Foundations of Clustering

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Theoretical Foundations of Artificial Intelligence

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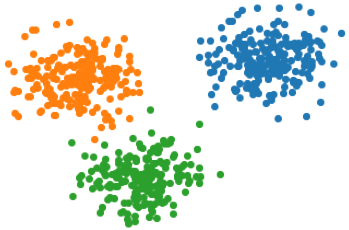
What is clustering?

Whats are clusters?



Closely packed points

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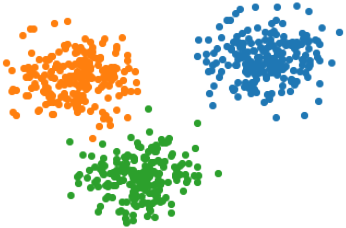

Closely packed points

Points in same pattern

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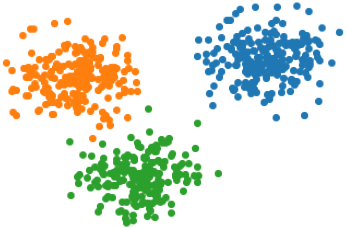

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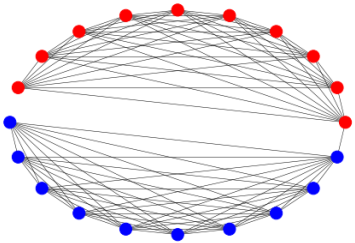

Similar / connected entities

. . . and others

Definition of cluster analysis

- Cambridge dictionary
  A way of studying or examining large amounts of data to find groups that are **more like each other** than they are like the data in other group

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- *Clustering: Science or Art?* [Luxburg et al 2012]
  Clustering should not be treated as an application-independent mathematical problem, but should always be studied in the context of its end-use

Clustering vs classification / estimation

- Formal objective

  Classification: Yes, reduce number of errors

  Clustering: None

Clustering vs classification / estimation

- Formal objective

  Classification: Yes, reduce number of errors

  Clustering: None

- Solved using optimisation

  Classification: Mostly, via training

  Clustering: Not clear for most algorithms / heuristics

Goal of this lecture

- Few popular clustering approaches
  - k-means and more (centroid based clustering)
  - Linkage methods (hierarchical clustering)
  - GMM, DBSCAN (density based clustering)
  - Deep networks
- What do these algorithms solve (formally)?
- How do we measure the goodness of clustering?

Practical guides

- Software documentation
- Blogs (easier than papers, reliability issues)
- Tutorial videos

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- Software documentation
  - Python: sklearn clustering
  - HDBSCAN documentation. Comparing Python Clustering Algorithms
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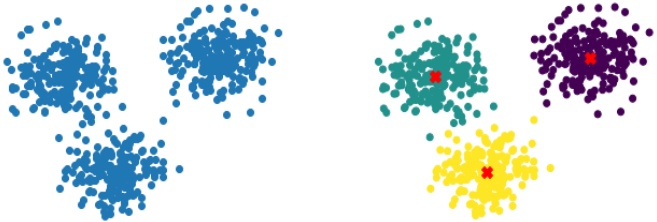
  - towards data science
  - G. Seif. The 5 Clustering Algorithms Data Scientists Need to Know
- Tutorial videos

Centroid based clustering

Basic setup

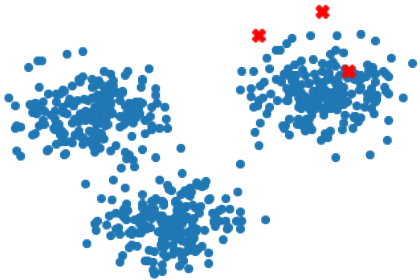
- Given n points, and number of clusters k
- Goal: Data compression
  - Find k centers that best represent the n points
  - Associate each point with nearest center



k-means algorithm

[Lloyd 1982]

1. Choose any k locations as potential centers



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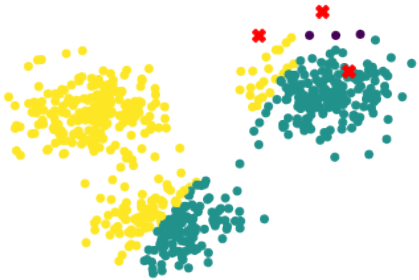

