CSC 411: Lecture 12: Clustering

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Today

- Unsupervised learning
- Clustering
  - k-means
  - Soft k-means

Motivating Examples

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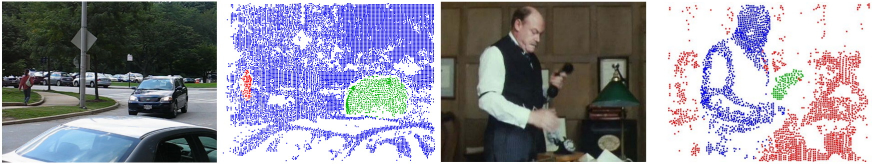

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- Key utility
  - Compress data
  - Detect outliers
  - Facilitate other learning

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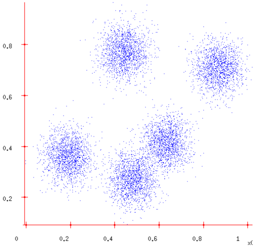
  2. Clustering: represent each input case using a prototype example (e.g., k-means, mixture models)
  3. Density estimation: estimating the probability distribution over the data space

Clustering

- Grouping N examples into K clusters one of canonical problems in unsupervised learning



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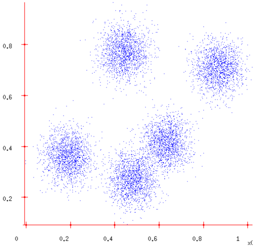

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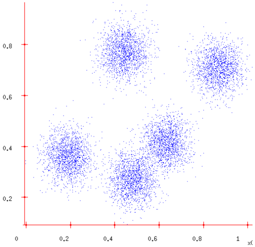

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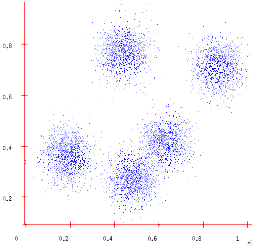

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- What is the objective function that is optimized by sensible clustering?

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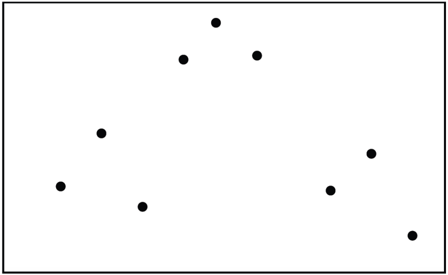

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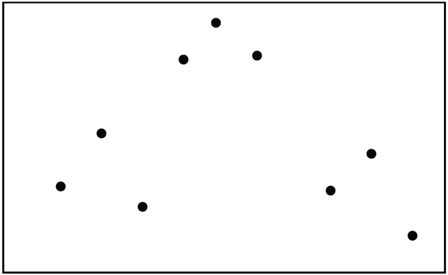

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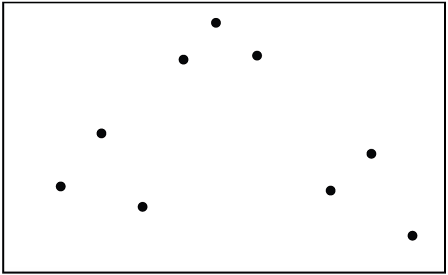

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- How can we identify those classes (data points that belong to each class)?

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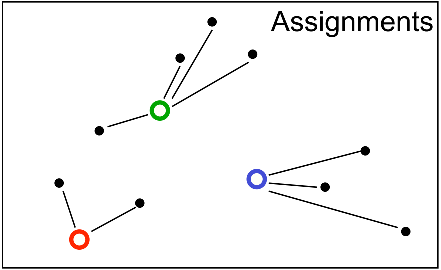

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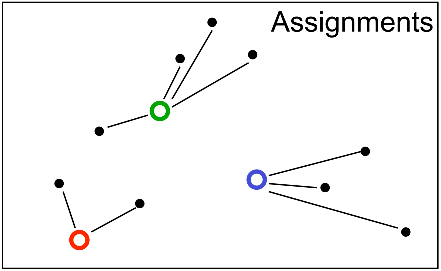

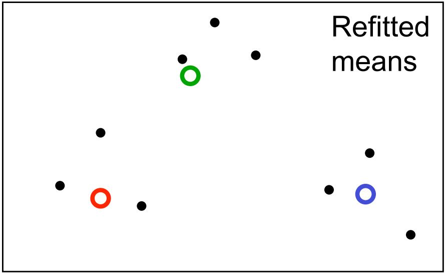

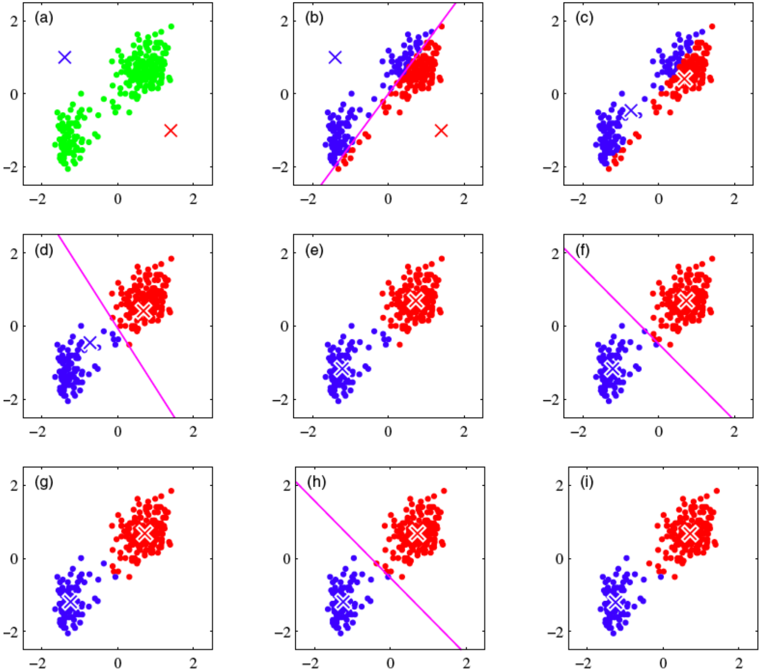

Figure from Bishop

Simple demo: http://syskall.com/kmeans.js/

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  - Fix assignments, optimize means (average of assigned datapoints)

