CSE 446
K-means / GMM

Natasha Jaques

CSE 446

- Supervised learning
  - Linear models
    - Linear regression
    - Ridge regression
    - LASSO regression
    - Logistic regression
  - Non-linear models
    - Kernel methods
    - Neural Networks
    - Non-parametric methods
- **Unsupervised learning**
  - PCA/SVD
  - **Clustering**
    - **k-means**
    - **Gaussian Mixture Models (GMM)**
    - **Spectral Clustering**
- Modern machine learning / Advanced topics

Clustering

a fundamental unsupervised task

Clustering images

Unsupervised

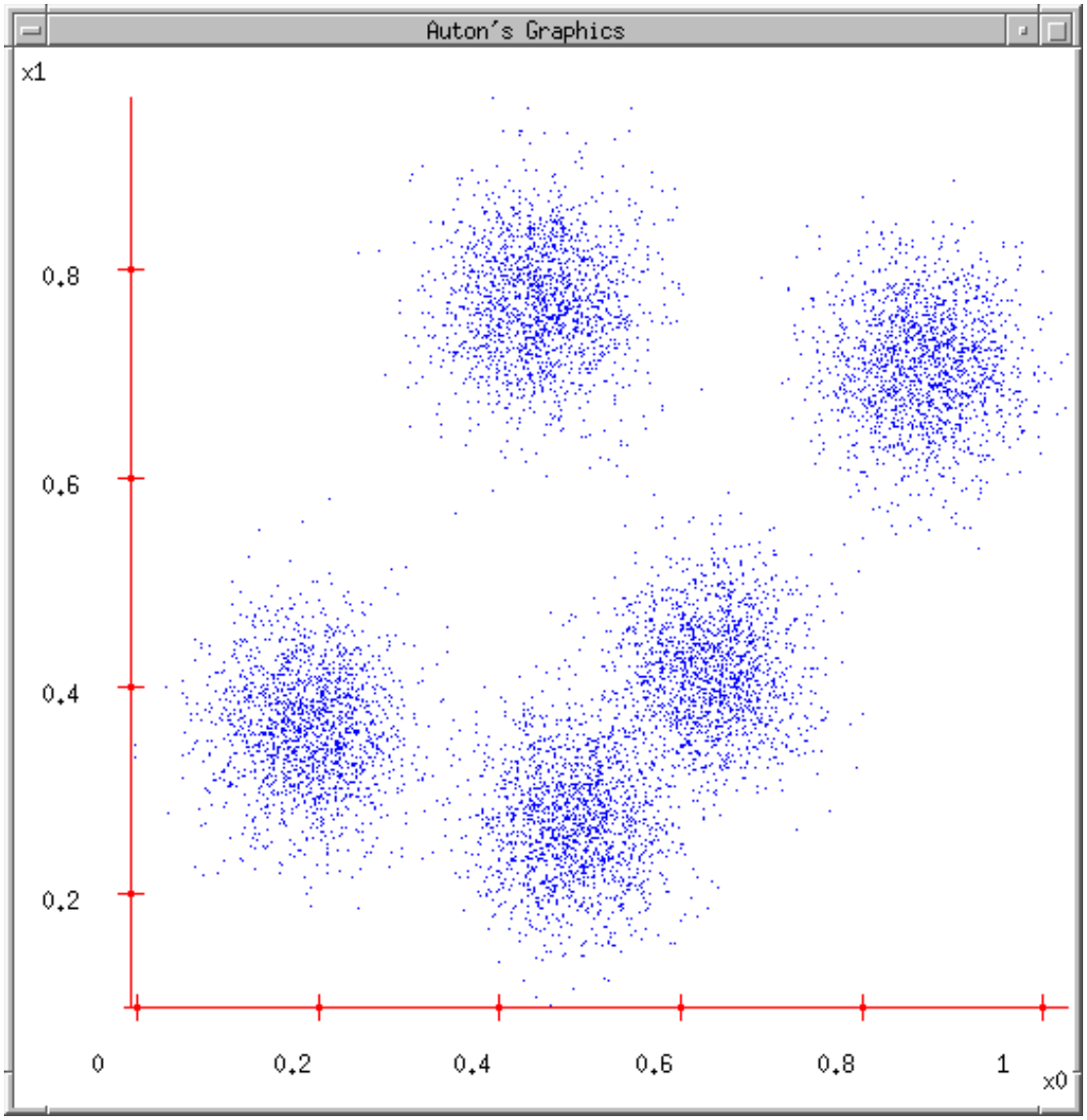
no labels

group similar images

[Goldberger et al.]

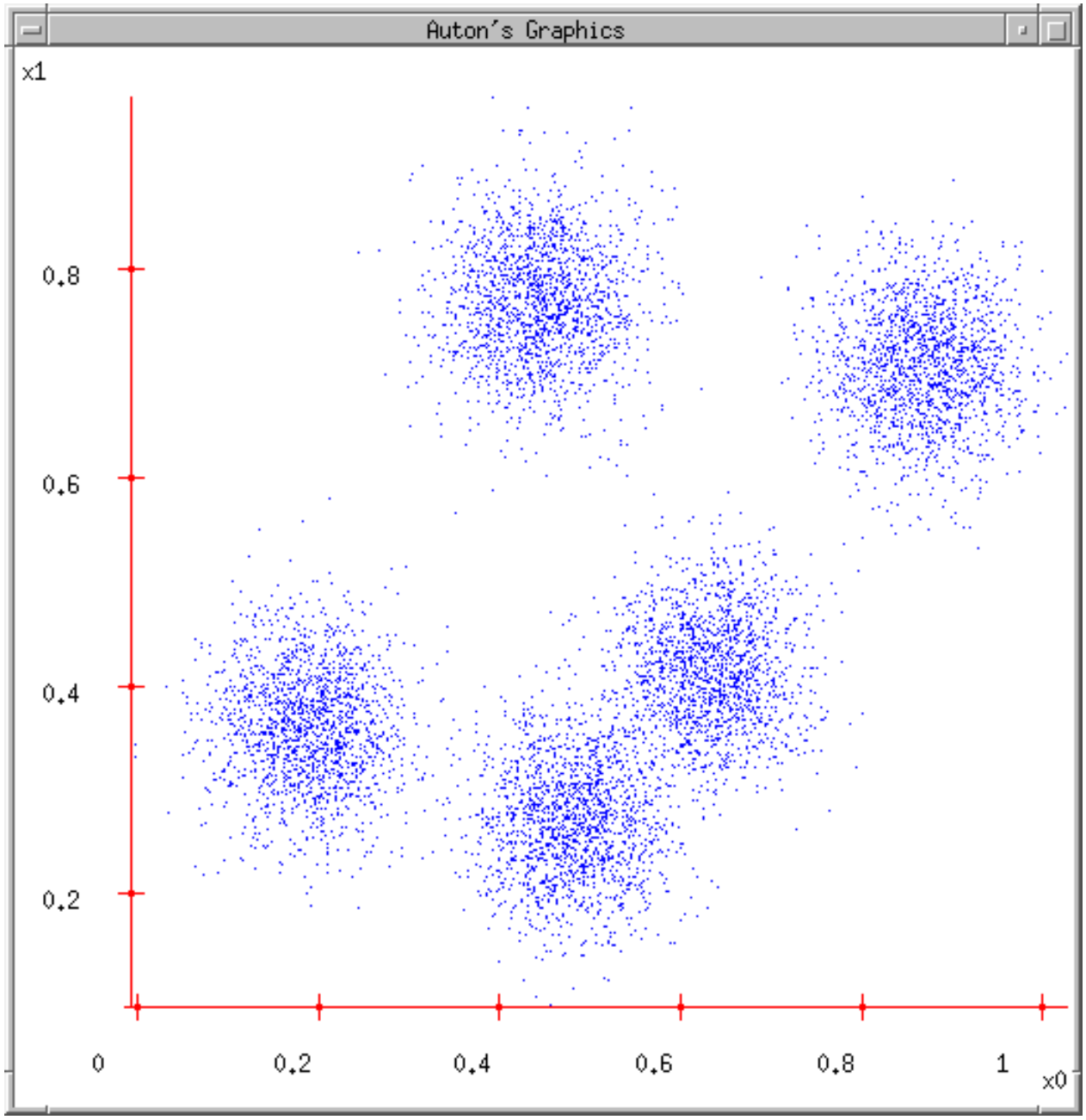
Example of 2-dimensional data points

- k-**means** algorithm assumes this kind of **structured** data, which will be clear once we learn what the algorithm does



