Model Learning and Clustering

CPS170
Ron Parr

material from: Lise Getoor, Andrew Moore, Tom Dietterich, Sebastian Thrun, Rich Maclin

Unsupervised Learning

- Supervised learning: Data <x1, x2, … xn, y>
- Unsupervised Learning: Data <x1, x2, … xn>

- So, what's the big deal?
- Isn't y just another feature?
- No explicit performance objective
  - Bad news: Problem not necessarily well defined without further assumptions
  - Good news: Results can be useful for more than predicting y

Model Learning

- Produce a global summary of the data
- Not an exact copy
- Consider space of models M and dataset D
- One approach: Maximize P(M|D)
- How to do this? Bayes Rule:

$$P(M \mid D) = \frac{P(D \mid M)P(M)}{P(D)}$$

Example: Modeling Coin Flips

- Suppose we have observed: D=HTTHT
- Which is a better model?
  - P(H=0.4)
  - P(H=0.5)

$$P(M \mid D) = \frac{P(D \mid M)P(M)}{P(D)}$$

$$P(D \mid (P(H = 0.5)) = 0.5^5 = 0.312$$
$$P(D \mid (P(H = 0.4)) = 0.4^2 * 0.6^3 = 0.3456$$

What about P(D) and P(M)???

Model Learning With Bayes Rule

$$P(M \mid D) = \frac{P(D \mid M)P(M)}{P(D)}$$

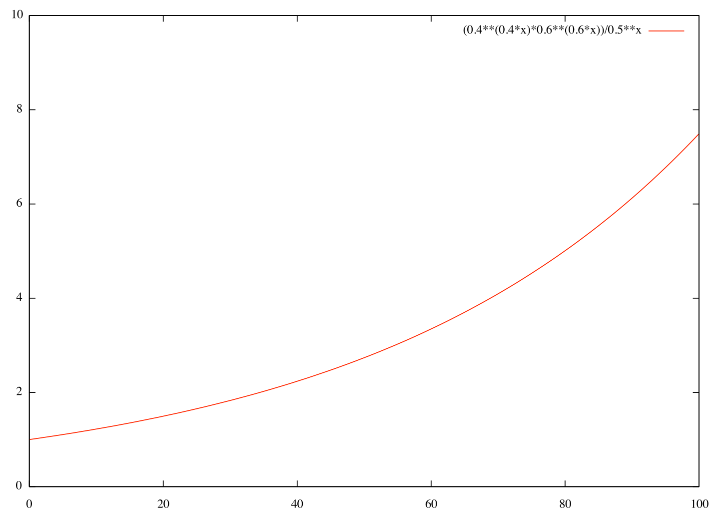
- We call P(D|M) the ***likelihood***
- We can ignore P(D)… Why?
- What about P(M)?
  - Call this a our ***prior probability*** on models
  - If P(M) is uniform (all models equally likely) then maximizing P(D|M) is equivalent to maximizing P(M|D) (Call this the ***maximium likelihood*** approach.)

Using Priors

- Suppose we have good reason to expect that the coin is fair
- Should we really conclude P(H)=0.4?
- Suppose we think P(P(H=0.5)) = 2 x P(P(H=0.4))
- This means P(D|P(H=0.4)) must be 2X larger than P (D|P(H=0.5)) to compensate if P(H=0.4) is to maximize the ***posterior probability***

$$\boxed{P(M \mid D)} = \frac{P(D \mid M)P(M)}{P(D)}$$

Data Can Overwhelm a Prior



Specifying Priors

- In our coin example, we considered just two models P(H=0.4) and P(H=0.5)
- In general, we might want to specify a distribution over all possible coin probabilities

- This introduces complications:
  - P(M) is now a distribution over a continuous parameter
  - Need to use calculus to find maximizer of P(D|M)P(M)

Conjugate Priors

- A likelihood and prior are said to be ***conjugate*** if their product has the same parametric form as the prior
- (This is outside the scope of the class, but we provide one nice example.)
- The beta distribution is conjugate to the binomial distribution
  - Can think of the beta distribution as specifying a number of “imagined” heads and tails
  - Maximum of the posterior adds together observed heads and tails with imagined heads and tails
  - Examples:
    - Prior of 100 heads and 100 tails is a strong prior towards fairness
    - Prior of 1 head and 1 tail is a weak prior towards fairness