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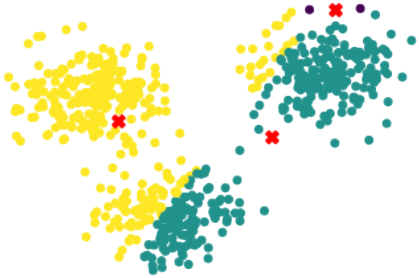
3. Update centers to be means of clusters



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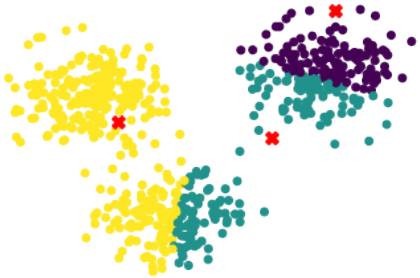

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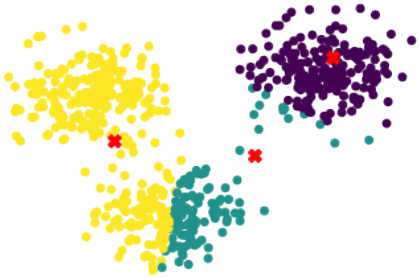

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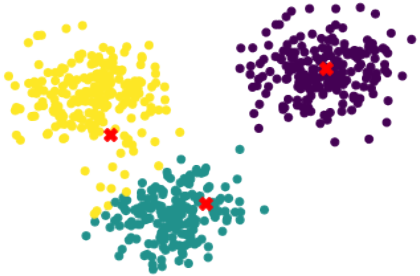

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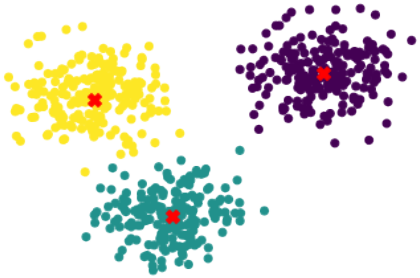

Questions

- Do the iterations converge?
- If yes, how long can it take to converge?

- What formal problem does k-means solve?
- Is the solution always ‘good’?

k-means problem

[Lloyd 1982]

- Given $\mathcal{X} = \{x_1, x_2, \ldots, x_n\} \in \mathbb{R}^p$
- For any k centers $c_1, \ldots, c_k \in \mathbb{R}^p$

$$\text{k-means cost:} \quad f(c_1, \ldots, c_k) = \sum_{j=1}^{k} \sum_{x_i \in C_j} \|x_i - c_j\|^2$$

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$\|x_i - c_j\| =$ Euclidean distance

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- Can we converge to the global minimum (or close to it)?
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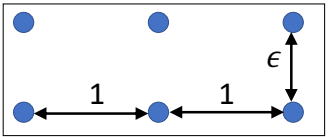
- How long does it take to converge?
  - No non-trivial bound on number of iterations

Exercise: Sub-optimality of Lloyd's algorithm

- Consider 6 points in $\mathbb{R}^2$ ($\epsilon \ll 1$)



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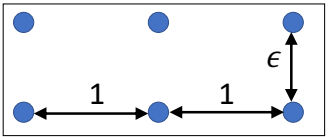

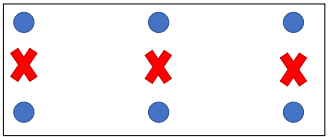

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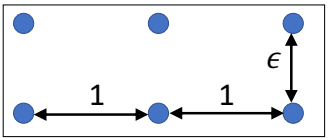
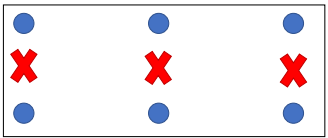
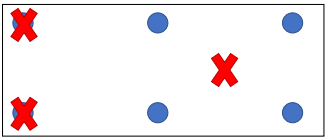
- No updates if we initialise with configuration on right
  - Cost $f = 2\sqrt{1+\epsilon^2} \quad \gg f_{opt}$



Six points



Optimal centers



Local optimum

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- Standard implementations of k-means
  - Run k-means++, follows by few iterations of k-means

