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Machine Learning

IT3190E

Lecture: Introduction

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CS771: Intro to ML

Contents

- Lecture 1: Introduction to Machine Learning
- Lecture 2: Linear regression
- **Lecture 3+4: Clustering**
- Lecture 5: Decision tree and Random forest
- Lecture 6: Neural networks
- Lecture 7: Support vector machines
- Lecture 8: Performance evaluation
- Lecture 9: Probabilistic models
- Lecture 10: Ensemble learning
- Lecture 11: Reinforcement learning
- Lecture 12: Regularization
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Unsupervised Learning: k-means

Dam Quang Tuan

Unsupervised Learning

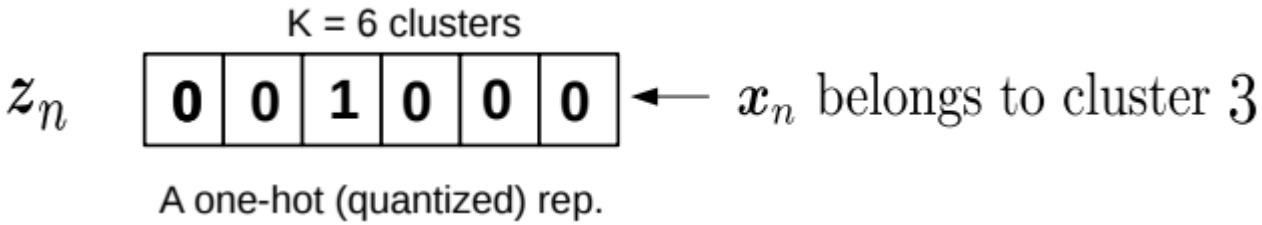
- It's about learning interesting/useful structures in the data (unsupervisedly!)
- There is no supervision (no labels/responses), only inputs $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N$
- Some examples of unsupervised learning
  - Clustering: Grouping similar inputs together (and dissimilar ones far apart)
  - Dimensionality Reduction: Reducing the data dimensionality
  - Estimating the probability density of data (which distribution "generated" the data)

e.g., estimating a Gaussian given observed data

- Most unsup. learning algos can also be seen as learning a new representation of data
  - For example, hard clustering can be used to get a one-hot representation

Each point belongs deterministically to a single cluster

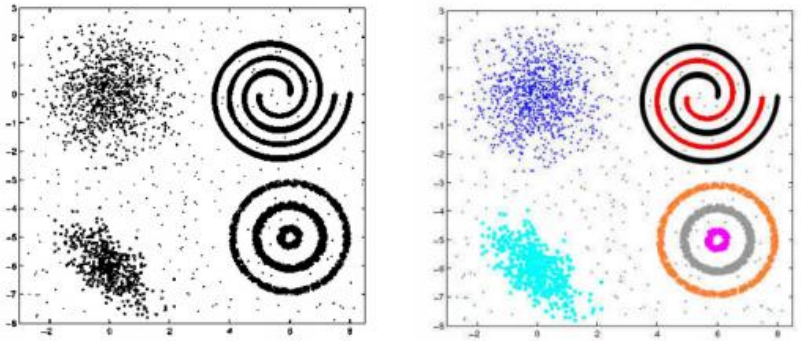
In contrast, there is also soft/probabilistic clustering in which $\boldsymbol{z}_n$ will be be probability vector that sums to 1 (will see later)



Clustering

In some cases, we may not know the right number of clusters in the data and may want to learn that (technique exists for doing this but beyond the scope)

- Given: N unlabeled examples $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N$; desired no. of partitions K
- Goal: Group the examples into K "homogeneous" partitions



(a) Input data (b) Desired clustering

Picture courtesy: "Data Clustering: 50 Years Beyond K-Means", A.K. Jain (2008)

- Loosely speaking, it is classification without ground truth labels
- A good clustering is one that achieves
  - High within-cluster similarity
  - Low inter-cluster similarity

Similarity can be Subjective

- Clustering only looks at similarities b/w inputs, since no labels are given
- Without labels, similarity can be hard to define

- Thus using the right distance/similarity is very important in clustering
- In some sense, related to asking: "Clustering based on what"?

Picture courtesy: http://www.guy-sports.com/humor/videos/powerpoint presentation dogs.htm

Clustering: Some Examples

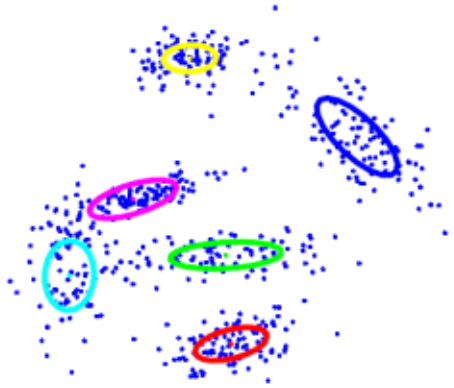
- Document/Image/Webpage Clustering
- Image Segmentation (clustering pixels)

- Clustering web-search results
- Clustering (people) nodes in (social) networks/graphs
- .. and many more..

