Clustering by fast search and find of density peaks

Alex Rodriguez, Alessandro Laio

Presenter: Honglei Zhuang

Rodriguez, Alex, and Alessandro Laio. "Clustering by fast search and find of density peaks." *Science* 344.6191 (2014): 1492-1496.

Existing Clustering Algorithms

- K-means, K-medoids
  - Data points are assigned to nearest cluster centers
  - Not applicable for nonspherical clusters
- Distribution-based
  - Assuming a generative (mixture) distribution for data
  - Requiring pre-defined distribution

Existing Clustering Algorithms

- Density-based
  - DBSCAN
    - Given a density threshold, assigns to different clusters disconnected regions of high density
    - Sensitive to the density threshold
  - Mean-Shift
    - Define a density field
    - Points converged to the same local maximum of the density field are assigned to the same clusters
    - Works only for data defined by a set of coordinates

Proposed Algorithm

- Basic Idea
  - Cluster centers are surrounded by neighbors with lower local density
  - Cluster centers are far away from other points with a higher local density
- Advantages
  - Based only on distance between data points
  - Can produce nonspherical clusters

Basic Definitions

- Local Density

$$\rho_i = \sum_j \chi\left(d_{ij} - d_c\right)$$

  where $\chi\left(x\right) = \mathbf{1}_{\{x<0\}}$ and d_c is a given cutoff

  – Basically is the number of points closer than the cutoff to the point.

- Define $\delta_i = \min\limits_{j:\rho_j>\rho_i}\left(d_{ij}\right)$

  – The minimum distance to other points with a higher local density

  – Defined as $\delta_i = \max\limits_j\left(d_{ij}\right)$ is the density is largest