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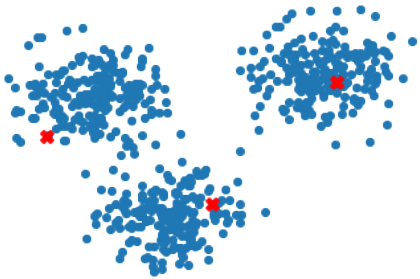

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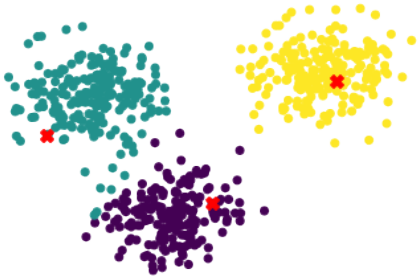

Theory for k-means

- Worst-case approximation guarantee (definition):

  An algorithm is b-factor approximation if, for any data, solution $c_1, \ldots, c_k$ satisfies

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- Impossibility result: [Lee et at 2017]

  NP-Hard to find a worst-case approximation $b \leq 1.0013$

Clustering in metric spaces

$$\text{k-means problem:} \quad \underset{c_1,\ldots,c_k}{\text{minimise}} \sum_{j=1}^{k} \sum_{x_i \in C_j} \|x_i - c_j\|^2$$

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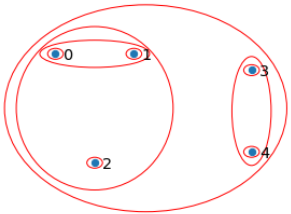
- Means can only be defined in vector spaces
  - It minimises squared distance to all points only in Hilbert space
- General metric space
  - Restrict centers to be points in data set $\mathcal{X}$, and replace Euclidean distance by metric d

$$\text{k-medoid problem:} \quad \underset{c_1,\dots,c_k \in \mathcal{X}}{\text{minimise}} \sum_{j=1}^{k} \sum_{x_i \in C_j} d(x_i, c_j)$$

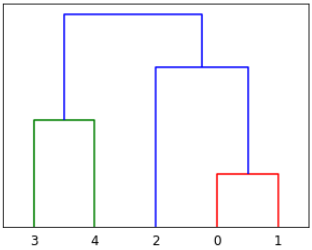
Hierarchical clustering

Hierarchical clustering

- Group data $\mathcal{X}$ at different levels of granularity
  - Hierarchy of clusters
  - One can derive k large clusters or many small clusters
- Dendrogram: Binary tree depicting hierarchy of clusters



Clusters at different levels



Dendrogram / Tree

Average linkage

- Average linkage between two clusters C, C'

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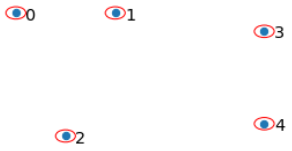

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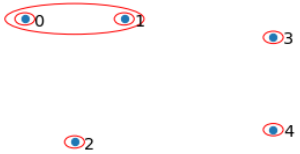

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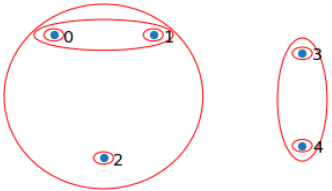

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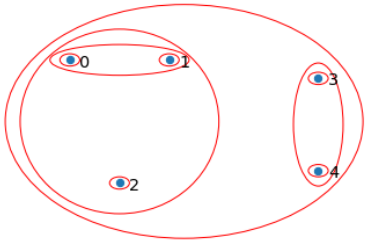

Agglomerative vs divisive clustering

- Agglomerative clustering
  - Initialisation: Each cluster contains a single data
  - Recursion: Merge most similar clusters at each level
  - Example: Average linkage

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- Agglomerative clustering
  - Initialisation: Each cluster contains a single data
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- Divisive clustering
  - Initialisation: Entire set is a single cluster
  - Recursion: Split each cluster into smaller clusters
  - Example: Recursive k-means

Analysing hierarchical clustering

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- Is hierarchical clustering an optimisation problem?

