CS722/822: Machine Learning

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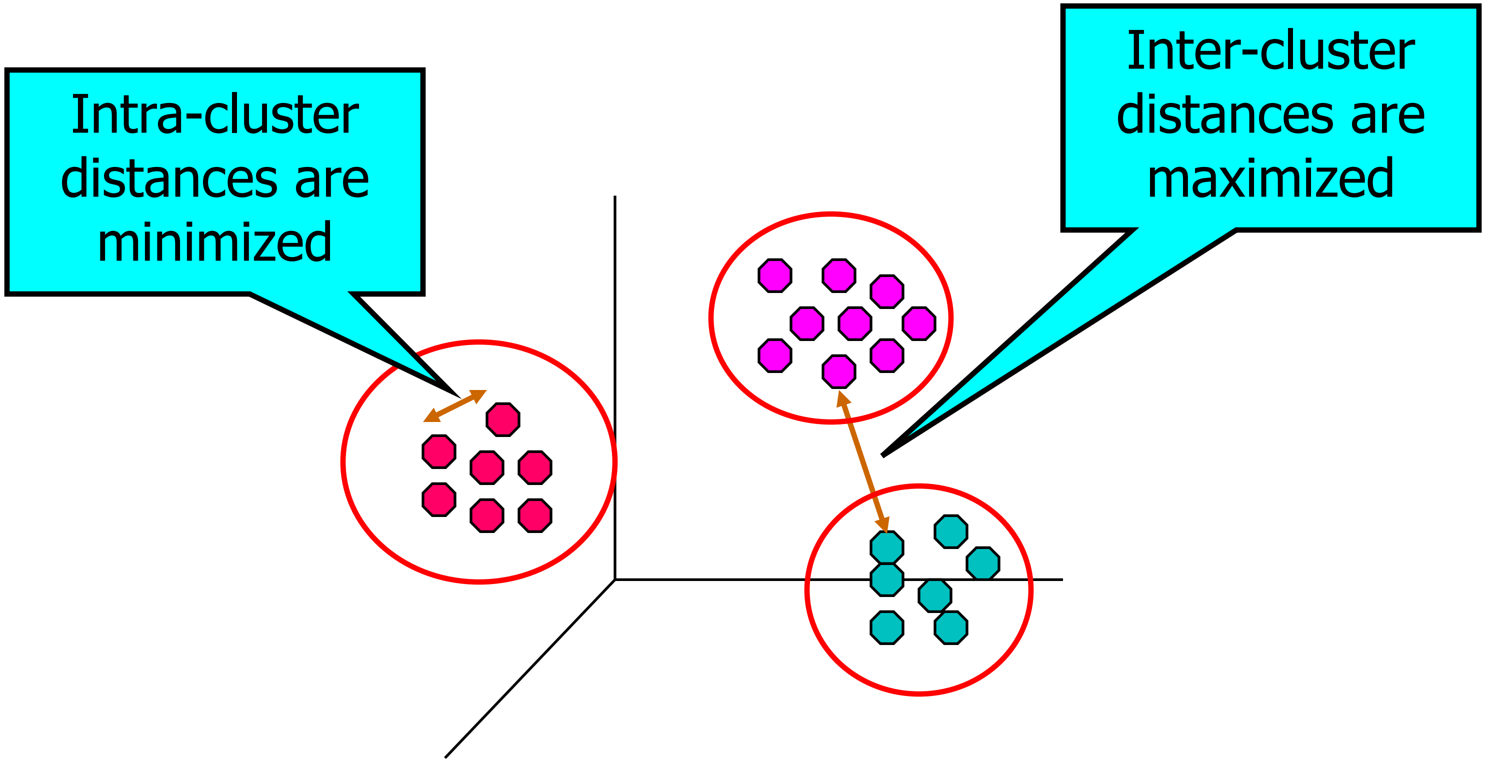
Unsupervised Learning

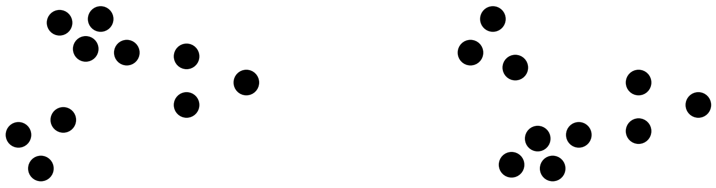
- Draw inferences from the data for exploratory analysis, such as finding hidden patterns or grouping of examples
  - Given a collection of examples, each consisting of a set of features, but without a clear target, i.e., $\{\mathrm{x}_1, \mathrm{x}_2, \cdots, \mathrm{x}_N\}$
  - Examples:
    - Principal component analysis (PCA)
    - Clustering (cluster analysis)

What is Cluster Analysis?

