

Machine Learning

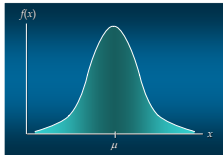
10-701/15-781, Fall 2006

Tutorial on Basic Probability

Eric Xing

Lecture 2, September 14, 2006

Reading: Chap. 1&2, CB & Chap 5,6, TM



Eric Xing, ML/CMU



What is this?



Uncertainty!

- Classical AI and ML research ignored this phenomena
- The Problem (an example):
 - you want to catch a flight at 10:00am from Pitt to SF, can I make it if I leave at 7am and take a 28X at CMU?
- partial observability (road state, other drivers' plans, etc.)
- noisy sensors (radio traffic reports)
- uncertainty in action outcomes (flat tire, etc.)
- immense complexity of modeling and predicting traffic
- Reasoning under uncertainty!

Eric Xing, ML/CMU

2

Basic Probability Concepts



- A **sample space** $\mathcal{S}$ is the set of all possible outcomes of a conceptual or physical, repeatable experiment. ($\mathcal{S}$ can be finite or infinite.)
 - E.g., $\mathcal{S}$ may be the set of all possible outcomes of a dice roll: $\mathcal{S} \equiv \{1, 2, 3, 4, 5, 6\}$
 - E.g., $\mathcal{S}$ may be the set of all possible nucleotides of a DNA site: $\mathcal{S} \equiv \{A, T, C, G\}$
 - E.g., $\mathcal{S}$ may be the set of all possible positions time-space positions of an aircraft on a radar screen: $\mathcal{S} \equiv \{0, R_{\max}\} \times \{0, 360^\circ\} \times \{0, +\infty\}$
- An **event** $\mathcal{A}$ is the any subset $\mathcal{S}$:
 - Seeing "1" or "6" in a roll; observing a "G" at a site; UA007 in space-time interval X
- An **event space** $\mathcal{E}$ is the possible worlds the outcomes can happen
 - All dice-rolls, reading a genome, monitoring the radar signal



Eric Xing, ML/CMU

3

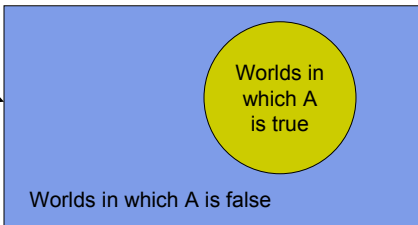
Visualizing Probability Space



- A **probability space** is a sample space of which, for every subset $\mathcal{S} \in \mathcal{S}$, there is an assignment $P(\mathcal{S}) \in \mathcal{S}$ such that:
 - $0 \leq P(\mathcal{S}) \leq 1$ ✓
 - $\sum_{\mathcal{S} \in \mathcal{S}} P(\mathcal{S}) = 1$ ✓
- $P(\mathcal{S})$ is called the probability (or probability mass) of $\mathcal{S}$

Event space of all possible worlds.

Its area is 1



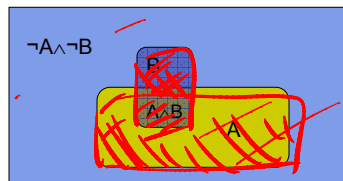
$P(A)$ is the area of the oval

Eric Xing, ML/CMU

4

Kolmogorov Axioms

- All probabilities are between 0 and 1 ✓
 - $0 \leq P(X) \leq 1$ ✓
- $P(\text{true}) = 1$ ✓
 - regardless of the event, my outcome is true
- $P(\text{false}) = 0$
 - no event makes my outcome true
- The probability of a disjunction is given by
 - $P(A \vee B) = P(A) + P(B) - P(A \wedge B)$



Eric Xing, ML/CMU

5

Why use probability?

- There have been attempts to develop different methodologies for uncertainty:
 - Fuzzy logic
 - Qualitative reasoning (Qualitative physics)
 - ...
- "Probability theory is nothing but common sense reduced to calculation"
 - — Pierre Laplace, 1812.
- In 1931, de Finetti proved that it is irrational to have beliefs that violate these axioms, in the following sense:
 - If you bet in accordance with your beliefs, but your beliefs violate the axioms, then you can be guaranteed to lose money to an opponent whose beliefs more accurately reflect the true state of the world. (Here, "betting" and "money" are proxies for "decision making" and "utilities".)
- What if you refuse to bet? This is like refusing to allow time to pass: every action (including inaction) is a bet

Eric Xing, ML/CMU

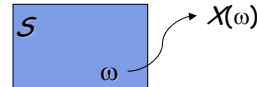
6

Random Variable

PL →



- A **random variable** is a function that associates a unique numerical value (a token) with every outcome of an experiment. (The value of the r.v. will vary from trial to trial as the experiment is repeated)



- Discrete r.v.:
 - The outcome of a dice-roll X
 - The outcome of reading a nt at site i : X_i
- Binary event and indicator variable:
 - Seeing an "A" at a site $\Rightarrow X=1$, o/w $X=0$.
 - This describes the true or false outcome a **random event**.
 - Can we describe richer outcomes in the same way? (i.e., $X=1, 2, 3, 4$, for being A, C, G, T) --- think about what would happen if we take **average** of X .
- Unit-Base Random vector

$X_i = [X_{iA}, X_{iT}, X_{iG}, X_{iC}]$, $X_i \in [0, 0, 1, 0] \Rightarrow$ seeing a "G" at site i
- Continuous r.v.:
 - The outcome of **recording** the **true** location of an aircraft: X_{true}
 - The outcome of **observing** the **measured** location of an aircraft X_{obs}