Picture courtesy: http://people.cs.uchicago.edu/~pff/segment/

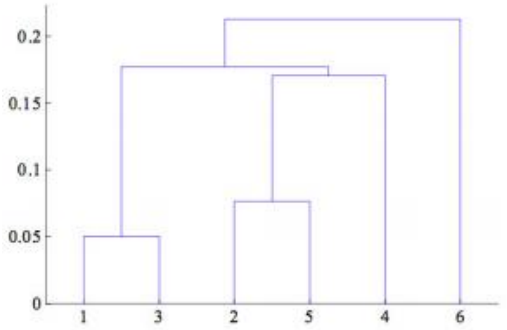
Types of Clustering

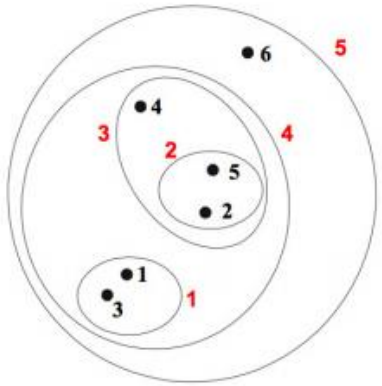
- Flat or Partitional clustering
  - Partitions are independent of each other



- Hierarchical clustering
  - Partitions can be visualized using a tree structure (a dendrogram)

In hierarchical clustering, we can look at a clustering for any given number of cluster by "cutting the dendrogram at an appropriate level (so K does not have to be specified)





Hierarchical clustering gives us a clustering at multiple levels of granularity

Flat Clustering: *K*-means algorithm (Lloyd, 1957)

- **Input:** N unlabeled examples $\boldsymbol{x_1, x_2, \ldots, x_N}$; $\boldsymbol{x_n} \in \mathbb{R}^D$; desired no. of partitions K
- **Desired Output:** Cluster assignments of these N examples and K cluster means
- **Initialize:** The K cluster means denoted by $\boldsymbol{\mu_1, \mu_2, \ldots, \mu_K}$; with each $\boldsymbol{\mu_k} \in \mathbb{R}^D$
  - Usually initialized randomly, but good initialization is crucial; many smarter initialization heuristics exist (e.g., *K*-means++, Arthur & Vassilvitskii, 2007)
- **Iterate:**
  - (Re)-Assign each input $\boldsymbol{x_n}$ to its closest cluster center (based on the smallest Eucl. distance)

$\mathcal{C}_k$: Set of examples assigned to cluster k with center $\boldsymbol{\mu_k}$

$$\mathcal{C}_k = \{n : \quad k = \arg\min_k ||\boldsymbol{x}_n - \boldsymbol{\mu}_k||^2\}$$

  - Update the cluster means

$$\mu_k = \text{mean}(\mathcal{C}_k) = \frac{1}{|\mathcal{C}_k|} \sum_{n \in \mathcal{C}_k} \boldsymbol{x}_n$$

  - Repeat until not converged

Some ways to declare convergence if between two successive iterations:
- Cluster means don't change
- Cluster assignments don't change
- Clustering "loss" doesn't change by much

K-means algorithm: Summarized Another Way

- Notation: $z_n \in \{1,2,\ldots,K\}$ or $\boldsymbol{z}_n$ is a K-dim one-hot vector
  - ($z_{nk} = 1$ and $z_n = k$ mean the same)

K-means algo can also be seen as doing a compression by "quantization": Representing each of the N inputs by one of the $K < N$ means

K-means Algorithm

1. Initialize K cluster means $\mu_1, \ldots, \mu_K$
2. For $n = 1, \ldots, N$, assign each point $\boldsymbol{x}_n$ to the closest cluster

$$z_n = \arg\min_{k \in \{1,\ldots,K\}} ||\boldsymbol{x}_n - \mu_k||^2$$

3. Suppose $\mathcal{C}_k = \{\boldsymbol{x}_n : z_n = k\}$. Re-compute the means

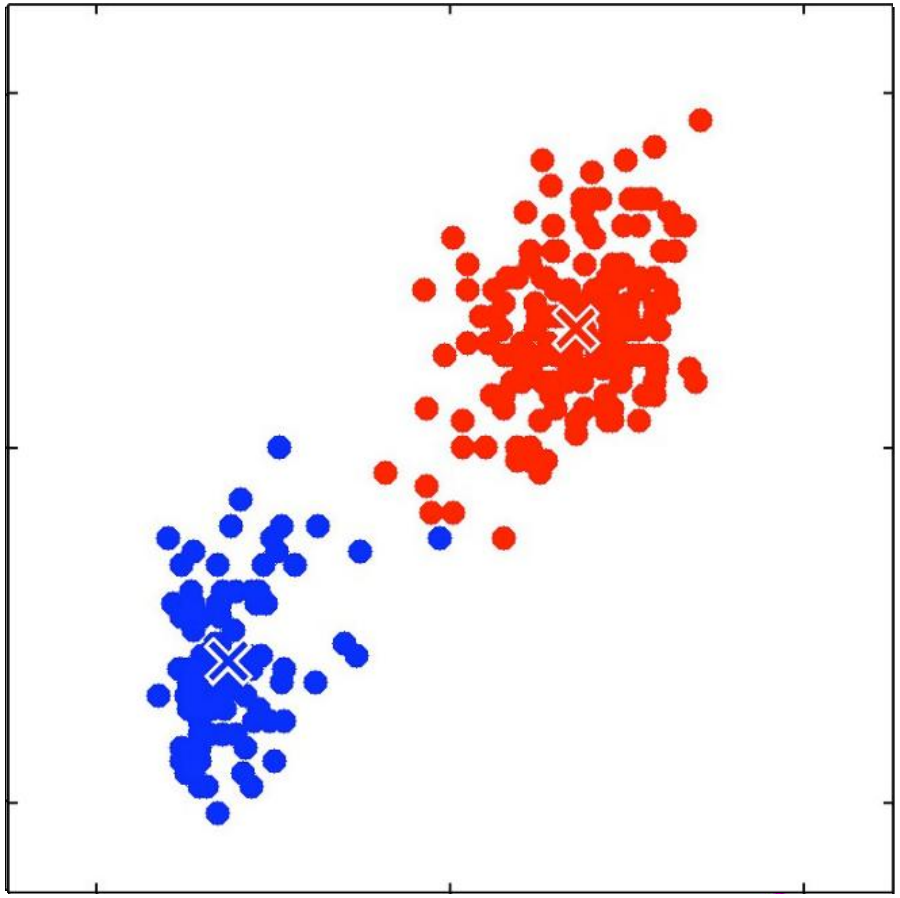
$$\mu_k = \text{mean}(\mathcal{C}_k), \quad k = 1, \ldots, K$$