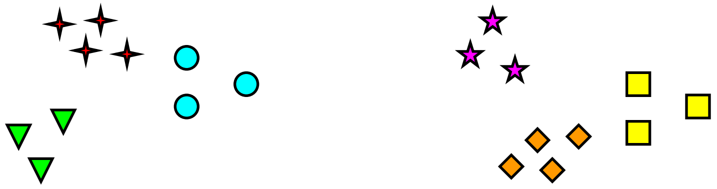
- Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups


Intra-cluster distances are minimized
Inter-cluster distances are maximized

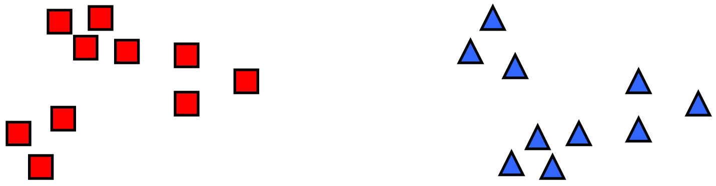
Notion of a Cluster can be Ambiguous



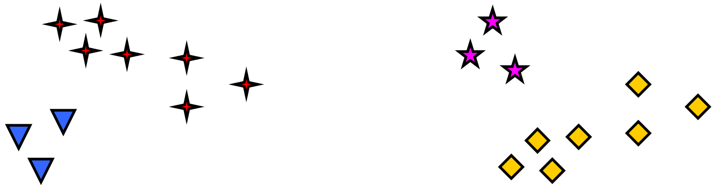
How many clusters?



Six Clusters



Two Clusters

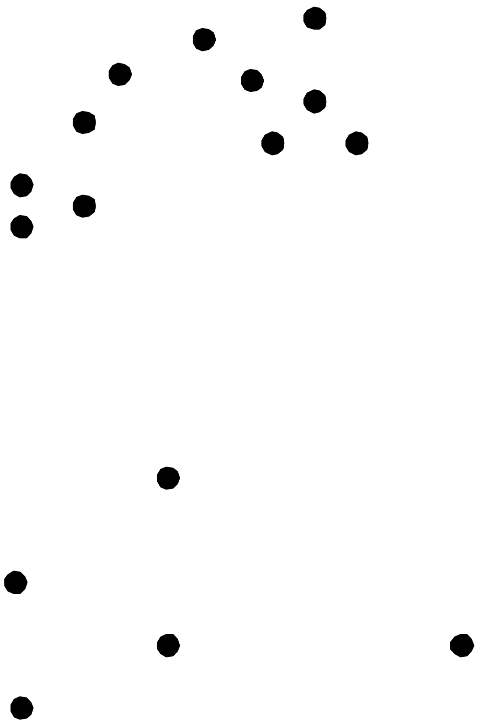


Four Clusters

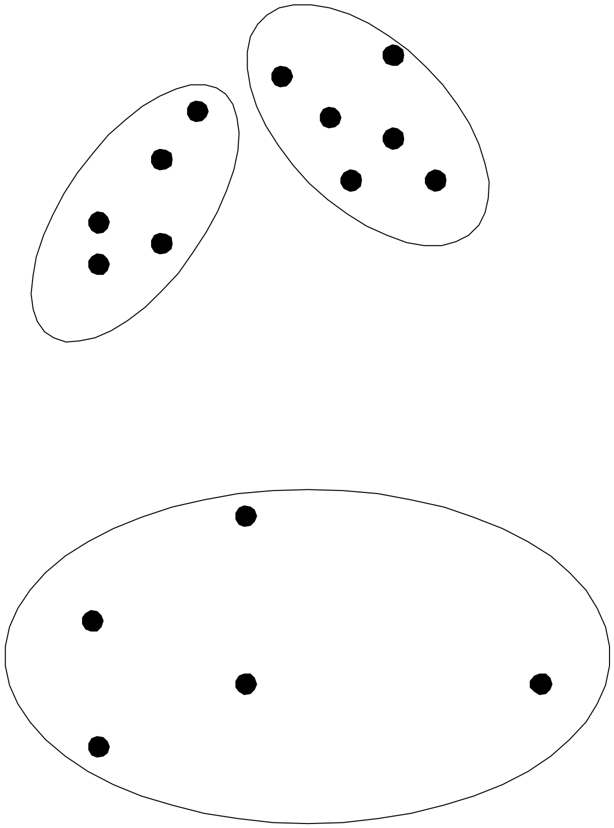
Types of Clusterings

- A clustering is a set of clusters
- Important distinction between hierarchical and partitional sets of clusters
- Partitional Clustering
  - A division data objects into **non-overlapping** subsets (clusters) such that each data object is in exactly **one** subset
- Hierarchical clustering
  - A set of nested clusters organized as a hierarchical tree