Eric Xing, ML/CMU

7

Discrete Prob. Distribution



- (In the discrete case), a probability distribution P on S (and hence on the domain of X) is an assignment of a non-negative real number $P(s)$ to each $s \in S$ (or each valid value of x) such that $\sum_{s \in S} P(s) = 1$. ($0 \leq P(s) \leq 1$)
 - intuitively, $P(s)$ corresponds to the **frequency** (or the likelihood) of getting s in the experiments, if repeated many times
 - call $\theta_s = P(s)$ the **parameters** in a discrete probability distribution
- A probability distribution on a sample space is sometimes called a **probability model**, in particular if several different distributions are under consideration
 - write models as M_1, M_2 , probabilities as $P(X|M_1), P(X|M_2)$
 - e.g., M_1 may be the appropriate prob. dist. if X is from "fair dice", M_2 is for the "loaded dice".
 - M is usually a two-tuple of {dist. family, dist. parameters}

Eric Xing, ML/CMU

8

Discrete Distributions

- Bernoulli distribution: $\text{Ber}(p)$

$$p(x) = \begin{cases} 1-p & \text{for } x=0 \\ p & \text{for } x=1 \end{cases} \Rightarrow p(x) = p^x (1-p)^{1-x}$$



- Multinomial distribution: $\text{Mult}(1, \theta)$

- Multinomial (indicator) variable:

$$X = \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \end{bmatrix}, \quad \text{where } X_j \in [0,1], \text{ and } \sum_{j=1}^6 X_j = 1$$

$$X_j = 1 \text{ w.p. } \theta_j, \quad \sum_{j=1}^6 \theta_j = 1$$



$$p(x(j)) = \prod_{j=1}^6 \theta_j^{x_j} = \theta_1^{x_1} \times \theta_2^{x_2} \times \theta_3^{x_3} \times \theta_4^{x_4} \times \theta_5^{x_5} \times \theta_6^{x_6} = \prod_k \theta_k^{x_k} = \theta^x$$

Eric Xing, ML/CMU

9

Discrete Distributions

- Multinomial distribution: $\text{Mult}(n, \theta)$

- Count variable:

$$X = \begin{bmatrix} x_1 \\ \vdots \\ x_K \end{bmatrix}, \quad \text{where } \sum_j x_j = n$$

$$p(x) = \frac{n!}{x_1! x_2! \dots x_K!} \theta_1^{x_1} \theta_2^{x_2} \dots \theta_K^{x_K} = \frac{n!}{x_1! x_2! \dots x_K!} \theta^x$$

"Arts"	"Budgets"	"Children"	"Education"
NEW FILM	MILITARY	CHILDREN	SCHOOL
MOVIE	TAX	WOMEN	STUDENTS
MUSIC	FEDERAL	PEOPLE	TEACHERS
MOVIE	BUDGET	CHILD	EDUCATION
PLAY	MILITARY	YEAR	TEACHERS
MUSICAL	FEDERAL	FAMILY	TEACHER
REST	SPENDING	PARENTS	TEACHER
ACTION	NEW	SAYS	BENNETT
FIRST	STATE	FAMILY	MANGAT
YORK	PLAN	WELFARE	NAMERY
OPERA	MONEY	MEN	STATE
THEATRE	PROGRAMS	PERCENT	PRESIDENT
ACTRESS	GOVERNMENT	CARE	ELEMENTARY
LOVE	CONGRESS	DATE	

The *William Randolph Hearst Foundation* will give \$1.25 million to Lincoln Center, Metropolitan Opera Co., New York Philharmonic and Juilliard School. "Our board felt that we had a real opportunity to make a mark on the future of the performing arts with these grants and set every bit as important as our traditional areas of support in health, medical research, education and the social services," Hearst Foundation President Randolph A. Hearst said today. In announcing the grants, Lincoln Center's share will be \$500,000 for its new building, which will house grand opera and provide new public facilities. The Metropolitan Opera Co. and New York Philharmonic will receive \$400,000 each. The Juilliard School, whose opera and the performing arts are equally well served, will get \$350,000. The Hearst Foundation, a leading supporter of the Lincoln Center Consortium Corporate Fund, will make its total annual \$100,000 donation, too.

Eric Xing, ML/CMU

10

Continuous Prob. Distribution

- A **continuous random variable** X can assume any value in an interval on the real line or in a region in a high dimensional space
 - X usually corresponds to a real-valued measurements of some property, e.g., length, position, ...
 - It is not possible to talk about the probability of the random variable assuming a particular value -- $P(x) = 0$
 - Instead, we talk about the probability of the random variable assuming a value within a given interval or half interval
 - $P(X \in [x_1, x_2])$,
 - $P(X < x) = P(X \in [-\infty, x])$
 - Arbitrary Boolean combination of basic propositions



Continuous Prob. Distribution

- The probability of the random variable assuming a value within some given interval from x_1 to x_2 is defined to be the area under the graph of the probability density function between x_1 and x_2 .

- Probability mass: $P(X \in [x_1, x_2]) = \int_{x_1}^{x_2} p(x) dx$,

note that $\int_{-\infty}^{+\infty} p(x) dx = 1$.

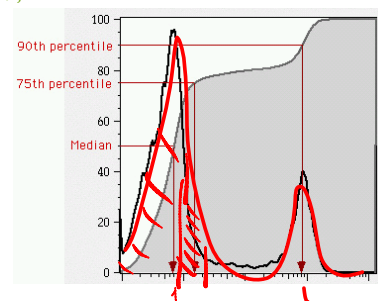
- Cumulative distribution function (CDF):

$$P(x) = P(X < x) = \int_{-\infty}^x p(x') dx'$$

- Probability density function (PDF):

$$p(x) = \frac{d}{dx} P(x)$$

$$\int_{-\infty}^{+\infty} p(x) dx = 1; \quad p(x) > 0, \forall x$$



Car flow on Liberty Bridge (cooked up!)