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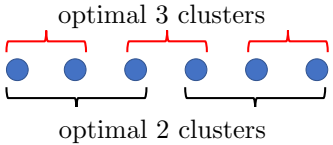
  - Example: No tree optimal for both $k = 2, 3$

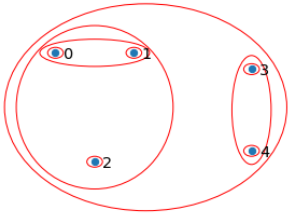


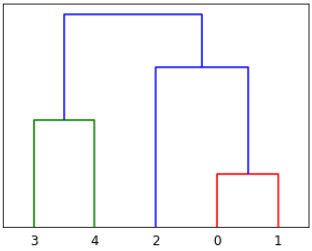
Analysing hierarchical clustering

- How can we measure goodness of obtained tree / dendrogram?
- Is hierarchical clustering an optimisation problem?
- Approach 2:
  - Define new cost / value function for a dendrogram
  - Formulate hierarchical clustering as optimisation over all dendrograms

Cost / value of dendrogram

[Dasgupta 2016; Cohen-Addad et al 2018]





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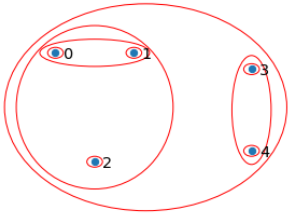
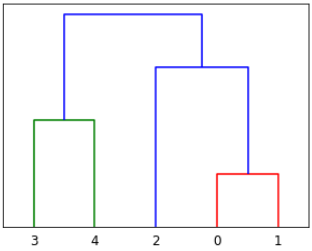
  - value(T) = measure of goodness of clusters in the tree

Cost / value of dendrogram

[Dasgupta 2016; Cohen-Addad et al 2018]





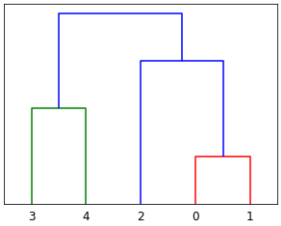
- T = binary tree / dendrogram
  - value(T) = measure of goodness of clusters in the tree
- N = node in tree = corresponding cluster
  - N_1, N_2 = children of N

Value function of dendrogram

[Cohen-Addad et al 2018]

- Distance between two nodes

$$d(N_1, N_2) = \sum_{x \in N_1} \sum_{x' \in N_2} d(x, x')$$



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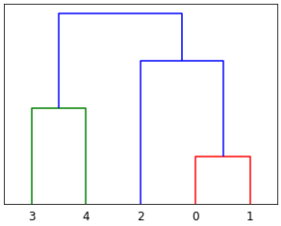

- Value function for T

$$\begin{aligned} \text{value}(T) &= \sum_{N \in T} d(N_1, N_2) \cdot |N| \\ &= \sum_{x \neq x'} d(x, x') \cdot |\text{lca}(x, x')| \end{aligned}$$

- $\text{lca}(x, x')$ = smallest cluster / node containing both x, x' (least common ancestor)

Hierarchical clustering as optimisation

- High value(T) if

$$\begin{aligned} \text{high } d(x, x') &\implies x, x' \text{ merged higher in } T \\ \text{closer } x, x' &\implies x, x' \text{ merged towards bottom of } T \end{aligned}$$

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- Formal hierarchical clustering problem

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- Approximation guarantee for average linkage

$$\text{value}\left(\widehat{T}_{avg-linkage}\right) \ \geq \ \frac{1}{2} \cdot \max_{T} \ \text{value}(T)$$

Deep clustering

Motivation

- Drawback of k-means:
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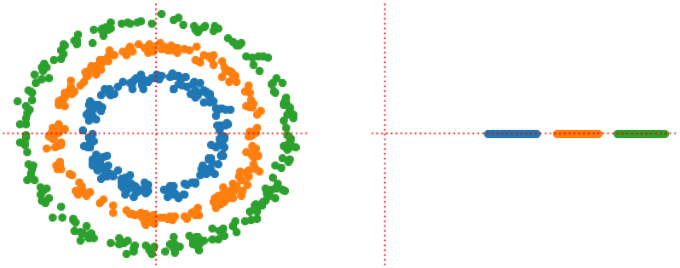
- Sometimes we can transform the data to get this



