Iterative Consensus Clustering: An Algorithm We Can All Agree On

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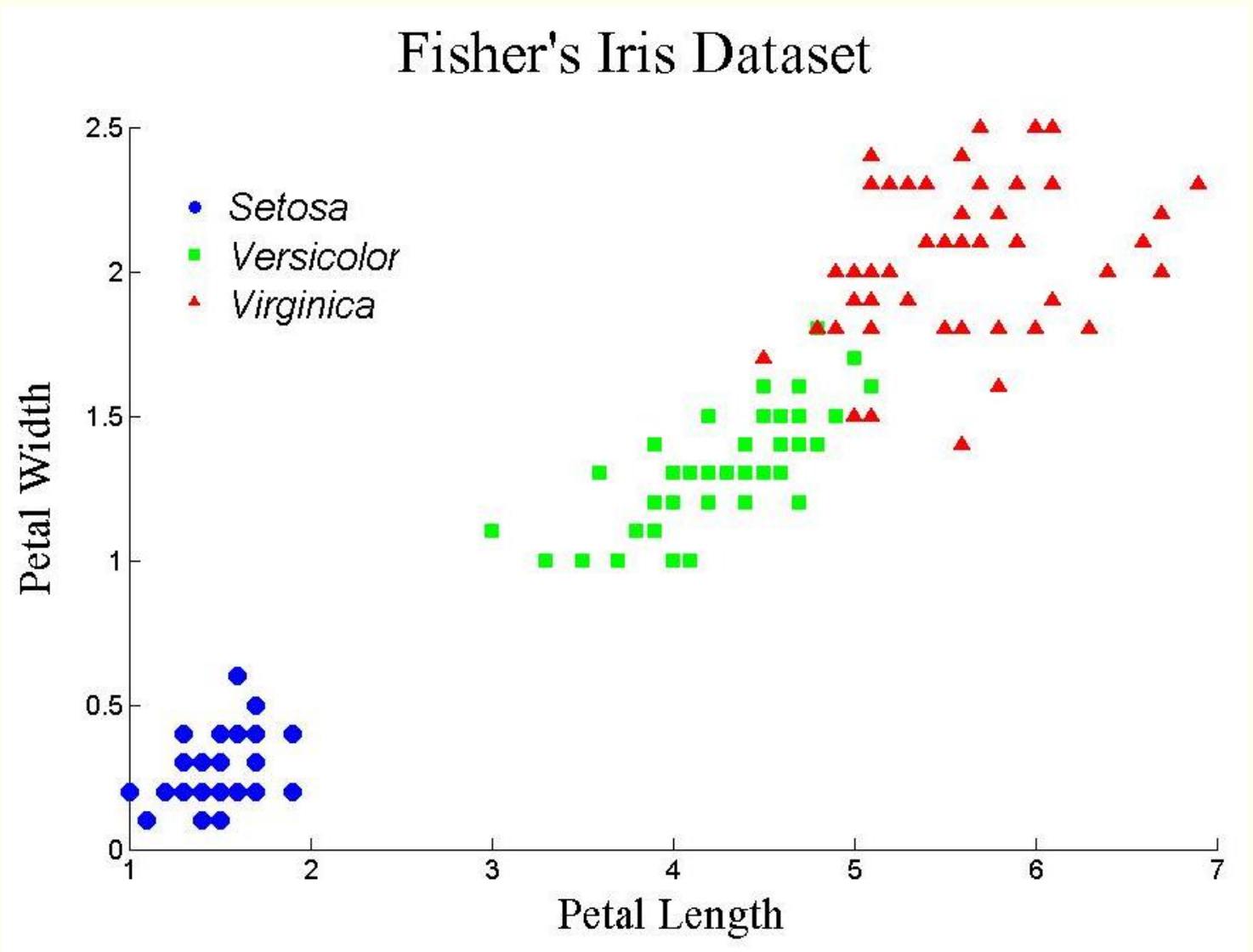
Background Information

Clustering : Grouping data based on a predefined metric of similarity.

Why Cluster?