4. Go to step 2 if not yet converged

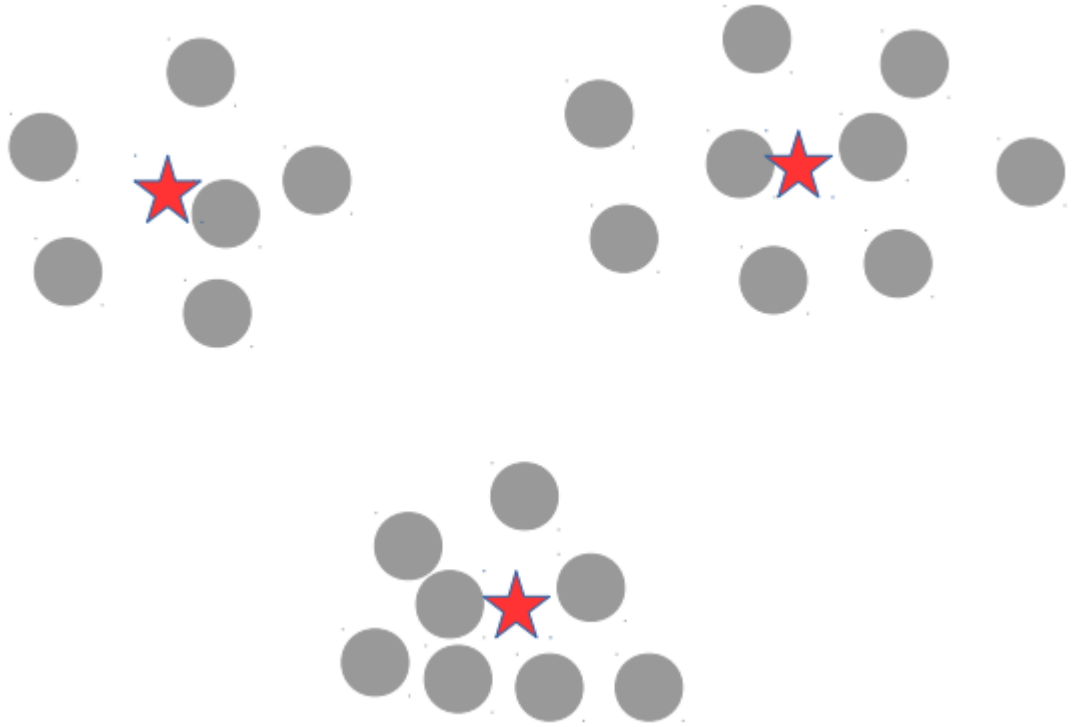
Can be fixed by modeling each cluster by a probability distribution, such as Gaussian (e.g., Gaussian Mixture Model; will see later)

This basic K-means models each cluster by a single mean μ_k. Ignores size/shape of clusters

K-means: An Illustration



K-means = LwP with Unlabeled Data



- Guess the means
- Predict the labels (cluster ids)
- Recompute the means using these predicted labels
- Repeat until not converged

The *K*-means Algorithm: Some Comments

- One of the most popular clustering algorithms
- Very widely used, guaranteed to converge (to a local minima; will see a proof)
- Can also be used as a sub-routine in graph clustering (in the Spectral Clustering algorithm): Inputs are given as an $N \times N$ adjacency matrix A ($A_{nm} = 0/1$)
  - Perform a spectral decomposition of the graph Laplacian of A to get F (an $N \times K$ matrix)
  - Run K-means using rows of the F matrix as the inputs
- Has some shortcomings but can be improved upon, e.g.,
  - Can be kernelized (using kernels or using kernel-based landmarks/random features)
  - More flexible cluster sizes/shapes via probabilistic models (e.g., every cluster is a Gaussian)
  - Soft-clustering (fractional/probabilistic memberships): z_n is not one-hot but a probability vector
  - Overlapping clustering – an input can belong to multiple clusters: z_n is a binary vector
  - .. even deep learning based K-means (use a deep network to extract features and run K-means on those)
- Let's look at K-means in some more detail now..

What Loss Function is *K*-means Optimizing?

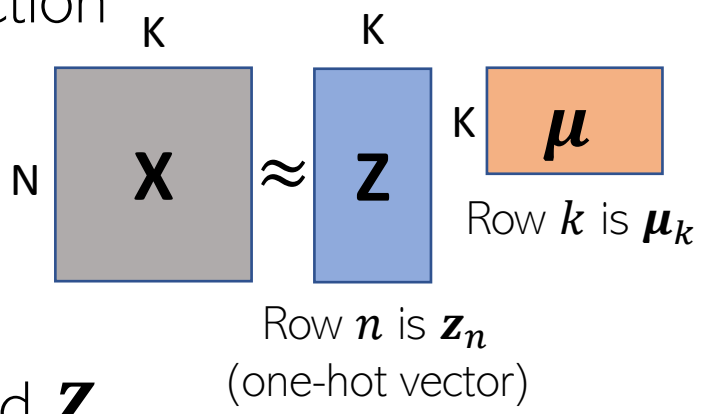
$\boldsymbol{z}_n = [z_{n1}, z_{n2}, \ldots, z_{nK}]$ denotes a length K one-hot encoding of $\boldsymbol{x}_n$