Example

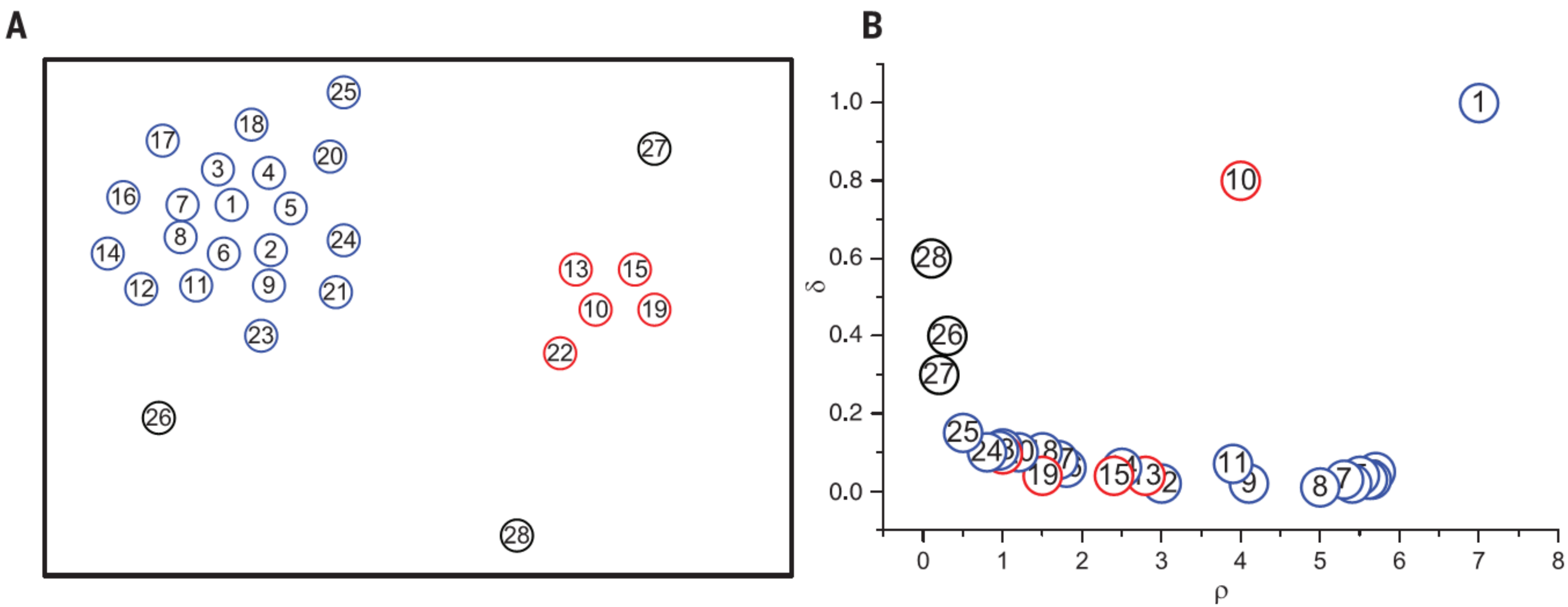
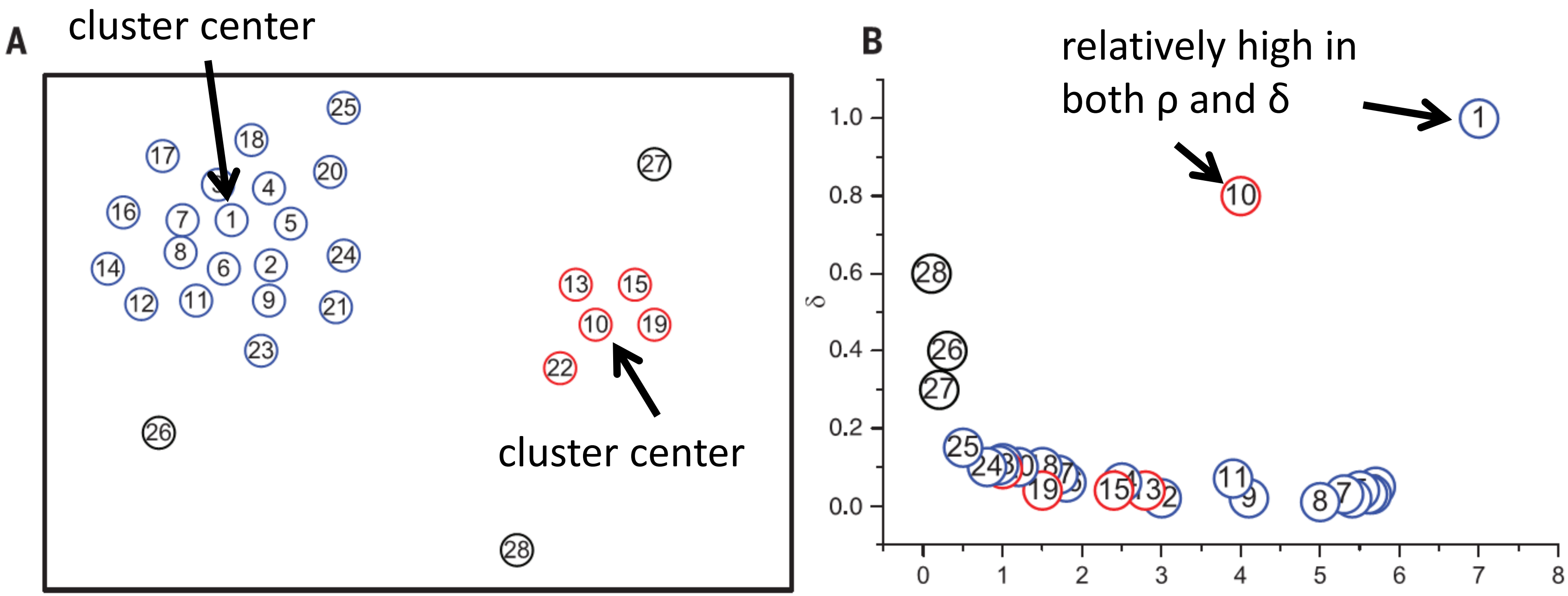


Fig. 1. The algorithm in two dimensions. (**A**) Point distribution. Data points are ranked in order of decreasing density. (**B**) Decision graph for the data in (A). Different colors correspond to different clusters.

