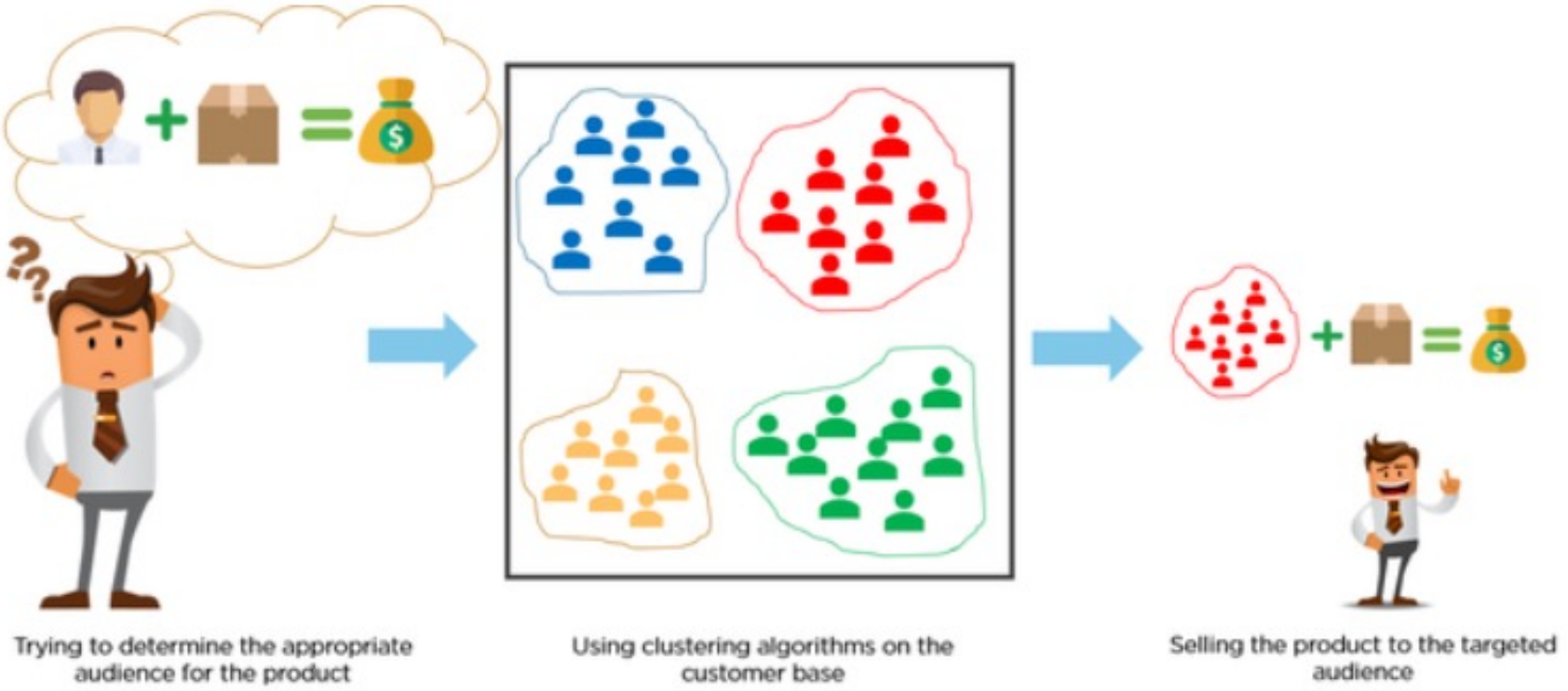
Clustering

David I. Inouye

Clustering application:
Market segmentation to group customers



https://medium.com/analytics-vidhya/customer-segmentation-for-differentiated-targeting-in-marketing-using-clustering-analysis-3ed0b883c18b

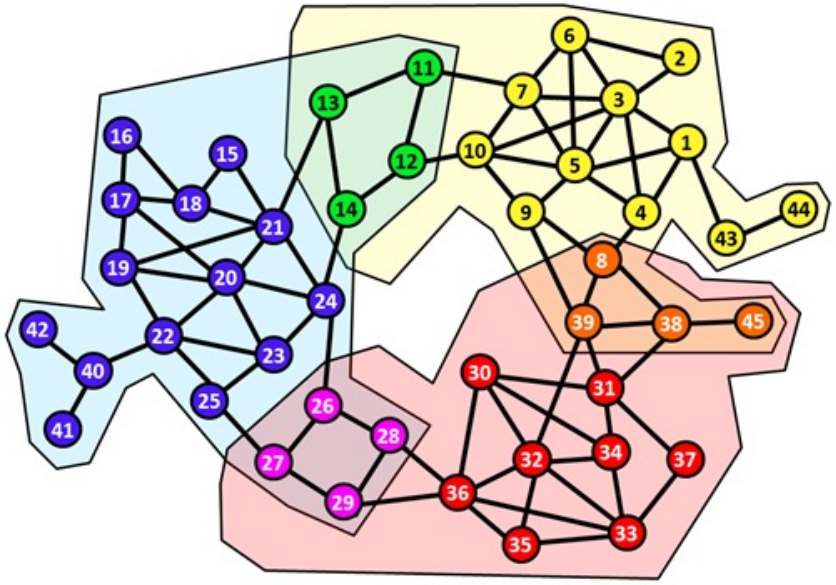
Clustering applications: Discretization of colors for compression

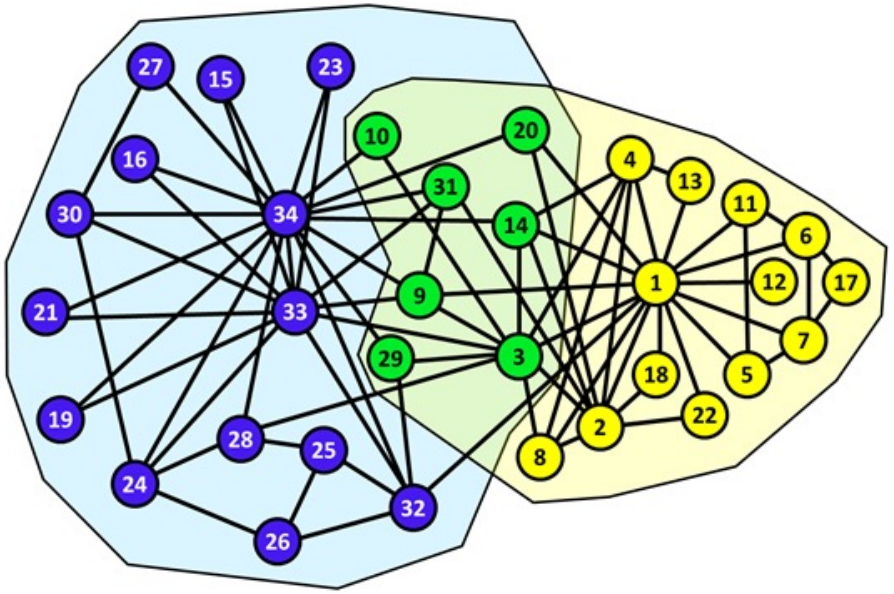
https://docs.opencv.org/3.4/d1/d5c/tutorial_py_kmeans_opencv.html

Clustering applications: Unsupervised image segmentation

R. Achanta, A. Shaji, K. Smith, A. Lucchi, P. Fua and S. Süsstrunk, "SLIC Superpixels Compared to State-of-the-Art Superpixel Methods," in *IEEE Transactions on Pattern Analysis and Machine Intelligence*, vol. 34, no. 11, pp. 2274-2282, Nov. 2012, doi: 10.1109/TPAMI.2012.120.