- Let $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_K$ be the K cluster centroids/means
- Let $z_{nk} \in \{0, 1\}$ be s.t. $z_{nk} = 1$ if $\boldsymbol{x}_n$ belongs to cluster $\boldsymbol{k}$, and 0 otherwise
- Define the distortion or "loss" for the cluster assignment of $\boldsymbol{x}_n$

$$\ell(\boldsymbol{\mu}, \boldsymbol{x}_n, \boldsymbol{z}_n) = \sum_{k=1}^{K} z_{nk} ||\boldsymbol{x}_n - \boldsymbol{\mu}_k||^2$$

- Total distortion over all points defines the K-means "loss function"

$$L(\boldsymbol{\mu}, \mathbf{X}, \mathbf{Z}) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} ||\boldsymbol{x}_n - \mu_k||^2 = \underbrace{||\mathbf{X} - \mathbf{Z}\boldsymbol{\mu}||_F^2}_{\text{matrix factorization view}}$$



- The K-means problem is to minimize this objective w.r.t. $\boldsymbol{\mu}$ and $\boldsymbol{Z}$
  - Alternating optimization on this loss would give the K-means (Lloyd's) algorithm we saw earlier!

K-means Loss: Several Forms, Same Meaning!

- Notation: $\boldsymbol{X}$ is $N \times D$
- $\boldsymbol{Z}$ is $N \times K$ (each row is a one-hot z_n or equivalently $z_n \in \{1,2,\ldots,K\}$)
- $\boldsymbol{\mu}$ is K × D (each row is a μ_k)

Replacing the ℓ_2 (Euclidean) squared by ℓ_1 distances givesn the K-medoids algorithm (more robust to outliers)

Distortion on assigning x_n to cluster z_n

$$\mathcal{L}(\mathbf{X},\mathbf{Z},\boldsymbol{\mu}) = \sum_{n=1}^{N} ||\boldsymbol{x}_n - \mu_{z_n}||^2$$

$$\mathcal{L}(\mathbf{X},\mathbf{Z},\boldsymbol{\mu}) = \sum_{k=1}^{K} \underbrace{\sum_{n:z_n=k} ||\boldsymbol{x}_n - \mu_k||^2}_{\text{within cluster variance}}$$

$$\mathcal{L}(\mathbf{X},\mathbf{Z},\boldsymbol{\mu}) = \sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}||\boldsymbol{x}_n - \mu_k||^2$$

$$\mathcal{L}(\mathbf{X},\mathbf{Z},\boldsymbol{\mu}) = \underbrace{||\mathbf{X} - \mathbf{Z}\boldsymbol{\mu}||_F^2}_{\text{as matrix factorization}}$$

$$\{\hat{\mathbf{Z}},\hat{\boldsymbol{\mu}}\} = \arg\min_{\mathbf{Z},\boldsymbol{\mu}} \mathcal{L}(\mathbf{X},\mathbf{Z},\boldsymbol{\mu})$$

Total "distortion" or reconstruction error

- Note: Most unsup. learning algos try to minimize a distortion or recon error

Optimizing the *K*-means Loss Function

- So the K-means problem is

$$\{\hat{\mathbf{Z}}, \hat{\boldsymbol{\mu}}\} = \arg\min_{\mathbf{Z},\boldsymbol{\mu}} \mathcal{L}(\mathbf{X}, \mathbf{Z}, \boldsymbol{\mu}) = \arg\min_{\mathbf{Z},\boldsymbol{\mu}} \sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}||\boldsymbol{x}_n - \mu_k||^2$$

- Can't optimize it jointly for $\boldsymbol{Z}$ and $\boldsymbol{\mu}$. Let's try alternating optimization for $\boldsymbol{Z}$ and $\boldsymbol{\mu}$

Alternating Optimization for *K*-means Problem

1. Fix $\boldsymbol{\mu}$ as $\hat{\boldsymbol{\mu}}$ and find the optimal $\mathbf{Z}$ as

$$\hat{\mathbf{Z}} = \arg\min_{\mathbf{Z}} \mathcal{L}(\mathbf{X}, \mathbf{Z}, \hat{\boldsymbol{\mu}}) \quad \text{(still not easy - next slide)}$$

2. Fix $\mathbf{Z}$ as $\hat{\mathbf{Z}}$ and find the optimal $\boldsymbol{\mu}$ as

$$\hat{\boldsymbol{\mu}} = \arg\min_{\boldsymbol{\mu}} \mathcal{L}(\mathbf{X}, \hat{\mathbf{Z}}, \boldsymbol{\mu})$$

3. Go to step 1 if not yet converged

Solving for Z

- Solving for $\boldsymbol{Z}$ with $\boldsymbol{\mu}$ fixed at $\hat{\boldsymbol{\mu}}$

$$\hat{\mathbf{Z}} = \arg\min_{\mathbf{Z}} \mathcal{L}(\mathbf{X}, \mathbf{Z}, \hat{\mu}) = \arg\min_{\mathbf{Z}} \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} ||\boldsymbol{x}_n - \hat{\mu}_k||^2$$

- Still not easy. $\boldsymbol{Z}$ is discrete and above is an NP-hard problem
  - Combinatorial optimization: K^N possibilities for $\boldsymbol{Z}$ ($N \times K$ matrix with one-hot rows)

- Greedy approach: Optimize $\boldsymbol{Z}$ one row (z_n) at a time keeping all others z_n's (and the cluster means $\mu_1, \mu_2, \ldots, \mu_K$) fixed

$$\hat{\boldsymbol{z}}_n = \arg\min_{\boldsymbol{z}_n} \sum_{k=1}^{K} z_{nk} ||\boldsymbol{x}_n - \hat{\mu}_k||^2 = \arg\min_{\boldsymbol{z}_n} ||\boldsymbol{x}_n - \hat{\mu}_{z_n}||^2$$

- Easy to see that this is minimized by assigning $\boldsymbol{x}_n$ to the closest mean
  - This is exactly what the K-means (Lloyd's) algo does!