x $f(x) = \|x\|$

Few characteristics of deep learning

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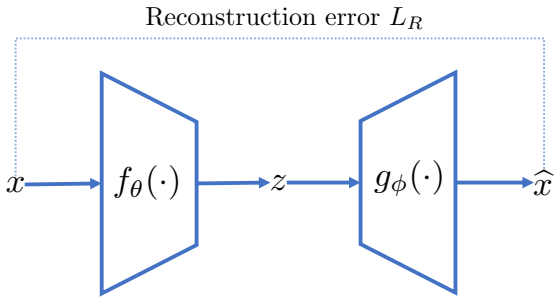
- Every problem boils down to a large optimisation

Clustering with Autoencoder

[Xie et al 2016; Dizaji et al 2017]

- Autoencoder finds low dimensional representation by minimising reconstruction error



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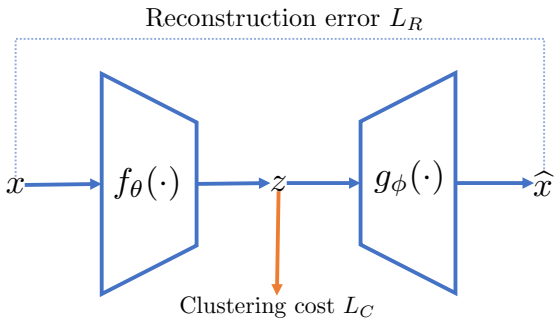

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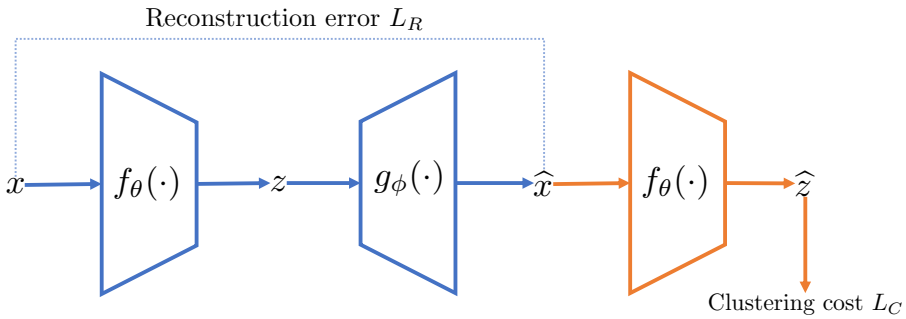

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- No theoretical guarantee
- Nice overview: P. Dahal. Deep clustering

Density based clustering

Statistical view of clustering

- Previous perspective:
  - Observed data are some fixed entities
  - Clustering = optimisation problems

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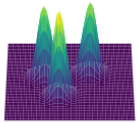
    ... model has cluster structure (mixture model)
  - Clustering = (part of) model estimation

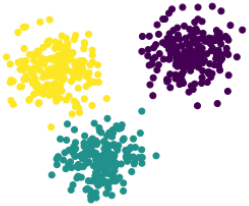
Gaussian mixture model

Data

Fitted GMM



Clusters



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Gaussian mixture model

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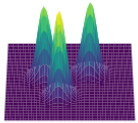

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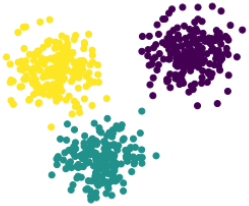

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- Fit GMM model: $\mathcal{D}_x = w_1\mathcal{N}_d(\mu_1, \Sigma_1) + w_2\mathcal{N}_d(\mu_2, \Sigma_2) + \ldots + w_k\mathcal{N}_d(\mu_k, \Sigma_k)$

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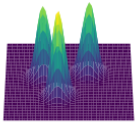

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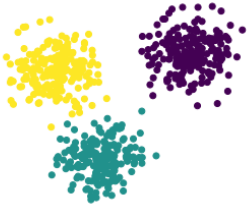

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- Typically solved via Expectation Maximisation (EM)