Another clustering application: Clustering people in social networks





Zachary's Karate Club Network

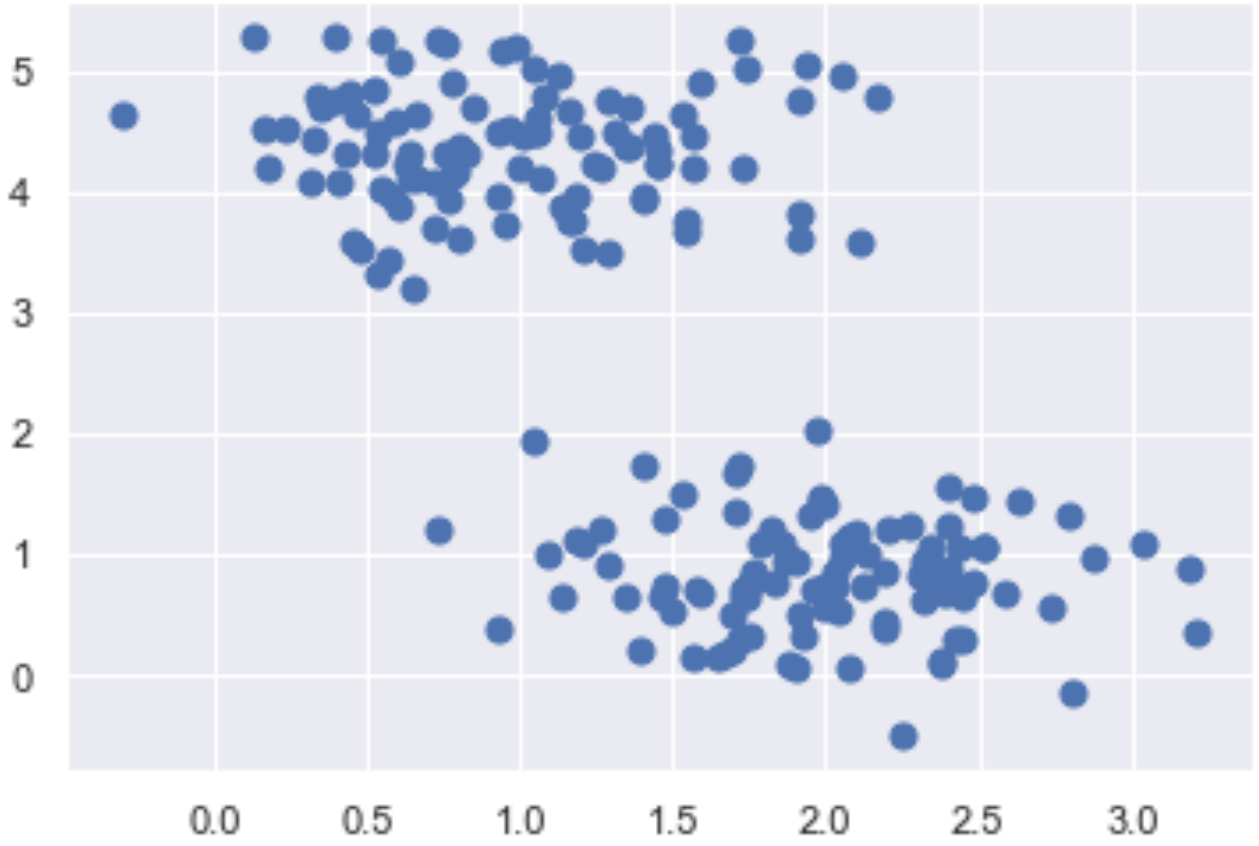
https://en.wikipedia.org/wiki/Zachary%27s_karate_club

https://bigdata.oden.utexas.edu/project/graph-clustering/

Outline

- Clustering applications
- Clustering objective
- K-means
  - Algorithm (Python demo)
  - Relation to PCA
- Graph clustering
- Spectral clustering

Can you put these points into two clusters?



How can we formalize what you can do visually?

One clustering objective is to minimize the pairwise distances between points in the same cluster

- Let the input dataset be $\{x_i\}_{i=1}^n$
- The goal of clustering is to find cluster labels $\{y_i\}_{i=1}^n$, where $y_i \in \{1,2,\dots,k\}$
- Given cluster labels y_i, let clusters be defined:

$$\mathcal{C}_j = \{x_i : y_i = j\}$$

- Like MSE for regression, the most common clustering objective is:

$$\min_{\mathcal{C}_1,\cdots,\mathcal{C}_k} \sum_{j=1}^{k} \frac{1}{|\mathcal{C}_j|} \sum_{x \in \mathcal{C}_j, \tilde{x} \in \mathcal{C}_j} \|x - \tilde{x}\|_2^2$$

The clustering objective can be reformulated as finding centers and clusters simultaneously

- Original pairwise objective

$$\min_{\mathcal{C}_1,\cdots,\mathcal{C}_k} \sum_{j=1}^{k} \frac{1}{|\mathcal{C}_j|} \sum_{x\in\mathcal{C}_j,\tilde{x}\in\mathcal{C}_j} \|x-\tilde{x}\|_2^2$$

- Equivalent objective via free parameters μ_j

$$\min_{\substack{\mathcal{C}_1,\cdots,\mathcal{C}_k \\ \mu_1,\cdots,\mu_k}} \sum_{j=1}^{k} \sum_{x\in\mathcal{C}_j} \|x-\mu_j\|_2^2$$

- In general, this is an NP-hard problem to solve

(i.e., you might have to enumerate an exponentially large number of possibilities to solve)

For proof, see https://www.math.ucdavis.edu/~strohmer/courses/180BigData/180lecture_kmeans.pdf

However, if the clusters OR the centers are fixed, the optimization problem is simple

- If $\mu_1, \cdots, \mu_k$ are fixed, then the clustering assignment is simple:

$$x_i \in \mathcal{C}_j \Leftrightarrow j = \text{argmin}_j \left\| x_i - \mu_j \right\|_2^2$$

- If $\mathcal{C}_1, \cdots, \mathcal{C}_k$ are fixed, then the optimal centers are merely the mean:

$$\mu_j = \frac{1}{\left|\mathcal{C}_j\right|} \sum_{x_i \in \mathcal{C}_j} x_i \,, \qquad \forall j$$

The K-means algorithm simply alternates between solving each of these two steps

- Initialize centers $\mu_1, \cdots, \mu_j$ randomly

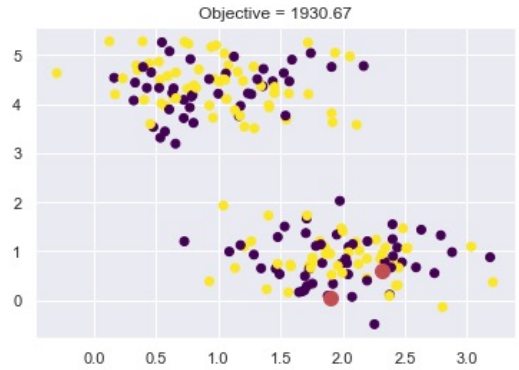
- Repeat the following until convergence
  1. Assign points to nearest center

$$x_i \in \mathcal{C}_J \Leftrightarrow j = \text{argmin}_j \left\| x_i - \mu_j \right\|_2^2$$

  2. Recompute centers as mean of assigned points

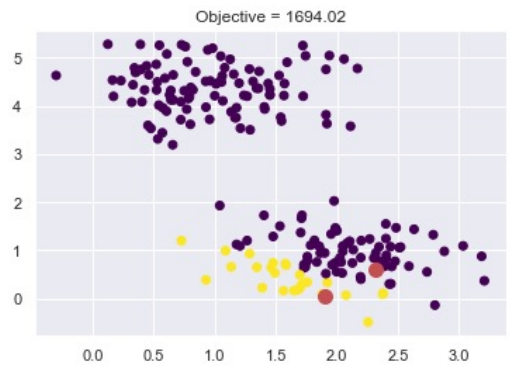
$$\mu_j = \frac{1}{\left|\mathcal{C}_j\right|} \sum_{x_i \in \mathcal{C}_j} x_i \,, \qquad \forall j$$