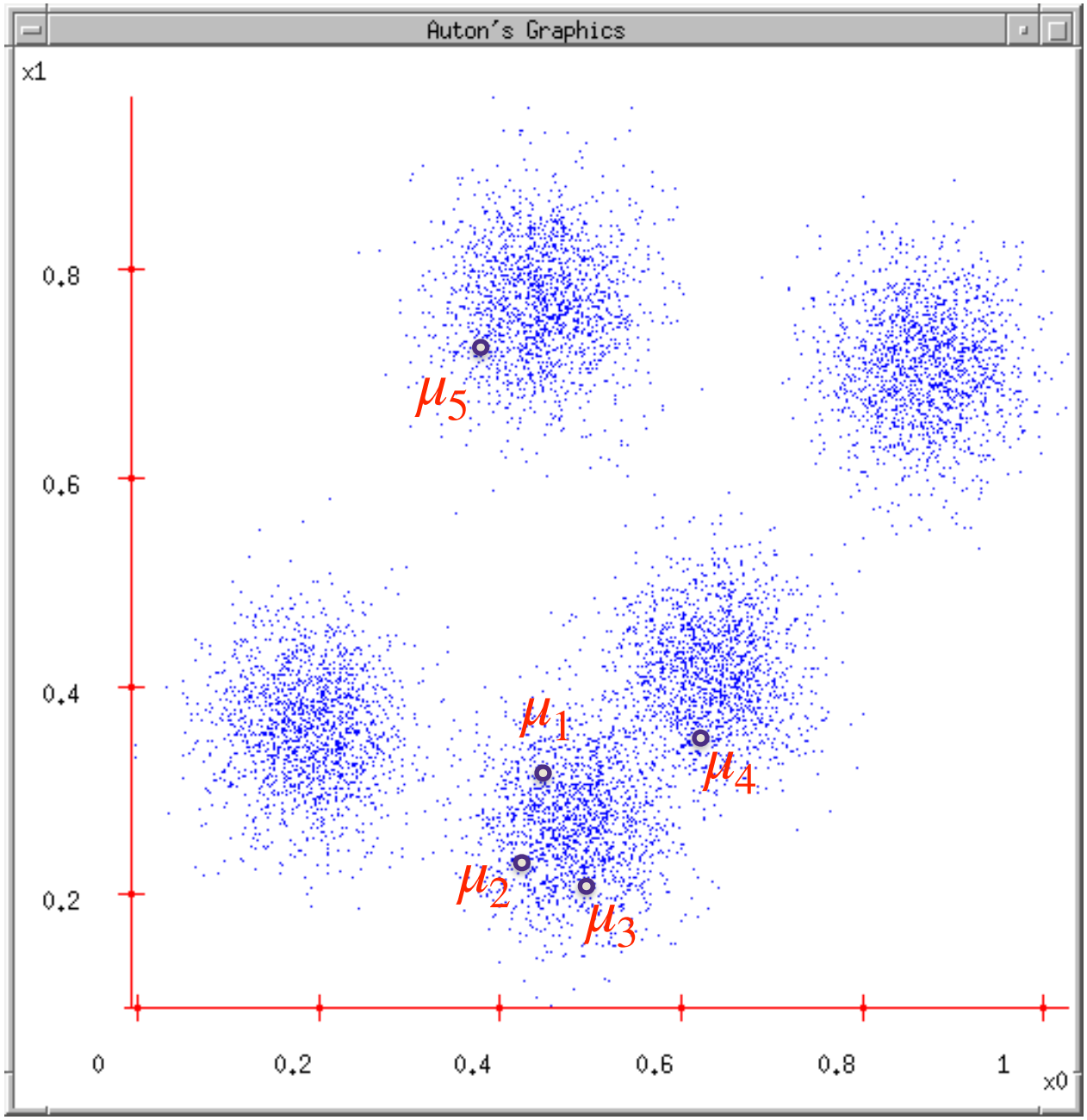
k-means

1. Ask user how many clusters they'd like. (e.g. k=5)



k-means

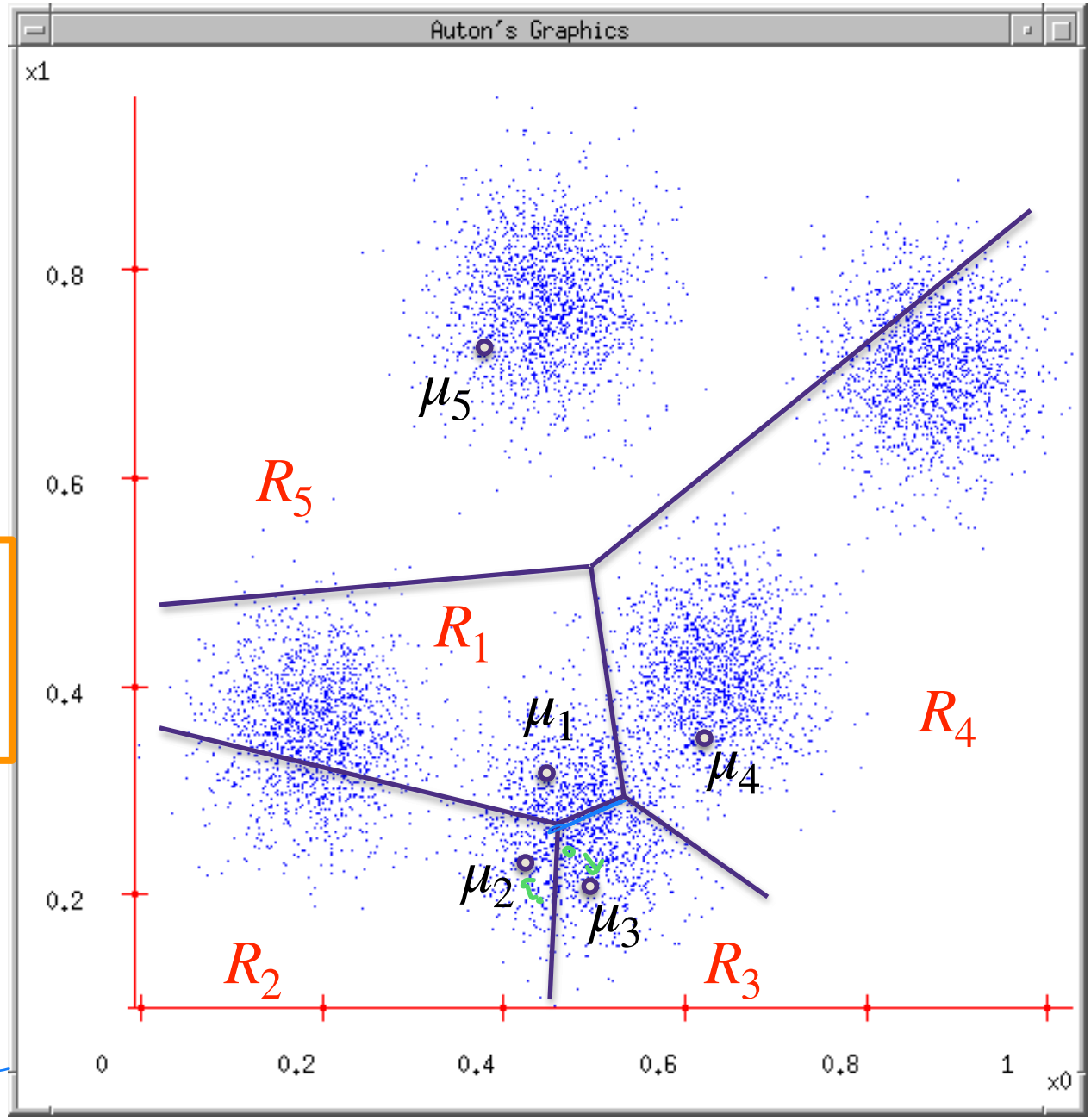
1. Ask user how many clusters they'd like. (e.g. k=5)
2. Randomly guess k cluster Center locations $\{\mu_1, \ldots, \mu_5\}$ init does matter



k-means

1. Ask user how many clusters they'd like. (e.g. k=5)
2. Randomly guess k cluster Center locations $\{\mu_1, \ldots, \mu_5\}$
3. Each datapoint finds out which Center it's closest to. (Thus each Center "owns" a set of datapoints)

Given $\{\mu_1 \ldots \mu_5\}$ → determine → Regions R → membership of each point in a cluster C



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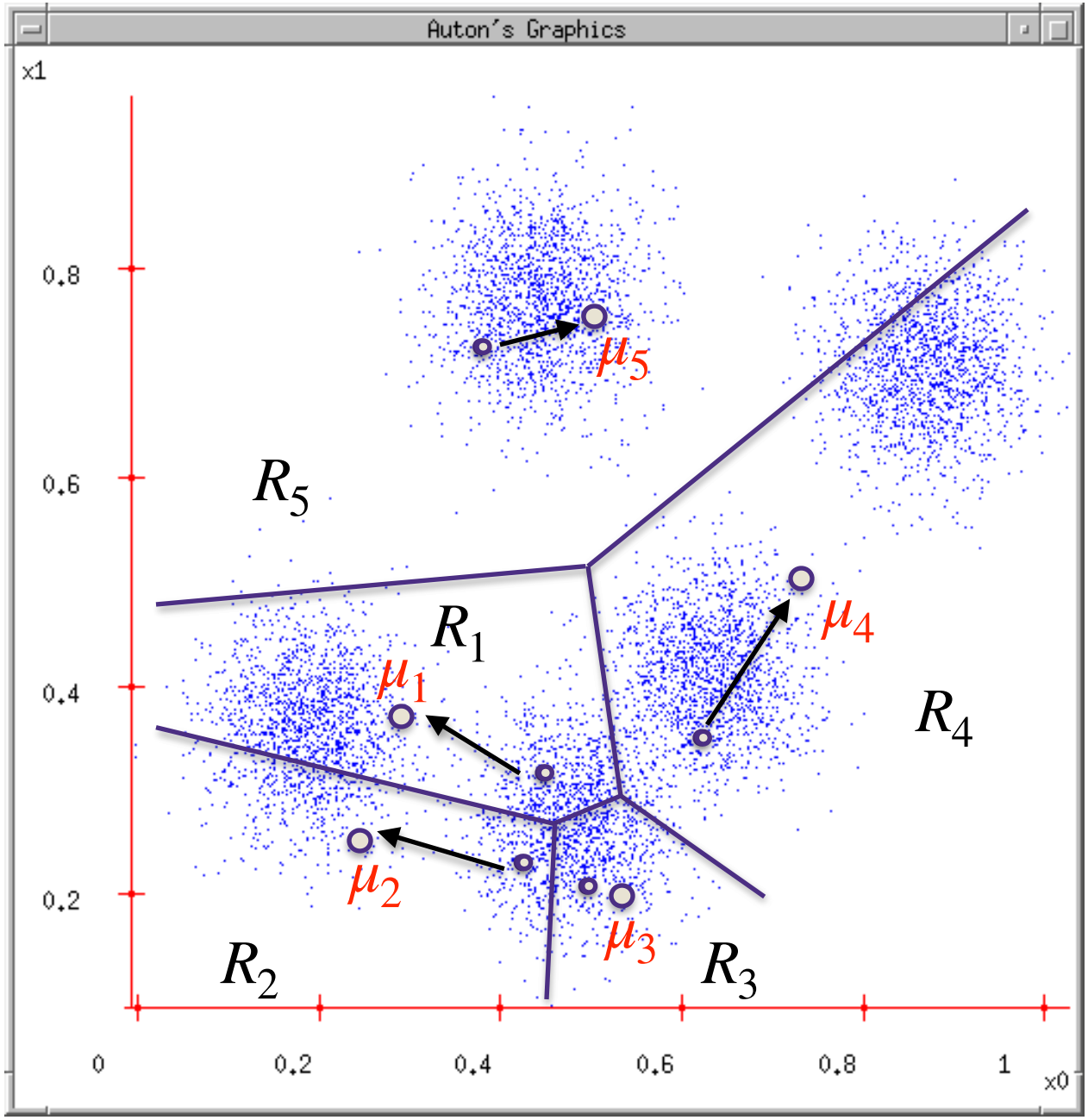
3. Each datapoint finds out which Center it's closest to.
4. Each Center finds a new centroid of the points it owns

$\{C_1 \ldots C_k\} \rightarrow \{\mu_1 \ldots \mu_5\}$

$\{R_1 \text{ in } R_5\}$



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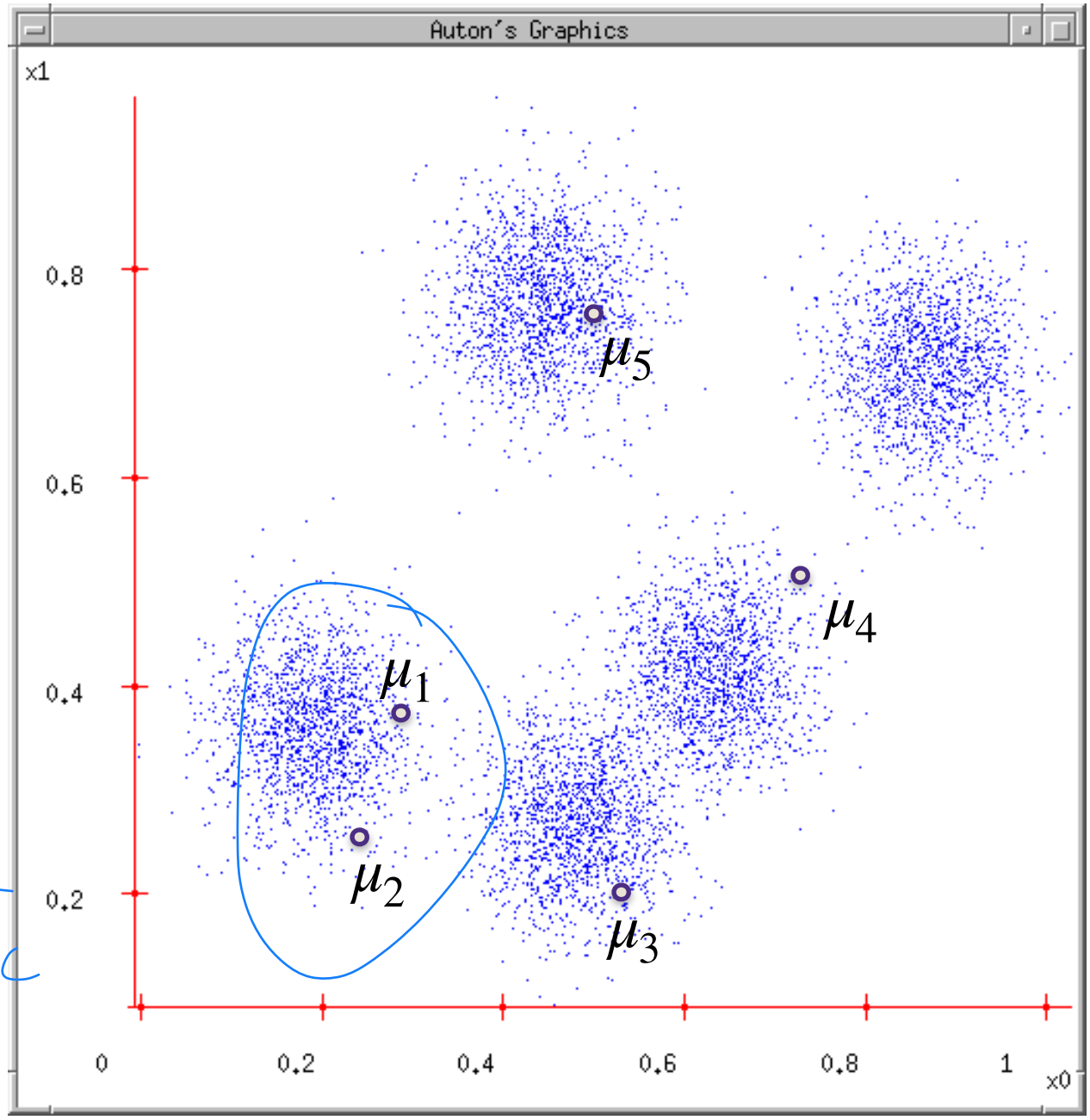
4. Each Center finds a new centroid of the points it owns…
5. …and jumps there
6. …Repeat until terminated!