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  - Update: Model parameters, means are adjusted to match sample means of data points they are responsible for:

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K-means for Vector Quantization

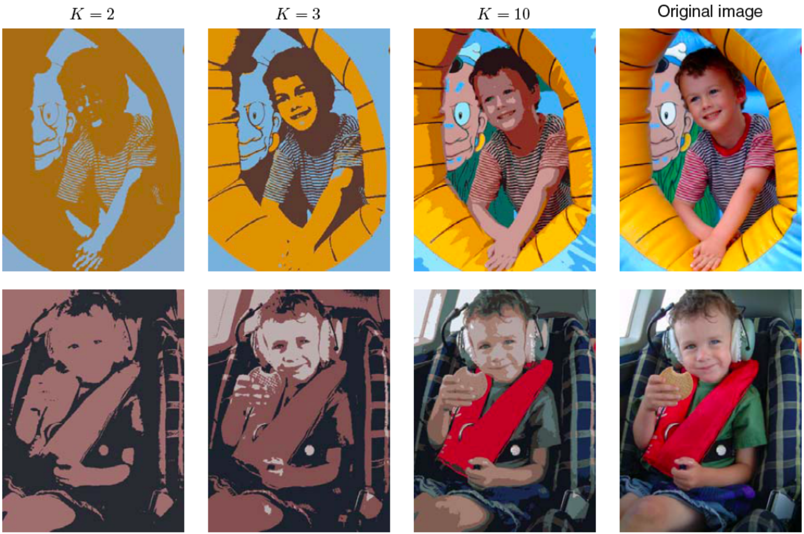
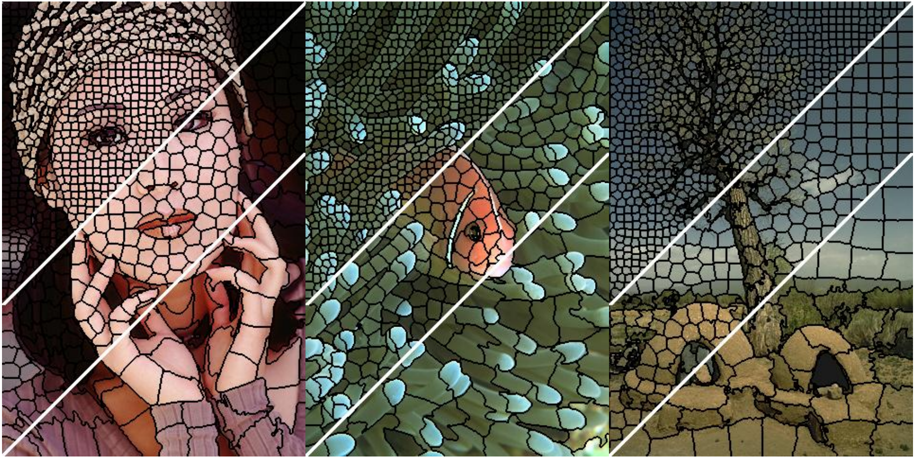


Figure from Bishop

K-means for Image Segmentation



- How would you modify k-means to get super pixels?

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Hard cases – unequal spreads, non-circular spreads, in-between points

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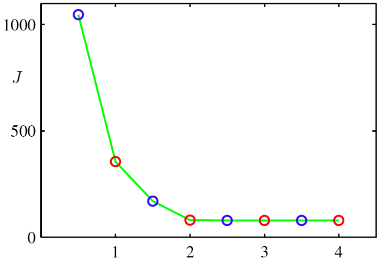
- Test for convergence: If the assignments do not change in the assignment step, we have converged (to at least a local minimum).

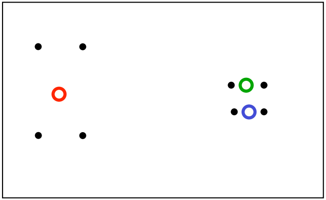


- K-means cost function after each E step (blue) and M step (red). The algorithm has converged after the third M step

Local Minima

- The objective J is non-convex (so coordinate descent on J is not guaranteed to converge to the global minimum)
- There is nothing to prevent k-means getting stuck at local minima.
- We could try many random starting points
- We could try non-local split-and-merge moves:
    - Simultaneously merge two nearby clusters
    - and split a big cluster into two

A bad local optimum



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  - What happens to our convergence guarantee?
  - How do we decide on the soft assignments?

Soft K-means Algorithm

- Initialization: Set K means $\{\mathbf{m}_k\}$ to random values
- Repeat until convergence (until assignments do not change):
  - Assignment: Each data point n given soft "degree of assignment" to each cluster mean k, based on responsibilities

$$r_k^{(n)} = \frac{\exp[-\beta d(\mathbf{m}_k, \mathbf{x}^{(n)})]}{\sum_j \exp[-\beta d(\mathbf{m}_j, \mathbf{x}^{(n)})]}$$

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    - It may make it possible to decide on the number of clusters.
- An obvious approach is to imagine that the data was produced by a generative model.
    - Then we can adjust the parameters of the model to maximize the probability that it would produce exactly the data we observed.