K-means Clustering and Extensions

Piyush Rai

Introduction to Machine Learning (CS771A)

September 13, 2018

Announcement: Mid-Sem Exam

- September 20 (Thursday) 13:00-15:00
- Venue: L17, L18, L19 (all OROS)

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- A review session: September 15/16/17 (timing/venue TBD)

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- Can extract "good" features $\psi(\boldsymbol{x}) \in \mathbb{R}^L$ from a kernel k (with mapping ϕ) such that

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- Landmark based approach: Using landmark points $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_L$ (selected or learned), compute
$$\psi(\boldsymbol{x}_n) = [k(\boldsymbol{z}_1, \boldsymbol{x}_n), k(\boldsymbol{z}_2, \boldsymbol{x}_n), \ldots, k(\boldsymbol{z}_L, \boldsymbol{x}_n)]$$

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- Some other approaches (that we didn't see): Nyström approx, other low-rank kernel matrix approx

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- Note: The basic K-means models each cluster only by a mean μ_k. Ignores size/shape of clusters

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- .. so it is worth looking a bit deeply into what K-means is doing

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Notation: $\mathbf{X}$ is $N \times D$, $\mathbf{Z}$ is $N \times K$ (each row is a one-hot $\boldsymbol{z}_n$), $\boldsymbol{\mu}$ is $K \times D$ (each row is a μ_k)

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Note: Replacing ℓ_2 squared (Euclidean) distance by absolute (ℓ_1) distance gives the K-medians algorithm (more robust to outliers)

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"distortion" on assignment to cluster z_n

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Total "distortion" or reconstruction error

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Note: Replacing ℓ_2 squared (Euclidean) distance by absolute (ℓ_1) distance gives the K-medians algorithm (more robust to outliers)

Note: Most unsup. learning algos try to minimize the distortion or reconstruction error of $\mathbf{X}$ from $\mathbf{Z}$

Optimizing the K-means Loss Function

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3. Go to step 1 if not yet converged

Solving for Z

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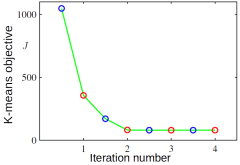
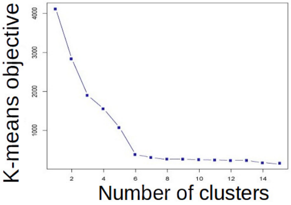
- Thus the K-means algorithm monotonically decreases the objective



(blue: after Z updated, red: after μ updated)

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"



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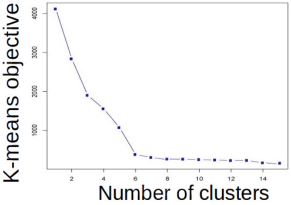

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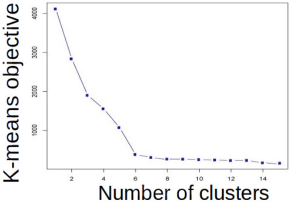

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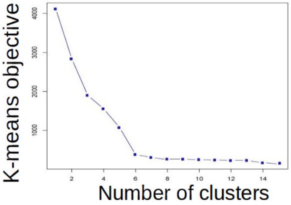

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- Several other approaches when using probabilistic models for clustering, e.g., comparing marginal likelihood $p(\mathbf{X}|K)$, using nonparametric Bayesian models, etc.

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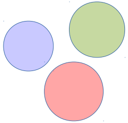

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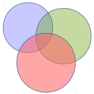

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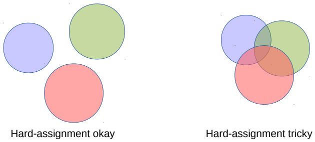

- A heuristic to get soft assignments: Transform distances from clusters into probabilities

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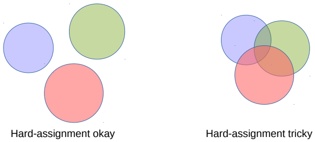

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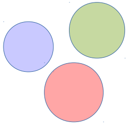

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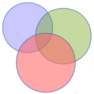

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- These heuristics are used in "fuzzy" or "soft" K-means algorithms
- Soft K-means μ_k updates are slightly different: $\mu_k = \frac{\sum_{n=1}^{N} \gamma_{nk} \boldsymbol{x}_n}{\sum_{n=1}^{N} \gamma_{nk}}$ (all points used, but fractionally)