Partitional Clustering

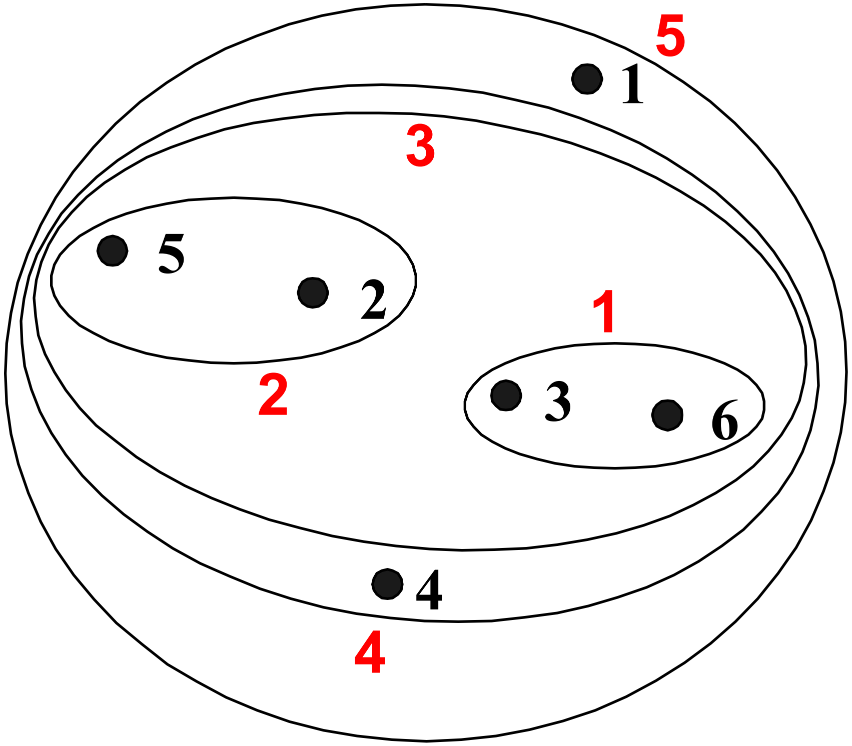


Original Points

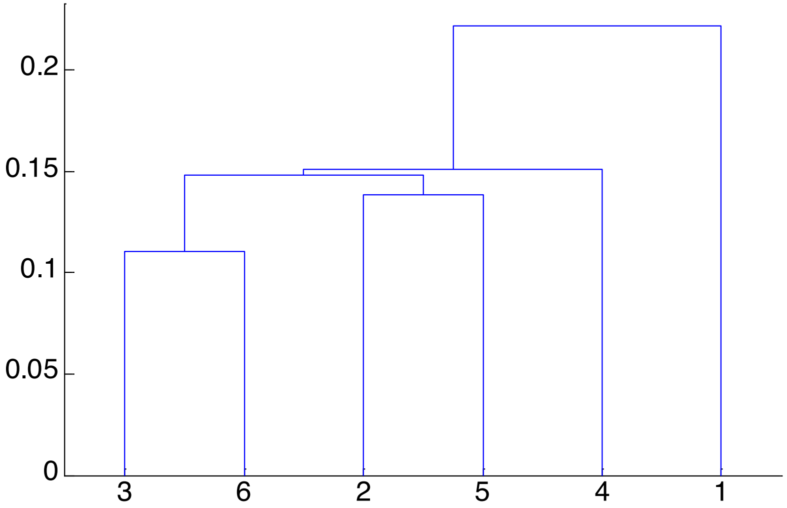


A Partitional Clustering

Hierarchical Clustering



Nested Clusters



Dendrogram

Other Distinctions Between Sets of Clusters

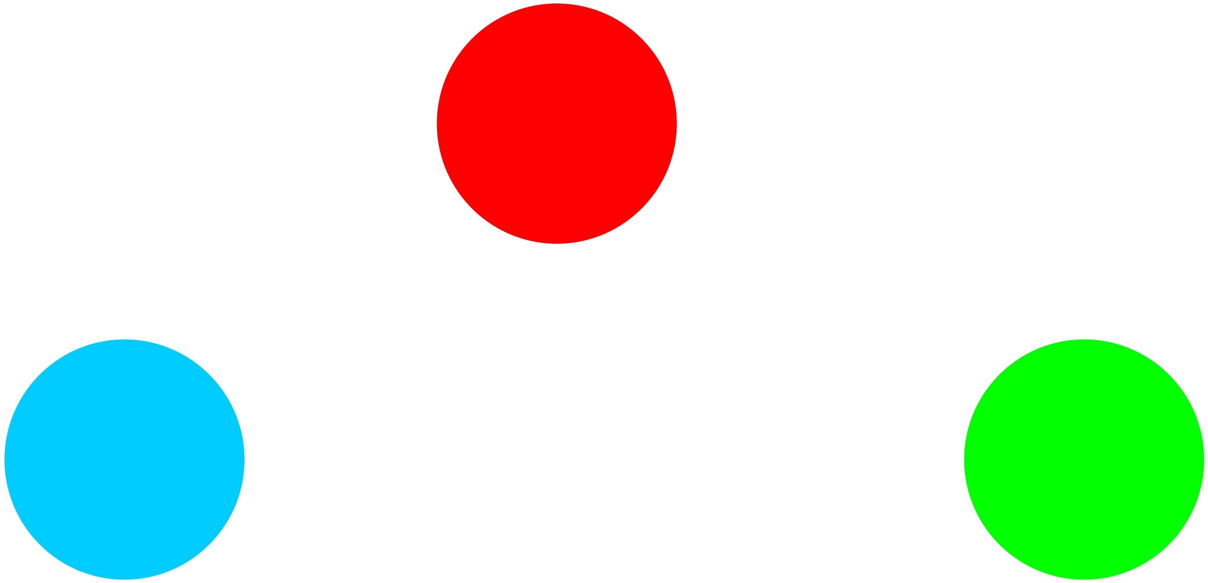
- Non-exclusive versus exclusive
  - In non-exclusive clustering, points may belong to multiple clusters.
  - Can represent multiple classes or ‘border’ points
- Fuzzy versus non-fuzzy, probability vs non-probability
  - In fuzzy clustering, a point belongs to every cluster with some weights
