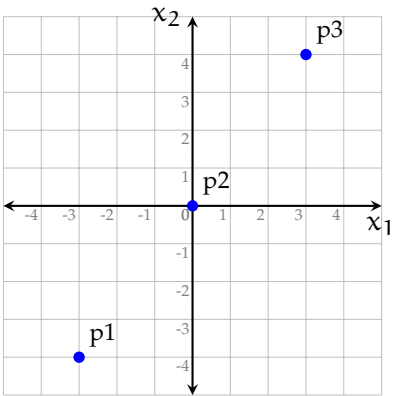
Questions:

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

$$\Sigma = \begin{bmatrix} \sigma^2_{x_1} & \sigma_{x_2,x_1} \\ \sigma_{x_1,x_2} & \sigma^2_{x_2} \end{bmatrix}$$

  - What is the correlation between x_1 and x_2?

PCA: a toy example



Questions:

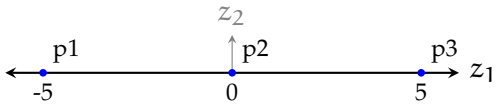
- How many dimensions do we have?
- How many dimensions do we need?
- Short divergence: calculate the covariance matrix

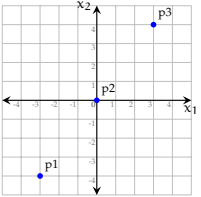
$$\Sigma = \begin{bmatrix} \frac{18}{3} & 8 \\ 8 & \frac{32}{3} \end{bmatrix}$$

  - What is the correlation between x_1 and x_2?

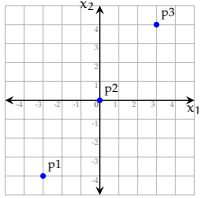
PCA: A toy example (2)

What if we reduce the data to:

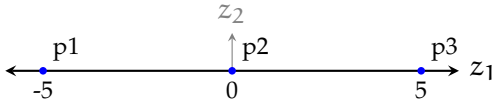




PCA: A toy example (2)



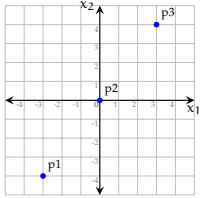
What if we reduce the data to:



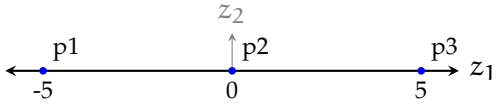
Going back to the original coordinates is easy, rotate using:

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

PCA: A toy example (2)



What if we reduce the data to:

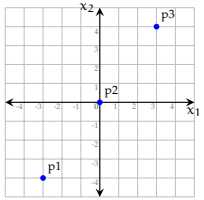


Going back to the original coordinates is easy, rotate using:

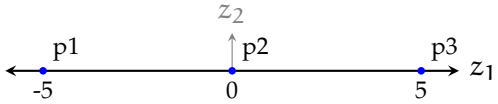
$$A = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} = \begin{bmatrix} \frac{3}{5} & -\frac{4}{5} \\ \frac{4}{5} & \frac{3}{5} \end{bmatrix}$$

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

PCA: A toy example (2)



What if we reduce the data to:



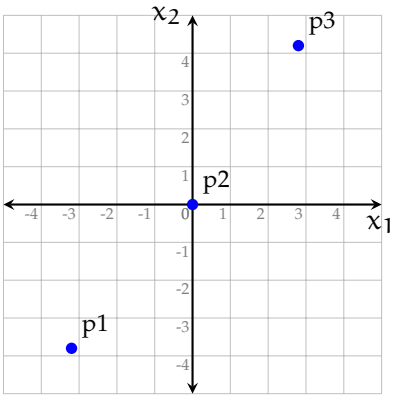
Going back to the original coordinates is easy, rotate using:

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

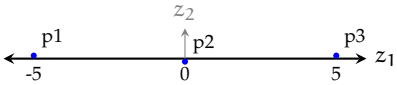
$$p1 = A \times \begin{bmatrix} -5 \\ 0 \end{bmatrix} = \begin{bmatrix} -3 \\ -4 \end{bmatrix} \quad p1 = A \times \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \; p1 = A \times \begin{bmatrix} 5 \\ 0 \end{bmatrix} = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$$

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:

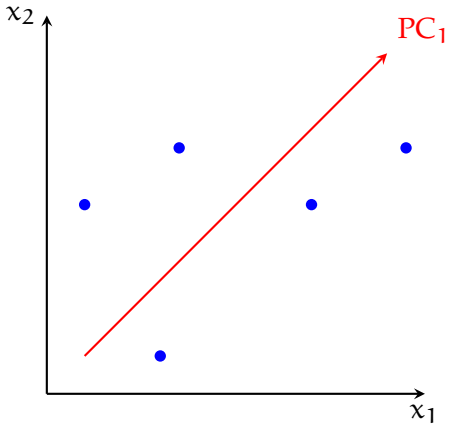
$$\text{p1} = \text{A} \times \begin{bmatrix} -5 \\ 0 \end{bmatrix} = \begin{bmatrix} -3 \\ -4 \end{bmatrix}$$

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

Why do we want to reduce the dimensionality

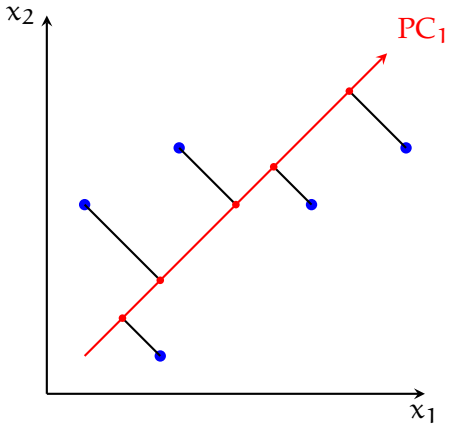
- Visualizing high-dimensional data becomes possible
- If we use the data for other ML methods,
  - we reduce the computation time
  - we may avoid 'the curse of dimensionality'
- Decorrelation is useful in some applications
- We compress the data (in a lossy way)
- We eliminate noise (assuming a high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

Different views on PCA



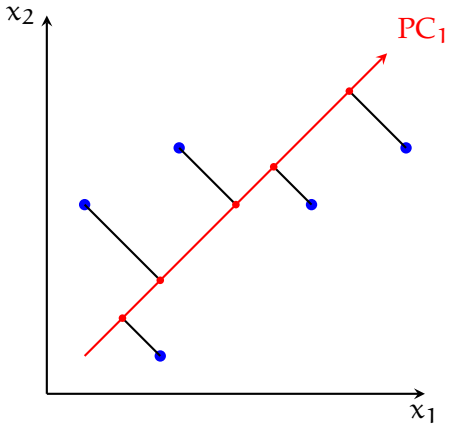
- Find the direction of the largest variance

Different views on PCA



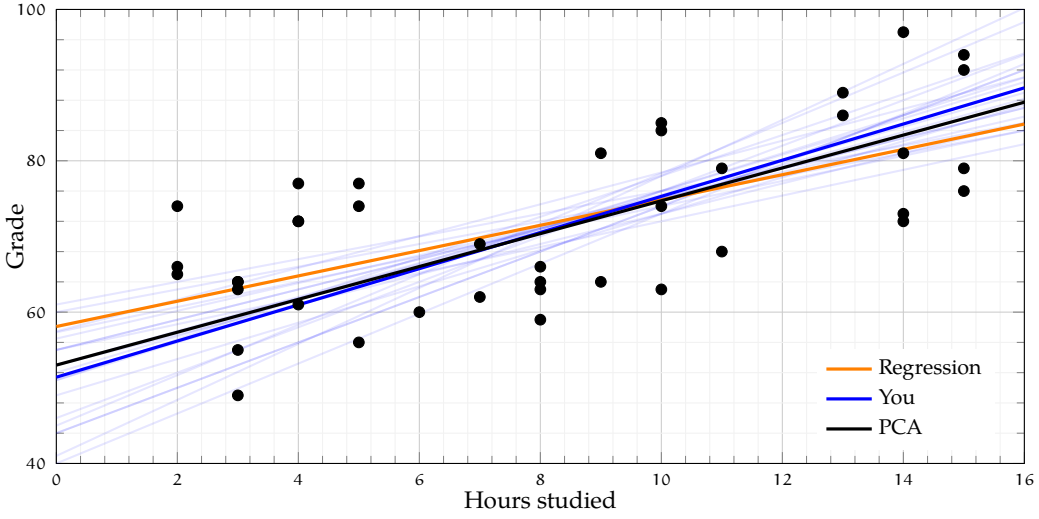
- Find the direction of the largest variance
- Find the projection with the least reconstruction error

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 $\Sigma = X^T X$)

$$\Sigma = U \Lambda U^T$$

  - the columns of U are the principal components (eigenvectors)
  - Λ is a diagonal matrix of eigenvalues

- Another option is SVD, which factorizes the input vector (k variables $\times$ n data points) as

$$X = U D V^*$$

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

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

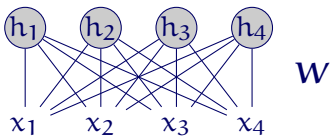
Some practical notes on PCA

- 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

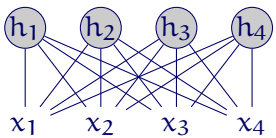
Restricted Boltzmann machines (RBMs)



- 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.

