CMSC828G **Principles of Data Mining** Lecture #11

- Today's Reading:
  - HMS, 6.4, 9.2
- Today's Lecture:
  - Descriptive Modeling
  - Graphical Models
  - Class survey
- Upcoming Due Dates:
  - H2 due Thu 3/7

Describing Data

- The canonical descriptive strategy is to describe the data in terms of their underlying distribution
- As usual, we have a p-dimensional data matrix with variables $X_1, \ldots, X_p$
- The joint distribution is $P(X_1, \ldots, X_p)$
- The joint gives us complete information about the variables
- Given the joint distribution, we can answer any question about the relationships among any subset of variables
  - are X2 and X5 independent?
  - generating approximate answers to queries for large databases or **selectivity estimation**
    - Given a query (conditions that observations must satisfy), estimate the fraction of rows that satisfy this condition (the selectivity of the query)
    - These estimates are needed during query optimization
    - If we have a good approximation for the joint distribution of data, we can use it to efficiently compute approximate selectivities

Difficulty: Curse of Dimensionality

- consider joint distribution for multivariate categorical data
- p variables, each taking m values
- The joint distribution requires specifying $O(m^p)$ different probabilities.
- exponential # of parameters is problem for:
  - estimation
  - representation and reasoning

CoD: Estimation

- We can think of m^p cells, $\{c_1, \ldots, c_{m^p}\}$ each containing n_i observations
- The expected number of data points in cell i, given a random sample from p(x) of size n is $E_{p(x)}[n_i]=np_i$
- Suppose p(x) is uniform, i.e. $p(x_i) \approx 1/m^p$
- Then

$$E_{p(x)}[n_i] \approx \frac{n}{m^p}$$

- if $n < 0.5m^p$ then the expected number of points in any cell is closer to 0 then 1.
- if we use MLE estimator, $p_i=0$ for each empty cell
- fundamental problem:

if we have a data set of size n over p variables and we want to increase the number of variables from p to 2p, in order to keep the expected number of data points in each cell the same, we must increase the size of the data set by a factor of m^p!!

CoD: Reasoning

- Even if we can reliably estimate a full joint distribution from the data, it is exponential in both space and time to manipulate it directly.
- For example if we want to determine the marginal distribution of any single variable x_j, we calculate it as follows:

$$p(x_j) = \sum_{x_1,\ldots,x_{j-1},x_{j+1},\ldots,x_p} p(X_1, \ldots, X_{j-1}, X_{j+1}, \ldots, X_p)$$

- this requires summing over all the other variables and requires $O(m^p)$ summations.
- working directly with the ***full*** joint distribution is feasible for only relatively low-dimensional problems.

Models

- parametric
- nonparametric
- mixture distributions
- semi-parametric

Parametric Models

- assume a particular, relatively simple, functional form
- e.g., uniform distribution, normal distribution, exponential, Poisson
- typically relatively small number of parameters
- often closed form solutions for parameter estimates that require a single pass through the data
- important to test the assumptions made by the model:
  - using simple visualizations
  - using statistical goodness-of-fit tests

Nonparametric Models

- take a local data-driven weighted average of around the point of interest
- simplest version: histogram
  - estimate for density is just (scaled) number of points in bin
  - problems:
    - not smooth
    - choosing the number of bins, bin locations and widths
  - ok for large data sets, small p
  - regardless, generally useful to look at histograms with large number of bins, since can provide info on outliers, multmodality, skewness, tail behavior, etc.

Nonparametric Models cont.

- kernel density estimates
- density at any point x is proportional to a weighted sum of all points in the training data set
- weights are defined by an appropriately defined kernel function
- in 1-D:

$$f(x) = \frac{1}{n}\sum_{i=1}^{n} w_i \qquad w_i = K\left(\frac{x - x(i)}{h}\right)$$

$$K(t) = 1 - |t|,\ t \le 1;\ K(t) = 0 \text{ otherwise}$$

h determines smoothness; many possible choices for K

- we'll talk about this more when we discuss SVMs….

Mixture Distributions

- Assume a probability model for each component
- Mixture Model:

$$f(x) = \sum_{k=1}^{K} w_k f_k(x;\theta_k)$$

- distribution is linear combination of simpler distributions
- where f_k are component distributions
- components: gaussian, poisson, exponential
- unlike simple parametric models, typically no closed form solution for maximizing score; one approach: use EM

Semi-parametric Models

- general class of functional forms in which the number of adaptive parameters can be increased in a systematic way to build ever more flexible models, but where the total number of parameters in the model can be varied independently from the size of the data set. Bishop
- e.g., mixture-models (where k varies), neural networks, graphical models.

Graphical Models

- In the next 3-4 lectures, we will be studying graphical models
- e.g. Bayesian networks, Bayes nets, Belief nets, Markov networks, etc.
- We will study:
  - representation
  - reasoning
  - learning
- Materials based on upcoming book by Nir Friedman and Daphne Koller. Slides courtesy of Nir Friedman.

Probability Distributions

- Let $X_1,\ldots,X_p$ be random variables
- Let P be a joint distribution over $X_1,\ldots,X_p$

If the variables are binary, then we need $O(2^p)$ parameters to describe P

Can we do better?

