Hierarchical Clustering

36-350: Data Mining

25 September 2006

Last time...

- Unsupervised learning problems; finding clusters
- K means
  - divide into k clusters to minimize within-cluser variance*cluster size
  - local search, local minima

Limits of k-Means

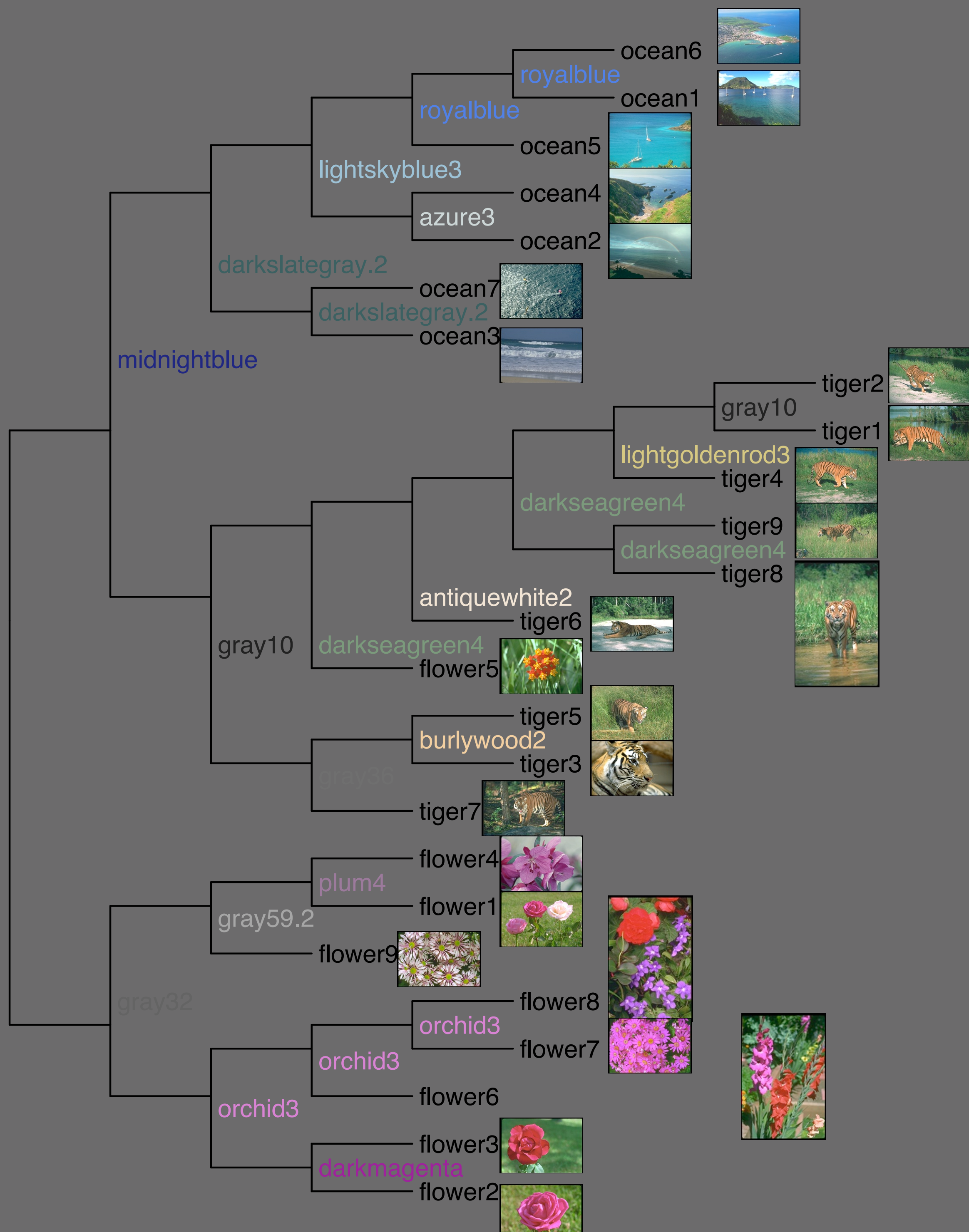
- Local search can get stuck
  - Random starts help
- Sum-of-squares likes ball-shaped clusters
- How to pick k?
- No relations between clusters

Hierarchical Clustering

- Basic idea: cluster the clusters
- High-level clusters contain multiple low-level clusters
- Clusters are now related
- Don’t need to chose k
- Assumes a hierarchy makes sense...