when membership of points → clusters stops changing



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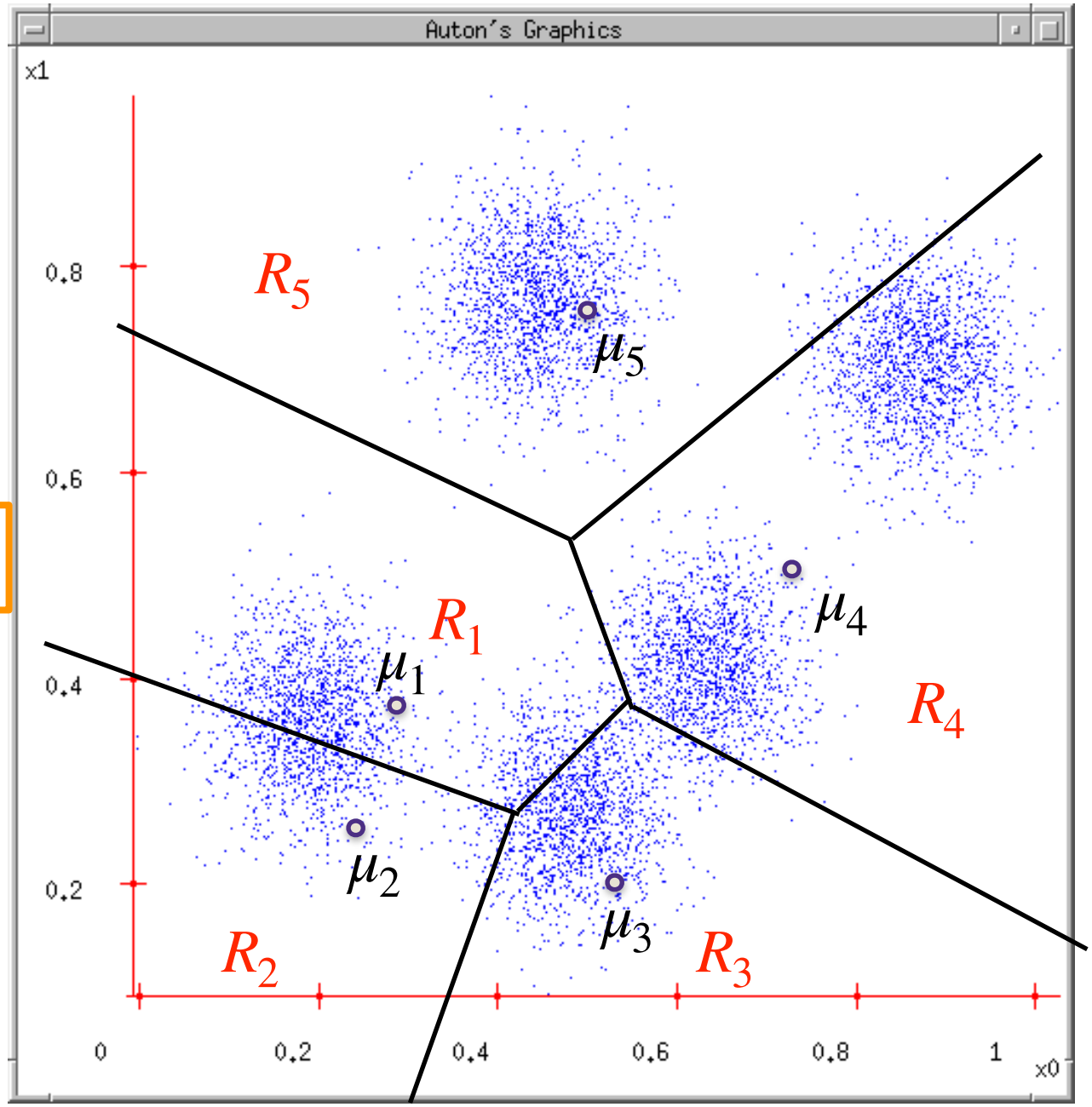

k-means

https://www.naftaliharris.com/blog/visualizing-k-means-clustering/

K-means algorithm

1. Choose k, how many clusters to find
2. Randomly initialize k centers
   - $\mu^{(0)} = [\mu_1^{(0)}, \ldots, \mu_k^{(0)}] \in \mathbb{R}^{d \times k}$
   - Usually randomly chosen from the data points, to make sure they are in the right domain

- For t=0,1,2,… repeat

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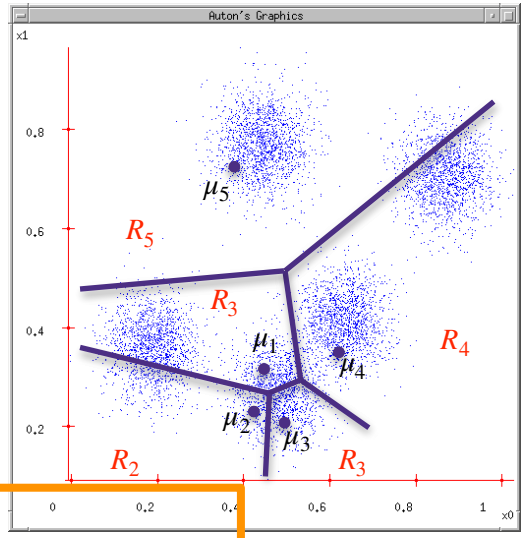
- For t=0,1,2,… repeat
3. Assign each point j∈{1,…,n} to its nearest center:

$$\underbrace{C_j^{(t)}}_{\text{Membership of the j-th data point}} \leftarrow \arg\min_{i \in \{1,2,\ldots,k\}} \|x_j - \mu_i^{(t)}\|^2$$

Assignment:



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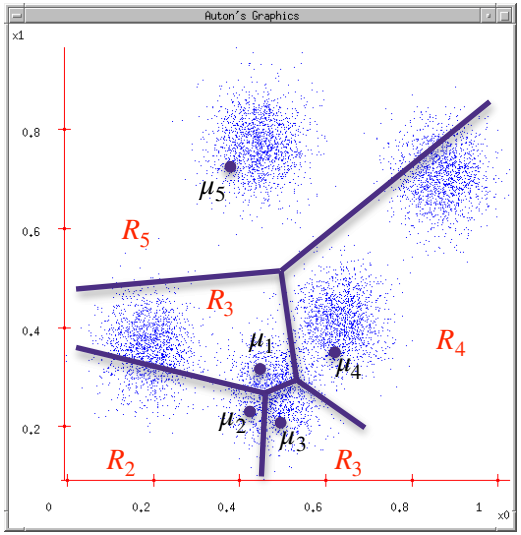
$$C_j^{(t)} \leftarrow \arg\min_{i \in \{1,2,\ldots,k\}} \|x_j - \mu_i^{(t)}\|^2$$

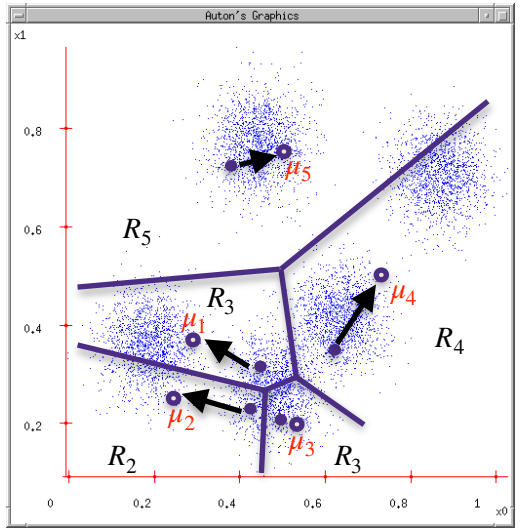
4. Recenter: μ_i becomes centroid of its point:

$$\mu_i^{(t+1)} \leftarrow \arg\min_{\mu} \sum_{j:C_j^{(t)}=i} \|\mu - x_j\|^2$$

Assignment:



Recenter:



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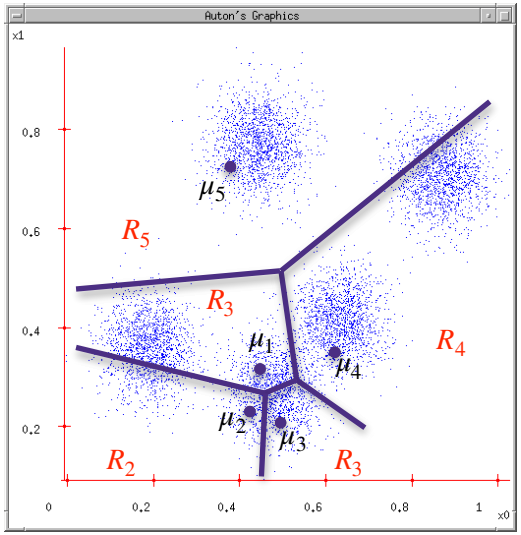
- Equivalent to
  $\mu_i^{(t+1)} \leftarrow$ average of all the points assigned to $\mu_i^{(t)}$

Assignment:



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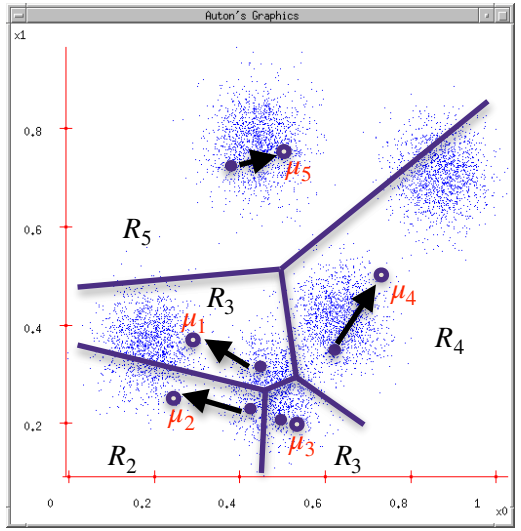
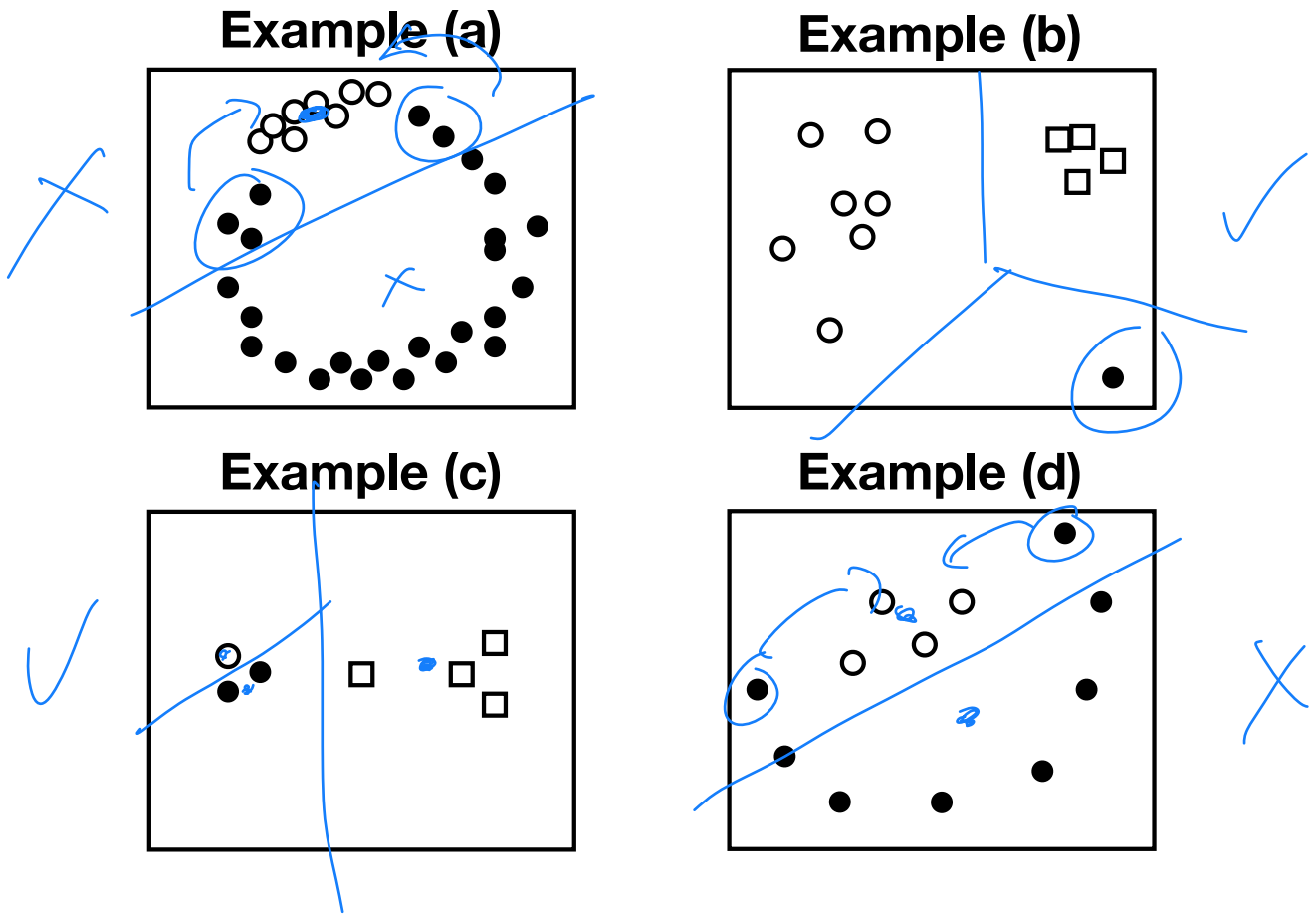


Which one is a snapshot of a converged k-means

When k-means is converged, there should be a set of centers and assignments that do not change when applying 1 step of k-means



Does k-means converge?

"Expectation maximization" ↳ GMM

- k-means is trying to minimize the following objective

$$\min_{\{\mu_i\}_{i=1}^{k}} \min_{\{C_\ell\}_{\ell=1}^{n}} \sum_{j=1}^{n} \|x_j - \mu_{C_j}\|^2$$

via alternating minimization
(equivalent to coordinate descent) → block coord. des.

- Fix μ, optimize C → convex
- Fix C, optimize μ → convex

- Does this converge? Does this terminate in finite time?

Does k-means converge?

- there is only a finite set of values that $\{C_j\}_{j=1}^{n} \in \{1,\ldots,k\}^n$ can take (k^n is large but finite)
- so there is only finite, k^n at most, values for cluster-centers, $\{\mu_i\}_{i=1}^{k}$, also
- each time we update them, we will never increase the objective function:

$$\sum_{j=1}^{n} \|x_j - \mu_{C_j}\|_2^2$$

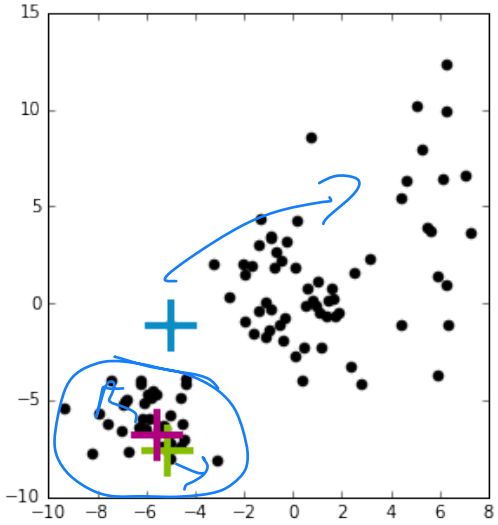
- the objective is lower bounded by zero
- after at most k^n steps, the algorithm must converge
  (as the assignments $\{C_j\}_{j=1}^{n}$ cannot return to previous assignments in the course of k-means iterations)

downsides of k-means

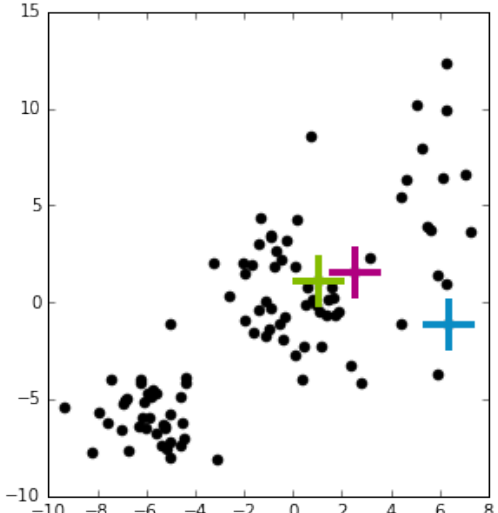
1. it requires the number of clusters k to be specified by us
2. the final solution depends on the initialization
   (does not find global minimum of the objective)

Initial position of centers

Trial 1



Trial 2



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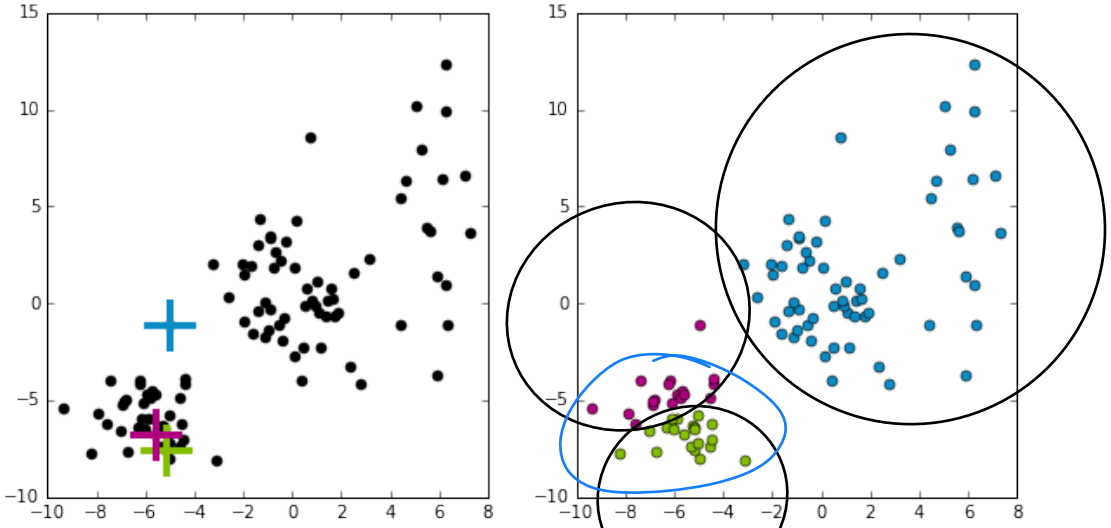
Initial position of centers final converged assignment

Trial 1



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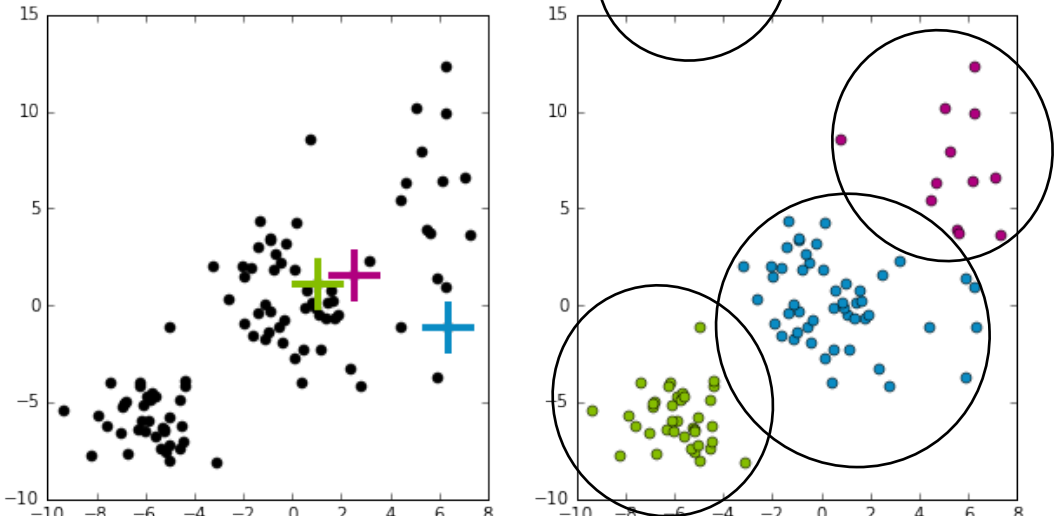


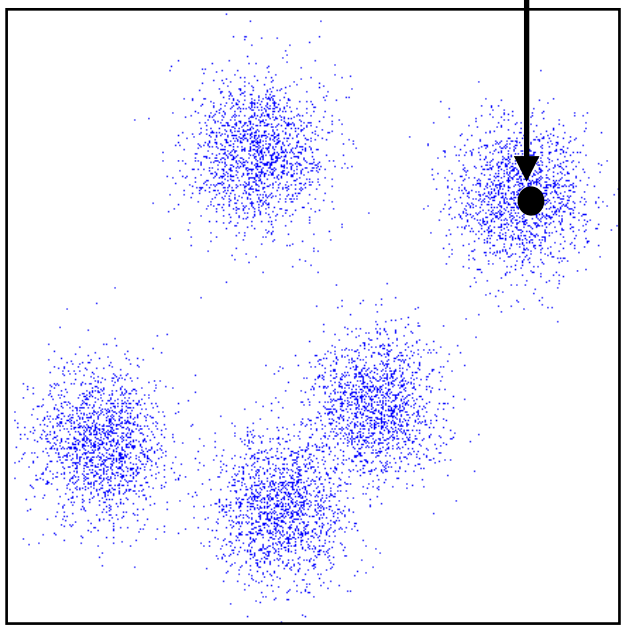
How to fix initialization?

