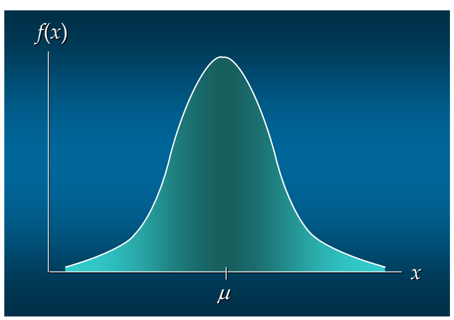
Machine Learning

10-701/15-781, Spring 2010

Probability 101

Aarti Singh

Lecture 2, January 13, 2010



Reading: **Bishop: Chap 1,2**

Slides courtesy: Eric Xing, Andrew Moore, Tom Mitchell

Announcements

Homework 1 is out!

Due: Wednesday, Jan 20, 2010 (beginning of class)

1^{st} Recitation

Jan 14, 2010 5:00-6:30 pm NSH 1305 Probability

Probability in Machine Learning

Machine Learning tasks involve reasoning under uncertainity

Sources of uncertainity/randomness:

- Noise – variability in sensor measurements, partial observability, incorrect labels
- Finite sample size - Training and test data are randomly drawn instances

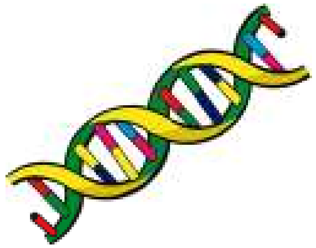
Hand-written digit recognition

Probability quantifies uncertainty!

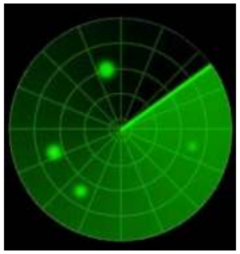
Basic Probability Concepts

Conceptual or physical, repeatable experiment with random outcome at any trial

Roll of dice



Nucleotide present at a DNA site



Time-space position of an aircraft on a radar screen

Sample space $\mathcal{S}$ - set of all possible outcomes. (can be finite or infinite.)

$$S \equiv \{1,2,3,4,5,6\} \qquad \mathcal{S} \equiv \{A, T, C, G\} \qquad \mathcal{S} \equiv \{0, R_{\max}\} \times \{0, 360^\circ\} \times \{0, +\infty\}$$

Event $\mathcal{A}$ - any subset of $\mathcal{S}$:

See “2“,”4” or “6” in a roll | observe a "G" at a site | UA007 in angular location {45°-60°}

Definition

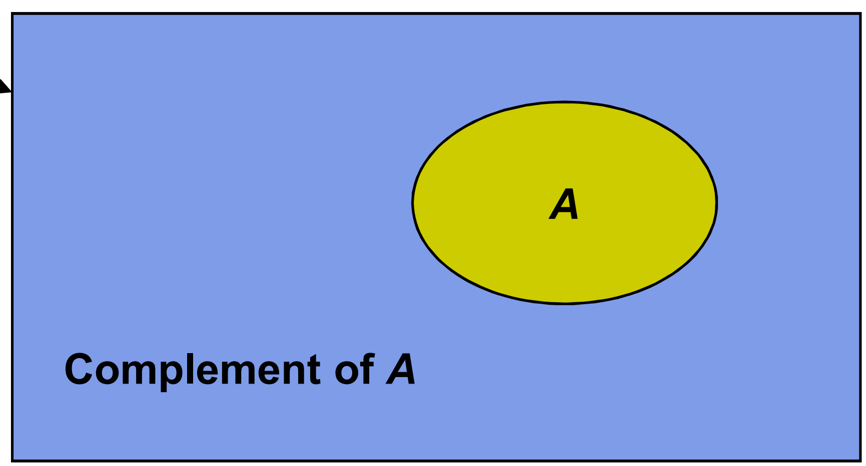
Classical: Probability of an event *A* is the relative frequency (limiting ratio of number of occurrences of event *A* to the total number of trials)