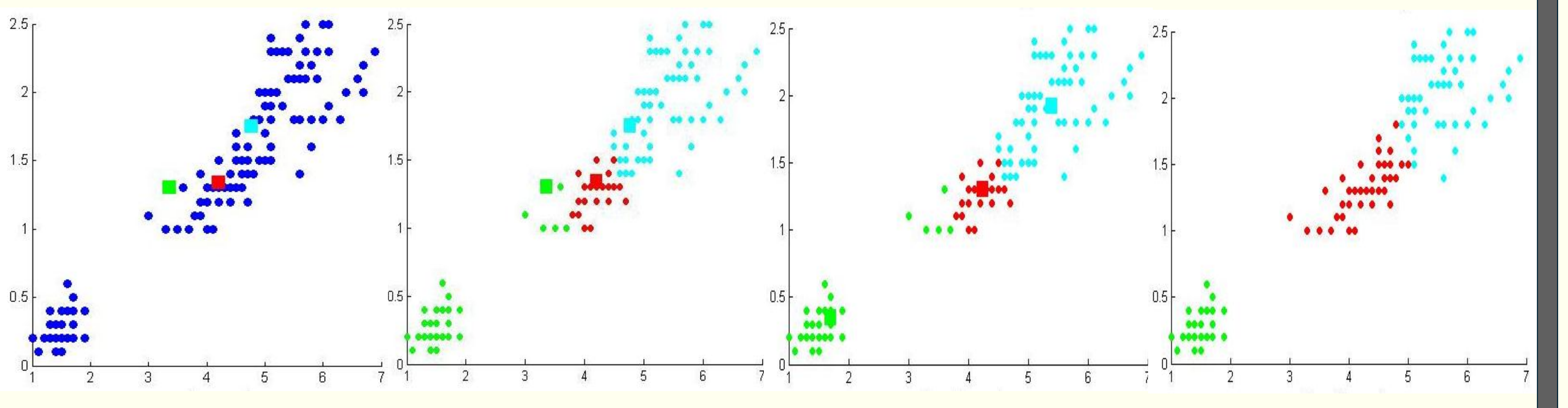
First step in interpreting large amounts of data