What is the intuitive meaning of $p(x)$



- If

$$p(x_1) = a \text{ and } p(x_2) = b,$$

then when a value X is sampled from the distribution with density $p(x)$, you are a/b times as likely to find that X is "very close to" x_1 than that X is "very close to" x_2 .

- That is:

$$\lim_{h \rightarrow 0} \frac{P(x_1 - h < X < x_1 + h)}{P(x_2 - h < X < x_2 + h)} = \frac{\int_{x_1-h}^{x_1+h} p(x) dx}{\int_{x_2-h}^{x_2+h} p(x) dx} = \frac{p(x_1) \times 2h}{p(x_2) \times 2h} = a/b$$

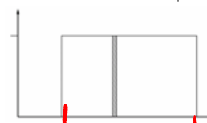
Continuous Distributions



- Uniform Probability Density Function

$$p(x) = 1/(b-a) \text{ for } a \leq x \leq b$$

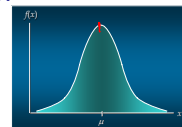
$$= 0 \text{ elsewhere}$$



- Normal (Gaussian) Probability Density Function

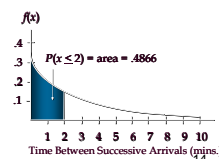
$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(x-\mu)^2 / 2\sigma^2}$$

- The distribution is symmetric, and is often illustrated as a bell-shaped curve.
- Two parameters, μ (mean) and σ (standard deviation), determine the location and shape of the distribution.
- The highest point on the normal curve is at the mean, which is also the median and mode.
- The mean can be any numerical value: negative, zero, or positive.



- Exponential Probability Distribution

$$\text{density: } p(x) = \frac{1}{\mu} e^{-x/\mu}, \quad \text{CDF: } P(x \leq x_0) = 1 - e^{-x_0/\mu}$$



Statistical Characterizations

- **Expectation:** the centre of mass, mean value, first moment):

$$E(X) = \begin{cases} \sum_{i \in S} x_i p(x_i) & \text{discrete} \\ \int_{-\infty}^{\infty} x p(x) dx & \text{continuous} \end{cases}$$

- **Sample mean:**

$$\mu = \frac{1}{N} \sum_{i=1}^N x_i$$

- **Variance:** the spreadness:

$$\text{Var}(X) = \begin{cases} \sum_{x \in S} [x_i - E(X)]^2 p(x_i) & \text{discrete} \\ \int_{-\infty}^{\infty} [x - E(X)]^2 p(x) dx & \text{continuous} \end{cases}$$

- **Sample variance**

$$\sigma^2 = \frac{1}{N-1} \sum_{i=1}^N (x_i - \mu)^2$$



Eric Xing, ML/CMU

15

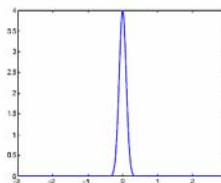
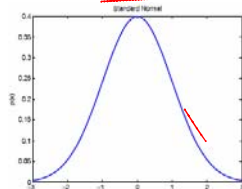
Gaussian (Normal) density in 1D

- If $X \sim N(\mu, \sigma^2)$, the probability density function (pdf) of X is defined as

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(x-\mu)^2 / (2\sigma^2)}$$

- We will often use the precision $\lambda = 1/\sigma^2$ instead of the variance σ^2 .
- Here is how we plot the pdf in matlab

```
xs=-3:0.01:3;
plot(xs, normpdf(xs, mu, sigma))
```



- Note that a density evaluated at a point can be bigger than 1!

Eric Xing, ML/CMU

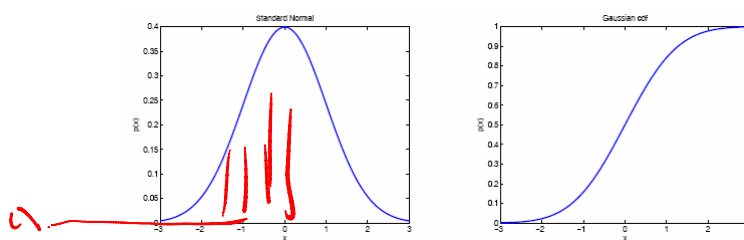
16

Gaussian CDF

- If $Z \sim N(0, 1)$, the cumulative density function is defined as

$$\begin{aligned}\Phi(x) &= \int_{-\infty}^x p(z) dz \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x e^{-z^2/2} dz\end{aligned}$$

- This has no closed form expression, but is built in to most software packages (eg. normcdf in matlab stats toolbox).



Eric Xing, ML/CMU

17

Use of the cdf

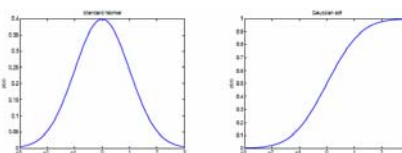
- If $X \sim N(\mu, \sigma^2)$, then $Z = (X - \mu)/\sigma \sim N(0, 1)$.
- How much mass is contained inside the $[-1.98\sigma, 1.98\sigma]$ interval?

$$P(a < X < b) = P\left(\frac{a-\mu}{\sigma} < Z < \frac{b-\mu}{\sigma}\right) = \Phi\left(\frac{b-\mu}{\sigma}\right) - \Phi\left(\frac{a-\mu}{\sigma}\right)$$