$$P(A) = \lim_{N \to \infty} \frac{N_A}{N}$$

E.g. $P(\{1\}) = 1/6$ $P(\{2,4,6\}) = 1/2$

Sample space S

Its area is 1, *P(S)* = 1

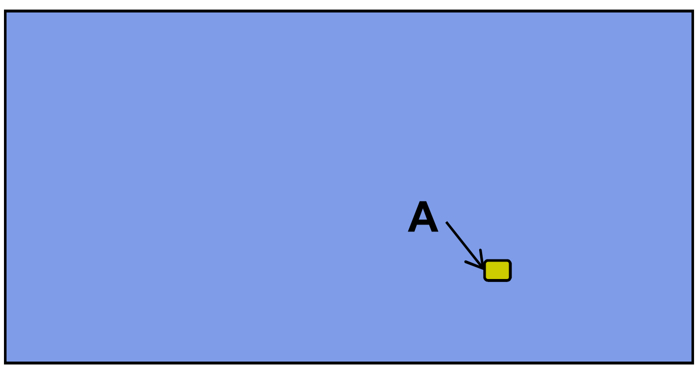


***P(A)* - area of the oval**

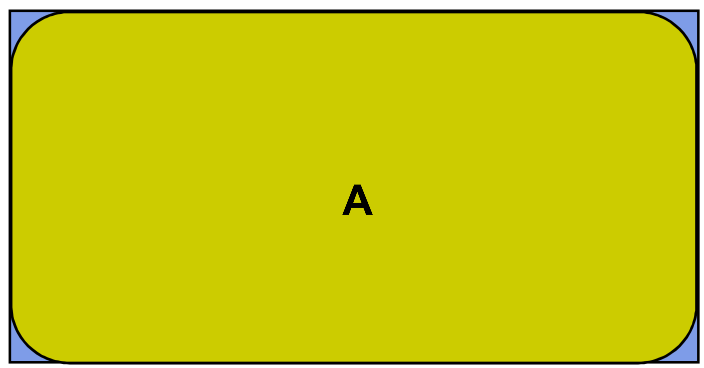
Definition

Axiomatic (Kolmogorov): Probability of an event *A* is a number assigned to this event such that

- $0 \le P(A) \le 1$ all probabilities are between 0 and 1



Area of A can't be smaller than 0

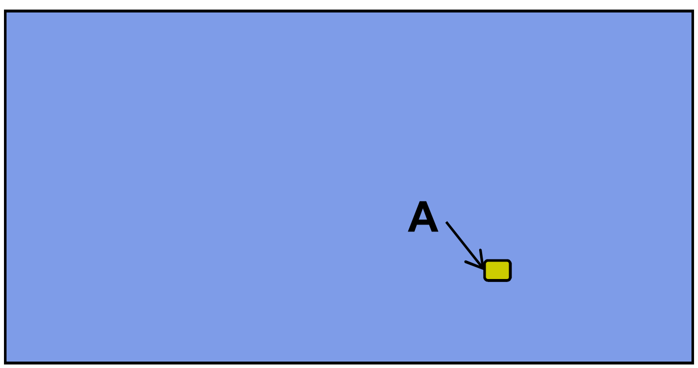


Area of A can't be larger than 1

Definition

Axiomatic (Kolmogorov): Probability of an event *A* is a number assigned to this event such that

- $0 \leq P(A) \leq 1$ all probabilities are between 0 and 1
- $P(\phi) = 0$ probability of no outcome is 0

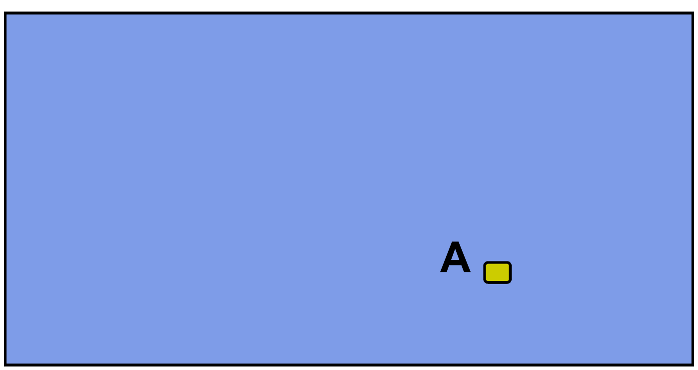


Area of A can't be smaller than 0

Definition

Axiomatic (Kolmogorov): Probability of an event *A* is a number assigned to this event such that