- Physical Observations
- Gene Expression
- Term Frequencies



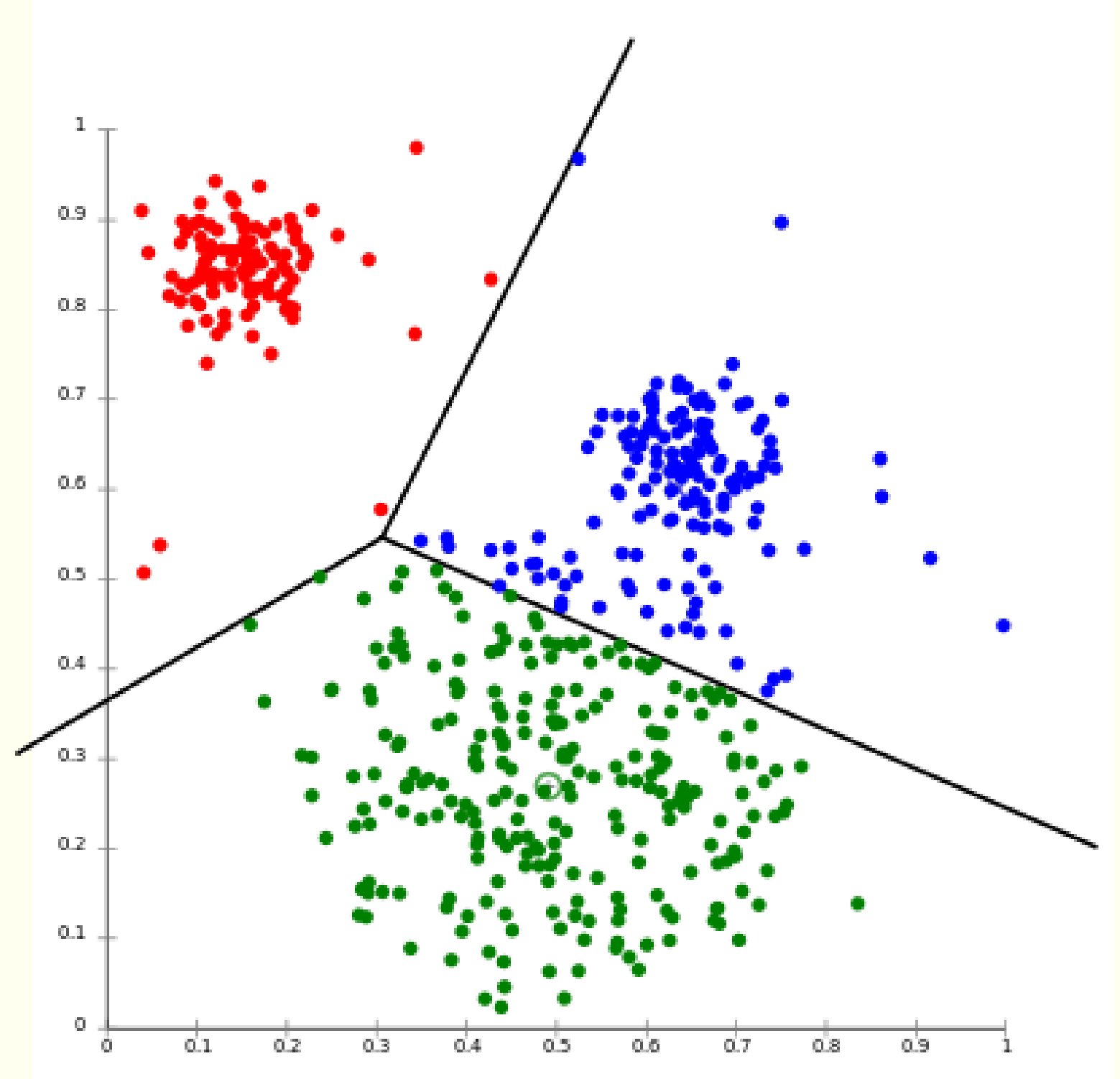
Example Algorithm : K-Means

1. Randomize centroids for each cluster
2. Cluster each point with its nearest centroid
3. Move centroid to mean of its cluster
4. Repeat steps 2 and 3 until equilibrium



Step 1: Initialize Step 2: Group Step 3: Center Step 4: Repeat

Problems



Picture by Chire

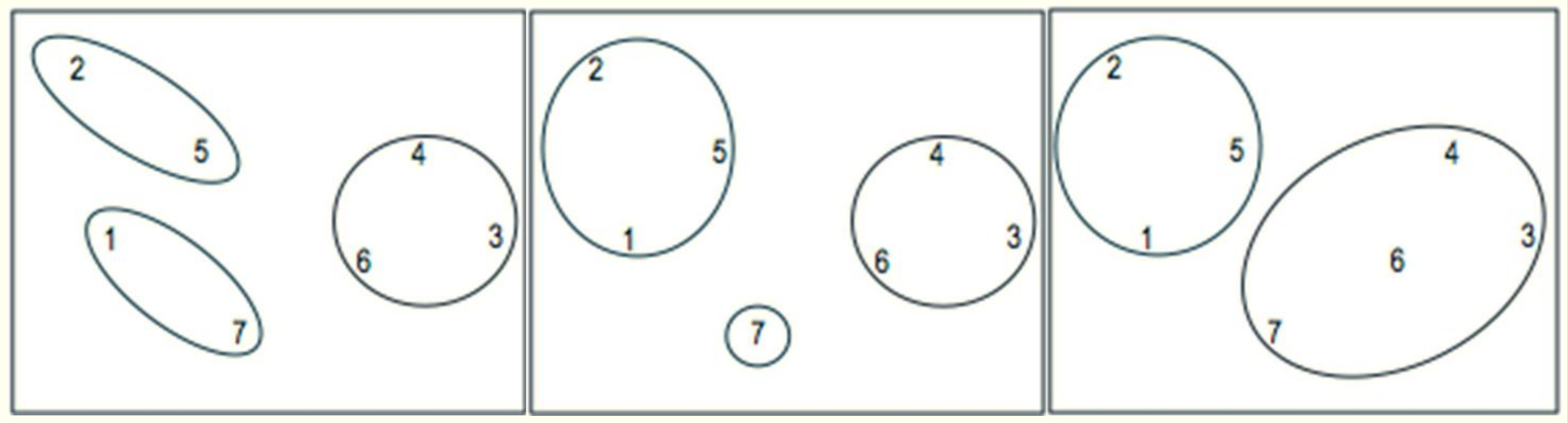
- Fundamental Problem of Clustering
  "There does not exist a best method, that is, one which is superior to all other methods" (Kogan).
- Determining the number of clusters, also known as *k*

Objectives

- Determining an accurate value for *k*
- Develop a technique that uses multiple algorithms to reach a consensus on a final clustering