- Since $p(Z \leq -1.96) = \text{normcdf}(-1.96) = 0.025$

we have

$$P(-2\sigma < X - \mu < 2\sigma) \approx 1 - 2 \times 0.025 = 0.95$$



Eric Xing, ML/CMU

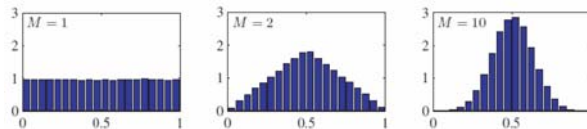
18

Central limit theorem

- If $(X_1, X_2, \dots, X_n)$ are i.i.d. (we will come back to this point shortly) continuous random variables
- Then define

$$\bar{X} = f(X_1, X_2, \dots, X_n) = \frac{1}{n} \sum_{i=1}^n X_i$$

- As $n \rightarrow \infty$,
 $p(\bar{X}) \rightarrow$ Gaussian with mean $E[X_i]$ and variance $\text{Var}[X_i]$



- Somewhat of a justification for assuming Gaussian noise is common

Eric Xing, ML/CMU

19

Elementary manipulations of probabilities

- Set probability of multi-valued r.v.

$$P(\{x=\text{Odd}\}) = P(1) + P(3) + P(5) = 1/6 + 1/6 + 1/6 = 1/2$$

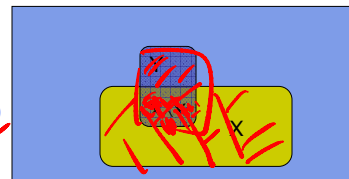
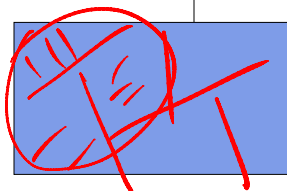
$$P(X = x_1 \vee X = x_2, \dots, \vee X = x_i) = \sum_{j=1}^i P(X = x_j)$$

- Multi-variant distribution:

$$\text{Joint probability: } P(X = \text{true} \wedge Y = \text{true})$$

$$P(Y \wedge \{X = x_1 \vee X = x_2, \dots, \vee X = x_i\}) = \sum_{j=1}^i P(Y \wedge X = x_j)$$

$$\text{Marginal Probability: } P(Y) = \sum_{j \in S} P(Y \wedge X = x_j)$$



Eric Xing, ML/CMU

20

Conditional Probability



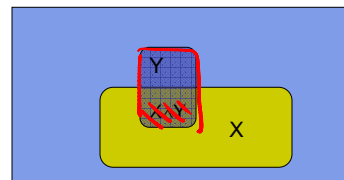
- $P(X|Y)$ = Fraction of worlds in which X is true that also have Y true
 - H = "having a headache"
 - F = "coming down with Flu"
 - $P(H)=1/10$
 - $P(F)=1/40$
 - $P(H|F)=1/2$
 - $P(H|F)$ = fraction of flu-inflicted worlds in which you have a headache
 $= P(H \wedge F)/P(F)$

- Definition:

$$P(X|Y) = \frac{P(X \wedge Y)}{P(Y)}$$

- Corollary: The Chain Rule

$$P(X \wedge Y) = P(X|Y)P(Y)$$



$$P(X_1, X_2, \dots, X_N) = P(X_N | X_1, X_2, \dots, X_{N-1})P(X_{N-1} | X_1, X_2, \dots, X_{N-2}) \dots P(X_2 | X_1)P(X_1)$$

Eric Xing, ML/CMU

21

Probabilistic Inference



- H = "having a Headache" ✓
- F = "coming down with Flu" ✓
 - $P(H)=1/10$
 - $P(F)=1/40$
 - $P(H|F)=1/2$
- One day you wake up with a headache. You come with the following reasoning: "since 50% of flues are associated with headaches, so I must have a 50-50 chance of coming down with flu"

Is this reasoning correct?

Eric Xing, ML/CMU

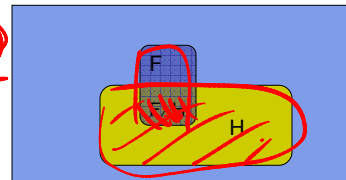
22

Probabilistic Inference

- H = "having a Headache"
- F = "coming down with Flu"
 - $P(H)=1/10$
 - $P(F)=1/40$
 - $P(H|F)=1/2$

- The Problem:

$$P(F|H) = ? \quad \frac{P(F \cdot H)}{P(H)} = \frac{P(H|F)P(F)}{P(H)}$$



Eric Xing, ML/CMU

23

The Bayes Rule

- What we have just did leads to the following general expression:

$$P(Y|X) = \frac{P(X|Y)p(Y)}{P(X)}$$

This is Bayes Rule

Bayes, Thomas (1763) An essay towards solving a problem in the doctrine of chances. *Philosophical Transactions of the Royal Society of London*, 53:370-418



Eric Xing, ML/CMU

24

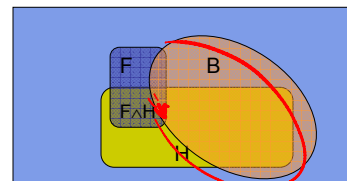
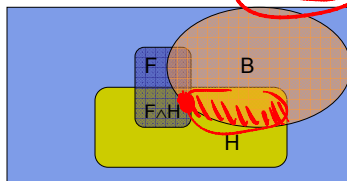
More General Forms of Bayes Rule

- $$P(Y|X) = \frac{P(X|Y)p(Y)}{P(X|Y)p(Y) + P(X|\neg Y)p(\neg Y)}$$

- $$P(Y = y_i | X) = \frac{P(X|Y)p(Y)}{\sum_{i \in S} P(X|Y = y_i)p(Y = y_i)}$$

- $$P(Y|X \wedge Z) = \frac{P(X|Y \wedge Z)p(Y \wedge Z)}{P(X \wedge Z)} = \frac{P(X|Y \wedge Z)p(Y \wedge Z)}{P(X|\neg Y \wedge Z)p(\neg Y \wedge Z) + P(X|Y \wedge Z)p(Y \wedge Z)}$$