Choose initial points by incorporating distance & # of points

k-means++: a smart initialization

Smart initialization:

1. Choose **first** cluster center μ_1 uniformly at random from data points



k-means++: a smart initialization

Smart initialization:

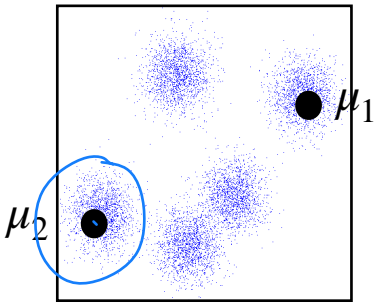
1. Choose **first** cluster center μ_1 uniformly at random from data points
2. For k=2,… K // For each initial cluster center

3. For each data point x_i, compute distance d_i to nearest cluster center
4. Choose new cluster center from amongst data points, with probability of x_i being chosen proportional to $(d_i)^2$

precisely,

$$d_i \leftarrow \min_{j \in \{1,\ldots k-1\}} \|\mu_j - x_i\|, \text{ for all } i \text{ that is not chosen already}$$

$$\text{Prob}(x_i \text{ chosen as the next center}) = \frac{(d_i)^2}{\sum_\ell (d_\ell)^2}$$



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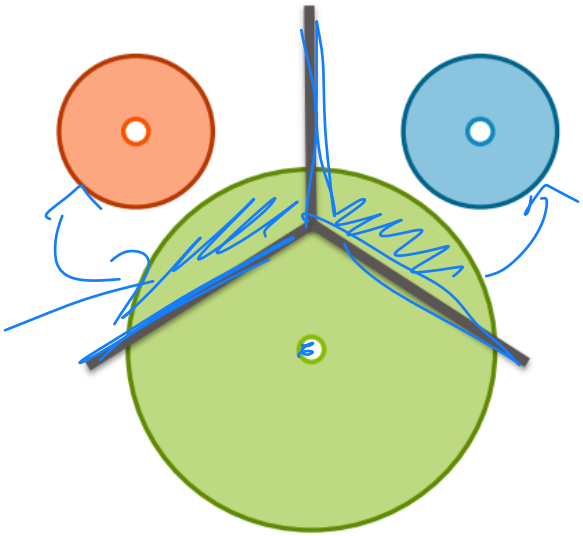
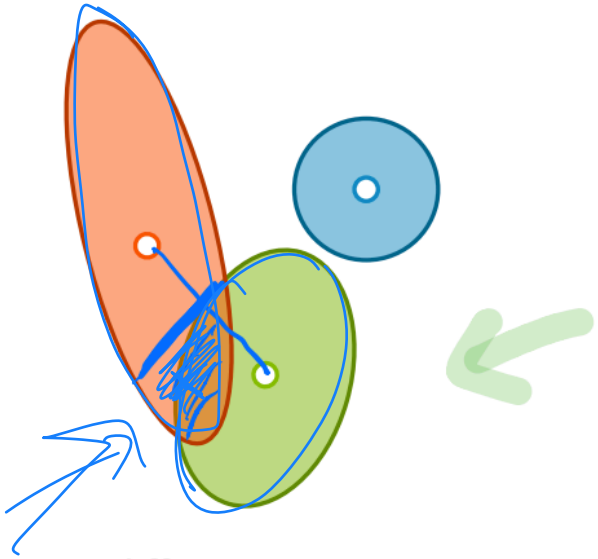
- apply standard K-means after this initialization

- K-means algorithm fails, when the data has:



disparate cluster sizes



different shaped/oriented clusters

- What can we do?

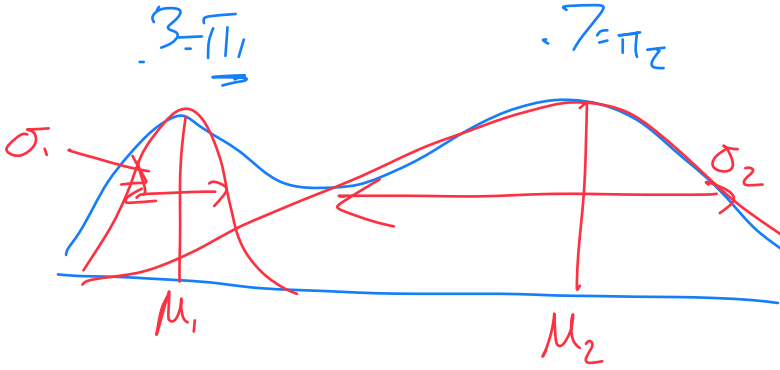
CSE 446/546 2025 winter

- Supervised learning
  - Linear models (lectures 1-9)
    - Linear regression
    - Ridge regression
    - LASSO regression
    - Logistic regression
  - Non-linear models (lectures 10-13)
    - Kernel methods
    - Neural Networks
    - Non-parametric methods
- **Unsupervised learning (lectures 14-16)**
  - PCA/SVD
  - **Clustering**
    - **k-means**
    - **Gaussian Mixture Models (GMM)**
    - **Spectral Clustering**
- Modern machine learning (lectures 17-19)

Gaussian Mixture Models

Extension of k-means

Gaussian Mixture Model



- input: data $\{x_i\}_{i=1}^n$ in $\mathbb{R}^d$
- parameters of a **Gaussian Mixture Model**
  - mixing weights:
    - $\pi_j = \mathbf{P}(\text{cluster membership} = j)$ for $j \in \{1, \ldots, K\}$
  - means:
    - $\mu_j \in \mathbb{R}^d$ for $j \in \{1, \ldots, K\}$
  - covariance matrices:
    - $\mathbf{\Sigma}_j \in \mathbb{R}^{d \times d}$ for $j \in \{1, \ldots, K\}$
- we suppose that the given data has been generated from a GMM, and try to find the best GMM parameters (this naturally will define clustering of the training data)

Gaussian Mixture Model

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- under the GMM, the i-th sample is drawn as follows
  - first sample a cluster $z_i \in \{1,\ldots,K\}$, from $\pi = [\pi_1, \ldots, \pi_K]$
  - conditioned on this cluster, x_i is sampled from

$$x_i \sim N(\mu_{z_i}, \mathbf{\Sigma}_{z_i})$$

demo: https://lukapopijac.github.io/gaussian-mixture-model/

Maximum likelihood estimation (MLE)

- we can find the best GMM for given data, by MLE
- for simplicity, suppose $d = 1$ and $K = 2$
- Model parameters are $\pi_1, \pi_2, \mu_1, \mu_2, \sigma_1^2, \sigma_2^2 \in \mathbb{R}$
- the probability of observing a sample x_i can be written as

$$\mathbf{P}(x_i; \pi_1, \pi_2, \mu_1, \mu_2, \sigma_1^2, \sigma_2^2) = \underbrace{\pi_1 \frac{1}{\sqrt{2\pi\sigma_1^2}} e^{-\frac{(x_i-\mu_1)^2}{2\sigma_1^2}}}_{\triangleq N(x_i;\mu_1,\sigma_1^2)} + \underbrace{\pi_2 \frac{1}{\sqrt{2\pi\sigma_2^2}} e^{-\frac{(x_i-\mu_2)^2}{2\sigma_2^2}}}_{\triangleq N(x_i;\mu_2,\sigma_2^2)}$$

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- MLE tries to find

$$\arg \max_{\pi_1,\pi_2,\mu_1,\mu_2,\mathbf{C}_1,\mathbf{C}_2} \sum_{i=1}^{n} \log \mathbf{P}(x_i; \pi_1, \pi_2, \mu_1, \mu_2, \sigma_1^2, \sigma_2^2)$$

- however, unlike least squared or logistic regression, this is not a concave function of the parameters (thus hard to find the optimal solution)
- in general, MLE of a mixture model is not convex/concave optimization

Recall lecture 1: fitting a single Gaussian model

- given $\{x_i\}_{i=1}^n \in \mathbb{R}$,fit the best Gaussian model with mean $\mu \in \mathbb{R}$ and variance $\sigma^2 \in \mathbb{R}$
- using MLE we want to solve

$$\text{maximize}_{\mu,\sigma^2} \; \mathscr{L}(\mu,\sigma^2) = \sum_{i=1}^n \underbrace{\left(-\frac{(x_i-\mu)^2}{2\sigma^2} - \log\left(\sqrt{2\pi\sigma^2}\right)\right)}_{\log N(x_i|\mu,\sigma^2)}$$

- we compute gradient and set it to zero:
  - $$\nabla_\mu \mathscr{L}(\mu,\sigma^2) = \frac{1}{\sigma^2}\sum_{i=1}^n (\mu - x_i) =$$

    which is zero for $\mu = \frac{1}{n}\sum_{i=1}^n x_i$

    (which makes sense as it is the empirical mean)

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    (which makes sense as it is the empirical mean)
  - $$\nabla_{\sigma^2} \mathscr{L}(\mu,\sigma^2) = \frac{\sum_{i=1}^n (x_i-\mu)^2}{2(\sigma^2)^2} - \frac{n}{2\sigma^2}$$

    which is zero for $\sigma^2 = \frac{1}{n}\sum_{i=1}^n (x_i-\mu)^2$

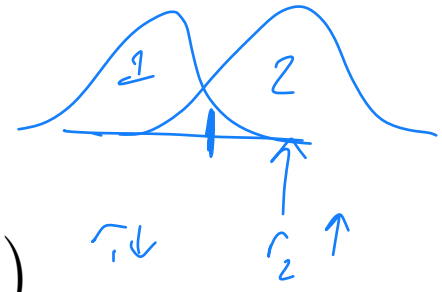
    (which makes sense as it is the empirical variance)

MLE for GMM

- we want to fit a model by solving

$$\max_{\pi_1,\pi_2,\mu_1,\mu_2,\sigma_1^2,\sigma_2^2} \sum_{i=1}^{n} \log\Bigg(\pi_1 \underbrace{\frac{1}{\sqrt{2\pi\sigma_1^2}} e^{-\frac{(x_i-\mu_1)^2}{2\sigma_1^2}}}_{\triangleq N(x_i;\mu_1,\sigma_1^2)} + \pi_2 \underbrace{\frac{1}{\sqrt{2\pi\sigma_2^2}} e^{-\frac{(x_i-\mu_2)^2}{2\sigma_2^2}}}_{\triangleq N(x_i;\mu_2,\sigma_2^2)} \Bigg)$$

MLE for GMM



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- define $r_{i1} = \mathbf{P}(z_i = 1 \mid x_i) = \dfrac{\mathbf{P}(z_i = 1, x_i)}{\mathbf{P}(z_i = 1, x_i) + \mathbf{P}(z_i = 2, x_i)}$

$$= \frac{\pi_1 N(x_i; \mu_1, \sigma_1^2)}{\pi_1 N(x_i; \mu_1, \sigma_1^2) + \pi_2 N(x_i; \mu_2, \sigma_2^2)}$$