Example



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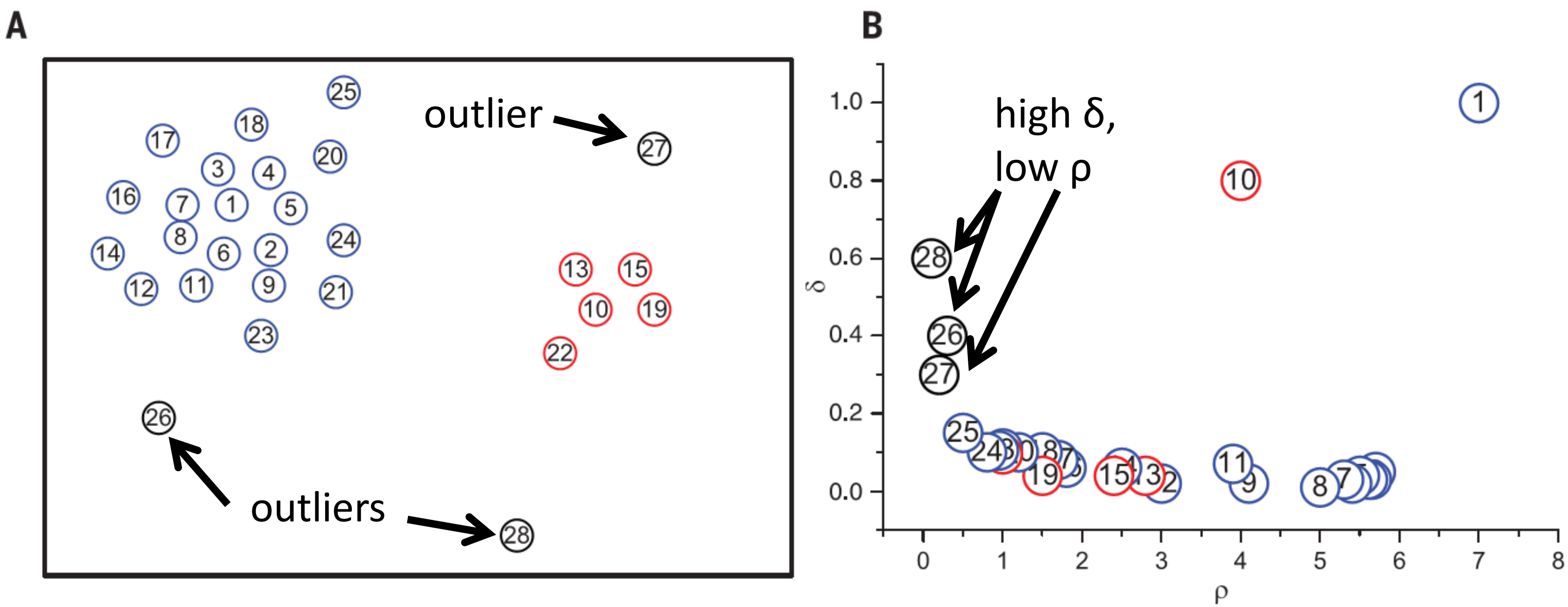