Clustering as Modeling

- Clustering assigns points in a space to clusters
- Example: By examining x-rays of cancer tumors, one might identify different subtypes of cancer based upon growth patterns
- Each cluster has its own probabilistic model describing how items of that cluster’s type behave

Examples of Clustering Applications

- Marketing: Help marketers discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs
- Land use: Identification of areas of similar land use in an earth observation database
- Insurance: Identifying groups of motor insurance policy holders with similar claim cost
- City-planning: Identifying groups of houses according to their house type, value, and geographical location
- Earth-quake studies: Observed earth quake epicenters should be clustered along continent faults

Example of Subtleties in Clustering

- Household Dataset:

  location, income, number of children, rent/own, crime rate, number of cars

- Appropriate clustering may depend on use:
  - Goal to minimize delivery time $\Rightarrow$ cluster by location
  - Others?
  - Clustering work often suffers from mismatch between the clustering objective function and the performance criterion

Clustering Desiderata

- Decomposition or partition of data into groups so that
  - Points in one group are **similar** to each other
  - Are as **different** as possible from the points in other groups
- Measure of **distance** is fundamental
- Explicit representation:
  - D(x(i),x(j)) for each x
  - Only feasible for small domains
- Implicit representation by measurement:
  - Distance computed from features
  - Implement this as a function

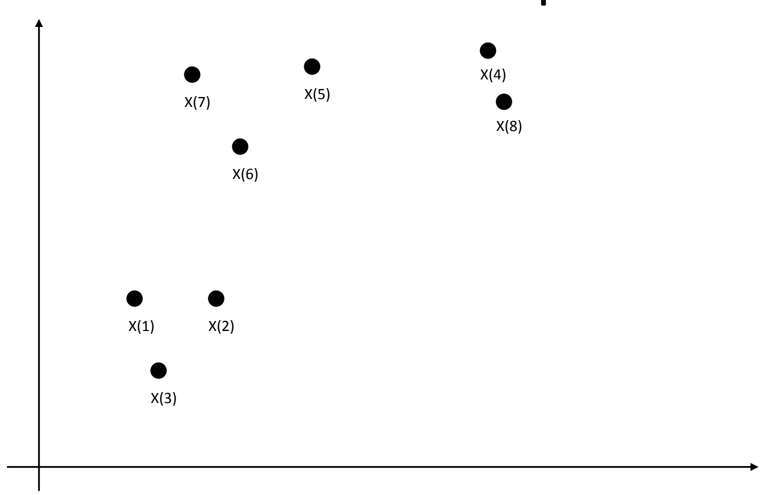
Families of Clustering Algorithms

- Partition-based methods
  - e.g., K-means
- Hierarchical clustering
  - e.g., hierarchical agglomerative clustering
- Probabilistic model-based clustering
  - e.g., mixture models
- Graph-based Methods
  - e.g., spectral methods

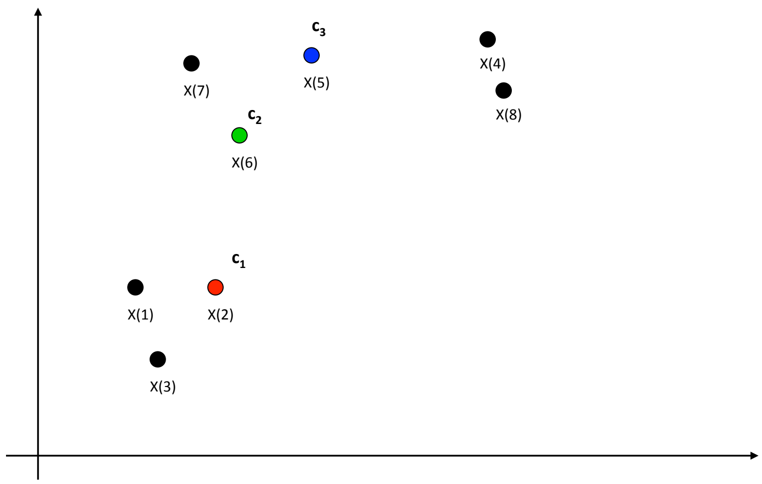
K-means

- Start with randomly chosen cluster centers
- Assign points to closest cluster
- Recompute cluster centers
- Reassign points
- Repeat until no changes