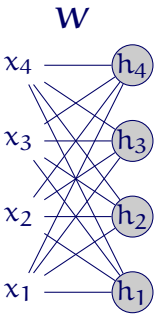
Restricted Boltzmann machines (RBMs)



- 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

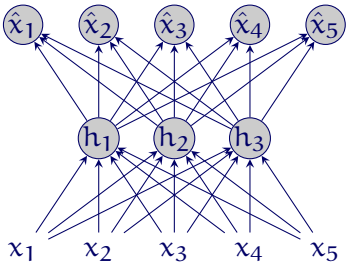
$$p(\mathbf{h}|\mathbf{x}) = \prod_j p(h_j|\mathbf{x}) \quad = \frac{1}{1 + e^{\mathbf{W}_j \mathbf{x}}}$$

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

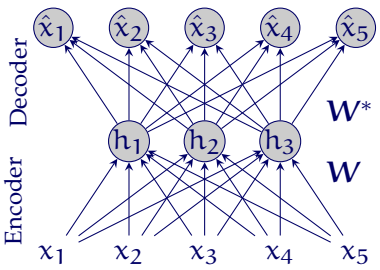
Learning in RBMs

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

Autoencoders

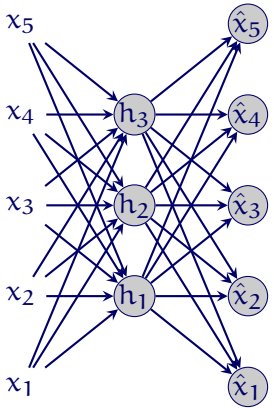


Autoencoders



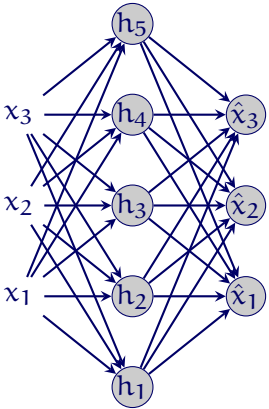
- Autoencoders are standard feed-forward networks
- The main difference is that they are trained to predict their input (they try to learn the identity function)
- The aim is to learn useful representations of input at the hidden layer
- Typically weights are tied ($W^* = W^\mathsf{T}$)

Under-complete autoencoders



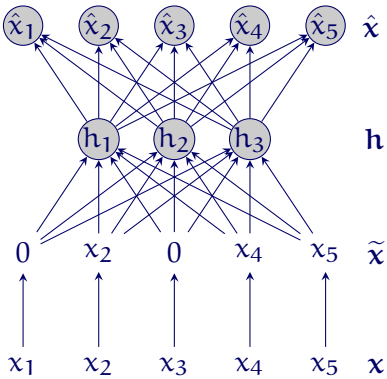
- An autoencoder is said to be *under-complete* if there are fewer hidden units than inputs
- The network is forced to learn a compact representation of the input (compress)
- An autoencoder with a single hidden layer approximates the PCA
- We need multiple layers for learning non-linear features

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

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:

Mon Artificial neural networks (ANNs)

Wed Deadline for assignment 3, assignment 4 will be out

Derivation of PCA by maximizing the variance

- We focus on the first PC (z_1), which maximizes the variance of the data onto itself
- We are interested only on the direction, so we choose z_1 to be a unit vector ($\|z_1\| = 1$)
- Remember that to project a vector onto another, we simply use dot product, So the projected data points are zx_i for $i = 1, \ldots, N$.
- The variance of the projected data points (that we want to maximize) is,

$$\sigma_{z_1} = \frac{1}{N} \sum_{i}^{N} (z_1 x_i - z_1 \bar{x}_i)^2 = z_1^T \Sigma z$$

where Σ_x is the covariance matrix of the unprojected data

Derivation of PCA by maximizing the variance (cont.)

- The problem becomes maximize

$$z_1^\top \Sigma z$$

  with the constraint $\|z_1\| = z_1^\top z_1 = 1$
- Turning it into a unconstrained optimization problem with Lagrange multipliers, we minimize

$$z_1^\top \Sigma z + \lambda_1 (1 - z_1^\top z_1)$$

- Taking the derivative and setting it to 0 gives us

$$\Sigma z_1 = \lambda_1 z_1$$

  Note: by definition, z_1 is an eigenvector of Σ, and λ_1 is the corresponding eigenvalue
- z_1 is the first principal component, we can now compute the second principal component with the constraint that it has to be orthogonal to the first one