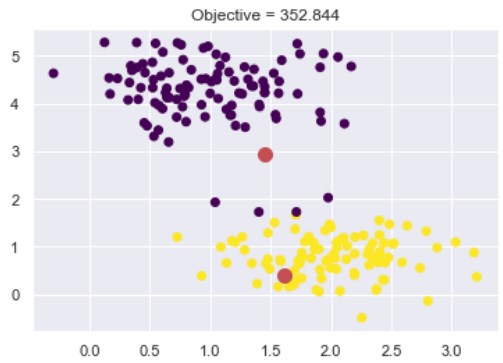
K-means demonstration

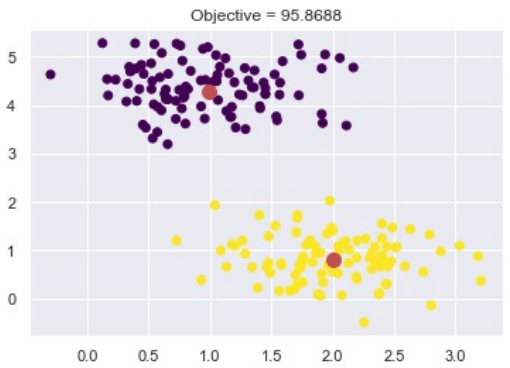


Initialize centers randomly

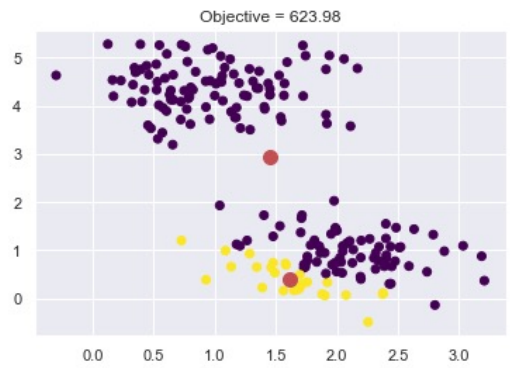
1. Assign

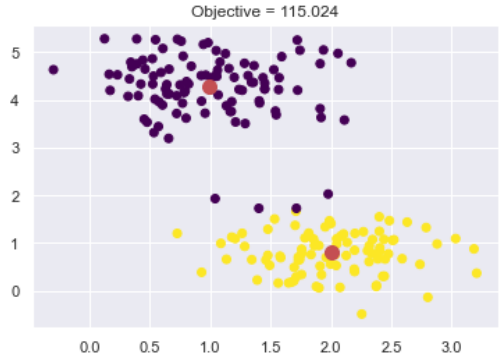


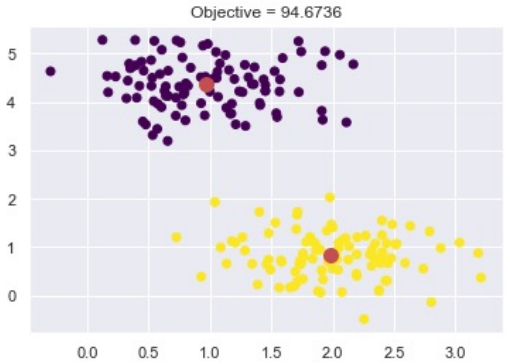




2. Compute centers







Reformulation of k-means objective in terms of matrices

- $y_i \in \{1, \dots, k\}$ is the cluster label for each instance
- z_i is the corresponding one hot vector to y_i
- $M = \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_k \end{bmatrix} \in \mathbb{R}^{k \times d}$ is the matrix of mean vectors
- $\sum_{j=1}^{k} \sum_{x \in \mathcal{C}_j} \|x - \mu_j\|_2^2$ (Original objective)
- $= \sum_{i=1}^{n} \|x_i - \mu_{y_i}\|_2^2$ (Using y_i notation)
- $= \sum_{i=1}^{n} \|x_i^T - z_i^T M\|_2^2$ (row vector form)
- $= \sum_{i=1}^{n} \sum_{s=1}^{d} \left(x_{is} - z_i^T m_s\right)^2$ (m_s is a column of M)
- $= \left(\sqrt{\sum_{i=1}^{n} \sum_{s=1}^{d} \left(x_{is} - z_i^T m_s\right)^2} \right)^2$
- $= \|X - ZM\|_F^2$ What does this look like?

Recap: Principal Component Analysis (PCA) can be formalized as minimizing the linear reconstruction error of the data using only $k \leq d$ dimensions

- PCA can be formalized as

$$\min_{Z,W} \|X_c - ZW^T\|_F^2$$

  - where
    $X_c = X - \mathbf{1}_n \mu_x^T \in \mathbb{R}^{n \times d}$ (centered input data)
    $Z \in \mathbb{R}^{n \times k}$ (latent representation or "scores")
    $W^T \in \mathbb{R}^{k \times d}$ (principal components)
    $w_s^T w_t = 0, w_s^T w_s = \|w_s\|_2 = 1, \forall s, t$ (orthogonal constraint)
- Solution
  - $W^T = V_{1:k}^T$ where $X_c = USV^T$ is the **SVD** of X_c
  - $Z = X_c W$

K-means relation to PCA: One-hot vectors vs continuous vectors

- k-means clustering can be seen as reducing the dimensionality to k latent categories
  - Each category can be represented by a one-hot vector of length k
    e.g., if $k = 3$, $z_i \in \{[1,0,0], [0,1,0], [0,0,1]\}, \forall i$
  - Every instance can only "belong" to one category
- In dimensionality reduction techniques, the latent vectors can have non-zeros for all k latent dimensions
  - e.g., if $k = 3$, $z_i \in \mathbb{R}^3, \forall i$

K-means objective can be reformulated as seeking the best approximation to X with one-hot latents

- Original k-means objective

$$\min_{\substack{\mathcal{C}_1,\ldots,\mathcal{C}_k \\ \mu_1,\ldots,\mu_k}} \sum_{j=1}^{k} \sum_{x \in \mathcal{C}_j} \|x - \mu_j\|_2^2$$

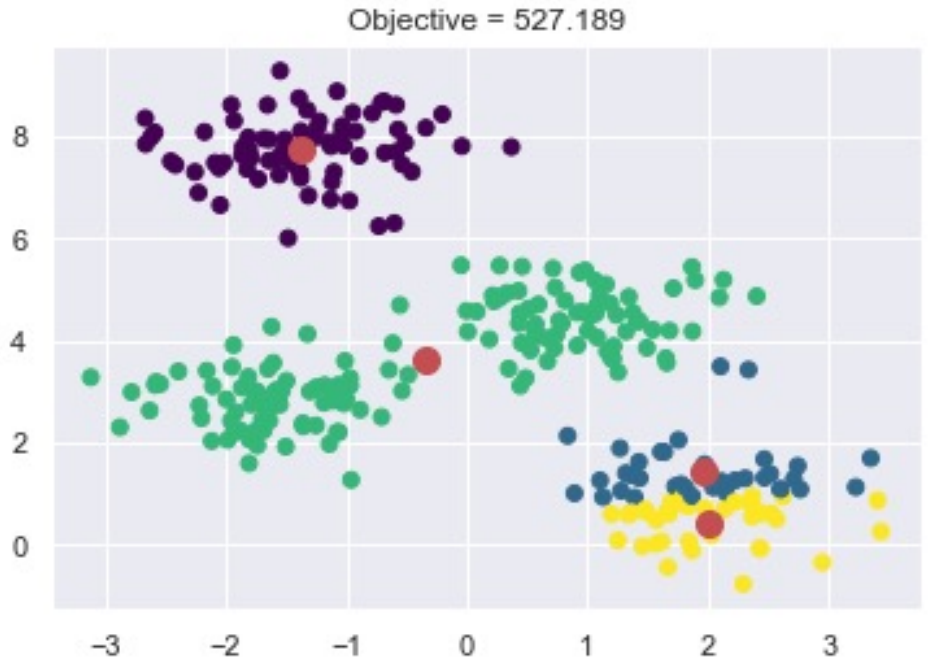
- Equivalent to the following objective

$$\min_{Z,M} \|X - ZM\|_F^2$$
$$\text{where } Z \in \{0,1\}^{n \times k}, \sum_j z_{ij} = 1, \forall i$$
$$\text{and } M \in \mathbb{R}^{k \times d}$$

- K-means can be seen as **alternating** between solving for Z with M fixed, and solving for M with Z fixed

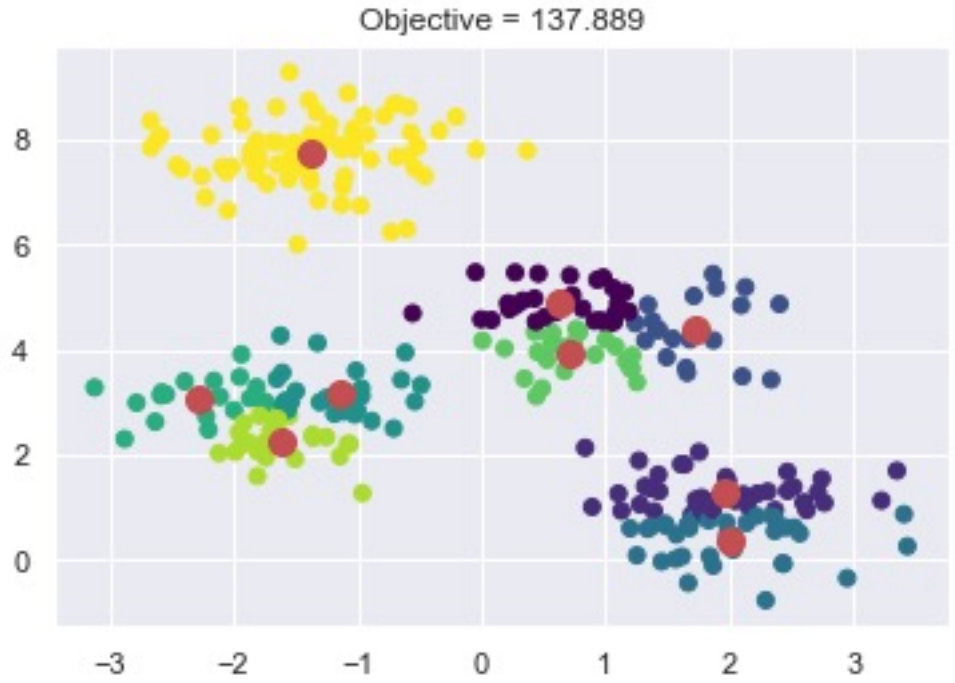
While k-means is fast and can give good solutions in practice, it has some issues