GMM estimation via k-means

- Data $= x_1, \ldots, x_n$
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Σ-update: $\quad \Sigma_j = \dfrac{\sum_{i=1}^{n} Z_{ij}(x_i - \mu_j)(x_i - \mu_j)^T}{\sum_{i=1}^{n} Z_{ij}}$ $\qquad$ w-update: $\quad w_j = \dfrac{\sum_{i=1}^{n} Z_{ij}}{n}$

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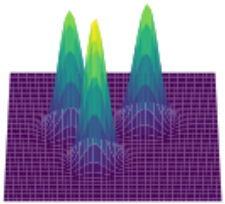

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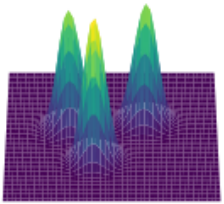

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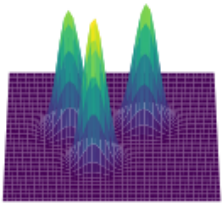

- Z-update in EM: $$Z_{ij} = \frac{w_j \exp\left(-(x_i - \mu_j)^T \Sigma_j^{-1} (x_i - \mu_j)\right)}{\sum_{l=1}^{k} w_j \exp\left(-(x_i - \mu_l)^T \Sigma_l^{-1} (x_i - \mu_l)\right)}$$

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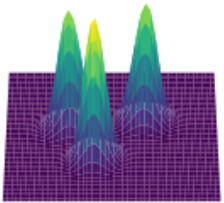

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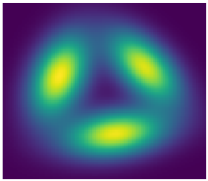
- w, μ and Σ updates in EM: Same as previous slide

Limitations of GMM (and k-means)

- Finds only elliptical clusters



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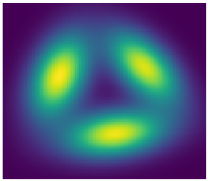

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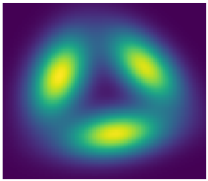

- Cannot deal with outliers

- Need to know number of clusters

Nonparametric clustering

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- Examples: [?] GMM [?] k-means [?] average linkage

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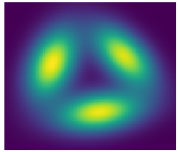
  - Example: DBSCAN [Ester et al 1996]
    Density-based Spatial Clustering of Applications with Noise

Philosophy behind DBSCAN

- Clusters are high density regions

  . . . and points in low density region are outliers



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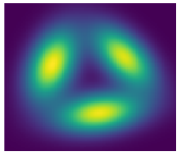

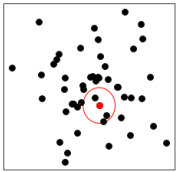

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- Estimate the density locally, around a point
  - Exercise: Consider ball $B(x, \epsilon)$ centred at x and radius ϵ

$$x \sim \mathcal{D} \quad \Longrightarrow \quad \text{pdf}_{\mathcal{D}}(x) \approx \frac{\#\text{points in } B(x,\epsilon)}{\text{total } \#\text{points}} \cdot \frac{1}{\text{volume}(B(x,\epsilon))}$$

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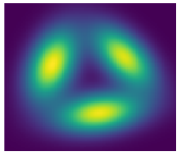
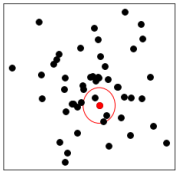
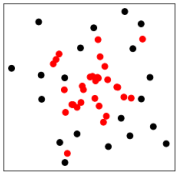
- Can threshold $\text{pdf}_{\mathcal{D}}(x)$ to decide if point inside cluster or outlier

  ... or threshold based on #points in $B(x, \epsilon)$







DBSCAN

[Ester et al 1996]

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DBSCAN

[Ester et al 1996]

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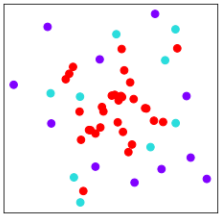
- Types of points
  - Core point: #points in $B(x, \epsilon) \geq$ `minPts`
  - Border point: #points in $B(x, \epsilon) <$ `minPts`, but lies in ball of core point
  - Outlier: neither core or border point