- $0 \leq P(A) \leq 1$ all probabilities are between 0 and 1
- $P(\phi) = 0$ probability of no outcome is 0
- $P(S) = 1$ probability of some outcome is 1



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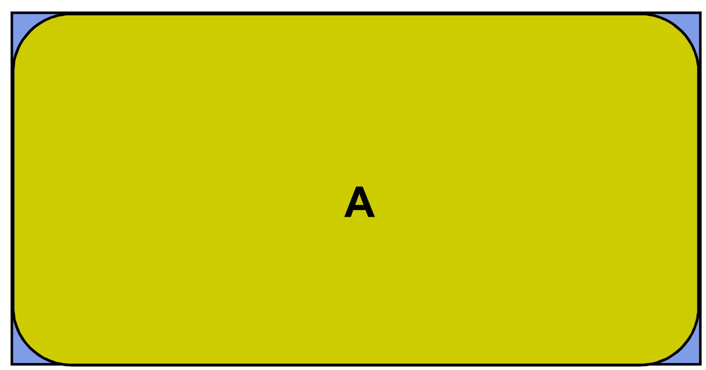
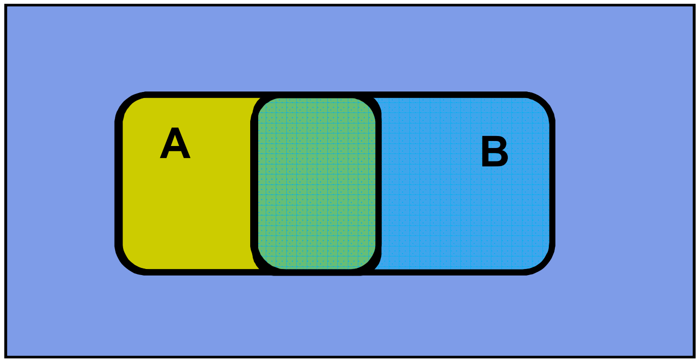


Area of A can't be larger than 1

Definition

Axiomatic (Kolmogorov): Probability of an event *A* is a number assigned to this event such that

- $0 \leq P(A) \leq 1$ — all probabilities are between 0 and 1
- $P(\phi) = 0$ — no outcome has 0 probability
- $P(S) = 1$ — some outcome is bound to occur
- $P(A \cup B) = P(A) + P(B) - P(A \cap B)$ — probability of union of two events



Area of A U B = Area of A + Area of B – Area of A ∩ B

Definition

Axiomatic (Kolmogorov): Probability of an event *A* is a number assigned to this event such that

- $0 \le P(A) \le 1$ — all probabilities are between 0 and 1
- $P(\phi) = 0$ — no outcome has 0 probability
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- $P(A \cup B) = P(A) + P(B) - P(A \cap B)$ — probability of union of two events

Probability space is a sample space equipped with an assignment *P(A)* to every event $A \subset S$ such that *P* satisfies the Kolmogorov axioms.