- $P(\text{Flu} | \text{Headache} \wedge \text{DrankBeer})$



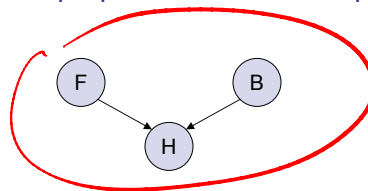
Eric Xing, ML/CMU

25

Prior Distribution

- Support that our propositions about the possible has a "causal flow"

- e.g.,



- Prior or unconditional probabilities of propositions

e.g., $P(\text{Flu} = \text{true}) = 0.025$ and $P(\text{DrankBeer} = \text{true}) = 0.2$

correspond to belief prior to arrival of any (new) evidence

- A probability distribution gives values for all possible assignments:

- $P(\text{DrankBeer}) = [0.01, 0.09, 0.1, 0.8]$

- (normalized, i.e., sums to 1)

Eric Xing, ML/CMU

26

Joint Probability



- A joint probability distribution for a set of RVs gives the probability of every atomic event (sample point)

- $P(Flu, DrinkBeer)$ = a 2×2 matrix of values:

	B	$\neg B$
F	0.005	0.02
$\neg F$	0.195	0.78

- $P(Flu, DrinkBeer, Headache) = ?$
- Every question about a domain can be answered by the joint distribution, as we will see later.

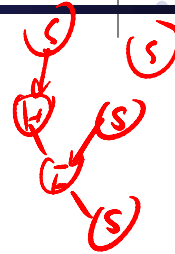
Eric Xing, ML/CMU

27

Posterior conditional probability



- Conditional or posterior (see later) probabilities
 - e.g., $P(Flu|Headache) = 0.178$
 - given that Headache is all I know
 - NOT "if Headache then 17.8% chance of Flu"
- Representation of conditional distributions:
 - $P(Flu|Headache)$ = 2-element vector of 2-element vectors
- If we know more, e.g., DrinkBeer is also given, then we have
 - $P(Flu|Headache, DrinkBeer) = 0.070$ This effect is known as explain away!
 - $P(Flu|Headache, Flu) = 1$
 - Note: the less or more certain belief remains valid after more evidence arrives, but is not always useful
- New evidence may be irrelevant, allowing simplification, e.g.,
 - $P(Flu|Headache, StealerWin) = P(Flu|Headache)$
 - This kind of inference, sanctioned by domain knowledge, is crucial



Eric Xing, ML/CMU

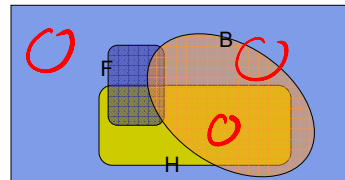
28

Inference by enumeration

- Start with a Joint Distribution
- Building a Joint Distribution of M=3 variables

- Make a truth table listing all combinations of values of your variables (if there are M Boolean variables then the table will have 2^M rows).
- For each combination of values, say how probable it is.
- Normalized, i.e., sums to 1

F	B	H	Prob
0	0	0	0.4
0	0	1	0.1
0	1	0	0.17
0	1	1	0.2
1	0	0	0.05
1	0	1	0.05
1	1	0	0.015
1	1	1	0.015



Eric Xing, ML/CMU

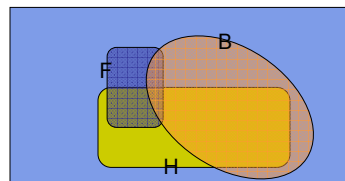
29

Inference with the Joint

- Once you have the JD you can ask for the probability of any atomic event consistent with you query

$$P(E) = \sum_{i \in E} P(\text{row}_i)$$

$\neg F$	$\neg B$	$\neg H$	0.4	
$\neg F$	$\neg B$	H	0.1	
$\neg F$	B	$\neg H$	0.17	
$\neg F$	B	H	0.2	
F	$\neg B$	$\neg H$	0.05	
F	$\neg B$	H	0.05	
F	B	$\neg H$	0.015	
F	B	H	0.015	



Eric Xing, ML/CMU

30

Inference with the Joint

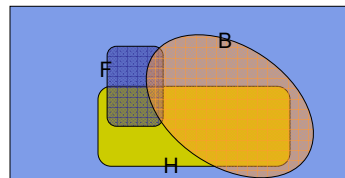
- Compute Marginals

$$P(\text{Flu} \wedge \text{Headache}) =$$

$$0.05 + 0.01$$

$$= .065$$

¬F	¬B	¬H	0.4	
¬F	¬B	H	0.1	
¬F	B	¬H	0.17	
¬F	B	H	0.2	
F	¬B	¬H	0.05	
F	¬B	H	0.05	
F	B	¬H	0.015	
F	B	H	0.015	



Eric Xing, ML/CMU

31

Inference with the Joint

- Compute Marginals

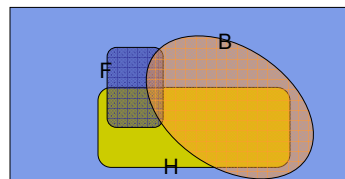
$$P(\text{Headache}) =$$

$$.1 + .2 + .05$$

$$+ .015$$

$$0.385$$

¬F	¬B	¬H	0.4	
¬F	¬B	H	0.1	
¬F	B	¬H	0.17	
¬F	B	H	0.2	
F	¬B	¬H	0.05	
F	¬B	H	0.05	
F	B	¬H	0.015	
F	B	H	0.015	



Eric Xing, ML/CMU

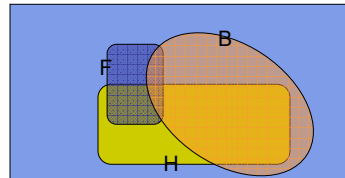
32

Inference with the Joint

- Compute Conditionals

$$P(E_1|E_2) = \frac{P(E_1 \wedge E_2)}{P(E_2)} = \frac{\sum_{i \in E_1 \cap E_2} P(\text{row}_i)}{\sum_{i \in E_2} P(\text{row}_i)}$$