Methods

Consensus Clustering

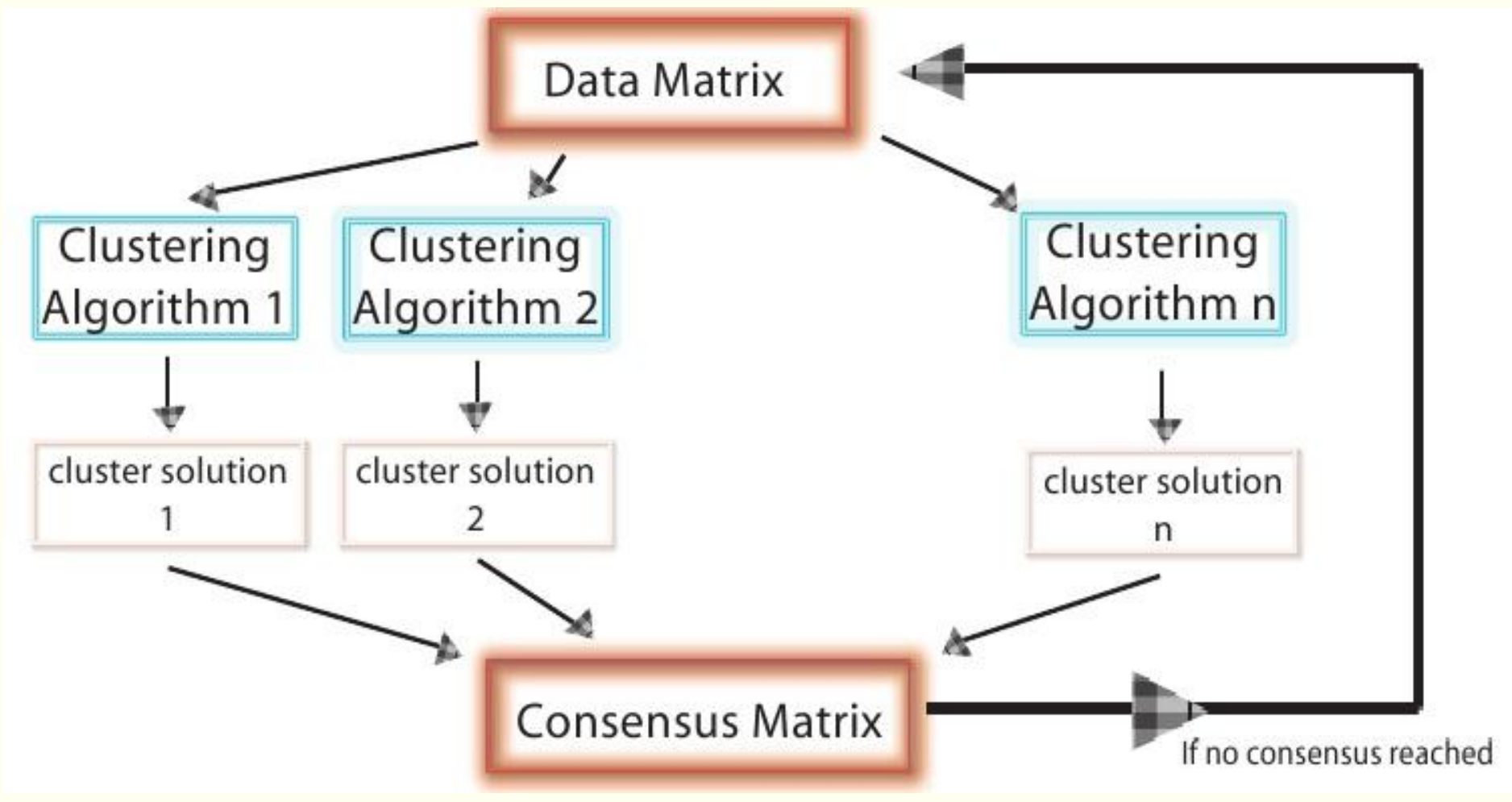


$$\begin{array}{c|ccccccc} & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ \hline 1 & 0 & 2 & 0 & 0 & 2 & 0 & 1 \\ 2 & 2 & 0 & 0 & 0 & 3 & 0 & 0 \\ 3 & 0 & 0 & 0 & 3 & 0 & 3 & 1 \\ 4 & 0 & 0 & 3 & 0 & 0 & 3 & 1 \\ 5 & 2 & 3 & 0 & 0 & 0 & 0 & 0 \\ 6 & 0 & 0 & 3 & 3 & 0 & 0 & 1 \\ 7 & 1 & 0 & 1 & 1 & 0 & 1 & 0 \end{array}$$