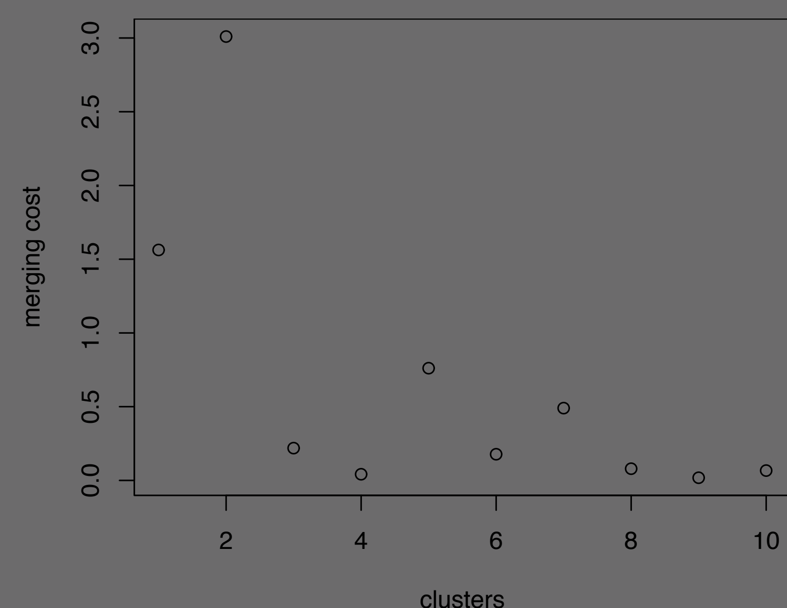
Ward’s Method

1. Start with every point in its own cluster
2. For each pair of clusters, calculate “merging cost” = increase in sum of squares
3. Merge least-costly pair
4. Stop when merging cost takes a big jump



Ward's method applied to the images from lecture 3: ocean, tigers, flowers

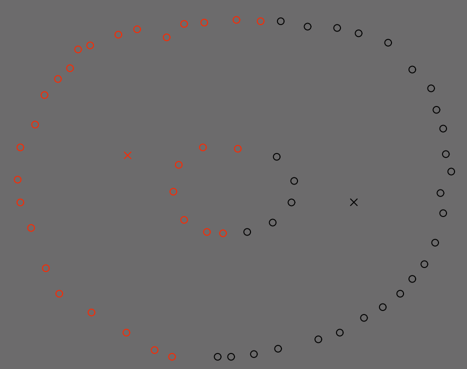
Jump in merging cost suggests 3 clusters - almost exactly right ones, too (but thinks flower5 is a tiger)



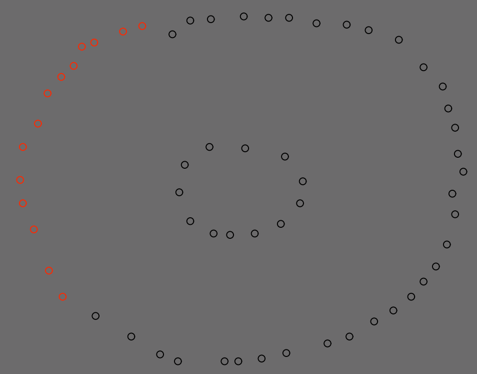
- Don’t have to chose k
- Sum of squares is worse, generally, than k-means (for equal k)
    - more constrained search
    - prefers to merge small clusters, all else equal

Minimizing the mean distance from the center tends to make spheres, which can be silly