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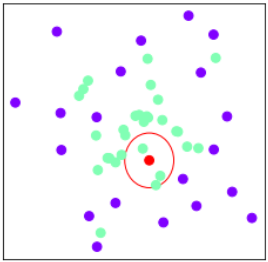

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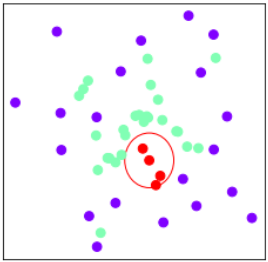
   i. Assign all points in $B(x, \epsilon)$ to same cluster



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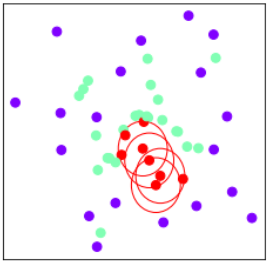

DBSCAN

[Ester et al 1996]

1. Select any **core point** x that is not clustered yet
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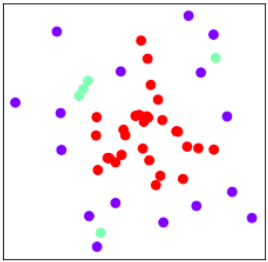

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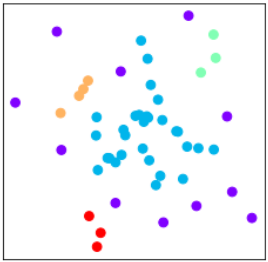
3. Repeat steps 1-2 till there is no more unclustered core point



Theoretical analyses

- GMM is theoriticians' favourite model [Dasgupta 1999; Vankadara & Ghoshdastidar 2020]
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- Huge literature on performance / convergence of EM algorithm
- DBSCAN finds level sets of probability distributions [Sriperumbudur & Steinwart 2012]

Semidefinite programming and similarity based clustering

Reformulating k-means problem

- Co-occurrence matrix $M \in \mathbb{R}^{n \times n}$ for clusters $C_1, \ldots, C_k$

$$M_{ij} = \begin{cases} \dfrac{1}{|C_\ell|} & \text{if both } x_i, x_j \in C_\ell \\ 0 & \text{if } x_i \text{ and } x_j \text{ in different clusters} \end{cases}$$

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- Define $X \in \mathbb{R}^{n \times p}$ where rows are data points $x_1, \ldots, x_n$

- Rewriting k-means cost (exercise)

$$\sum_{j=1}^{k} \sum_{x_i \in C_j} \|x_i - c_j\|^2 \quad = \quad \|X - MX\|_F^2 \qquad\qquad \|A\|_F^2 := \sum_{i,j} A_{ij}^2$$

Reformulating k-means problem

- Equivalent k-means optimisation

$$\underset{M \in \mathbb{R}^{n \times n}}{\text{maximise}} \quad \text{trace}\left(XX^T M\right) \qquad \text{trace}(A) = \sum_i A_{ii}$$

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- Relaxation: Replace constraint by simpler condition satisfied by co-occurrence matrix

(i) M has non-negative entries

(ii) M is positive semi-definite

(iii) $\text{trace}(M) = k$

(iv) M has row sum 1

Semidefinite programming (SDP)

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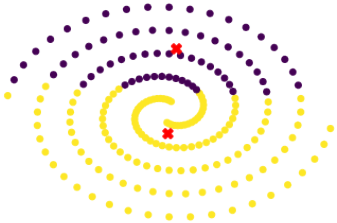
- SDP relaxation of k-means: [Peng & Wei, 2007]

$$\begin{aligned} \underset{M \text{ is psd}}{\text{maximise}} \quad & \operatorname{trace}\left(XX^T M\right) \\ \text{s.t.} \quad & M_{ij} \geq 0, \qquad \textstyle\sum_j M_{ij} = 1, \qquad \operatorname{trace}(M) = k \end{aligned}$$

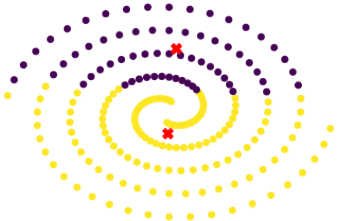
Drawbacks of k-means problem

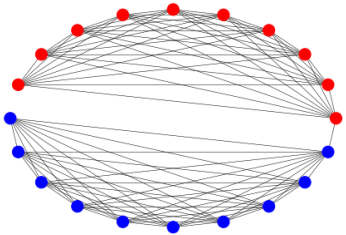
- k-means produces linear cluster boundaries
  - Can only find convex non-overlapping clusters



Drawbacks of k-means problem

- k-means produces linear cluster boundaries
  - Can only find convex non-overlapping clusters
- k-means requires data representation $x_1, \ldots, x_n$
  - What happens if we can only observe similarity between two items?