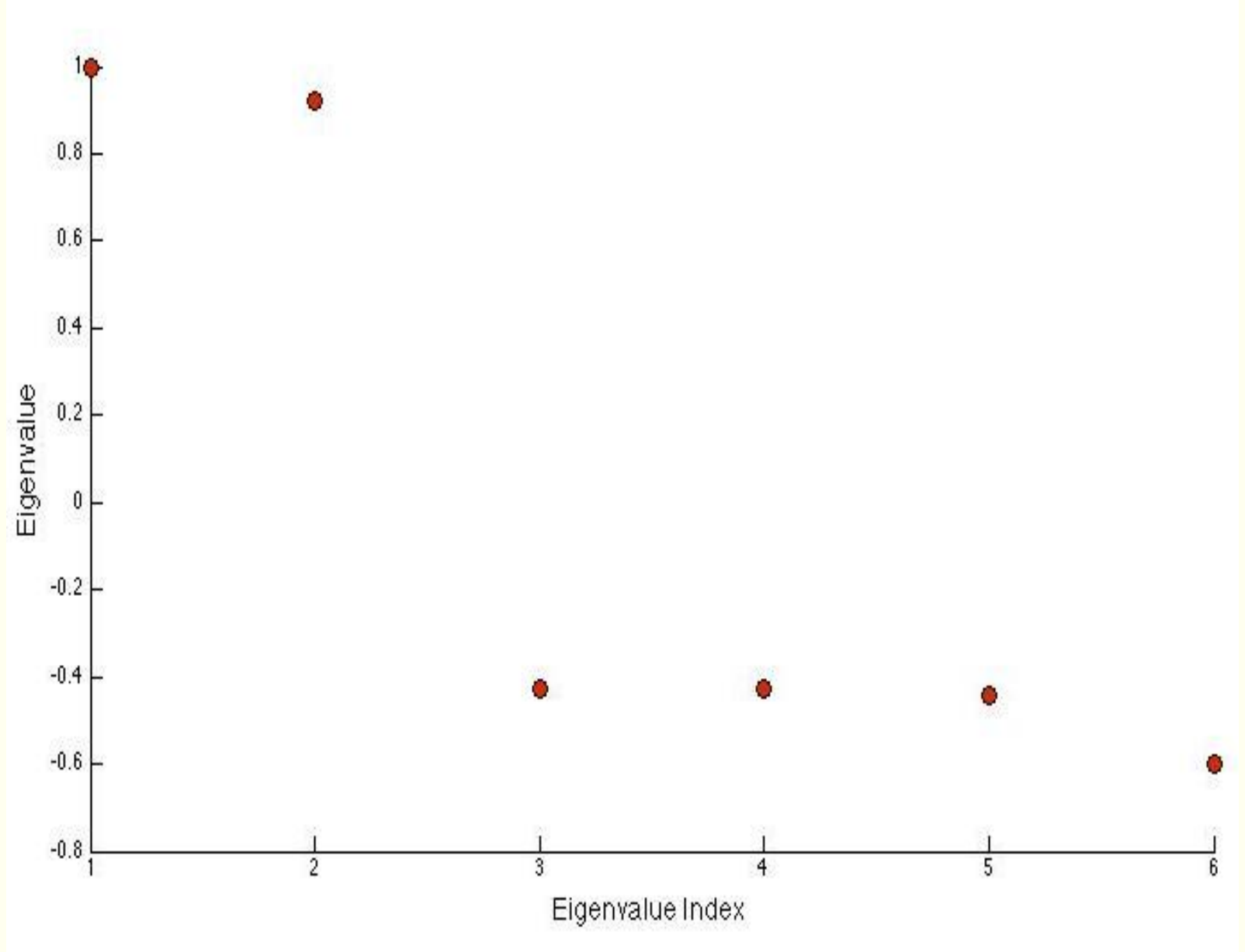
- Each row and column represent a point
- Each matrix entry is the number of times its corresponding row and column are clustered together

Iterated Consensus Clustering

- Treats consensus matrix as a new set of data
- Clusters consensus matrix based on similarities in previous groupings
- Terms in consensus matrix below a certain threshold are dropped
- Iterates this process until convergence