Solving for $\boldsymbol{\mu}$

- Solving for $\boldsymbol{\mu}$ with $\boldsymbol{Z}$ fixed at $\widehat{\boldsymbol{Z}}$

$$\hat{\boldsymbol{\mu}} = \arg\min_{\boldsymbol{\mu}} \mathcal{L}(\mathbf{X}, \hat{\mathbf{Z}}, \boldsymbol{\mu}) = \arg\min_{\boldsymbol{\mu}} \sum_{k=1}^{K} \sum_{n:\hat{z}_n=k} ||\boldsymbol{x}_n - \mu_k||^2$$

- Not difficult to solve (each $\boldsymbol{\mu_k}$ is a real-valued vector, can optimize easily)

$$\hat{\mu}_k = \arg\min_{\mu_k} \sum_{n:\hat{z}_n=k} ||\boldsymbol{x}_n - \mu_k||^2$$

- Note that each $\boldsymbol{\mu_k}$ can be optimized for independently

- (Verify) This is minimized by setting $\widehat{\boldsymbol{\mu_k}}$ to be mean of points currently in cluster $\boldsymbol{k}$
  - This is exactly what the $\boldsymbol{K}$-means (Lloyd's) algo does!

Convergence of *K*-means algorithm

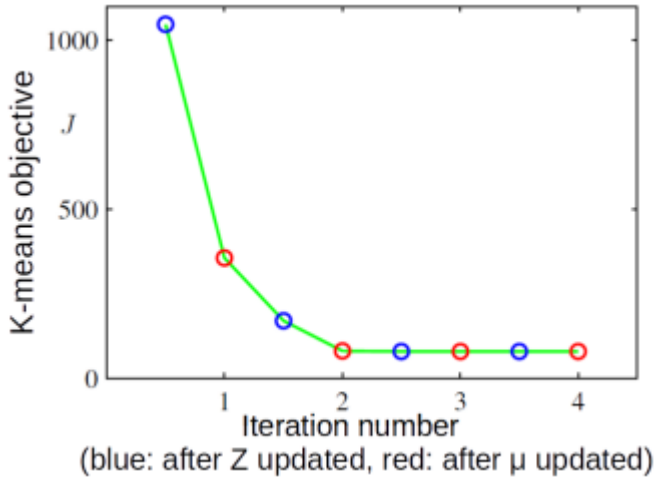
- Each step (updating $\boldsymbol{Z}$ or $\boldsymbol{\mu}$) can never increase the K-means loss
- When we update $\boldsymbol{Z}$ from $\boldsymbol{Z}^{(t-1)}$ to $\boldsymbol{Z}^{(t)}$

$$\mathcal{L}(\mathbf{X}, \mathbf{Z}^{(t)}, \boldsymbol{\mu}^{(t-1)}) \leq \mathcal{L}(\mathbf{X}, \mathbf{Z}^{(t-1)}, \boldsymbol{\mu}^{(t-1)}) \quad \text{because} \quad \mathbf{Z}^{(t)} = \arg\min_{\mathbf{Z}} \mathcal{L}(\mathbf{X}, \mathbf{Z}, \boldsymbol{\mu}^{(t-1)})$$

- When we update $\boldsymbol{\mu}$ from $\boldsymbol{\mu}^{(t-1)}$ to $\boldsymbol{\mu}^{(t)}$

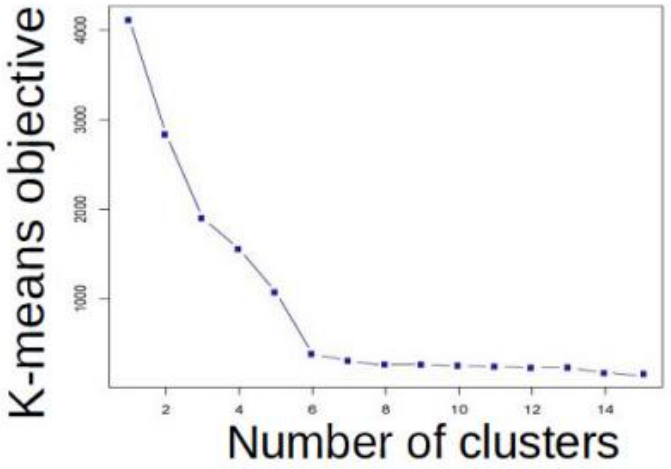
$$\mathcal{L}(\mathbf{X}, \mathbf{Z}^{(t)}, \boldsymbol{\mu}^{(t)}) \leq \mathcal{L}(\mathbf{X}, \mathbf{Z}^{(t)}, \boldsymbol{\mu}^{(t-1)}) \quad \text{because} \quad \boldsymbol{\mu}^{(t)} = \arg\min_{\boldsymbol{\mu}} \mathcal{L}(\mathbf{X}, \mathbf{Z}^{(t)}, \boldsymbol{\mu})$$