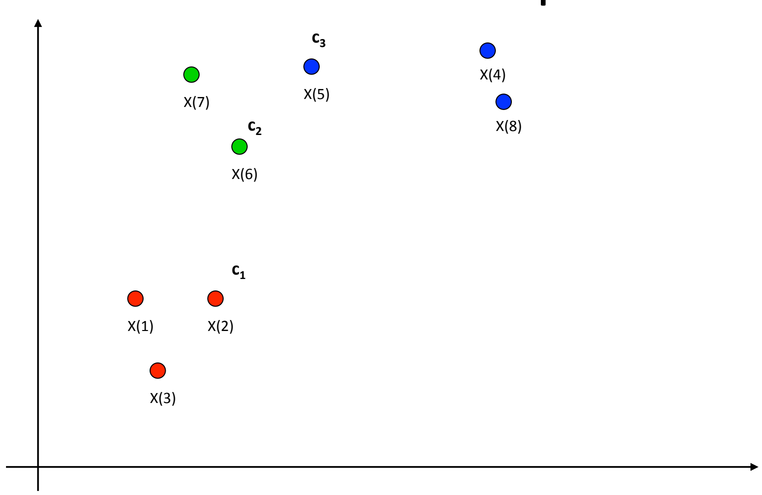
K-means example



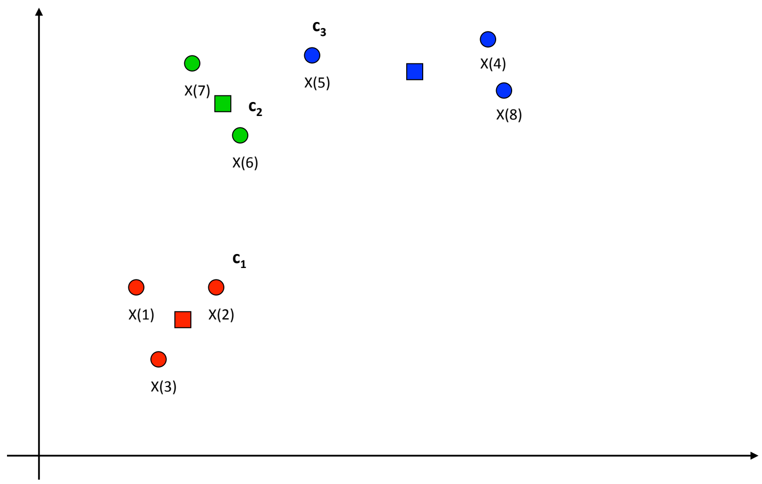
K-means example



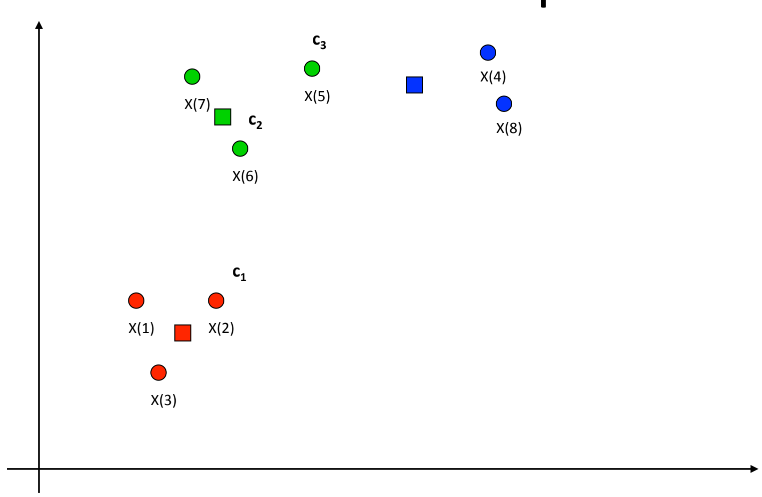
K-means example



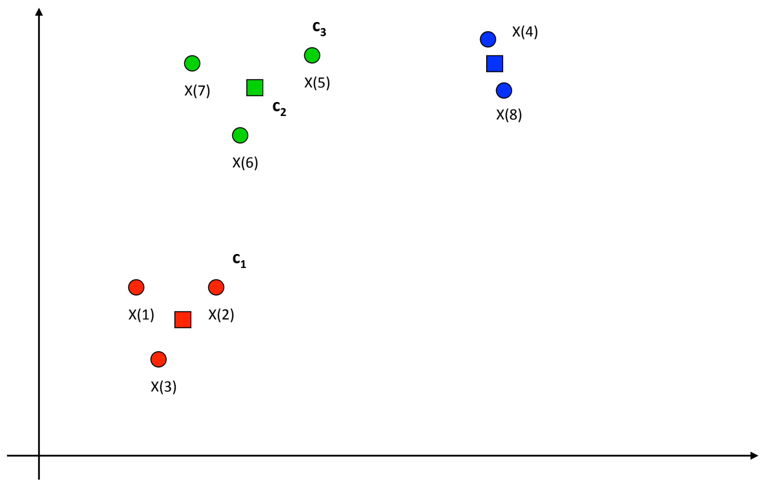
K-means example



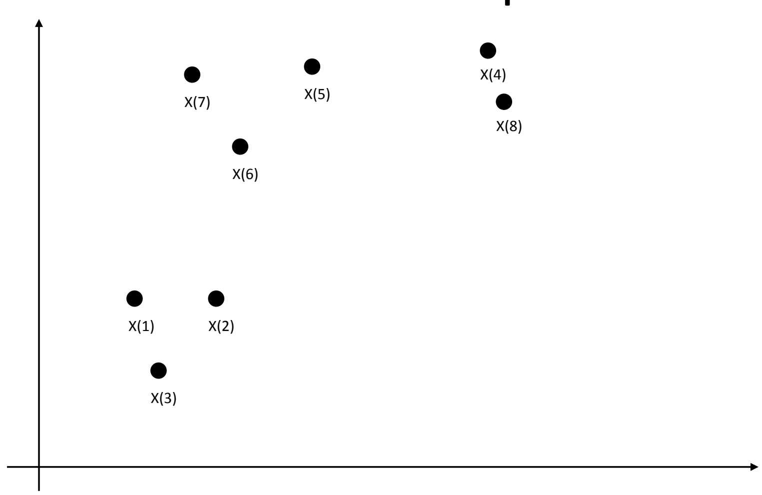
K-means example



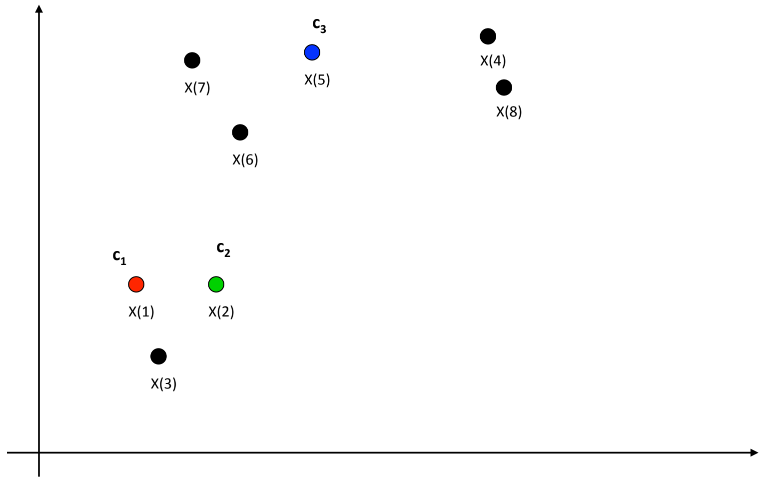
K-means example



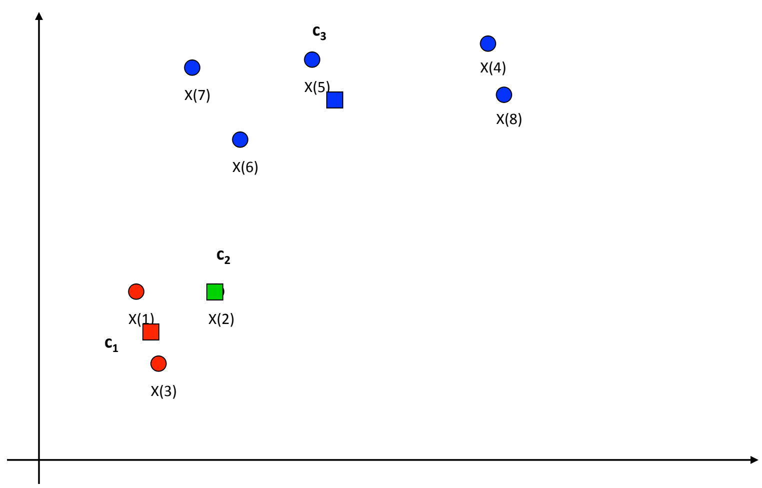
K-means example #2



K-means example #2



K-means example #2



Demo

http://home.dei.polimi.it/matteucc/Clustering/tutorial_html/AppletKM.html

Complexity

- Does algorithm terminate?

  yes

- Does algorithm converge to optimal clustering?

  Can only guarantee local optimum

- Time complexity one iteration?

  nk

Understanding k-Means

- Implicitly models data as coming from a Gaussian distribution centered at cluster centers
- log P(data) ~ sum of squared distances

$$P(x_i \in c_j) \propto e^{-\|(x_i - c_j)\|^2}$$

$$P(data) = \prod_i P(x_i \in c_{clustering(i)})$$

$$\log(P(data)) = \alpha \sum_i (x_i - c_{clustering(i)})^2$$

Understanding k-Means II

- Each step of k-Means increases P(data)