Eigengap Method

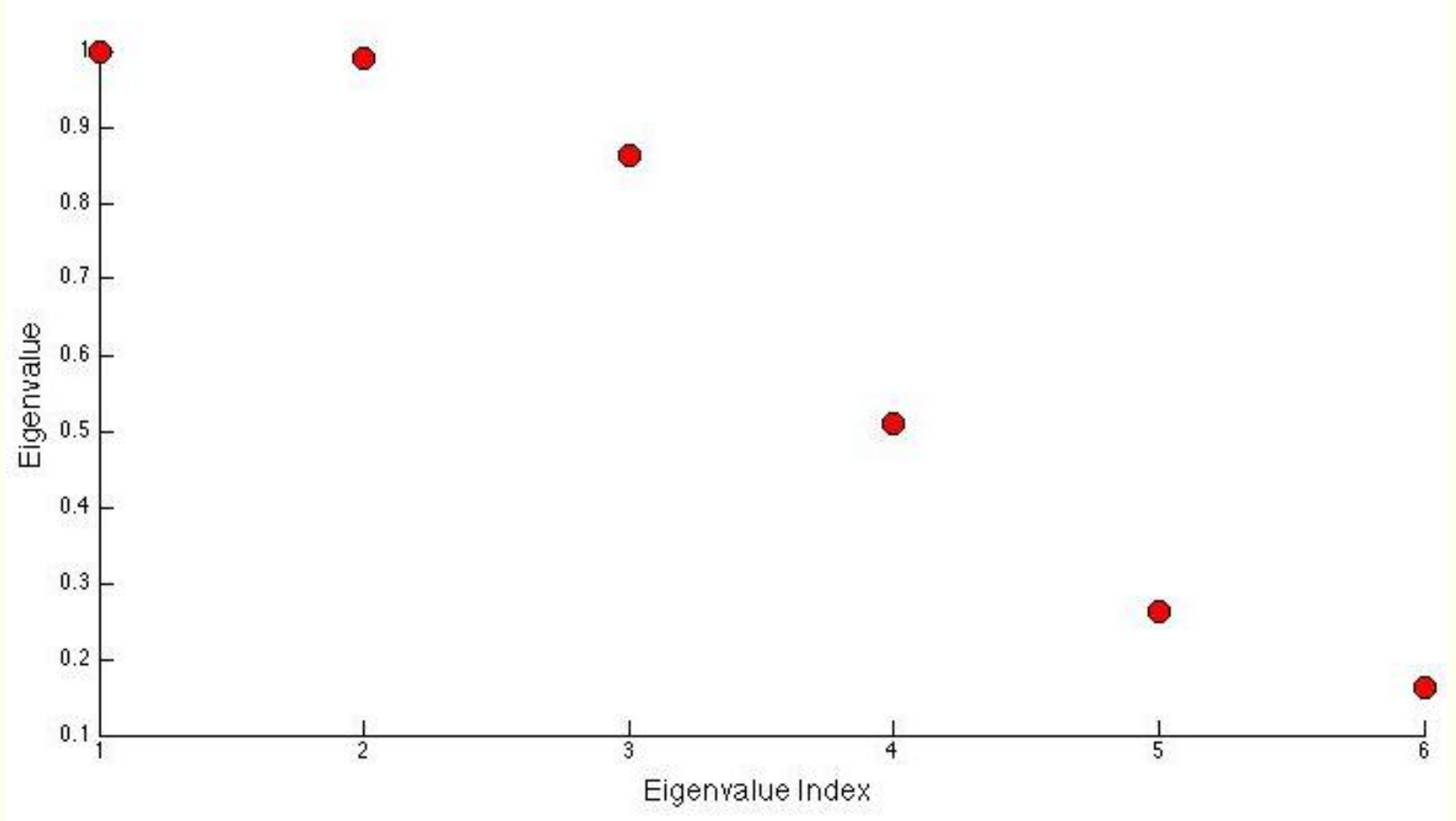


- Eigengap : the largest difference between consecutive eigenvalues
- Create a special "P Matrix" using the consensus matrix
- Sort the P Matrix eigenvalues
- The index of the eigenvalue before the eigengap is an approximation for k