- Does not always converge to the optimal/best solution



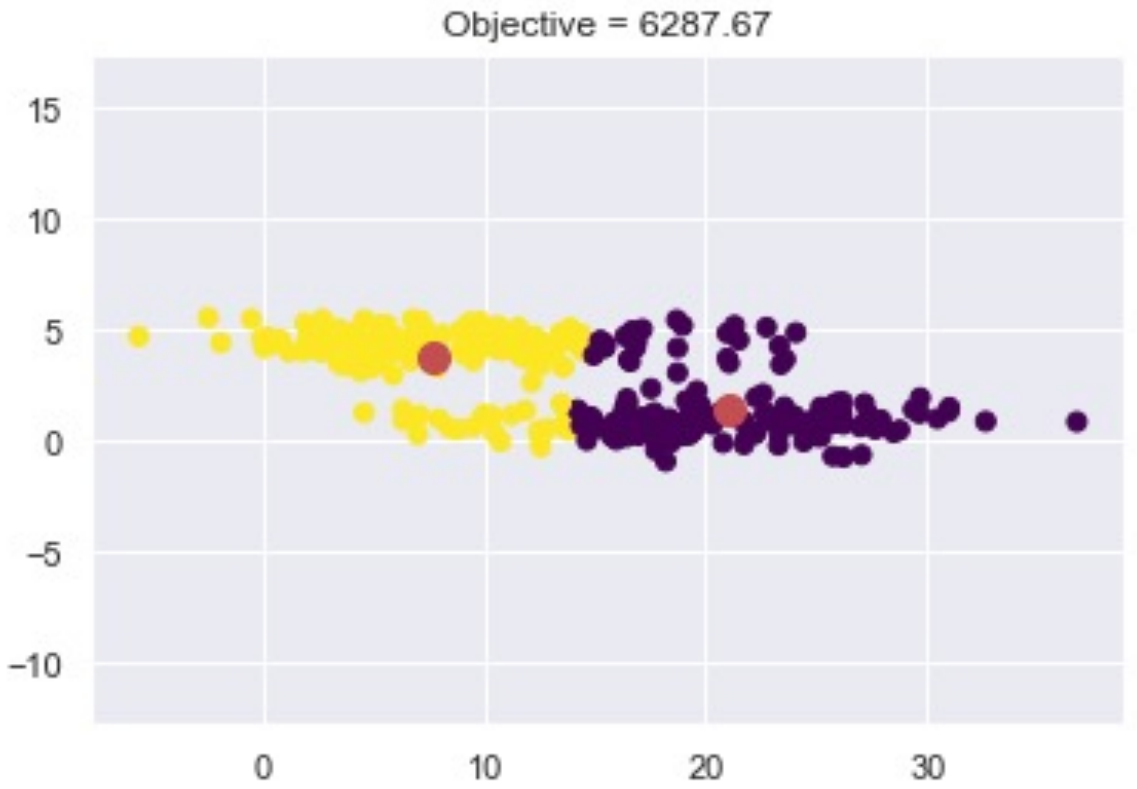
While k-means is fast and can give good solutions in practice, it has some issues

- Choosing the number of clusters is not obvious



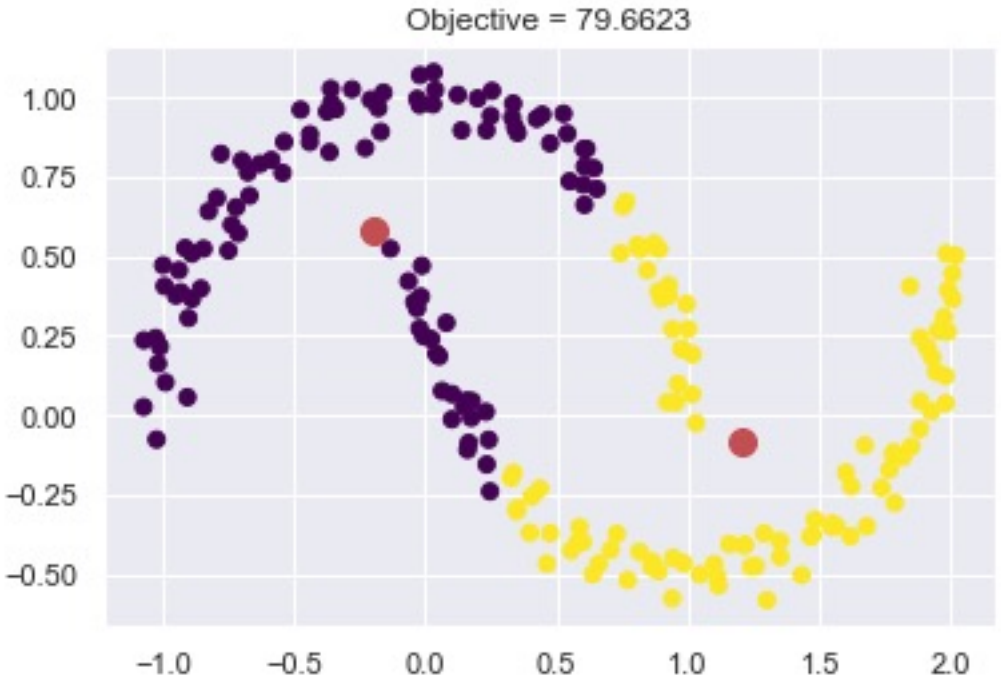
While k-means is fast and can give good solutions in practice, it has some issues

- Scaling of variables and clusters matters

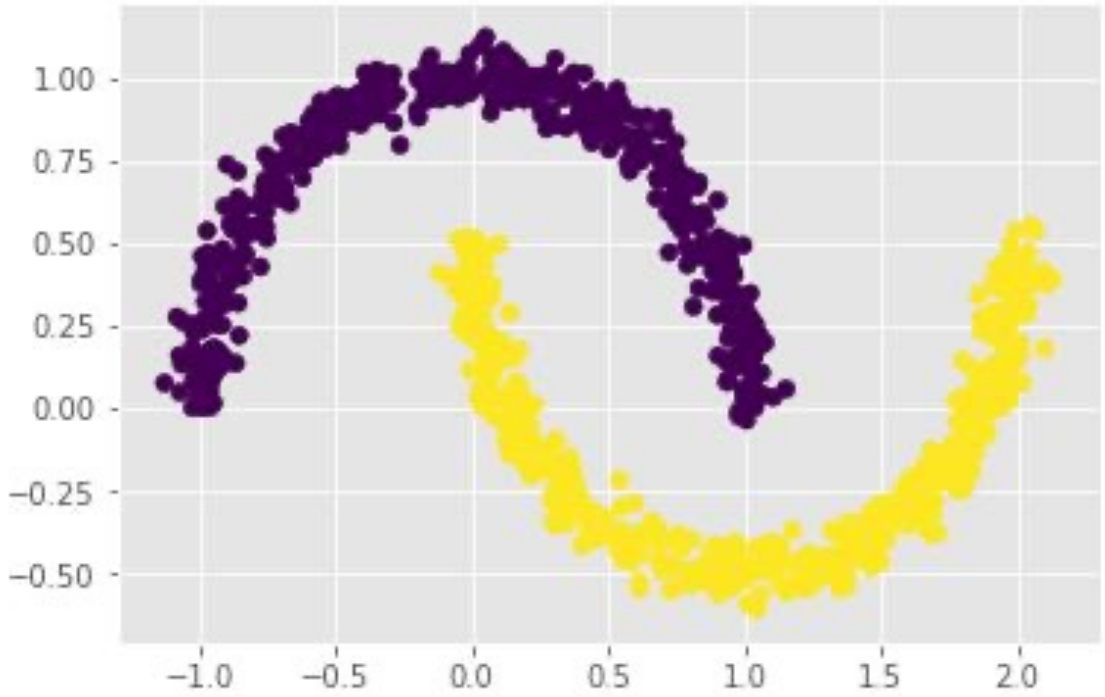


While k-means is fast and can give good solutions in practice, it has some issues