¬F	¬B	¬H	0.4	
¬F	¬B	H	0.1	
¬F	B	¬H	0.17	
¬F	B	H	0.2	
F	¬B	¬H	0.05	
F	¬B	H	0.05	
F	B	¬H	0.015	
F	B	H	0.015	



Eric Xing, ML/CMU

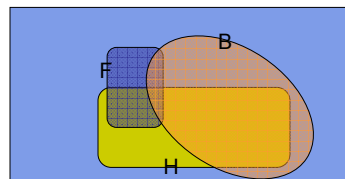
33

Inference with the Joint

- Compute Conditionals

$$P(\text{Flu}|\text{Headhead}) = \frac{P(\text{Flu} \wedge \text{Headhead})}{P(\text{Headhead})} = \frac{0.015}{0.365}$$

¬F	¬B	¬H	0.4	
¬F	¬B	H	0.1	
¬F	B	¬H	0.17	
¬F	B	H	0.2	
F	¬B	¬H	0.05	
F	¬B	H	0.05	
F	B	¬H	0.015	
F	B	H	0.015	



- General idea: compute distribution on query variable by **fixing** evidence variables and **summing** over hidden variables

Eric Xing, ML/CMU

34

Summary: Inference by enumeration



- Let X be all the variables. Typically, we want
 - the posterior joint distribution of the query variables Y
 - given specific values e for the evidence variables E .
 - We write the hidden variables as $H = X - Y - E$
- Then the required summation of joint entries is done by summing out the hidden variables:

$$P(Y|E=e) = \alpha P(Y, E=e) = \alpha \sum_H P(Y, E=e, H=h)$$

- The terms in the summation are joint entries because Y , E , and H together exhaust the set of random variables
- Obvious problems:
 - Worst-case time complexity $O(d^n)$ where d is the largest arity
 - Space complexity $O(d^n)$ to store the joint distribution
 - How to find the numbers for $O(d^n)$ entries???

Eric Xing, ML/CMU

35

Conditional independence



- Write out full joint distribution using chain rule:

$$P(\text{Headache}; \text{Flu}; \text{Virus}; \text{DrinkBeer})$$

$$= P(\text{Headache} | \text{Flu}; \text{Virus}; \text{DrinkBeer}) P(\text{Flu}; \text{Virus}; \text{DrinkBeer})$$

$$= P(\text{Headache} | \text{Flu}; \text{Virus}; \text{DrinkBeer}) P(\text{Flu} | \text{Virus}; \text{DrinkBeer}) P(\text{Virus} | \text{DrinkBeer}) P(\text{DrinkBeer})$$

Assume independence and conditional independence

$$= P(\text{Headache} | \text{Flu}; \text{DrinkBeer}) P(\text{Flu} | \text{Virus}) P(\text{Virus}) P(\text{DrinkBeer})$$

I.e., ? independent parameters

- In most cases, the use of conditional independence reduces the size of the representation of the joint distribution from **exponential** in n to **linear** in n .
- Conditional independence is our most basic and robust form of knowledge about uncertain environments.

Eric Xing, ML/CMU

36

Rules of Independence --- by examples



- $P(\text{Virus} \mid \text{DrinkBeer}) = P(\text{Virus})$
iff **Virus** is independent of **DrinkBeer**
- $P(\text{Flu} \mid \text{Virus}; \text{DrinkBeer}) = P(\text{Flu} \mid \text{Virus})$
iff **Flu** is independent of **DrinkBeer**, given **Virus**
- $P(\text{Headache} \mid \text{Flu}; \text{Virus}; \text{DrinkBeer}) = P(\text{Headache} \mid \text{Flu}; \text{DrinkBeer})$
iff **Headache** is independent of **Virus**, given **Flu** and **DrinkBeer**

Marginal and Conditional Independence



- Recall that for events E (i.e. $X=x$) and H (say, $Y=y$), the conditional probability of E given H , written as $P(E|H)$, is

$$P(E \text{ and } H)/P(H)$$

(= the probability of both E and H are true, given H is true)

- E and H are (statistically) independent if

$$P(E) = P(E|H)$$

(i.e., prob. E is true doesn't depend on whether H is true); or equivalently

$$P(E \text{ and } H) = P(E)P(H).$$

- E and F are *conditionally* independent given H if

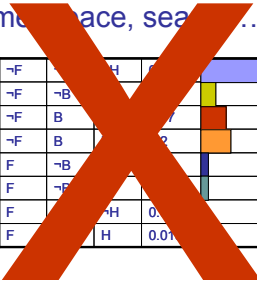
$$P(E|H, F) = P(E|H)$$

or equivalently

$$P(E, F|H) = P(E|H)P(F|H)$$

Why knowledge of Independence is useful



- Lower complexity (time, space, search, ...) 

¬F	¬B	¬H	0.4	
¬F	¬B	H	0.1	
¬F	B	¬H	0.17	
¬F	B	H	0.2	
F	¬B	¬H	0.05	
F	¬B	H	0.05	
F	B	¬H	0.015	
F	B	H	0.015	

- Motivates efficient inference for all kinds of queries
Stay tuned !!
- Structured knowledge about the domain
 - easy to learning (both from expert and from data)
 - easy to grow

Eric Xing, ML/CMU

39

Where do probability distributions come from?