Theorems from the Axioms

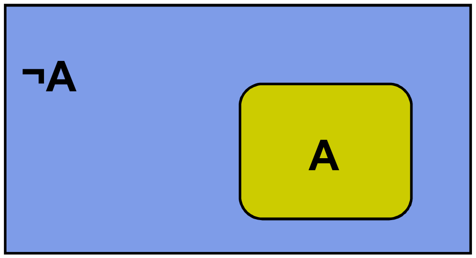
- $0 \le P(A) \le 1$
- $P(\phi) = 0$
- $P(S) = 1$
- $P(A \cup B) = P(A) + P(B) - P(A \cap B)$

$P(\neg A) = 1 - P(A)$

Proof: $P(A \cup \neg A) = P(S) = 1$

$P(A \cap \neg A) = P(\phi) = 0$

$1 = P(A) + P(\neg A) + 0 \quad \Rightarrow \quad P(\neg A) = 1 - P(A)$



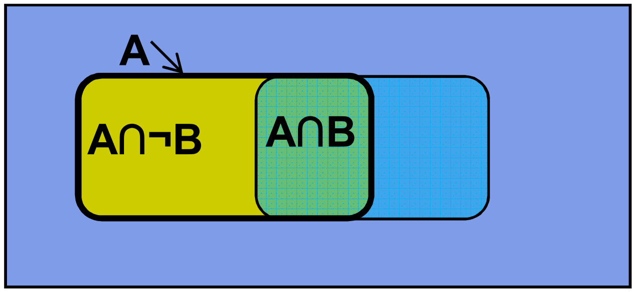
Theorems from the Axioms

- $0 \leq P(A) \leq 1$
- $P(\phi) = 0$
- $P(S) = 1$
- $P(A \cup B) = P(A) + P(B) - P(A \cap B)$

$$P(A) = P(A \cap B) + P(A \cap \neg B)$$

Proof:

$$\begin{aligned} P(A) &= P(A \cap S) = P(A \cap (B \cup \neg B)) = P((A \cap B) \cup (A \cap \neg B)) \\ &= P(A \cap B) + P(A \cap \neg B) - P((A \cap B) \cap (A \cap \neg B)) \\ &= P(A \cap B) + P(A \cap \neg B) - P(\phi) \\ &= P(A \cap B) + P(A \cap \neg B) \end{aligned}$$



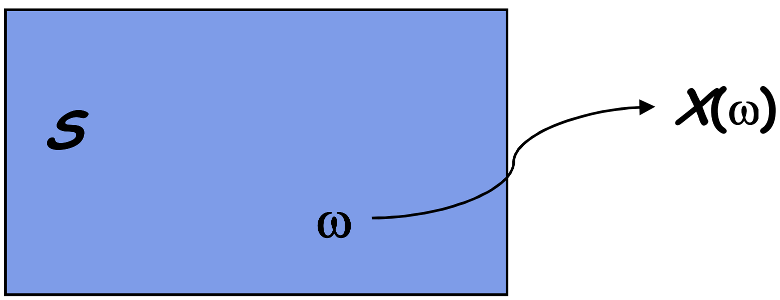
Why use probability?

- There have been many other approaches to handle uncertainty:
  - Fuzzy logic
  - Qualitative reasoning (Qualitative physics)
- "Probability theory is nothing but common sense reduced to calculation"
  - — Pierre Laplace, 1812.
- Any scheme for combining uncertain information really should obey these axioms
  - Di Finetti 1931 - If you gamble based on "uncertain beliefs" that satisfy these axioms, then you can't be exploited by an opponent

Random Variable

- A *random variable* is a function that associates a unique numerical value X(ω) with every outcome $\omega \in S$ of an experiment.

(The value of the r.v. will vary from trial to trial as the experiment is repeated)



P(X < 2) = P({ω: X(ω) < 2})

- Discrete r.v.:
  - The outcome of a coin-toss H = 1, T = 0 (Binary)
  - The outcome of a dice-roll 1-6
- Continuous r.v.:
  - The location of an aircraft
- Univariate r.v.:
  - The outcome of a dice-roll 1-6
- Multi-variate r.v.:
  - The time-space position of an aircraft on radar screen

$$X = \begin{bmatrix} R \\ \Theta \\ t \end{bmatrix}$$

Discrete Probability 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

$0 \leq P(X=x) \leq 1$ X – random variable

$\Sigma_x P(X = x) = 1$ x – value it takes

E.g. Bernoulli distribution with parameter θ

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

Discrete Probability Distribution

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$$0 \le P(X=x) \le 1 \qquad \text{X – random variable}$$

$$\Sigma_x P(X = x) = 1 \qquad \text{x – value it takes}$$

E.g. Multinomial distribution with parameters $\theta_1, \ldots, \theta_K$

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

$$P(x) = \frac{n!}{x_1! x_2! \cdots x_K!} \theta_1^{x_1} \theta_2^{x_2} \cdots \theta_K^{x_K}$$