- Thus the K-means algorithm monotonically decreases the objective



K-means: Choosing *K*

- One way to select K for the K-means algorithm is to try different values of K, plot the K-means objective versus K, and look at the "elbow-point"



K=6 is the elbow point

- Can also information criterion such as AIC (Akaike Information Criterion)

$$AIC = 2\mathcal{L}(\hat{\mu}, \mathbf{X}, \hat{\mathbf{Z}}) + KD$$

and choose K which gives the smallest AIC (small loss + large K values penalized)

- More advanced approaches, such as nonparametric Bayesian methods (Dirichlet Process mixture models also used, not within K-means but with other clustering algos)

Coming up next

- Improvements to K-means
  - Soft-assignments
  - Handling complex cluster shapes (basic K-means assumes spherical clusters)
- Evaluating clustering algorithms (how to evaluate without true labels)
- Probabilistic approaches to clustering

K-means algorithm: recap

- Notation: $z_n \in \{1,2,\ldots,K\}$ or $\boldsymbol{z}_n$ is a K-dim one-hot vector
  - ($z_{nk} = 1$ and $z_n = k$ mean the same)

K-means Algorithm

1. Initialize K cluster means $\mu_1, \ldots, \mu_K$
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3. Suppose $\mathcal{C}_k = \{\boldsymbol{x}_n : z_n = k\}$. Re-compute the means

$$\mu_k = \text{mean}(\mathcal{C}_k), \quad k = 1, \ldots, K$$

4. Go to step 2 if not yet converged

K-means loss function: recap

$\boldsymbol{z}_n = [z_{n1}, z_{n2}, \ldots, z_{nK}]$ denotes a length K one-hot encoding of $\boldsymbol{x}_n$

- Let $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_K$ be the K cluster centroids/means
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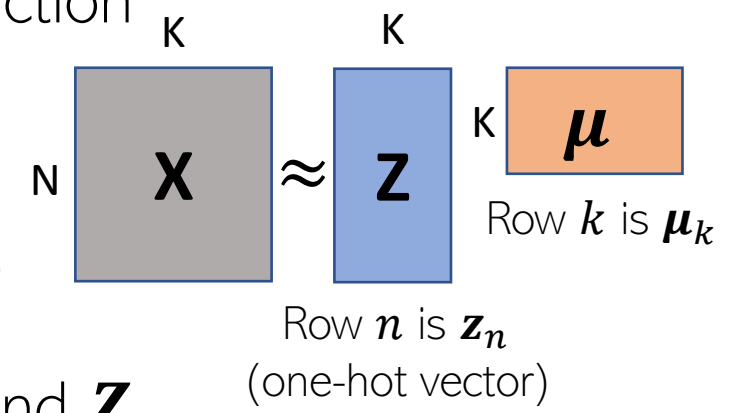
$$\ell(\boldsymbol{\mu}, \boldsymbol{x}_n, \boldsymbol{z}_n) = \sum_{k=1}^{K} z_{nk} ||\boldsymbol{x}_n - \boldsymbol{\mu}_k||^2$$

- Total distortion over all points defines the K-means "loss function"

$$L(\boldsymbol{\mu}, \mathbf{X}, \mathbf{Z}) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} ||\boldsymbol{x}_n - \mu_k||^2 = \underbrace{||\mathbf{X} - \mathbf{Z}\boldsymbol{\mu}||_F^2}_{\text{matrix factorization view}}$$

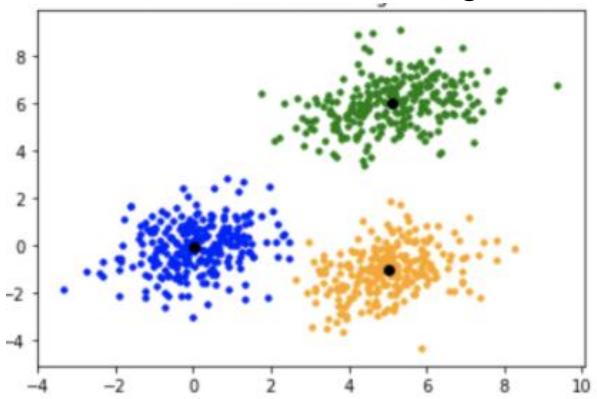


- The K-means problem is to minimize this objective w.r.t. $\boldsymbol{\mu}$ and $\boldsymbol{Z}$
  - Alternating optimization on this loss would give the K-means (Lloyd's) algorithm we saw earlier!

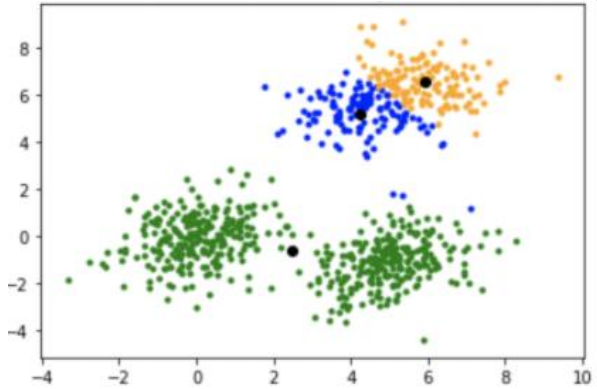
K-means++

- K-means results can be sensitive to initialization

Desired clustering



Poor initialization: bad clustering



- K-means++ (Arthur and Vassilvitskii, 2007) an improvement over K-means
  - Only difference is the way we initialize the cluster centers (rest of it is just K-means)
  - Basic idea: Initialize cluster centers such that they are reasonably far from each other
  - Note: In K-means++, the cluster centers are chosen to be K of the data points themselves