Estimated soft membership

MLE for GMM

- we want to fit a model by solving

$$\max_{\pi_1,\pi_2,\mu_1,\mu_2,\sigma_1^2,\sigma_2^2} \sum_{i=1}^{n} \log\Bigg(\pi_1 \underbrace{\frac{1}{\sqrt{2\pi\sigma_1^2}} e^{-\frac{(x_i-\mu_1)^2}{2\sigma_1^2}}}_{\triangleq N(x_i;\mu_1,\sigma_1^2)} + \pi_2 \underbrace{\frac{1}{\sqrt{2\pi\sigma_2^2}} e^{-\frac{(x_i-\mu_2)^2}{2\sigma_2^2}}}_{\triangleq N(x_i;\mu_2,\sigma_2^2)} \Bigg)$$

soft membership of a data point → n r_i's

- define $r_i = \mathbf{P}(z_i = 1 \mid x_i) = \dfrac{\mathbf{P}(z_i = 1, x_i)}{\mathbf{P}(z_i = 1, x_i) + \mathbf{P}(z_i = 2, x_i)}$

cluster 1

$$= \frac{\pi_1 N(x_i; \mu_1, \sigma_1^2)}{\pi_1 N(x_i; \mu_1, \sigma_1^2) + \pi_2 N(x_i; \mu_2, \sigma_2^2)}$$

← normalization over k clusters

- setting the gradient to zero, we get
  - $\pi_1 = \dfrac{N_1}{n}$ where $N_1 = \sum_{i=1}^{n} r_i$, and $\pi_2 = \dfrac{N_2}{n}$ where $N_2 = \sum_{i=1}^{n} (1 - r_i)$
  - $\mu_1 = \dfrac{1}{N_1} \sum_{i=1}^{n} r_i x_i$ and $\mu_2 = \dfrac{1}{N_2} \sum_{i=1}^{n} (1 - r_i) x_i$
  - $\sigma_1^2 = \dfrac{1}{N_1} \sum_{i=1}^{n} r_i (x_i - \mu_1)^2$ and $\sigma_2^2 = \dfrac{1}{N_2} \sum_{i=1}^{n} (1 - r_i)(x_i - \mu_2)^2$
- both LHS and RHS depend on the parameters, and no closed form solution exists
- **note that if we know r_i's it is trivial to compute parameters, and vice versa**

$\mu, \pi, \sigma \in \mathbb{R}^k$

Expectation Maximization (EM) algorithm to approximate the solution of MLE

- EM is a popular method to solve MLE for mixture models
- input: training data $\{x_i\}_{i=1}^n$
- output: $\pi_1, \pi_2, \mu_1, \mu_2, \sigma_1^2, \sigma_2^2 \in \mathbb{R}$ parameters of GMM

- initialization: randomly initialize the parameters

Expectation Maximization (EM) algorithm to approximate the solution of MLE

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- input: training data $\{x_i\}_{i=1}^n$
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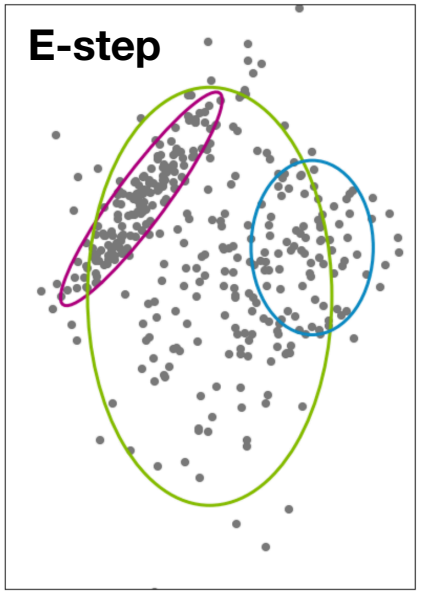
- initialization: randomly initialize the parameters
- repeat
  - **E-step** (Expectation): parameters → soft membership
    - $r_i = \dfrac{\pi_1 N(x_i; \mu_1, \sigma_1^2)}{\pi_1 N(x_i; \mu_1, \sigma_1^2) + \pi_2 N(x_i; \mu_2, \sigma_2^2)}$ for all $i \in \{1,2,\ldots,n\}$
  - **M-step** (Maximization): soft membership → parameters



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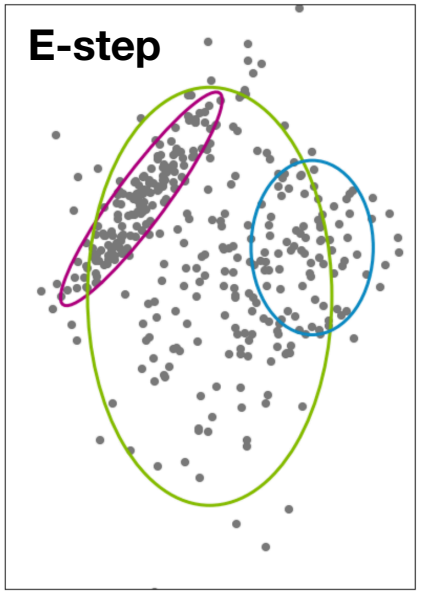
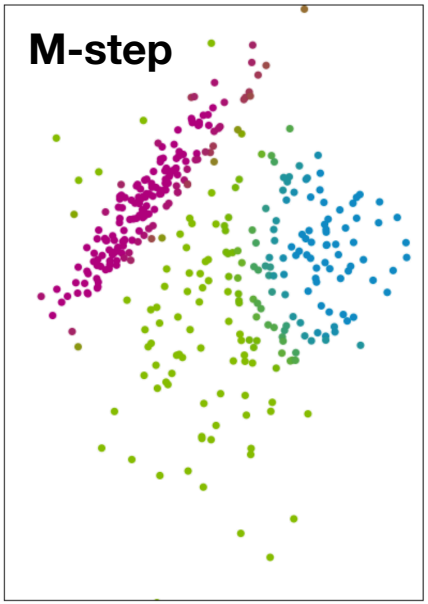
    - $\pi_1 = \dfrac{N_1}{n}$ where $N_1 = \sum_{i=1}^n r_i$, and $\pi_2 = \dfrac{N_2}{n}$ where $N_2 = \sum_{i=1}^n (1 - r_i)$
    - $\mu_1 = \dfrac{1}{N_1} \sum_{i=1}^n r_i x_i$ and $\mu_2 = \dfrac{1}{N_2} \sum_{i=1}^n (1 - r_i) x_i$
    - $\sigma_1^2 = \dfrac{1}{N_1} \sum_{i=1}^n r_i (x_i - \mu_1)^2$ and $\sigma_2^2 = \dfrac{1}{N_2} \sum_{i=1}^n (1 - r_i)(x_i - \mu_2)^2$





For general number of clusters K and dimension d

- we can derive EM for general case, in an analogous way
- Initialize parameters: $\pi_1, \ldots, \pi_K, \mu_1, \ldots, \mu_K, \Sigma_1, \ldots, \Sigma_K$

- **E-step**:
  - For k=1,…,K

$$r_{i,k} = \frac{\pi_k \, N(x_i \,|\, \mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \, N(x_i \,|\, \mu_j, \Sigma_j)}$$

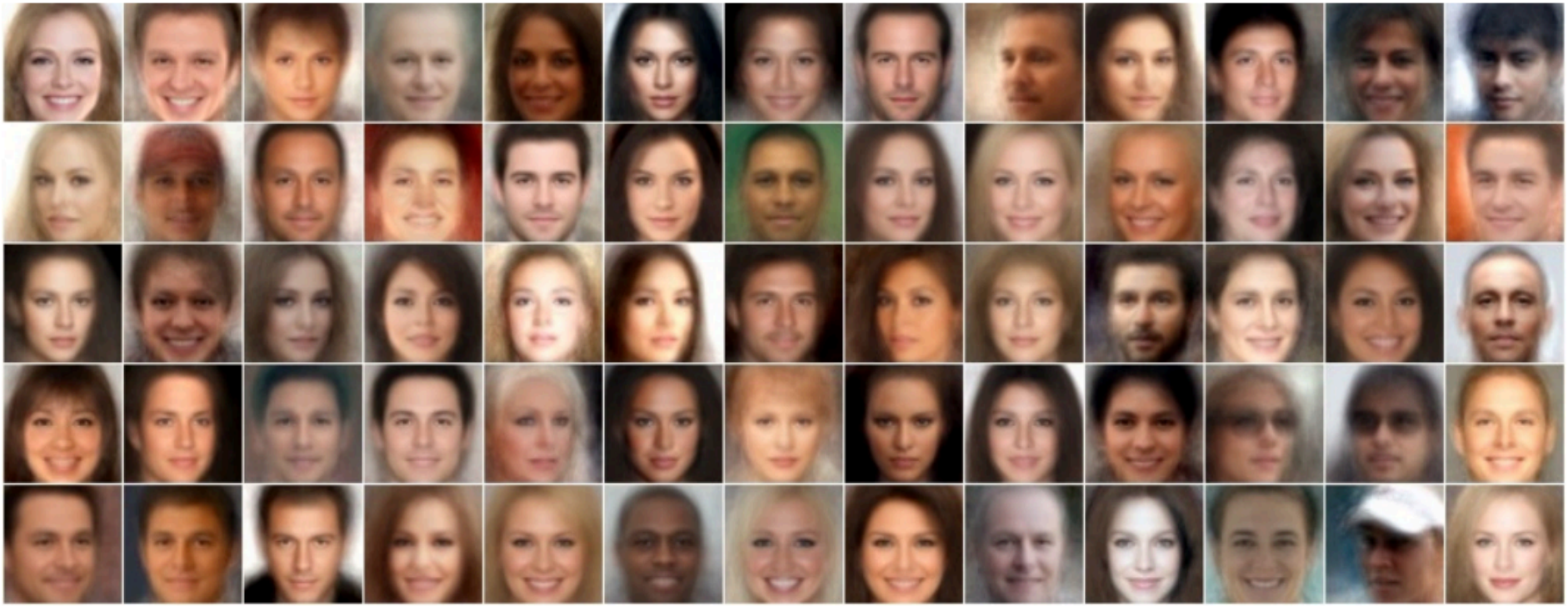
- **M-step**:
  - For k=1,..,K

$$\pi_k = \frac{N_k}{n} \quad \text{where} \quad N_k = \frac{\sum_{i=1}^{n} r_{i,k}}{n}$$

$$\mu_k = \frac{1}{N_k} \sum_{i=1}^{n} r_{i,k} x_i \quad \text{and} \quad \Sigma_k = \frac{1}{N_k} \sum_{i=1}^{n} r_{i,k} (x_i - \mu_k)(x_i - \mu_k)^T$$