- **Key idea**: use properties of independence

Independent Random Variables

- Two variables X and Y are **independent** if
  - P(X = x|Y = y) = P(X = x) for all values x,y
  - That is, learning the values of Y does not change prediction of X
- If X and Y are independent then
  - P(X,Y) = P(X|Y)P(Y) = P(X)P(Y)
- In general, if $X_1,\ldots,X_p$ are independent, then
  - $P(X_1,\ldots,X_p) = P(X_1)\ldots P(X_p)$
  - Requires O(n) parameters

Conditional Independence

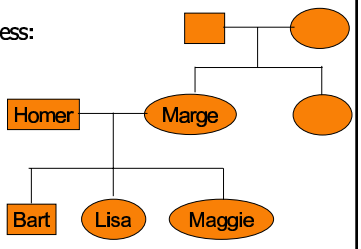
- Unfortunately, most of random variables of interest are not independent of each other
- A more suitable notion is that of **conditional independence**
- Two variables X and Y are **conditionally independent** given Z if
  - P(X = x|Y = y,Z=z) = P(X = x|Z=z) for all values x,y,z
  - That is, learning the values of Y does not change prediction of X once we know the value of Z
  - notation: I (X , Y | Z)

Example: Naïve Bayesian Model

- A common model in early diagnosis:
  - Symptoms are conditionally independent given the disease (or fault)
- Thus, if
  - $X_1,\ldots,X_p$ denote whether the symptoms exhibited by the patient (headache, high-fever, etc.) and
  - H denotes the hypothesis about the patients health
- then, $P(X_1,\ldots,X_p,H) = P(H)P(X_1|H)\ldots P(X_p|H)$,
- This **naïve Bayesian** model allows compact representation
  - It does embody strong independence assumptions

Example: Family trees

Noisy stochastic process:



Example: Pedigree

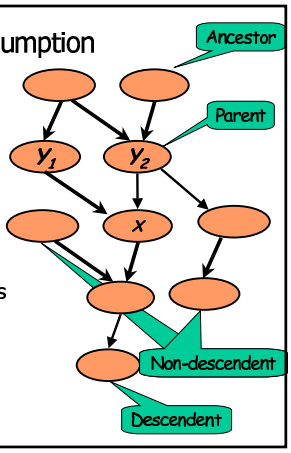
- A node represents an individual's genotype

Modeling assumptions:

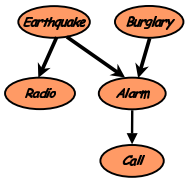
Ancestors can effect descendants' genotype only by passing genetic materials through intermediate generations

Markov Assumption

- We now make this independence assumption more precise for **directed acyclic graphs** (DAGs)
- Each random variable X, is independent of its non-descendents, given its parents Pa(X)
- Formally, I (X, NonDesc(X) | Pa(X))



Markov Assumption Example



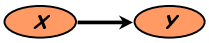
- In this example:
  - I (E, B)
  - I (B, {E, R})
  - I (R, {A, B, C} | E)
  - I (A, R | B,E)
  - I (C, {B, E, R} | A)

I-Maps

- A DAG G is an **I-Map** of a distribution P if the all Markov assumptions implied by G are satisfied by P
  (Assuming G and P both use the same set of random variables)

Examples:

x	y	P(x,y)
0	0	0.25
0	1	0.25
1	0	0.25
1	1	0.25



x	y	P(x,y)
0	0	0.2
0	1	0.3
1	0	0.4
1	1	0.1

Factorization

- Given that G is an I-Map of P, can we simplify the representation of P?
- Example:

- Since I(X,Y), we have that P(X|Y) = P(X)
- Applying the chain rule

  P(X,Y) = P(X|Y) P(Y) = P(X) P(Y)

- Thus, we have a simpler representation of P(X,Y)

Factorization Theorem

Thm: if G is an I-Map of P, then

$$P(X_1,\ldots,X_p) = \prod_i P(X_i \mid Pa(X_i))$$

Proof:

- By chain rule: $P(X_1,\ldots,X_p) = \prod_i P(X_i \mid X_1,\ldots,X_{i-1})$
- wlog. $X_1,\ldots,X_p$ is an ordering consistent with G

From assumption: $Pa(X_i) \subseteq \{X_1,\ldots,X_{i-1}\}$

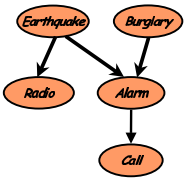
$$\{X_1,\ldots,X_{i-1}\} - Pa(X_i) \subseteq NonDesc(X_i)$$

- Since G is an I-Map, $I(X_i, NonDesc(X_i) \mid Pa(X_i))$
- Hence,

$$I(X_i, \{X_1,\ldots,X_{i-1}\} - Pa(X_i) \mid Pa(X_i))$$

- We conclude, $P(X_i \mid X_1,\ldots,X_{i-1}) = P(X_i \mid Pa(X_i))$

Factorization Example



P(C,A,R,E,B) = P(B)P(E|B)P(R|E,B)P(A|R,B,E)P(C|A,R,B,E)

versus

P(C,A,R,E,B) = P(B) P(E) P(R|E) P(A|B,E) P(C|A)

Consequences

- We can write P in terms of "local" conditional probabilities

If G is **sparse,**

- that is, $|Pa(X_i)| < k$,

⇒ each conditional probability can be specified compactly

- e.g. for binary variables, these require $O(2^k)$ params.

⇒ representation of P is **compact**

- linear in number of variables

Summary

- Probability distribution as descriptive model
- Difficulty: curse of dimensionality
- Categories of density estimation:
  - parametric
  - nonparametric
  - semi-parametric
- Graphical models tackle the curse of dimensionality by exploiting conditional independence

Next Time

- HW2 due

References

- *Principles of Data Mining*, Hand, Mannila, Smyth. MIT Press, 2001.
- *Neural Networks for Pattern Recognition*, Bishop. Clarendon Press, 1995.
- Nir Friedman's excellent lecture notes, http://www.cs.huji.ac.il/~pmai/
- Andrew Moore's excellent lecture notes, http://www-2.cs.cmu.edu/~awm/781/