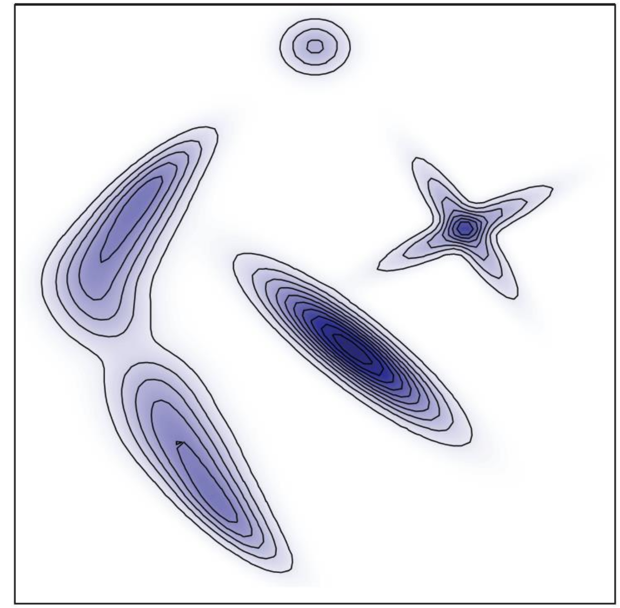
Fig. 1. The algorithm in two dimensions. (**A**) Point distribution. Data points are ranked in order of decreasing density. (**B**) Decision graph for the data in (A). Different colors correspond to different clusters.

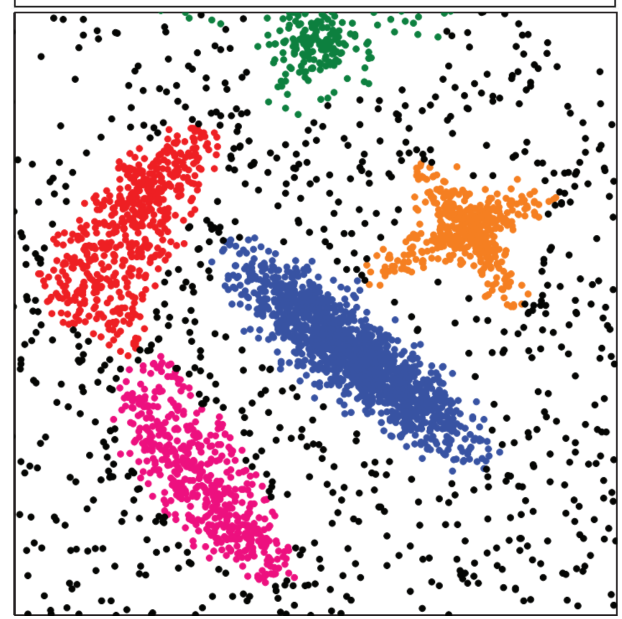
Proposed algorithm

- After cluster centers have been found,
  - Each remaining point is assigned to the cluster of nearest neighbor of higher density
  - No need to be optimized iteratively