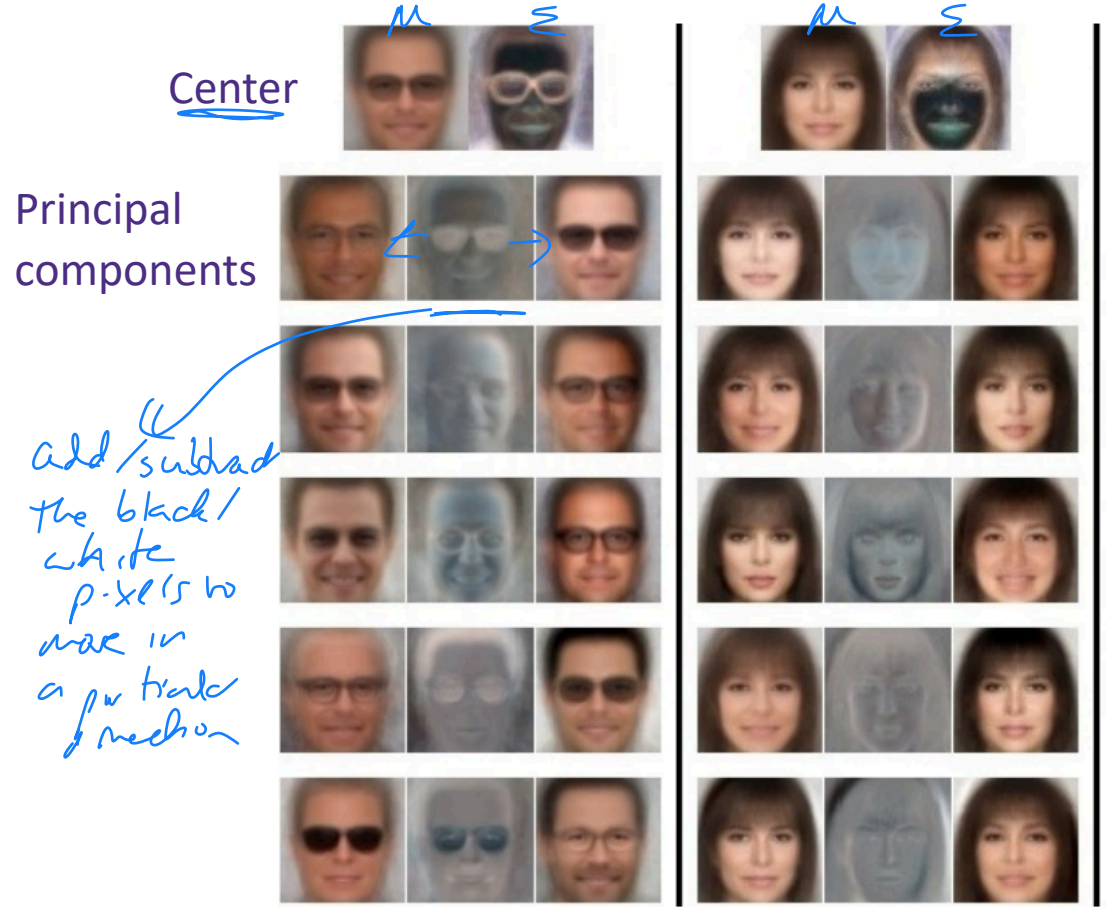
- **once GMM is learned, clustering is straight forward: cluster according to the $r_{i,k}$'s**

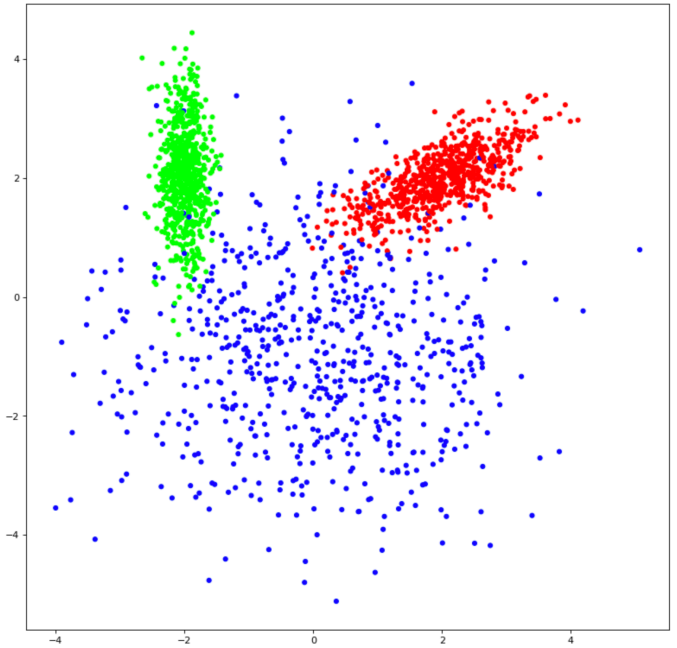
GMM for real data



- these are generated samples, from GMM trained on CelebA dataset
- image: 64*64*3=288 dimension
- covariance: restricted to rank-10 matrices
- mixture: K=1,000

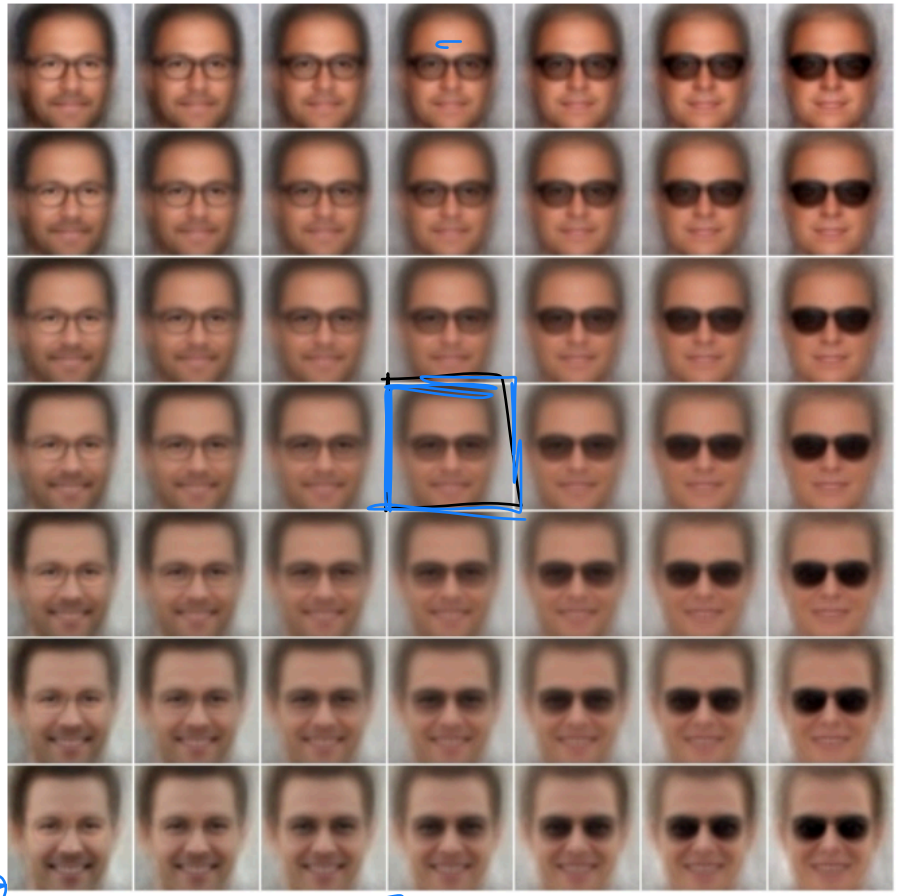
Images from "on GANs and GMMs", 2018, Richardson &Weiss





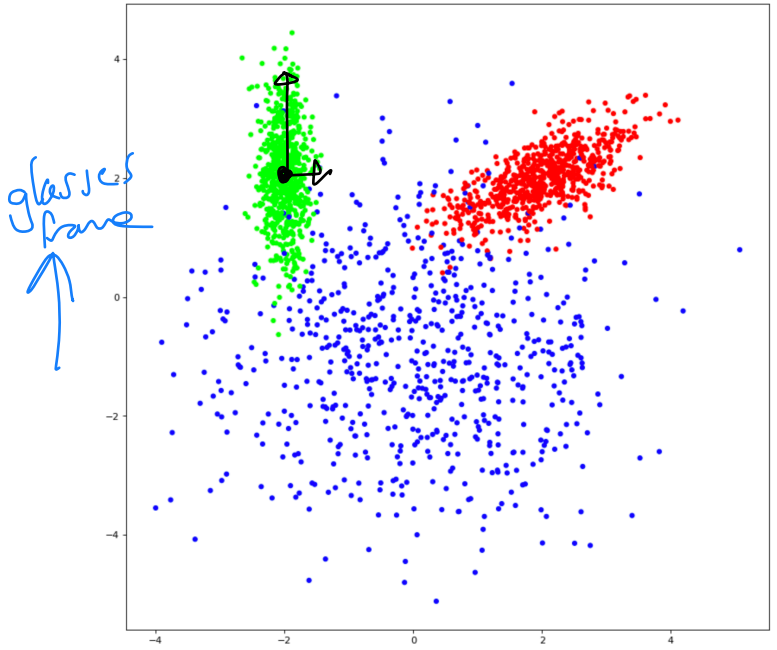
- **top**: center of a cluster μ_k and the diagonal entries of the covariance matrix Σ_k
- note that we have trained 10-dimensional covariance matrix $\Sigma_k = AA^T$, with $A \in \mathbb{R}^{288\times10}$, and let $A^{(j)}$ be the j-th column
- **bottom**: each row corresponds to different j, and we show $\mu_k + A^{(j)}$, $0.5 + A^{(j)}$, $\mu_k - A^{(j)}$

Images from "on GANs and GMMs", 2018, Richardson &Weiss



Principal Component direction 2

Principal Component direction 1

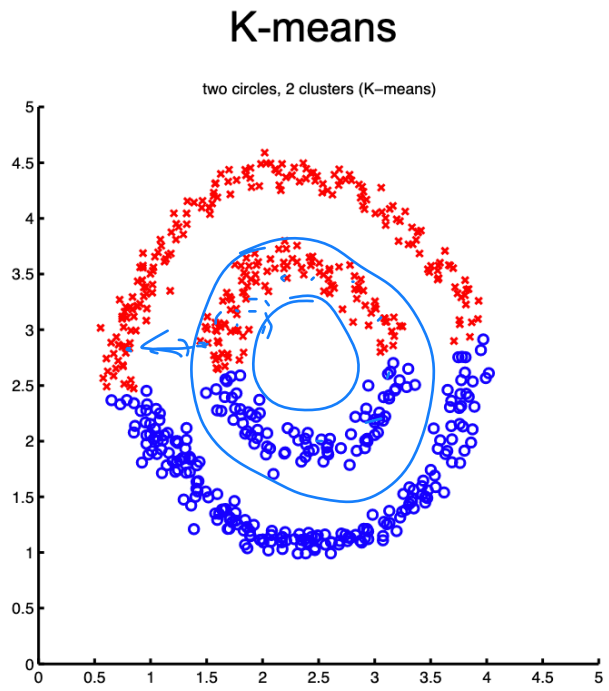


- middel: μ_k
- Each row: middel + $c \times A^{(1)}$
- Each column: middle + $c \times A^{(2)}$

Images from "on GANs and GMMs", 2018, Richardson &Weiss

k-means and GMMs are inherently linear

- It tries to find linear boundaries between centers
- It fails completely on non-linearly clustered datasets such as