  - Reassigning points moves points to clusters for which their coordinates have higher probability
  - Recomputing means moves cluster centers to increase the average probability of points in the cluster
- Fixed number of assignments and monotonic score implies convergence

Understanding k-Means III

$$P(M \mid D) = \frac{P(D \mid M)P(M)}{P(D)}$$

- Can view k-means as max likelihood method with a twist
  - Unlike the coin toss example, there is a hidden variable with each datum – the cluster membership
  - k-means iteratively improves its guesses about these hidden pieces of information
- k-means can be interpreted as an instance of a general approach to dealing with hidden variables called Expectation Maximization (EM)

But How Do We Pick k?

- Sometimes there will be an obvious choice given background knowledge or the intended use of the clustering output
- What if we just iterated over k?
  - Picking k=n will always maximize P(D|M)
  - We could introduce a prior over models using P(M) in Bayes rule
- Compare prior over models with regularization:
  - Regularization in regression penalized overly complex solutions
  - We can assign models with a high number of clusters low probability to achieve a similar effect
  - (In general, use of priors subsumes regularization.)

Is Clustering Well Defined?

- Clustering is not clearly axiomatized
- Can we define an "optimal" clustering w/o specifying an a priori preference (prior) on the cluster sizes or making additional assumptions?
- Kleinberg: Clustering is impossible under some plausible assumptions (IOW, union of unstated assumptions made by clustering algorithms is logically inconsistent)
- Recent efforts make progress putting clustering on more solid ground

Model Learning Conclusion

- Often seek to find the most likely model given the data
- Can be viewed as maximizing the posterior P(M|D) using Bayes rule
- Model learning can be applied to:
  - Coin flips
  - Clustering
  - Learning parameters of Bayes nets or HMMs
  - etc.
- Some care must go into formulation of modeling assumptions to avoid degenerate solutions, e.g., assigning every point to its own cluster
- Priors can help avoid degenerate solutions