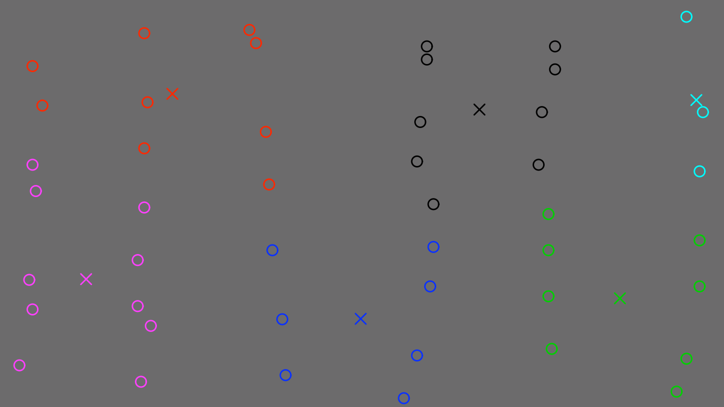
k-Means

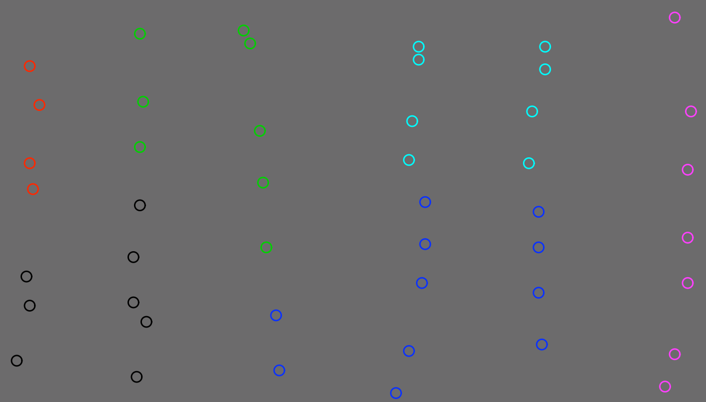


Ward's



note how Ward's is less balanced

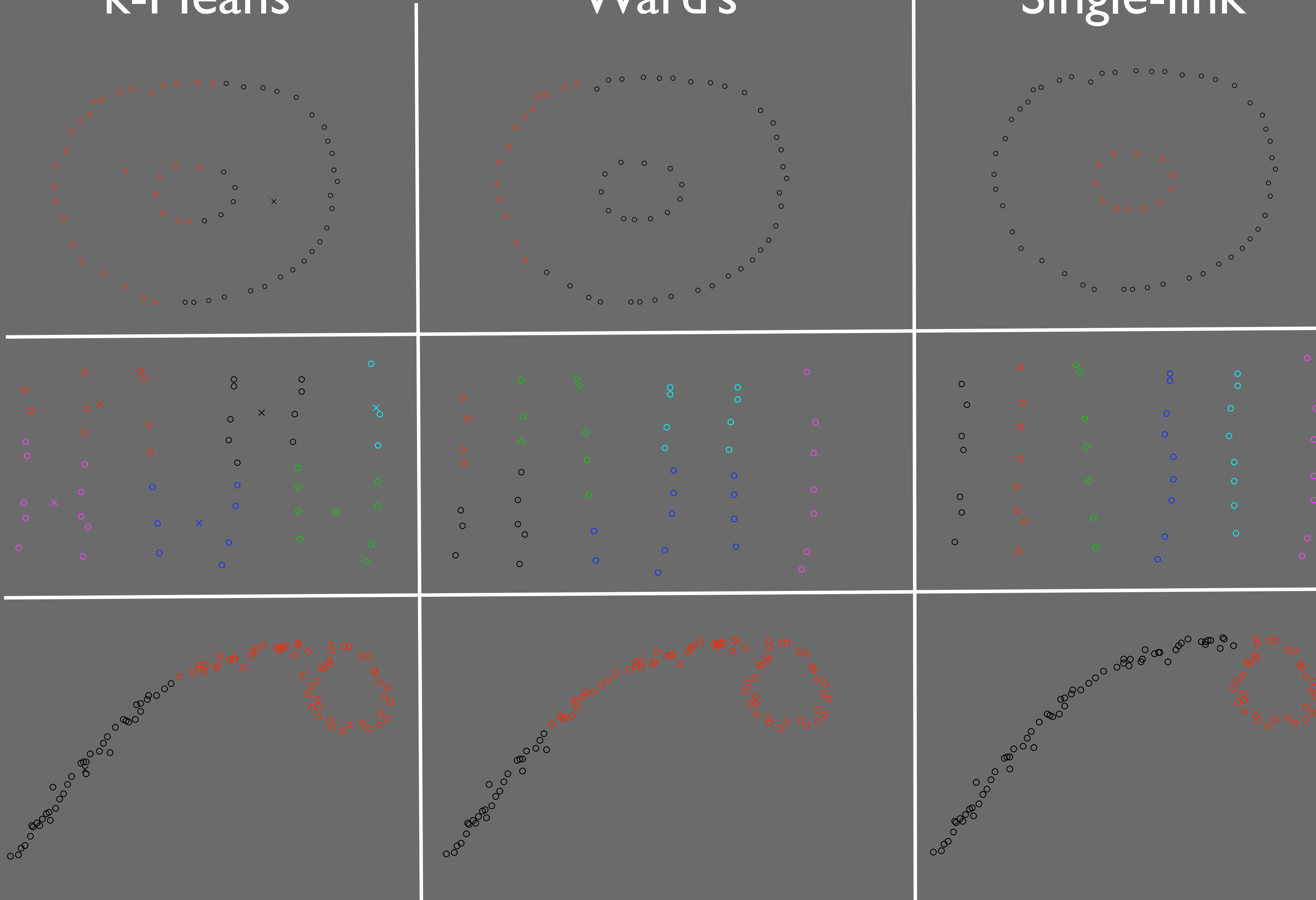




Single-link clustering

1. Start with every point in its own cluster
2. Calculate gaps between every pair of clusters = distance between 2 closest points in each cluster
3. Merge clusters with smallest gap

k-Means | Ward's | Single-link



Examples where single-link doesn't work so well

k-Means	Ward's	Single-link