Reliability

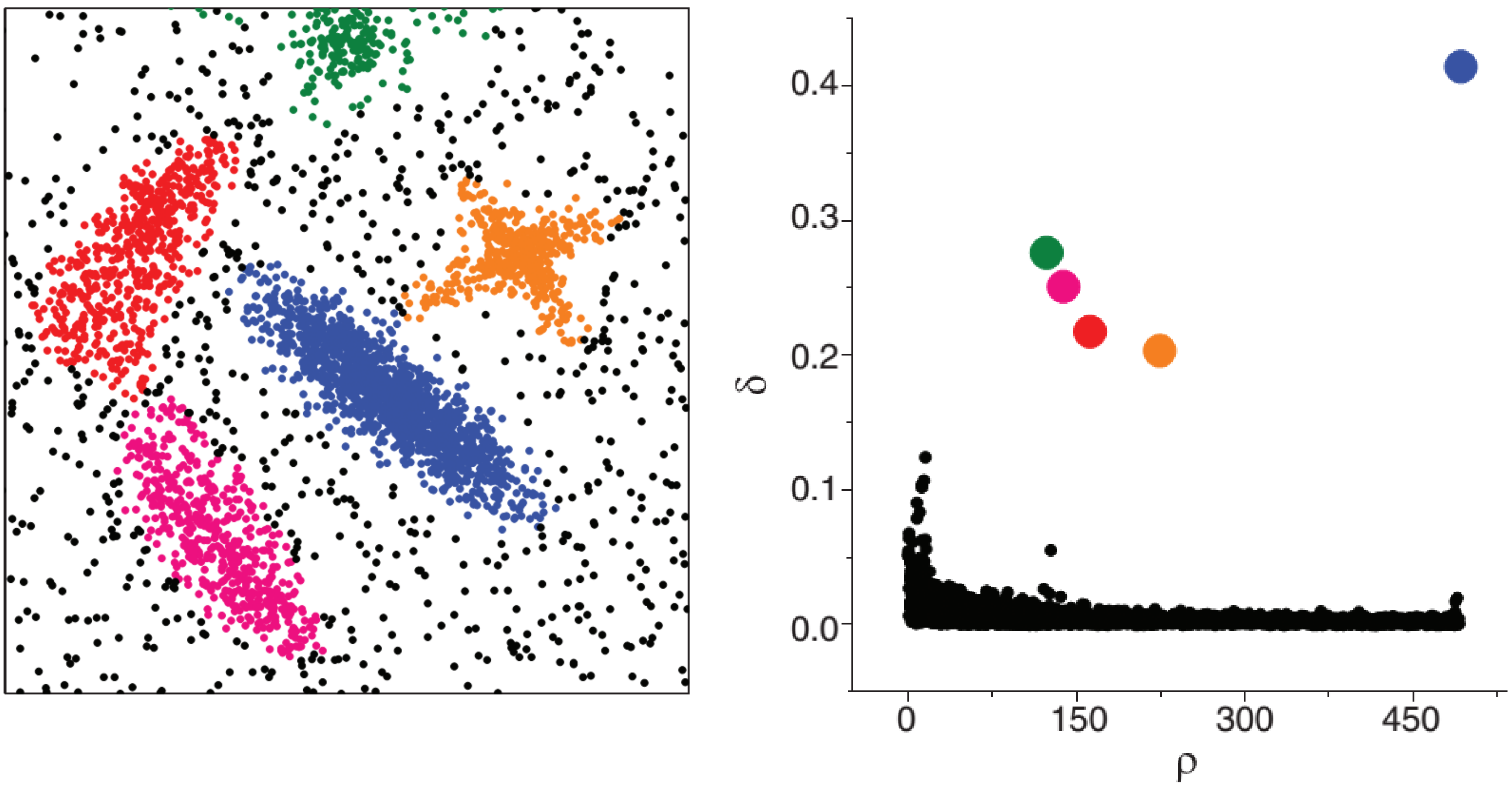
- When noise exists
- Define a "border region" for each cluster where points are within cutoff distance d_c from points of other clusters
- Define a highest density in the border region as the threshold density ρ_b
- Any points with a local density lower the threshold density is regarded as noise