  - Often with constraints that weights must sum to 1
  - Probabilistic clustering has similar characteristics
- Partial versus complete
  - In some cases, we only want to cluster some of the data
- Heterogeneous versus homogeneous
  - Cluster of widely different sizes, shapes, and densities

Types of Clusters

- Well-separated clusters
- Center-based clusters
- Contiguous clusters
- Density-based clusters
- Property or Conceptual
- Described by an Objective Function

Types of Clusters: Well-Separated

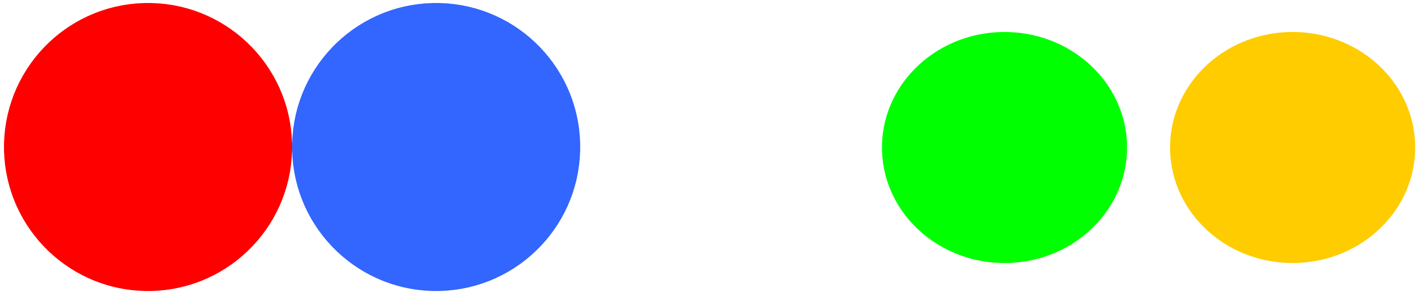
- Well-Separated Clusters:
  - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.