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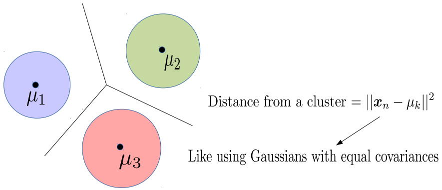

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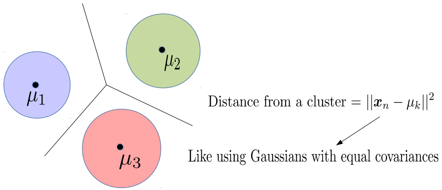

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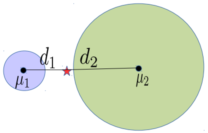

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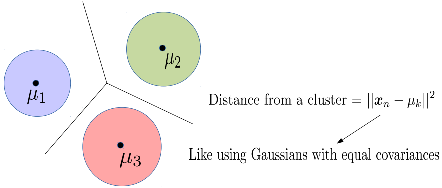

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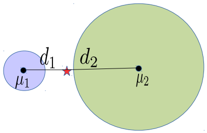

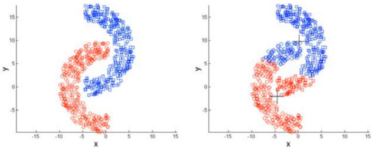

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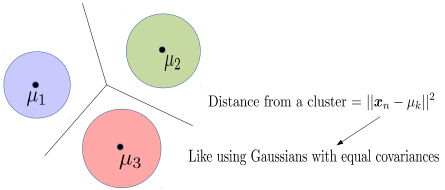

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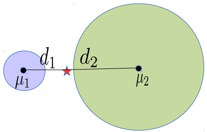

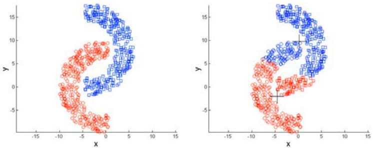

- Kernel K-means can help address some of these issues. Probabilistic models is another option

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

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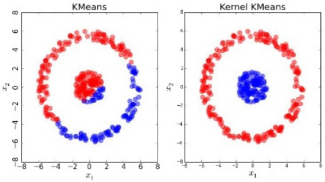

Pyclust: Open Source Data Clustering Pckage

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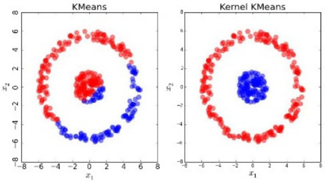

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- Can also use landmark or random features approach to make it faster
  - Can then simply run the basic K-means on those features!

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- A solution: Take an alternating approach (like K-means)

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- The above algorithm is an instance of a more general Expectation Maximization (EM) algorithm for latent variable models (we will see this post mid-sem)

Clustering vs Classification

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- Often "difficult" supervised learning problems can be seen as mixture of simpler models
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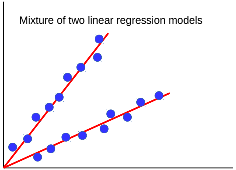

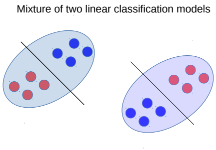

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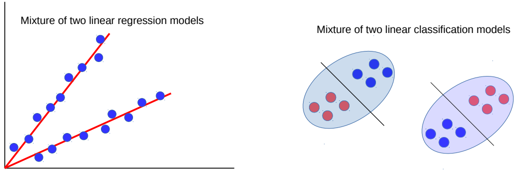

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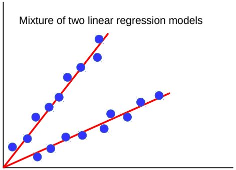

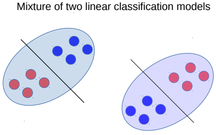

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  1. Initialize each linear model somehow (maybe randomly)
  2. Cluster the data by assigning each point to its "closest" linear model
  3. (Re-)Learn a linear model for each cluster's data. Go to step 2 if not converged.
- Often called Mixture of Experts models. Will look at these more formally after mid-sem