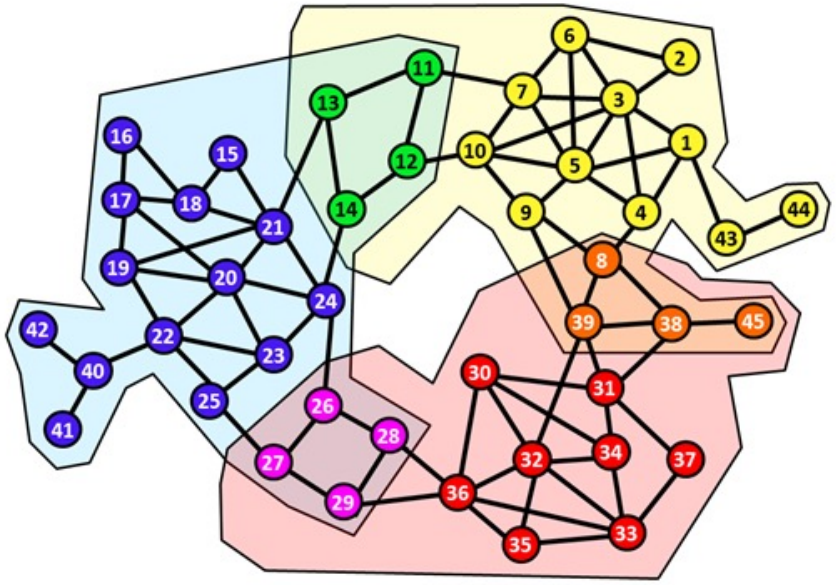
- Only linear boundaries between clusters

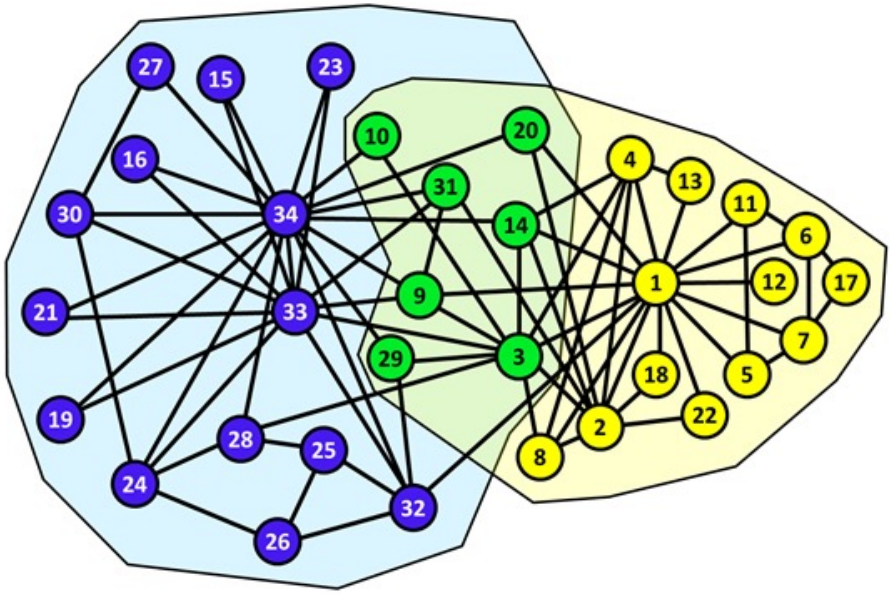


Graph-based clustering can enable non-linear clustering boundaries



How can we cluster the nodes of a network (a.k.a. a graph) instead of a set of points?





Zachary's Karate Club Network

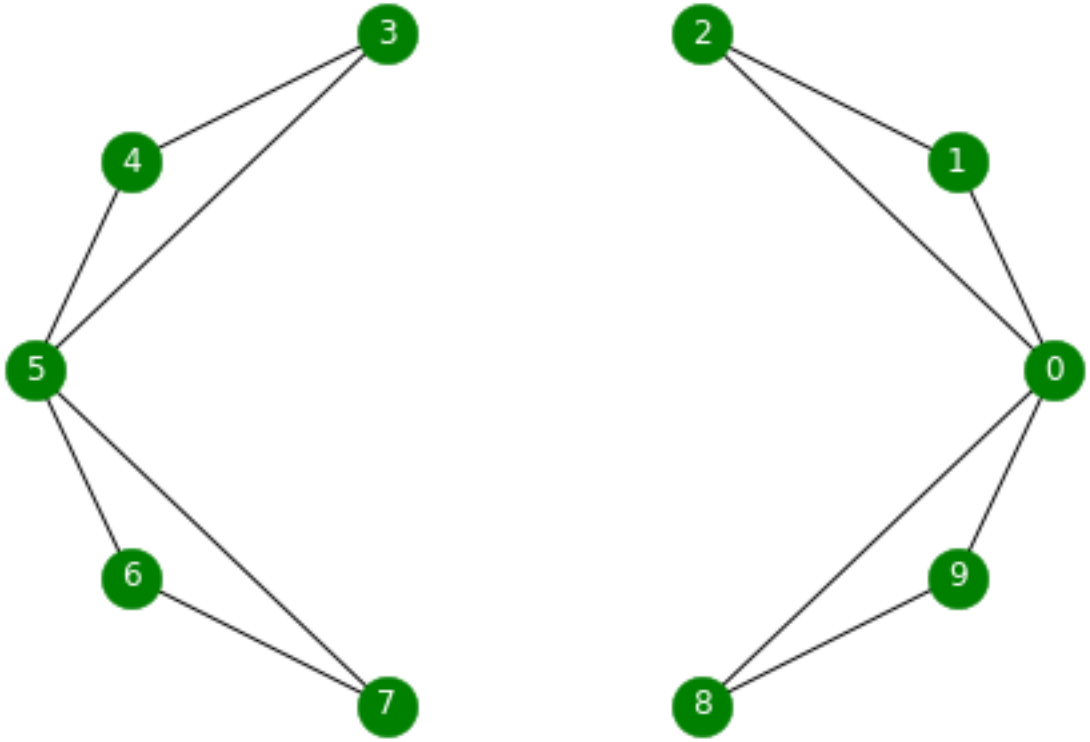
https://en.wikipedia.org/wiki/Zachary%27s_karate_club

https://bigdata.oden.utexas.edu/project/graph-clustering/

Graph clustering puts the nodes of a graph into clusters

- What is a graph?
- How do we represent a graph?
  - Adjacency matrix
  - Graph Laplacian
- How do we use graph Laplacian to cluster?

A graph/network is composed of nodes and weighted edges between the nodes

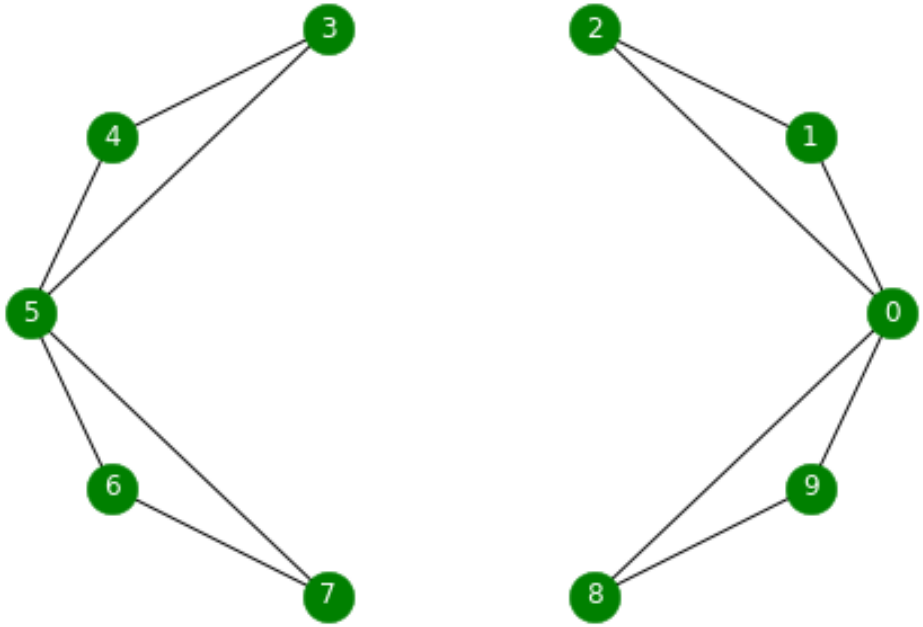


10 node graph with 2 connected components.