K-means++

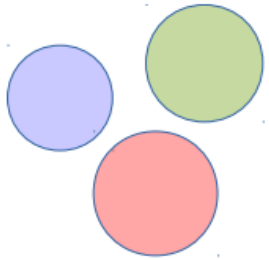
- K-means++ works as follows
  - Choose the first cluster mean uniformly randomly to be one of the data points
  - The subsequent $K-1$ cluster means are chosen as follows
    1. For each unselected point $\boldsymbol{x}$, compute its smallest distance $D(\boldsymbol{x})$ from already initialized means
    2. Select the next cluster mean unif. rand. to be one of the unselected points based on probability prop. to $D(\boldsymbol{x})^2$
    3. Repeat 1 and 2 until the $K-1$ cluster means are initialized
  - Now run standard K-means with these initial cluster means

Thus farthest points are most likely to be selected as cluster means

- K-means++ initialization scheme sort of ensures that the initial cluster means are located in different clusters

K-means: Soft Clustering

- *K*-means makes hard assignments of points to clusters
  - Hard assignment: A point either completely belongs to a cluster or doesn't belong at all



Hard-assignment okay

Hard-assignment tricky

A more principled extension of K-means for doing soft-clustering is via probabilistic mixture models such as the Gaussian Mixture Model

  - When clusters overlap, soft assignment is preferable (i.e., probability of being assigned to each cluster: say $K = 3$ and for some point $\boldsymbol{x}_n$, $p_1 = 0.7, p_2 = 0.2, p_3 = 0.1$)

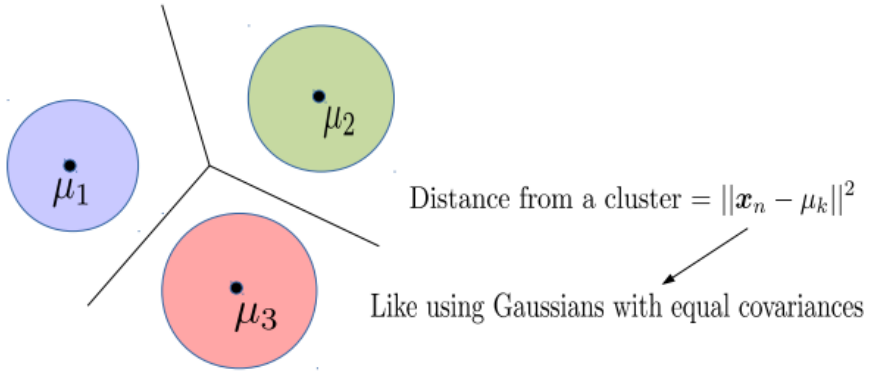
- A heuristic to get soft assignments: Transform distances from clusters into prob.

$$\sum_{k=1}^{K} \gamma_{nk} = 1 \qquad \gamma_{nk} = \frac{\exp(-||\boldsymbol{x}_n - \mu_k||^2)}{\sum_{\ell=1}^{K} \exp(-||\boldsymbol{x}_n - \mu_\ell||^2)} \quad \text{(prob. that } \boldsymbol{x}_n \text{ belongs to cluster } k\text{)}$$

- Cluster mean updates also change: $\mu_k = \frac{\sum_{n=1}^{N} \gamma_{nk} \boldsymbol{x}_n}{\sum_{n=1}^{N} \gamma_{nk}}$ (all points contribute, fractionally)

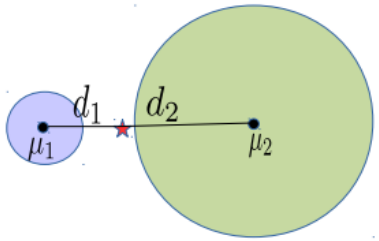
K-means: Decision Boundaries and Cluster Sizes/Shapes

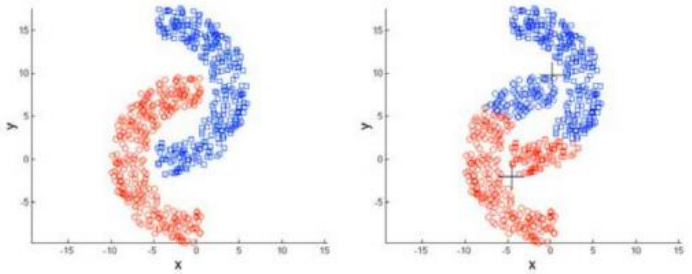
- K-mean assumes that the decision boundary between any two clusters is linear
- Reason: The K-means loss function implies assumes equal-sized, spherical clusters



Reason: Use of Euclidean distances

- May do badly if clusters are not roughly equi-sized and convex-shaped





Kernel *K*-means

Helps learn non-spherical clusters and nonlinear cluster boundaries

- Basic idea: Replace the Eucl. distances in K-means by the kernelized versions

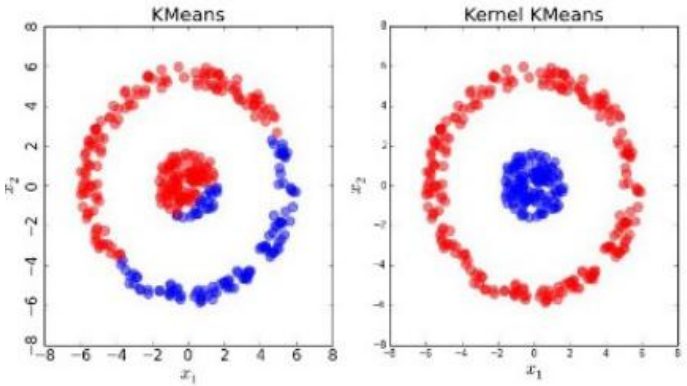
$$||\phi(\boldsymbol{x}_n) - \phi(\boldsymbol{\mu}_k)||^2 = ||\phi(\boldsymbol{x}_n)||^2 + ||\phi(\boldsymbol{\mu}_k)||^2 - 2\phi(\boldsymbol{x}_n)^\top \phi(\boldsymbol{\mu}_k)$$
$$= k(\boldsymbol{x}_n, \boldsymbol{x}_n) + k(\boldsymbol{\mu}_k, \boldsymbol{\mu}_k) - 2k(\boldsymbol{x}_n, \boldsymbol{\mu}_k)$$