Similarity (kernel) matrix

- $S = n \times n$ symmetric matrix

$$S_{ij} = \text{ similarity (kernel) function between } x_i \text{ and } x_j$$

- S could be computed from data or directly observed
- Examples:
  - Gaussian kernel: $S_{ij} = \exp\left(-\frac{\|x_i - x_j\|^2}{\sigma^2}\right)$
  - Graph: $S =$ adjacency matrix of a similarity graph

Similarity based clustering

- Given $S \in \mathbb{R}^{n \times n}$, find

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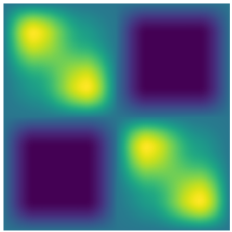
- Similarity / kernel SDP: [Vankadara & Ghoshdastidar 2020]

$$\begin{aligned} \underset{M \text{ is psd}}{\text{maximise}} \quad & \text{trace}\,(SM) \\ \text{s.t.} \quad & M_{ij} \geq 0, \quad \textstyle\sum_j M_{ij} = 1, \quad \text{trace}(M) = k \end{aligned}$$

Example

- S = similarity based on mutual 2-nearest neighbours (2-NN)

$$S_{ij} = \begin{cases} 1 & \text{if } i = j \\ 1 & \text{if } x_i \text{ is 2-NN of } x_j \text{ and } x_j \text{ is one of 2-NN of } x_i \\ 0 & \text{otherwise} \end{cases}$$



Co-occurrence matrix M

Obtained clusters

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- Getting clusters from M
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- Theoretical guarantees for similarity SDP
  - Graph / Ordinal data clustering [Yan et al 2018, Perrot et al 2020]

How good is the clustering?

Clustering metrics

- Implicit goodness of clustering

- Comparison with ground truth

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  - Define measure of goodness of clusters
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- Comparison with ground truth
  - Measure difference between two clustering / co-occurrences
  - Example: Classification error (up to permutation of labels)
    Adjusted Rand index (ARI)
    Normalsed mutual information (NMI)

Clustering stability [Ben-David et al 2006]

- If data is perturbed slightly, clustering should not change a lot
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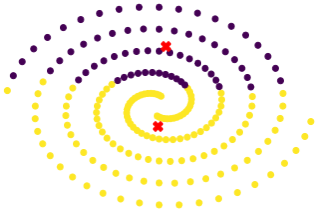

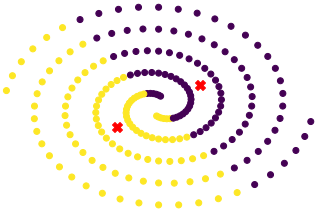

Different runs of k-means++ give different clusterings

Similarity SDP returns stable clustering

Finding good and stable clusters

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- How do we know if algorithm returns (good) stable clusters?
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- Measuring stability:
  - Verify if obtained clustering is good and stable [Meila 2018]

Verifying 'goodness' via optimisation [Meila 2018]

- Clustering via minimising cost (k-means)

$$\text{cost}(M) \;=\; \text{cost achieved by co-occurrence } M$$

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$$\text{cost}(M) \;=\; \text{cost achieved by co-occurrence } M$$

- Distance between clusterings $=$ $\|M - M'\|_F$

- Measure instability of solution M:

$$\epsilon(M) = \max_{\text{co-occurrence } M'} \left\{ \|M - M'\|_F \;:\; \text{cost}(M') \leq \text{cost}(M) \right\}$$

  - How far are other clusterings which are as good as M?
  - For some algorithms, this can be solved via SDP

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