- Idea One: Human, Domain Experts
- Idea Two: Simpler probability facts and some algebra

e.g., $P(F)$

$P(B)$

$P(H|\neg F, B)$

$P(H|F, \neg B)$

...



¬F	¬B	¬H	0.4	
¬F	¬B	H	0.1	
¬F	B	¬H	0.17	
¬F	B	H	0.2	
F	¬B	¬H	0.05	
F	¬B	H	0.05	
F	B	¬H	0.015	
F	B	H	0.015	

- Idea Three: Learn them from data!
 - A good chunk of this course is essentially about various ways of learning various forms of them!

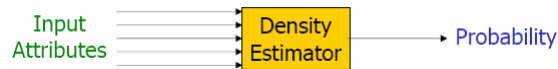
Eric Xing, ML/CMU

40

Density Estimation



- A Density Estimator learns a mapping from a set of attributes to a Probability



- Often know as parameter estimation if the distribution form is specified
 - Binomial, Gaussian ...
- Three important issues:
 - Nature of the data (iid, correlated, ...)
 - Objective function (MLE, MAP, ...)
 - Algorithm (simple algebra, gradient methods, EM, ...)
 - Evolution scheme (likelihood on test data, predictability, consistency, ...)

Eric Xing, ML/CMU

41

Parameter Learning from iid data



- Goal: estimate distribution parameters θ from a dataset of N independent, identically distributed (iid), fully observed, training cases

$$D = \{x_1, \dots, x_N\}$$

- Maximum likelihood estimation (MLE)
 1. One of the most common estimators
 2. With iid and full-observability assumptions, write $L(\theta)$ as the likelihood of the data:

$$\begin{aligned} L(\theta) &= P(x_1, x_2, \dots, x_N; \theta) \\ &= P(x_1; \theta) P(x_2; \theta), \dots, P(x_N; \theta) \\ &= \prod_{i=1}^N P(x_i; \theta) \end{aligned}$$

3. pick the setting of parameters most likely to have generated the data we saw:

$$\theta^* = \arg \max_{\theta} L(\theta) = \arg \max_{\theta} \log L(\theta)$$

Eric Xing, ML/CMU

42

Example 1: Bernoulli model

- Data:

- We observed *N* iid coin tossing: $D = \{1, 0, 1, \dots, 0\}$

- Representation:

Binary r.v: $x_n = \{0, 1\}$

- Model:

$$P(x) = \begin{cases} 1-p & \text{for } x=0 \\ p & \text{for } x=1 \end{cases} \Rightarrow P(x) = \theta^x (1-\theta)^{1-x}$$

- How to write the likelihood of a single observation x_i ?

$$P(x_i) = \theta^{x_i} (1-\theta)^{1-x_i}$$

- The likelihood of dataset $D = \{x_1, \dots, x_N\}$:

$$P(x_1, x_2, \dots, x_N | \theta) = \prod_{i=1}^N P(x_i | \theta) = \prod_{i=1}^N (\theta^{x_i} (1-\theta)^{1-x_i}) = \theta^{\sum_{i=1}^N x_i} (1-\theta)^{\sum_{i=1}^N 1-x_i} = \theta^{\text{\#head}} (1-\theta)^{\text{\#tails}}$$

Eric Xing, ML/CMU

43

MLE

- Objective function:

$$\ell(\theta; D) = \log P(D | \theta) = \log \theta^{n_h} (1-\theta)^{n_t} = n_h \log \theta + (N - n_h) \log(1-\theta)$$

- We need to maximize this w.r.t. θ

- Take derivatives wrt θ

$$\frac{\partial \ell}{\partial \theta} = \frac{n_h}{\theta} - \frac{N - n_h}{1-\theta} = 0 \quad \Rightarrow \quad \hat{\theta}_{MLE} = \frac{n_h}{N} \quad \text{or} \quad \hat{\theta}_{MLE} = \frac{1}{N} \sum_i x_i$$

Frequency as
sample mean

- Sufficient statistics

- The counts, n_h , where $n_k = \sum_i x_i$, are sufficient statistics of data D

Eric Xing, ML/CMU

44

MLE for discrete (joint) distributions



- More generally, it is easy to show that

$$P(\text{event}_i) = \frac{\text{\#records in which event}_i \text{ is true}}{\text{total number of records}}$$

- This is an important (but sometimes not so effective) learning algorithm!

$\neg F$	$\neg B$	$\neg H$	0.4	
$\neg F$	$\neg B$	H	0.1	
$\neg F$	B	$\neg H$	0.17	
$\neg F$	B	H	0.2	
F	$\neg B$	$\neg H$	0.05	
F	$\neg B$	H	0.05	
F	B	$\neg H$	0.015	
F	B	H	0.015	

Eric Xing, ML/CMU

45

Example 2: univariate normal



- Data:
 - We observed N iid real samples:
 $D = \{-0.1, 10, 1, -5.2, \dots, 3\}$
- Model: $P(x) = (2\pi\sigma^2)^{-1/2} \exp\{-(x - \mu)^2 / 2\sigma^2\}$

- Log likelihood:

$$\ell(\theta; D) = \log P(D | \theta) = -\frac{N}{2} \log(2\pi\sigma^2) - \frac{1}{2} \sum_{n=1}^N \frac{(x_n - \mu)^2}{\sigma^2}$$

- MLE: take derivative and set to zero:

$$\begin{aligned} \frac{\partial \ell}{\partial \mu} &= (1/\sigma^2) \sum_n (x_n - \mu) \\ \frac{\partial \ell}{\partial \sigma^2} &= -\frac{N}{2\sigma^2} + \frac{1}{2\sigma^4} \sum_n (x_n - \mu)^2 \end{aligned} \quad \Rightarrow \quad \begin{aligned} \mu_{MLE} &= \frac{1}{N} \sum_n (x_n) \\ \sigma_{MLE}^2 &= \frac{1}{N} \sum_n (x_n - \mu_{MLE})^2 \end{aligned}$$

Eric Xing, ML/CMU

46

Overfitting



- Recall that for Bernoulli Distribution, we have

$$\hat{\theta}_{ML}^{head} = \frac{n^{head}}{n^{head} + n^{tail}}$$

- What if we tossed too few times so that we saw zero head?
We have $\hat{\theta}_{ML}^{head} = 0$, and we will predict that the probability of seeing a head next is zero!!!