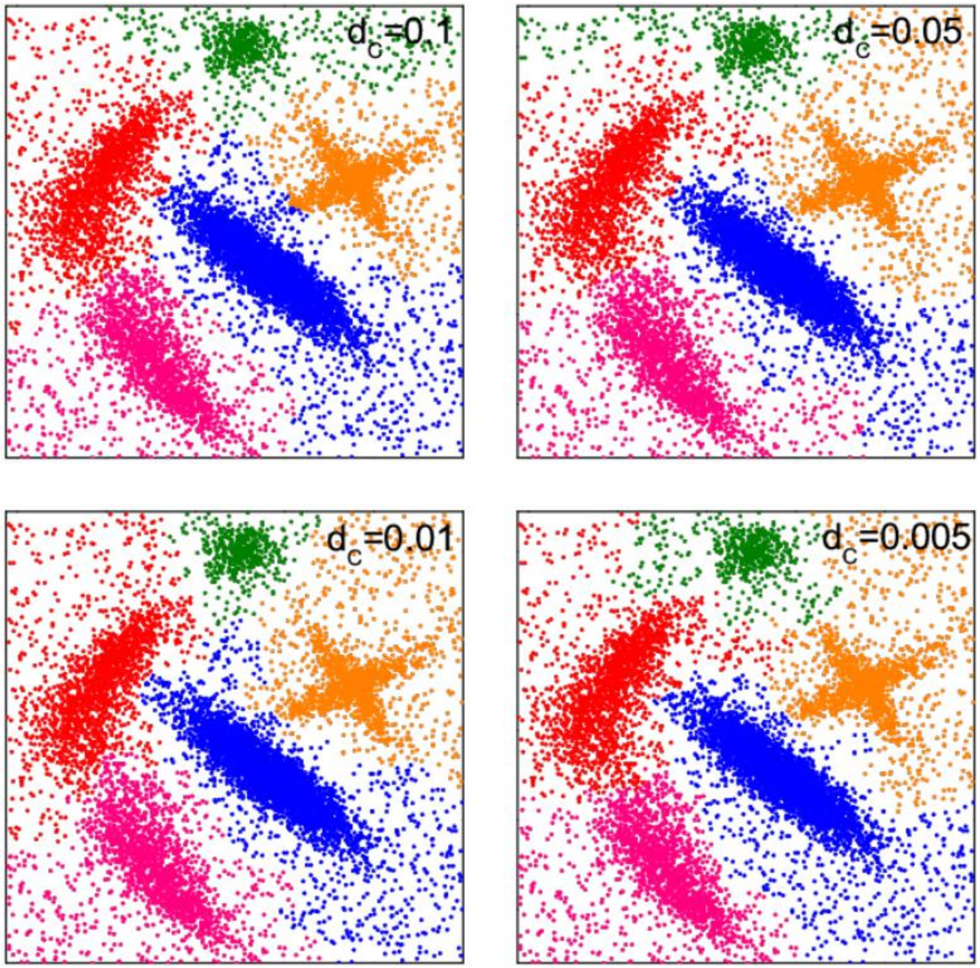


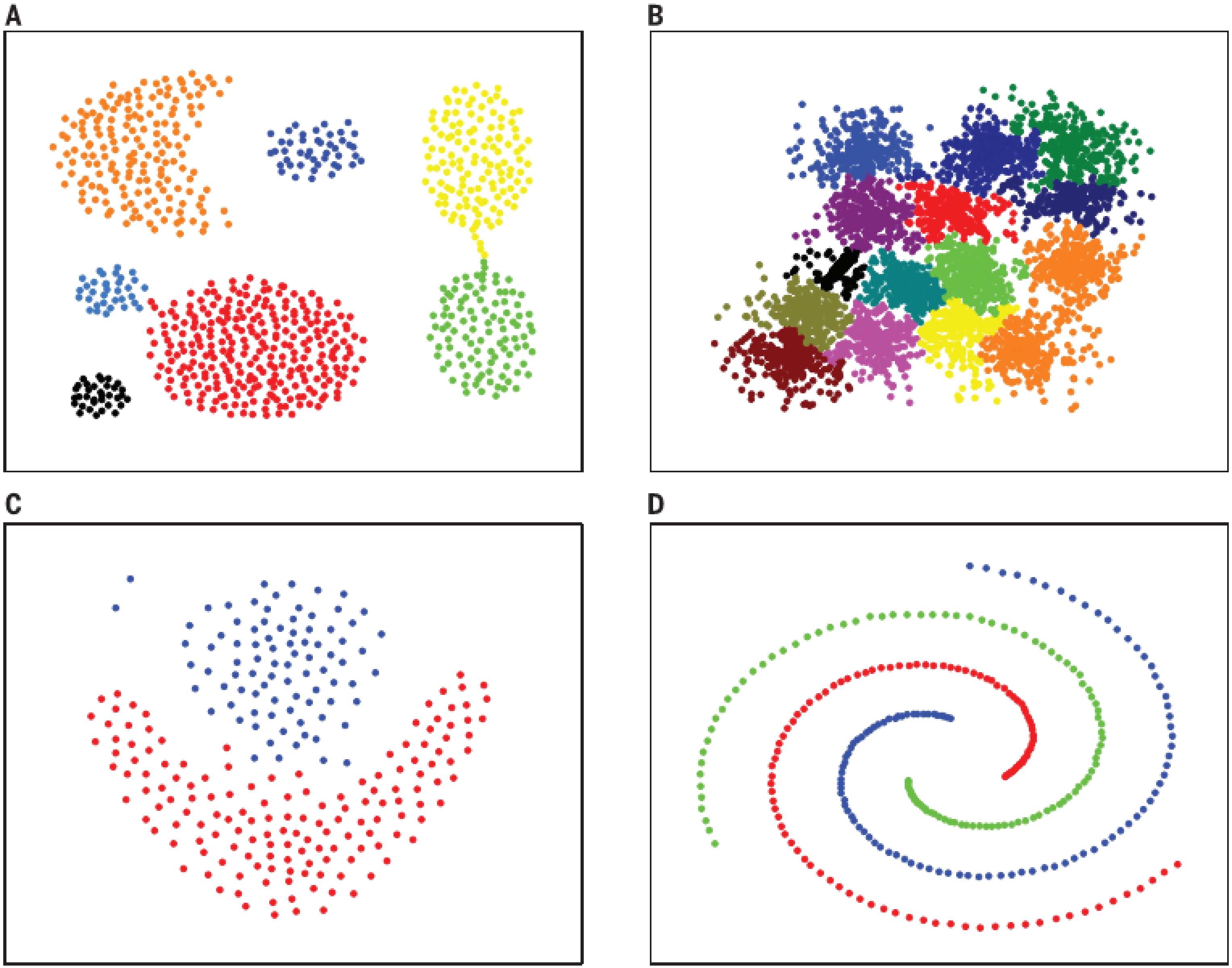
Experiments

- 4,000 points drawn



Parameter Sensitivity

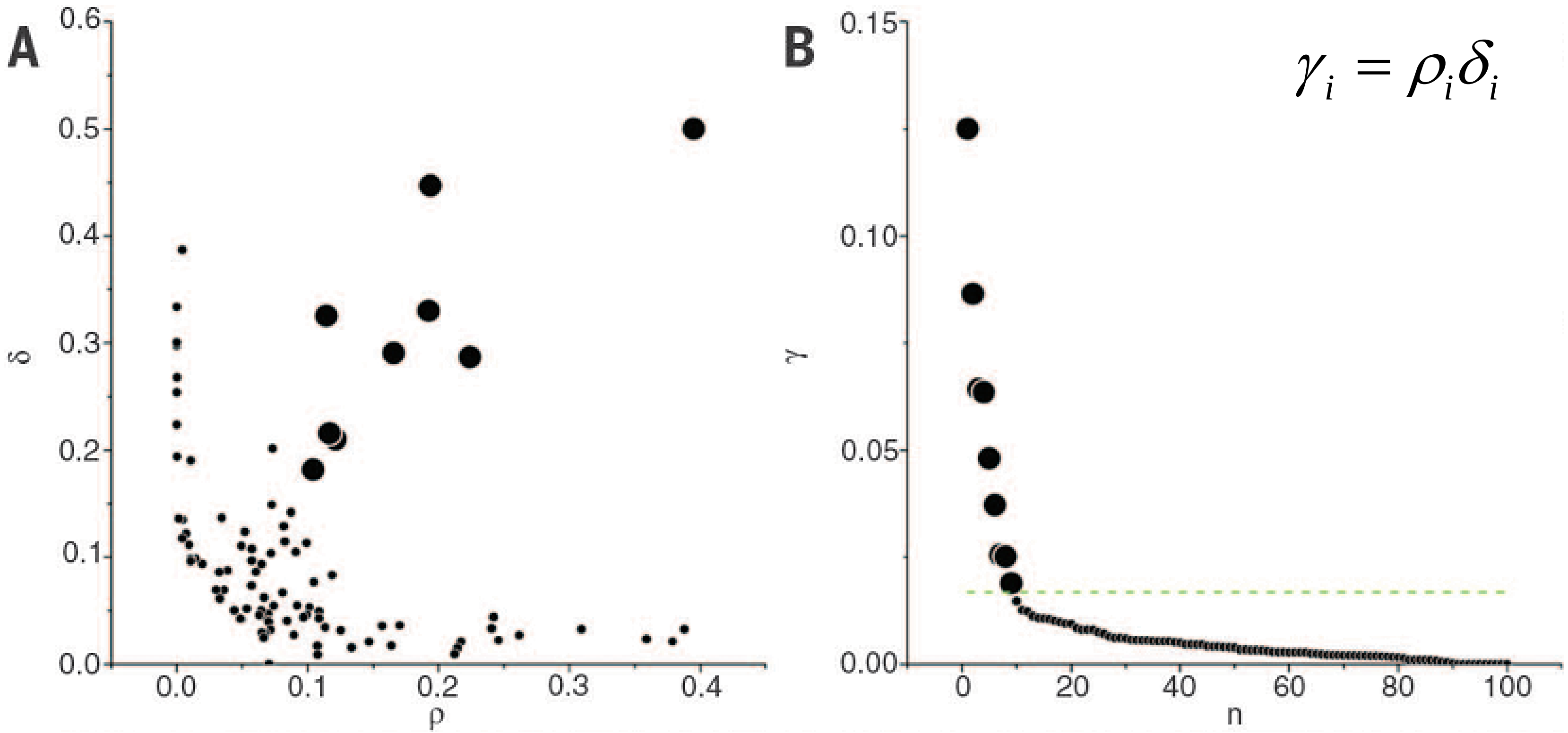



A
B
C
D

Experiments on Face Database

Experiments on Face Database

- Cannot clearly determine #clusters



$$\gamma_i = \rho_i \delta_i$$