https://towardsdatascience.com/spectral-clustering-aba2640c0d5b

A graph can be represented as an **adjacency matrix**

- Nodes are represented by rows/columns
- Edges are encoded as 1s




```
[[0 1 1 0 0 0 0 0 1 1]
 [1 0 1 0 0 0 0 0 0 0]
 [1 1 0 0 0 0 0 0 0 0]
 [0 0 0 0 1 1 0 0 0 0]
 [0 0 0 1 0 1 0 0 0 0]
 [0 0 0 1 1 0 1 1 0 0]
 [0 0 0 0 0 1 0 1 0 0]
 [0 0 0 0 0 1 1 0 0 0]
 [1 0 0 0 0 0 0 0 0 1]
 [1 0 0 0 0 0 0 0 1 0]]
```

https://towardsdatascience.com/spectral-clustering-aba2640c0d5b

The **graph Laplacian** is formed by subtracting the adjacency from the degree matrix

- The degree matrix is a diagonal matrix whose elements are the sum of the rows:

$$D = \text{diag}(A1)$$

- Graph Laplacian is defined as:

$$L = D - A$$

```
[[ 4 -1 -1  0  0  0  0  0 -1 -1]
 [-1  2 -1  0  0  0  0  0  0  0]
 [-1 -1  2  0  0  0  0  0  0  0]
 [ 0  0  0  2 -1 -1  0  0  0  0]
 [ 0  0  0 -1  2 -1  0  0  0  0]
 [ 0  0  0 -1 -1  4 -1 -1  0  0]
 [ 0  0  0  0  0 -1  2 -1  0  0]
 [ 0  0  0  0  0 -1 -1  2  0  0]
 [-1  0  0  0  0  0  0  0  2 -1]
 [-1  0  0  0  0  0  0  0 -1  2]]
```

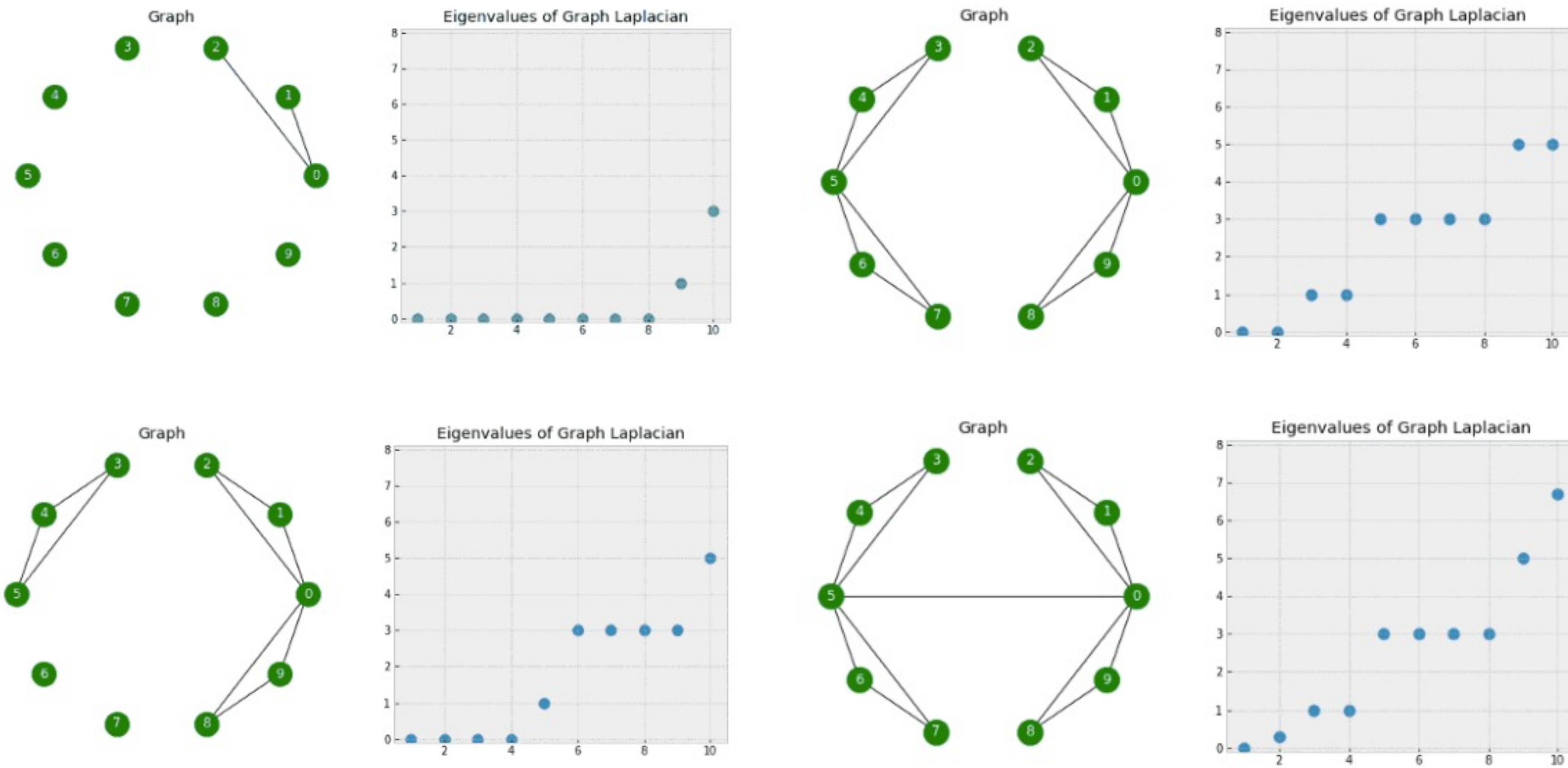
=

```
[[4 0 0 0 0 0 0 0 0 0]
 [0 2 0 0 0 0 0 0 0 0]
 [0 0 2 0 0 0 0 0 0 0]
 [0 0 0 2 0 0 0 0 0 0]
 [0 0 0 0 2 0 0 0 0 0]
 [0 0 0 0 0 4 0 0 0 0]
 [0 0 0 0 0 0 2 0 0 0]
 [0 0 0 0 0 0 0 2 0 0]
 [0 0 0 0 0 0 0 0 2 0]
 [0 0 0 0 0 0 0 0 0 2]]
```

−

```
[[0 1 1 0 0 0 0 0 1 1]
 [1 0 1 0 0 0 0 0 0 0]
 [1 1 0 0 0 0 0 0 0 0]
 [0 0 0 0 1 1 0 0 0 0]
 [0 0 0 1 0 1 0 0 0 0]
 [0 0 0 1 1 0 1 1 0 0]
 [0 0 0 0 0 1 0 1 0 0]
 [0 0 0 0 0 1 1 0 0 0]
 [1 0 0 0 0 0 0 0 0 1]
 [1 0 0 0 0 0 0 0 1 0]]
```