3 well-separated clusters

Types of Clusters: Center-Based

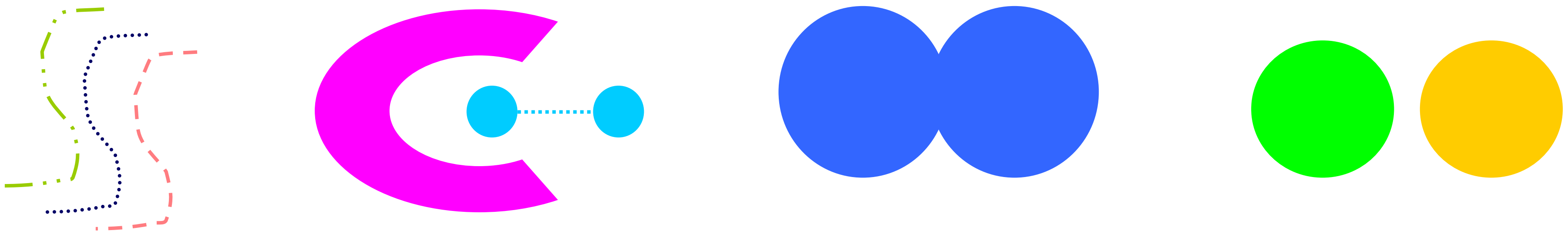
- Center-based
  - A cluster is a set of points such that any point in a cluster is closer (more similar) to the "center" of a cluster, than to the center of any other cluster
  - The center of a cluster is often the centroid, the average of all the points in the cluster, or the medoid, the most "representative" point of a cluster



4 center-based clusters

Types of Clusters: Contiguity-Based

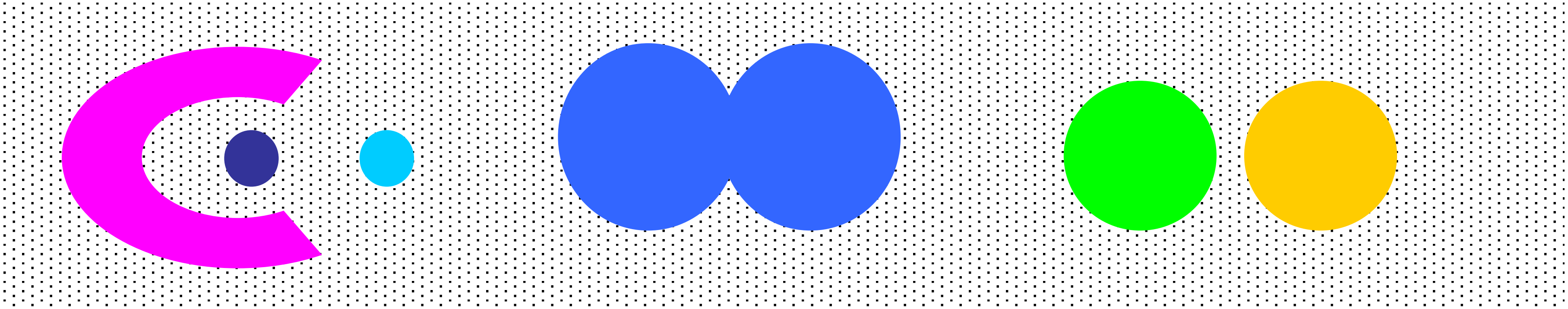
- Contiguous Cluster (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to **one or more** other points in the cluster than to any point not in the cluster.



8 contiguous clusters

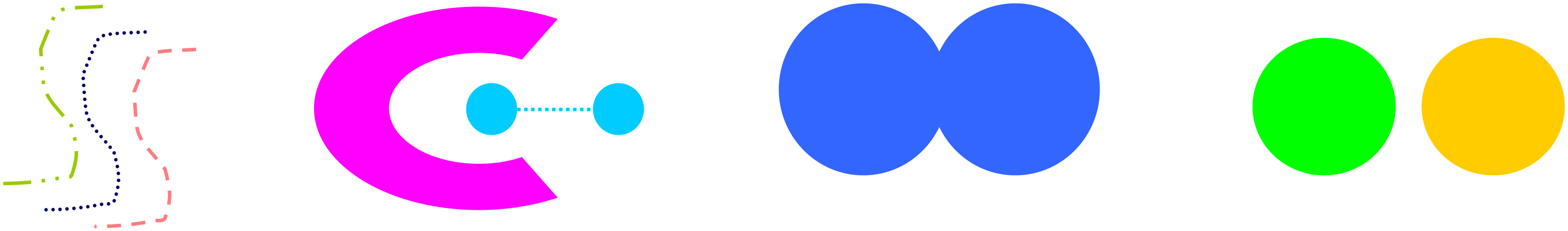
Types of Clusters: Density-Based

- Density-based
  - A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
  - Used when
    - the clusters are irregular or intertwined
    - noise and outliers are present