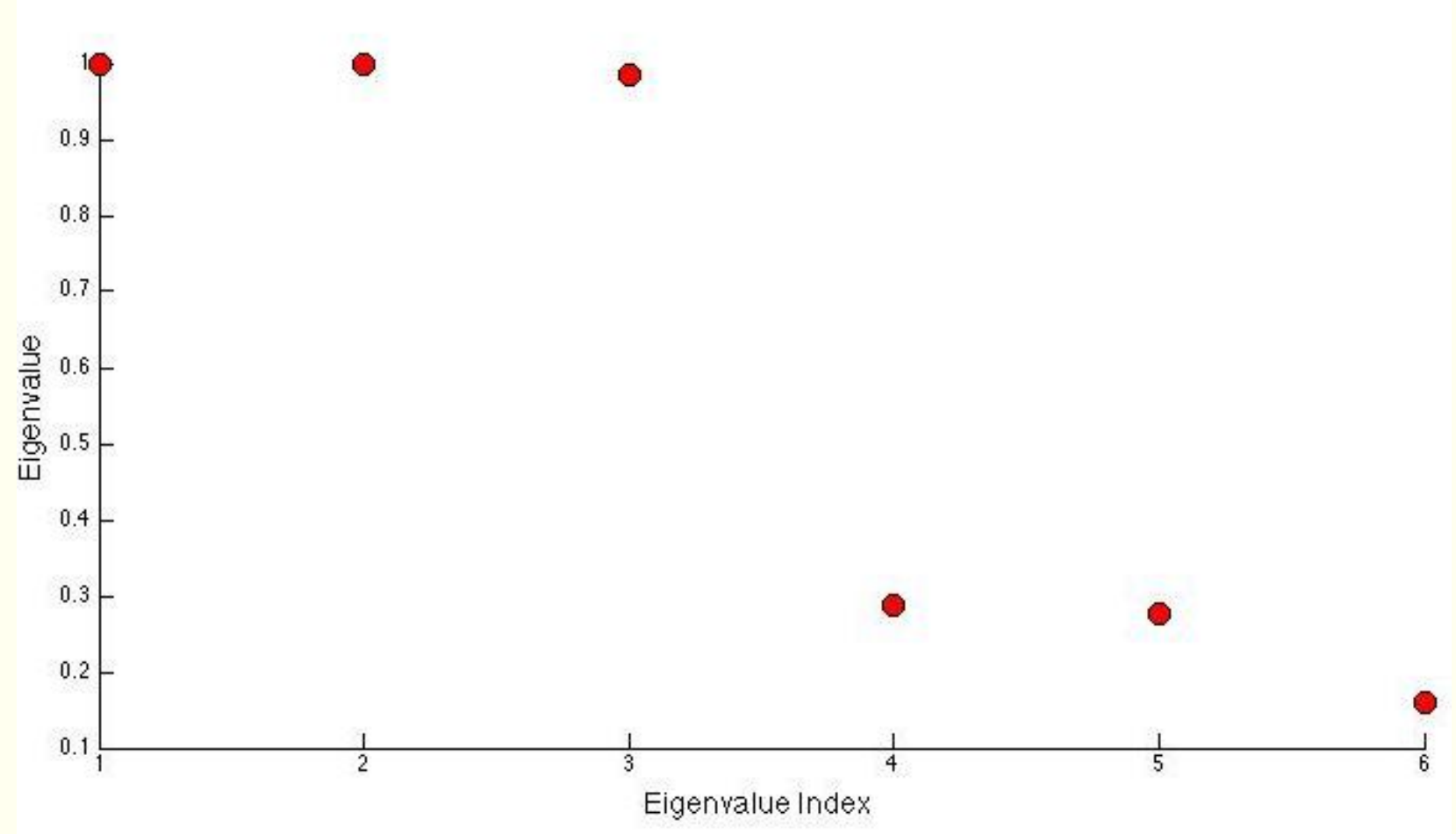
Results / Conclusion

Number of Clusters

Traditional Consensus Clustering



Iterated Consensus Clustering



- Iterated Consensus Clustering creates a larger eigengap, allowing for easier, and more confident, interpretation

Algorithm Consensus : Clustering Accuracy

Algorithm	1st Iteration	2nd Iteration	3rd Iteration
Alg 1	82%	89%	96%
Alg 2	79%	93%	96%
Alg 3	51%	88%	96%
Alg 4	89%	93%	96%
Alg 5	88%	95%	96%

- Errors are weeded out through iteration
- Most algorithms come to a consensus on the final clustering
- Final clustering improves upon many individual algorithms

Conclusion

- Iterated Consensus Clustering offers better results than traditional consensus clustering in:
  - Finding the number of clusters
  - Returning an appropriate clustering
- Calculations were done using the following techniques :
  Expectation Maximization, PDDP, k-Means, NMF, PCA, SVD

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