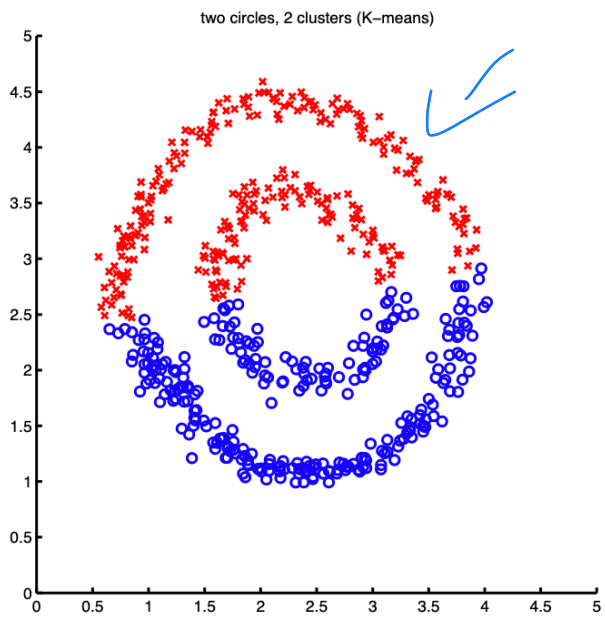


[Shi,Malik,'00],[Ng,Jordan,Weiss,'01]

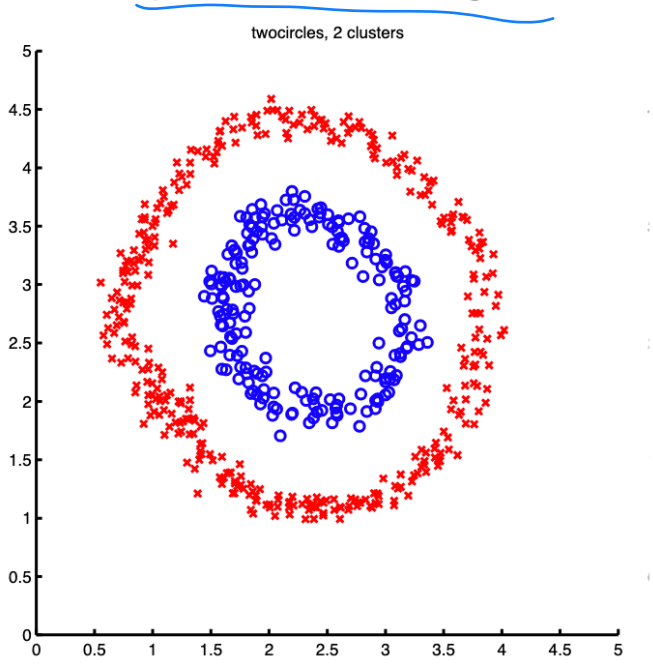
Spectral clustering

- Main idea:
  - Transform the dataset into a graph
  - Use eigenvalues (also called spectrum) and vectors of a graph to cluster

K-means



Spectral clustering



[Shi,Malik,'00],[Ng,Jordan,Weiss,'01]

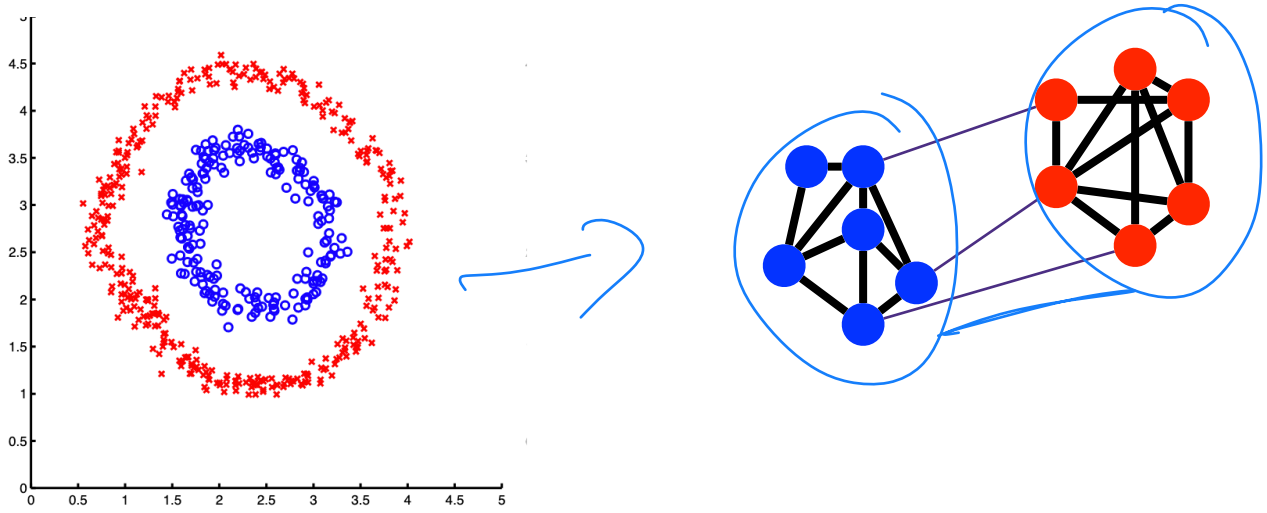
Step 1. From dataset to a graph

- Given $\mathscr{D} = \{x_i \in \mathbb{R}^d\}_{i=1}^n$, create a graph with n nodes and weighted edges $\{w_{ij}\}$, where each node represents each sample and each edge measures the similarity between the two nodes
  - Example 1: Gaussian kernel

$$w_{ij} = e^{-\frac{\|x_i - x_j\|_2^2}{\sigma^2}}$$

  - Example 2: k-nearest neighbor graph

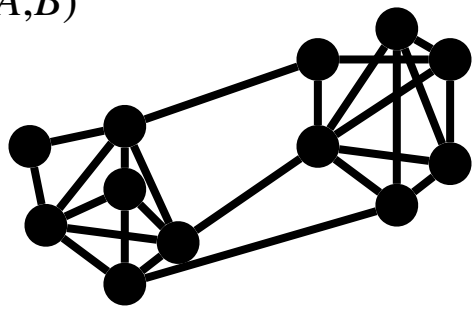
$$w_{ij} = 1 \text{ if } j \text{ is one of } k\text{-nearest neighbors of } i \text{ or}$$
$$i \text{ is one of } k\text{-nearest neighbors of } j$$



Step 2. Graph partitioning

- Once we have a similarity graph, how do we partition it?
- Can we use **minimum cut** for a graph $G(V, E)$?
  - Set of nodes $V = \{1, \ldots, n\}$
  - Set of edges $E = \{(i, j)\}$
  - If it is a weighted graph we have weights $\{w_{ij}\}_{(i,j)\in E}$
- **Minimum cut** of a graph is a partition $A \cup B = V$ and $A \cap B = \emptyset$ such that

$$\arg\min_{A,B} \underbrace{\sum_{i\in A}\sum_{j\in B} w_{i,j}}_{\text{cut}(A,B)}$$



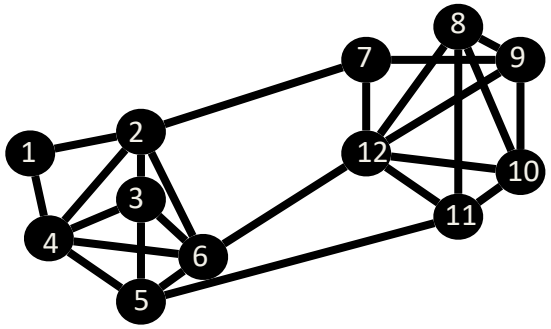
Step 2. Graph partition using Graph Laplacian

- Definitions (we will define it for unweighted graphs, but everything naturally generalizes to weighted graphs)
  - **Adjacency matrix** of a graph $A \in \mathbb{R}^{n \times n}$

    $A_{ij} = 1$ if $(i, j) \in E$

    0 otherwise
  - **Degree** of a node i, is $d_i = \sum_{j=1}^{n} A_{ij}$, which is number of edges connected to node i
  - Define $D \in \mathbb{R}^{n \times n}$ as a diagonal matrix with the degrees of each node in the diagonal
  - The **Graph Laplacian** of a graph is defined as

$$L_G = D - A$$

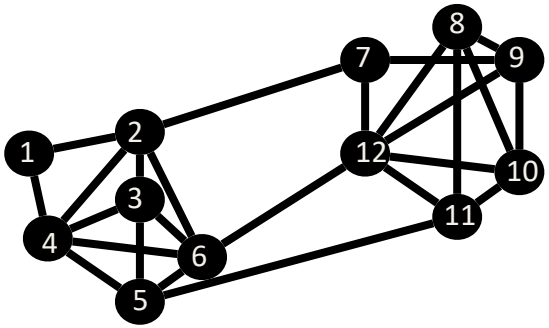


$$A = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \end{bmatrix}$$

$$D = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 5 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 \end{bmatrix}$$

Step 2. Graph partition using Graph Laplacian

- Graph Laplacian $L_G = D - A$ can capture some structure of the graph
- Consider placing each node in 1-dim line at positions $x = [x_1, x_2, \ldots, x_2]$



quadratic form of L_G is useful in capturing the structure of the graph:

$$
\begin{aligned}
x^T L_G x &= \sum_i d_i x_i^2 - \sum_{(i,j)\in E} 2x_i x_j \\
&= \sum_i \sum_{j:(i,j)\in E} x_i^2 - \sum_{(i,j)\in E} 2x_i x_j \\
&= \sum_{(i,j)\in E} 2x_i^2 - 2x_i x_j \\
&= \sum_{(i,j)\in E} x_i^2 + x_j^2 - 2x_i x_j \\
&= \sum_{(i,j)\in E} (x_i - x_j)^2
\end{aligned}
$$

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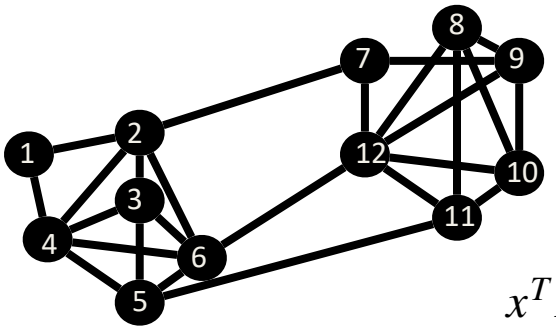

$$x^T L_G x = \sum_{(i,j)\in E} (x_i - x_j)^2$$

- If we want a good graph partition, we want to place nodes such that the distance between connected nodes are smaller
- This naturally leads to the following problem:

$$\arg\min_{x\in\mathbb{R}^n} x^T L_G x = \sum_{(i,j)\in E} (x_i - x_j)^2$$

- There is a trivial solution to this problem: $x_i = 1$ for all i, which achieves the minimum value of zero, so we change it to

$$\arg\min_{x\in\mathbb{R}^n} x^T L_G x = \sum_{(i,j)\in E} (x_i - x_j)^2 \qquad \text{subject to } x^T \mathbf{1} = 0$$

Step 2. Graph partition using Graph Laplacian

- To solve graph partitioning, we solve

$$\arg\min_{x \in \mathbb{R}^n} \; x^T L_G x = \sum_{(i,j) \in E} (x_i - x_j)^2$$

$$\text{subject to } x^T \mathbf{1} = 0$$
$$\|x\|_2 = 1$$

  and place nodes as per x, and find a partition using simple algorithms like k-means
- It turns out that the above optimization has a efficient solver, because The optimal x turns out to be the second smallest eigen vector of the graph Laplacian L_G
- Since, eigen values of a matrix is also called a spectrum, this is called a spectral clustering algorithm

Spectral clustering

- Step 1. Define a similarity graph $G(V, E, W)$
- Step 2. Compute the Graph Laplacian

$$L_G = D - W$$

where $D$is a diagonal matrix with $D_{ii} = \sum_{j=1}^{n} w_{ij}$

  - let x be the Eigen vector corresponding to the second smallest Eigen value
  - Place samples according to x and apply k-means clustering

- instead of using just the second smallest Eigen pair, you can use multiple smallest Eigen pairs