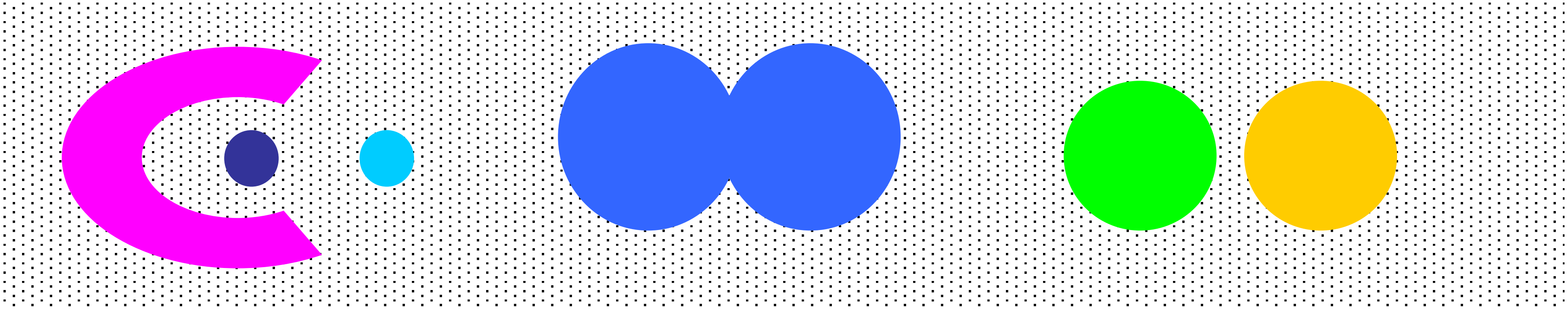


6 density-based clusters

Contiguity Based vs Density-Based



8 contiguous clusters



6 density-based clusters

Types of Clusters: Conceptual Clusters

- Shared Property or Conceptual Clusters
  - Finds clusters that share some common property or represent a particular concept.

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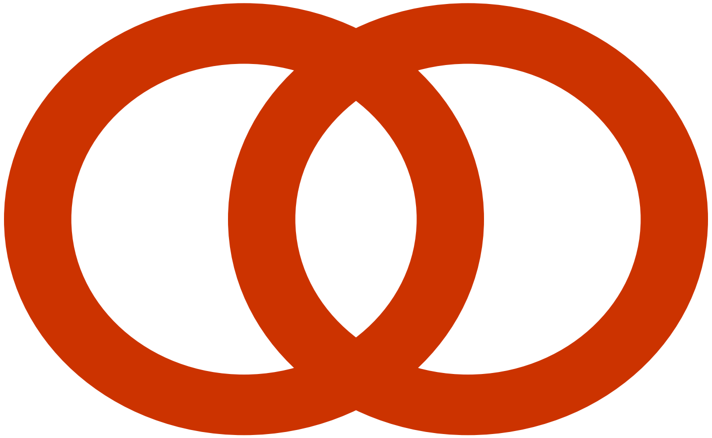

2 Overlapping Circles

Types of Clusters: Objective Function

- Clusters Defined by an Objective Function
  - Finds clusters that minimize or maximize an objective function.
  - Enumerate all possible ways of dividing the points into clusters and evaluate the `goodness' of each potential set of clusters by using the given objective function. (NP Hard)
  - Can have global or local objectives.
    - Hierarchical clustering algorithms typically have local objectives
    - Partitional algorithms typically have global objectives
  - A variation of the global objective function approach is to fit the data to a parameterized model.
    - Parameters for the model are determined from the data.
    - Mixture models assume that the data is a ‘mixture' of a number of statistical distributions.

Types of Clusters: Objective Function …

- Map the clustering problem to a different domain and solve a related problem in that domain
  - Proximity matrix defines a weighted graph, where the nodes are the points being clustered, and the weighted edges represent the proximities between points
  - Clustering is equivalent to breaking the graph into connected components, one for each cluster.
  - Want to minimize the edge weight between clusters and maximize the edge weight within clusters

Characteristics of the Input Data Are Important

- Type of proximity or density measure
  - This is a derived measure, but central to clustering
- Sparseness
  - Dictates type of similarity
  - Adds to efficiency
- Attribute (variable) type
  - Dictates type of similarity
- Type of Data
  - Dictates type of similarity
- Dimensionality
- Noise and Outliers
- Type of Distribution