- The rescue:
 - Where n' is known as the pseudo- (imaginary) count

$$\hat{\theta}_{ML}^{head} = \frac{n^{head} + n'}{n^{head} + n^{tail} + n'}$$

- But can we make this more formal?

Eric Xing, ML/CMU

47

The Bayesian Theory



- The Bayesian Theory: (e.g., for data D and model M)

$$P(M|D) = P(D|M)P(M)/P(D)$$

- the posterior equals to the likelihood times the prior, up to a constant.
- This allows us to capture uncertainty about the model in a principled way

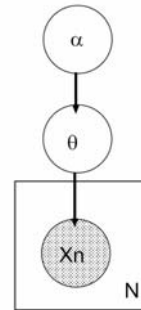
Eric Xing, ML/CMU

48

Hierarchical Bayesian Models

- θ are the parameters for the likelihood $p(x|\theta)$
- α are the parameters for the prior $p(\theta|\alpha)$.
- We can have hyper-hyper-parameters, etc.
- We stop when the choice of hyper-parameters makes no difference to the marginal likelihood; typically make hyper-parameters constants.
- Where do we get the prior?
 - Intelligent guesses
 - Empirical Bayes (Type-II maximum likelihood)
 - computing point estimates of α :

$$\hat{\alpha}_{MLE} = \arg \max_{\alpha} p(\tilde{n} | \alpha)$$



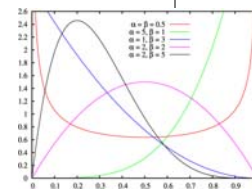
Eric Xing, ML/CMU

49

Bayesian estimation for Bernoulli

- Beta distribution:

$$P(\theta; \alpha, \beta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \theta^{\alpha-1} (1-\theta)^{\beta-1} = B(\alpha, \beta) \theta^{\alpha-1} (1-\theta)^{\beta-1}$$



- Posterior distribution of θ :

$$P(\theta | x_1, \dots, x_N) = \frac{p(x_1, \dots, x_N | \theta) p(\theta)}{p(x_1, \dots, x_N)} \propto \theta^{n_h} (1-\theta)^{n_t} \times \theta^{\alpha-1} (1-\theta)^{\beta-1} = \theta^{n_h + \alpha - 1} (1-\theta)^{n_t + \beta - 1}$$

- Notice the isomorphism of the posterior to the prior,
- such a prior is called a **conjugate prior**

Eric Xing, ML/CMU

50

Bayesian estimation for Bernoulli, con'd



- Posterior distribution of θ :

$$P(\theta | x_1, \dots, x_N) = \frac{p(x_1, \dots, x_N | \theta) p(\theta)}{p(x_1, \dots, x_N)} \propto \theta^{n_h} (1-\theta)^{n_t} \times \theta^{\alpha-1} (1-\theta)^{\beta-1} = \theta^{n_h+\alpha-1} (1-\theta)^{n_t+\beta-1}$$

- Maximum *a posteriori* (MAP) estimation:

$$\theta_{MAP} = \arg \max_{\theta} \log P(\theta | x_1, \dots, x_N)$$

- Posterior mean estimation:

$$\theta_{Bayes} = \int \theta p(\theta | D) d\theta = C \int \theta \times \theta^{n_h+\alpha-1} (1-\theta)^{n_t+\beta-1} d\theta = \frac{n_h + \alpha}{N + \alpha + \beta}$$

Bata parameters
can be understood
as pseudo-counts

- Prior strength: $A = \alpha + \beta$

- A can be interperated as the size of an imaginary data set from which we obtain the **pseudo-counts**

Eric Xing, ML/CMU

51

Effect of Prior Strength



- Suppose we have a uniform prior ($\alpha = \beta = 1/2$), and we observe $\vec{n} = (n_h = 2, n_t = 8)$

- Weak prior $A = 2$. Posterior prediction:

$$p(x = h | n_h = 2, n_t = 8, \vec{\alpha} = \vec{\alpha}' \times 2) = \frac{1+2}{2+10} = 0.25$$

- Strong prior $A = 20$. Posterior prediction:

$$p(x = h | n_h = 2, n_t = 8, \vec{\alpha} = \vec{\alpha}' \times 20) = \frac{10+2}{20+10} = 0.40$$

- However, if we have enough data, it washes away the prior. e.g., $\vec{n} = (n_h = 200, n_t = 800)$. Then the estimates under weak and strong prior are $\frac{1+200}{2+1000}$ and $\frac{10+200}{20+1000}$, respectively, both of which are close to 0.2

Eric Xing, ML/CMU

52

Bayesian estimation for normal distribution



- Normal Prior:

$$P(\mu) = (2\pi\tau^2)^{-1/2} \exp\{-(\mu - \mu_0)^2 / 2\tau^2\}$$

- Joint probability:

$$P(\mathbf{x}, \mu) = (2\pi\sigma^2)^{-N/2} \exp\left\{-\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2\right\} \\ \times (2\pi\tau^2)^{-1/2} \exp\{-(\mu - \mu_0)^2 / 2\tau^2\}$$

- Posterior:

Homework!!!