The number of 0 eigenvalues of the Laplacian is the number of connected components



https://towardsdatascience.com/spectral-clustering-aba2640c0d5b

The Fiedler vector (2nd to last eigenvector) can be used to create 2 clusters

- Intuitively, we could 0 the 2nd to last eigenvalue to get 2 components instead

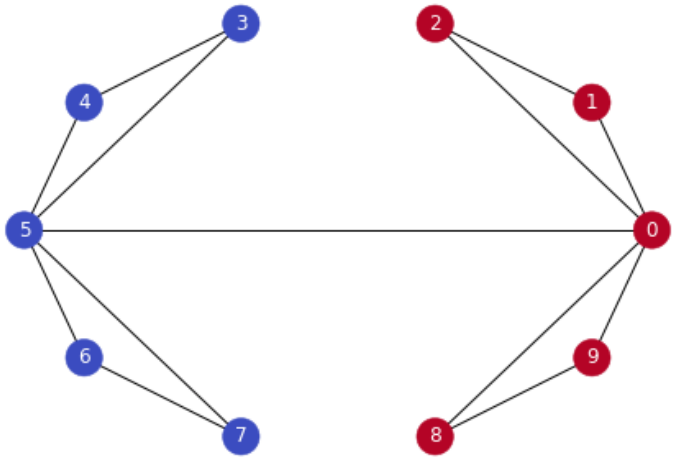
- Nodes are clustered based on whether their values in the Fiedler vector

$$y = 1(f > 0)$$

- In theory, this is known as the **minimal cut**

Fiedler vector

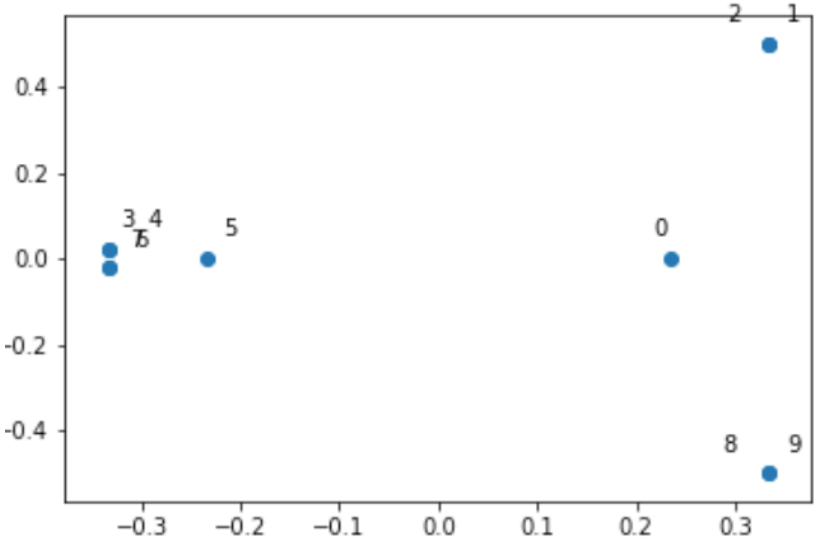
0	0.234
1	0.333
2	0.333
3	-0.333
4	-0.333
5	-0.234
6	-0.333
7	-0.333
8	0.333
9	0.333

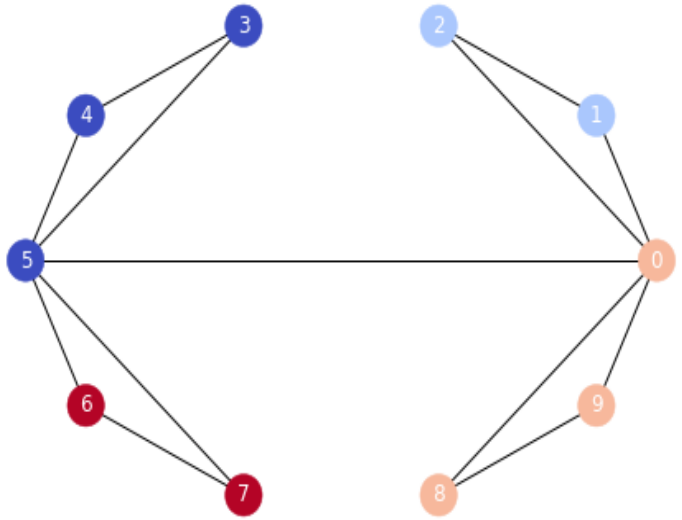


Spectral clustering generalizes to $k > 2$ clusters by taking the lowest eigenvectors as a new node representation and then doing K-means

- We take the m-lowest eigenvectors to represent the data
- Then just run K-means

2 lowest eigenvector representations of nodes

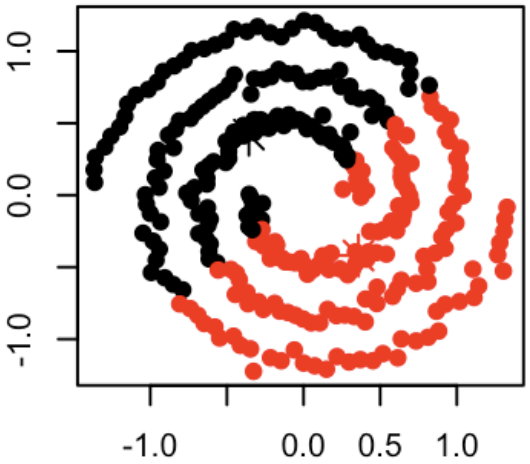


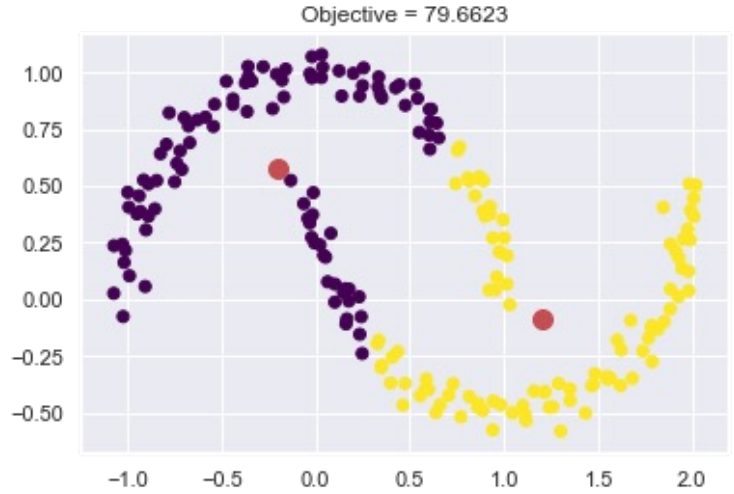


https://towardsdatascience.com/spectral-clustering-aba2640c0d5b

Standard K-means clustering is limited to circular clusters with linear boundaries between clusters

- K-means is based on the clustering assumption of "compactness"
  - Points in a cluster are close to one another
  - Squared error objective within cluster
- This assumption may not be appropriate

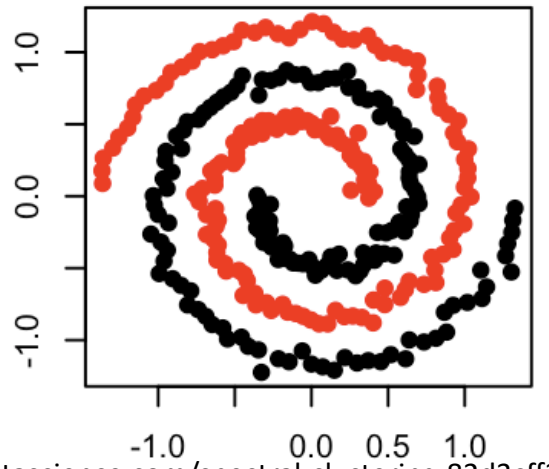


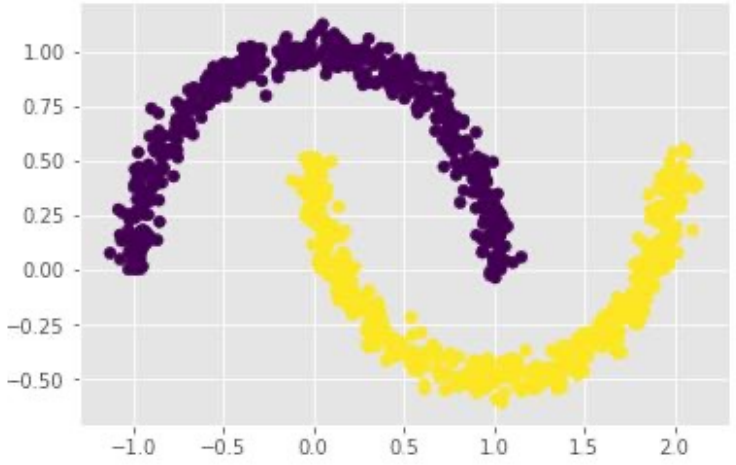


https://towardsdatascience.com/spectral-clustering-82d3cff3d3b7

Spectral clustering applied to vector data can be used to learn clusters based on "connectivity"

- Points that are "connected" to each other are clustered together
- This allows non-circular clustering