Kernelized distance between input $\boldsymbol{x}_n$ and mean of cluster k

- Here $k(.,.)$ denotes the kernel function and ϕ is its (implicit) feature map
- Note: $\phi(\mu_k)$ is the mean of ϕ mappings of the data points assigned to cluster k

Not the same as the ϕ mapping of the mean of the data points assigned to cluster k

$$\phi(\mu_k) = \frac{1}{|\mathcal{C}_k|} \sum_{n:z_n=k} \phi(\boldsymbol{x}_n)$$



Can also used landmarks or kernel random features idea to get new features and run standard k-means on those

Note: Apart from kernels, it is also possible to use other distance functions in K-means. Bregman Divergence* is such a family of distances (Euclidean and Mahalanobis are special cases)

*Clustering with Bregman Divergences (Banerjee et al, 2005)

Overlapping Clustering

Kind of unsupervised version of multi-label classification (just like standard clustering is like unsupervised multi-class classification)

Example: Clustering people based on the interests they may have (a person may have multiple interests; thus may belong to more than one cluster simultaneously)

- Have seen hard clustering and soft clustering
- In hard clustering, z_n is a one-hot vector
- In soft clustering, z_n is a vector of probabilities
- Overlapping Clustering: A point can simultaneously belong to multiple clusters
  - This is different from soft-clustering
  - z_n would be a binary vector, rather than a one hot or probability vector, e.g.,

$$z_n = [1\ 0\ 0\ 1\ 0]$$

K=5 clusters with point x_n belonging (in whole, not in terms of probabilities) to clusters 1 and 4

- In general, more difficult than hard/soft clustering (for N data points and K clusters, the size of the space of possible solutions is not K^N but 2^{NK} - exp in both N and K)
- K-means has extensions* for doing overlapping clustering. There also exist latent variable models for doing overlapping clustering

*An extended version of the k-means method for overlapping clustering (Cleuziou, 2008); Non-exhaustive, Overlapping k-means (Whang et al, 2015)

Evaluating Clustering Algorithms

- Clustering algos are in general harder to evaluate since we rarely know the ground truth clustering (since clustering is unsupervised)

- If ground truth labels not available, use output of clustering for some other task
  - For example, use cluster assignment z_n (hard or soft) as a new feature representation
  - Performance on some task using this new rep. is a measure of goodness of clustering

- If ground truth labels are available, can compare them with clustering based labels
  - Not straightforward to compute accuracy since the label identities may not be the same, e.g.,

Ground truth = [1 1 1 0 0 0] Clustering = [0 0 0 1 1 1]

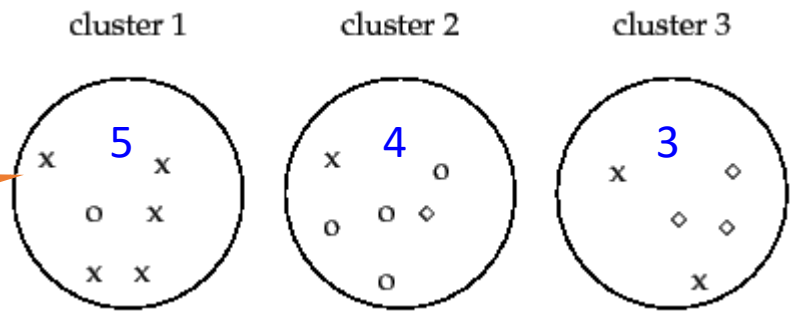
(Perfect clustering but zero "accuracy" if we just do a direct match)

  - There are various metrics that take into account the above fact
    - Purity, Rand Index, F-score, Normalized Mutual Information, etc

Evaluating Clustering Algorithms

- Purity: Looks at how many points in each cluster belong to the majority class in that cluster

3 classes (x, o ,Δ, assuming known ground truth labels)



Sum and divide by total number of points

Purity = (5+4+3)/17 ≈ 0.71

Close to 0 for bad clustering, 1 for perfect clustering

Also a bad metric if number of clusters is very large – each cluster will be kind of pure anyway

- Rand Index (RI): Can also look at what fractions of pairs of points with same (resp. different) label are assigned to same (resp. different) cluster

True Positive: No. of pairs with same true label and same cluster

True Negative: No. of pairs with diff true label and diff clusters

$$\mathrm{RI} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{FP} + \mathrm{FN} + \mathrm{TN}}$$

False Positive: No. of pairs with diff true label and same cluster

False Negative: No. of pairs with same true label and diff cluster

F_β score is also popular

$$P = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}} \qquad R = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}} \qquad F_\beta = \frac{(\beta^2 + 1)PR}{\beta^2 P + R}$$

Precision

Recall

References

CS771: Intro to Machine Learning (Fall 2021), Nisheeth Srivastava, IIT Kanpur

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Thanks