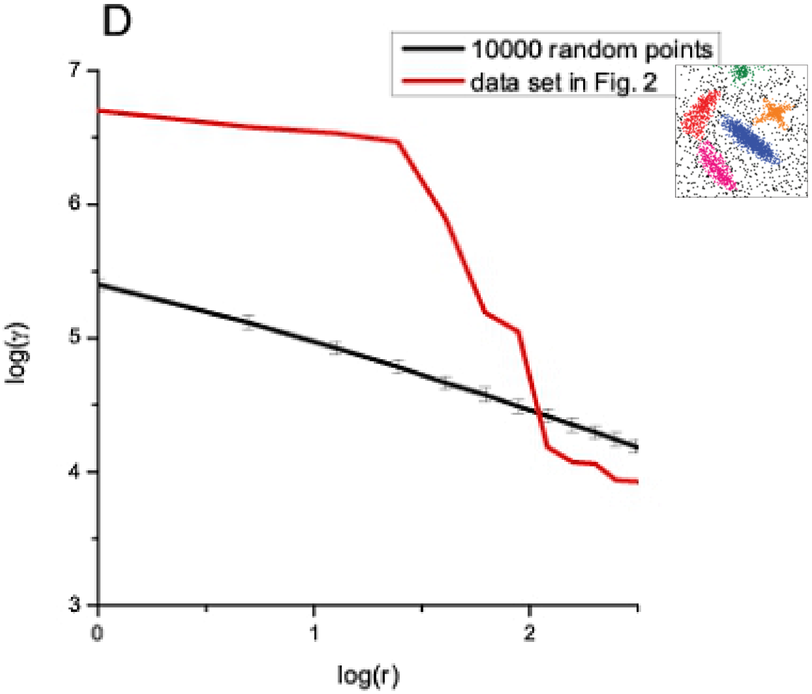
On Random Data Set

- A hint to determine the cluster centers is to calculate

$$\gamma_i = \rho_i \delta_i$$

where usually a gap exists

- In a (uniformly) randomly distributed data set, following a power law



Summary

- Algorithm Sketch
  - Calculate local density and minimum distance to data point with higher density
  - Determine cluster centers
  - Assign data points to cluster of the closest data point with higher density
- Advantages
  - Works for nonspherical clusters
  - Only requires distance
- Drawbacks
  - Sometimes hard to determine number of clusters

Thanks

Honglei Zhuang