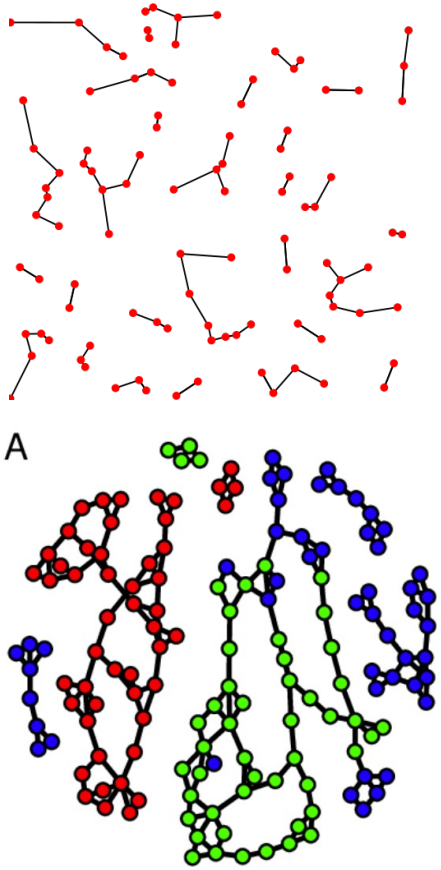
https://towardsdatascience.com/spectral-clustering-82d3cff3d3b7

Spectral clustering:
First create similarity graph based on data

- K-nearest neighbor graph
  - Add edge for all k-nearest neighbors

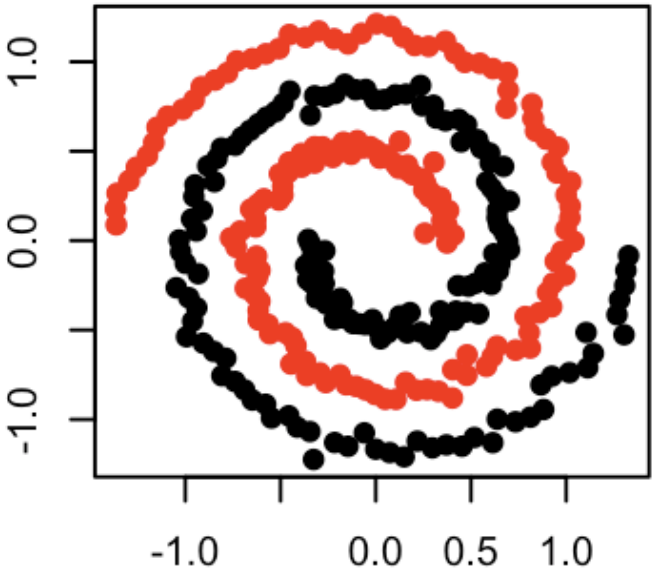
- General similarity graph
  - Compute all pairwise similarity between points such as:

$$s(x, y) = \exp\left(-\frac{\|x - y\|^2}{2\sigma^2}\right)$$

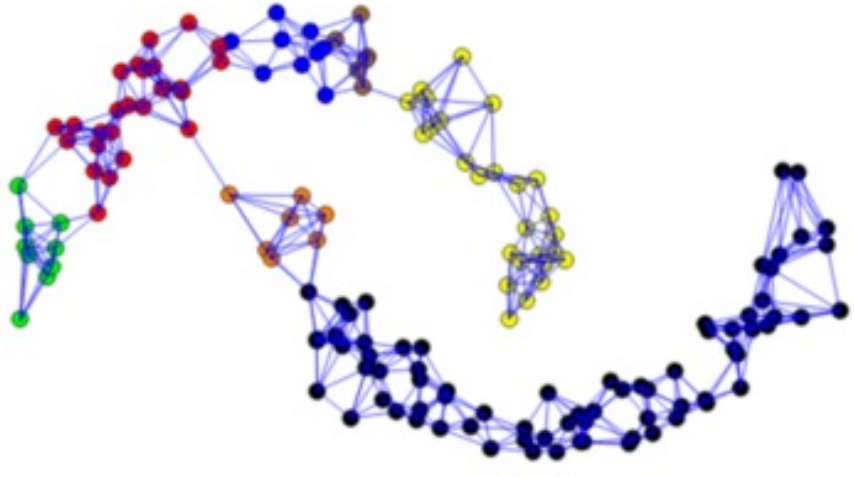


P. Veenstra, C. Cooper and S. Phelps, "Spectral clustering using the kNN-MST similarity graph," *2016 8th Computer Science and Electronic Engineering (CEEC)*, Colchester, 2016, pp. 222-227, doi: 10.1109/CEEC.2016.7835917.

Spectral clustering:
Second, apply spectral clustering to resulting graph

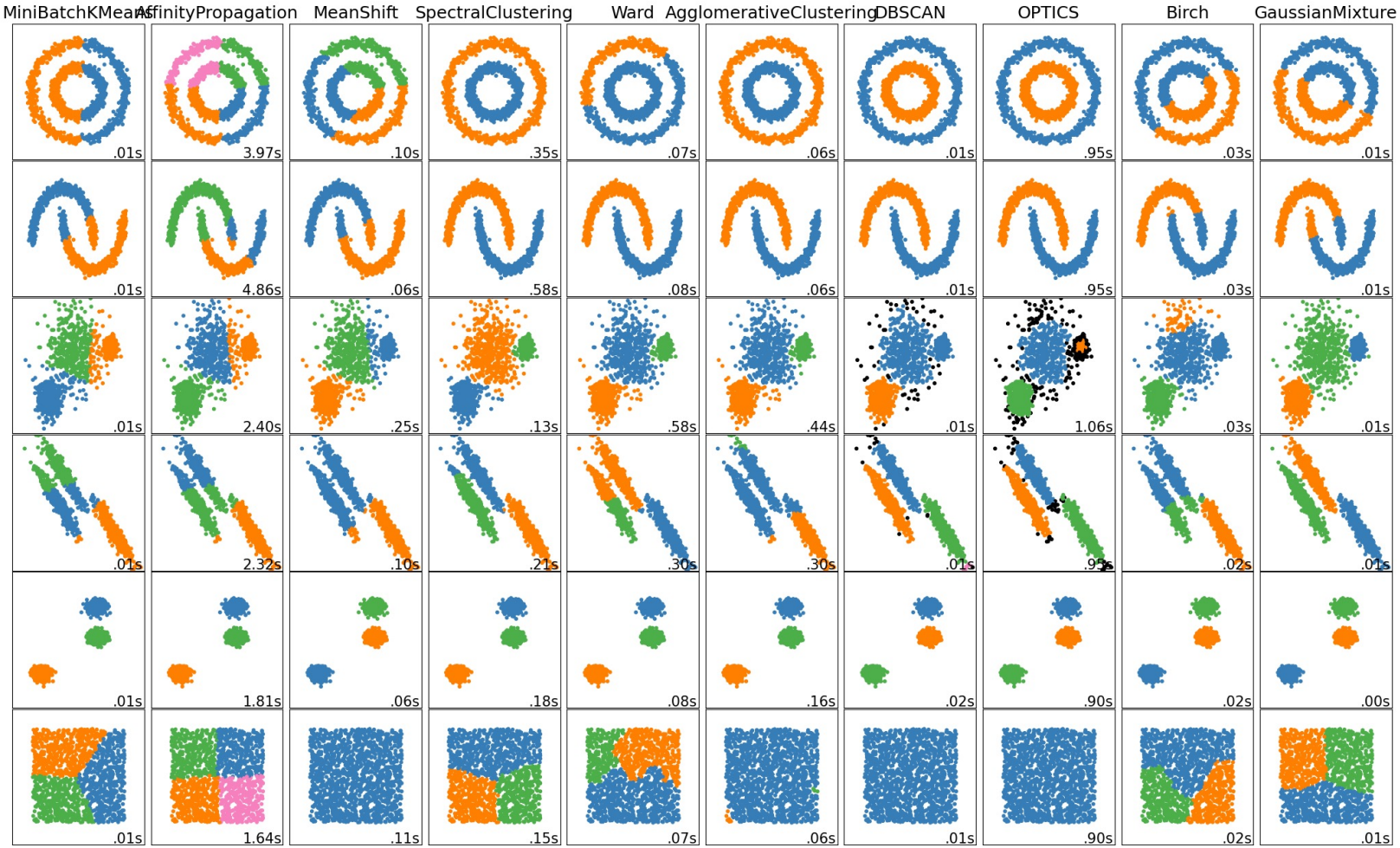


https://towardsdatascience.com/spectral-clustering-82d3cff3d3b7



http://math.ucdenver.edu/~sborgwardt/wiki/index.php/Spectral_clustering

Many other clustering algorithms exist



https://scikit-learn.org/stable/modules/clustering.html