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 --- $P(X=x) = 0$
  - Instead, we talk about the probability of the random variable assuming a value within a given interval, or half interval

$$P(X \in [x_1, x_2])$$

$$P(X < x) = P(X \in [-\infty, x])$$

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

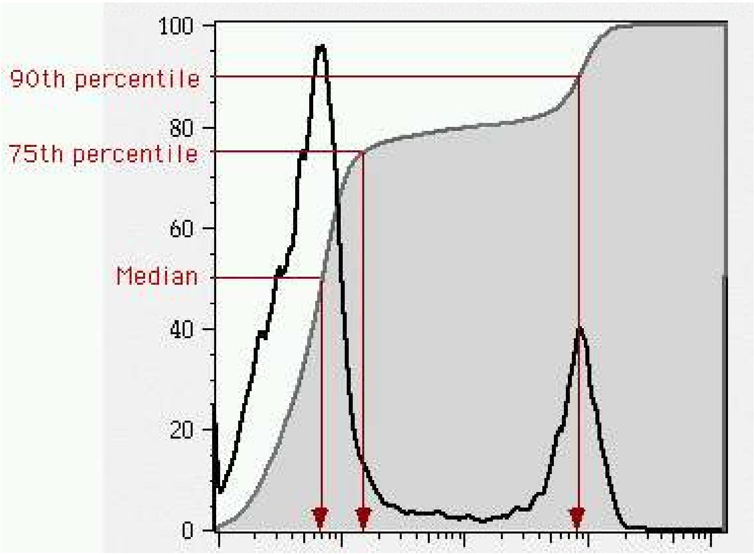
  - Cumulative distribution function (CDF):

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

  - Probability density function (PDF):

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

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



Car flow on Liberty Bridge (cooked up!)

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

- If

  $p(x_1) = a$ and $p(x_2) = b$,

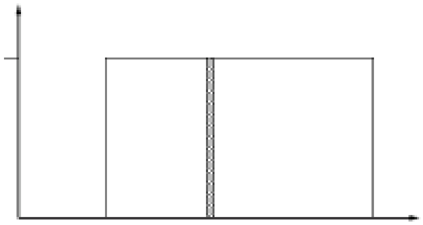
  then when a value X is sampled from the distribution with density p(x), you are a/b times as likely to find that X is "very close to" x_1 than that X is "very close to" x_2.

- That is:

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

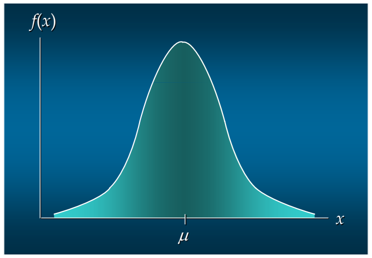
Continuous Distributions

- Uniform Probability Density Function



$$p(x) = 1/(b-a) \quad \text{for } a \le x \le b$$
$$= 0 \quad \text{elsewhere}$$

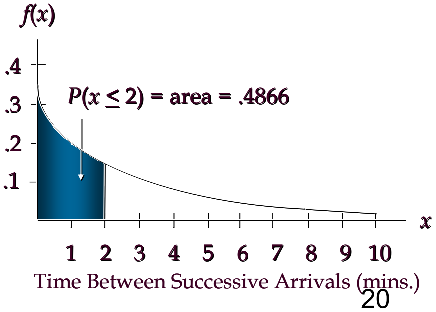
- Normal (Gaussian) Probability Density Function



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

  - 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.

- Exponential Probability Distribution



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

Statistical Characterizations

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

$$E(X) = \begin{cases} \sum_x xp(x) & \text{discrete} \\ \int_{-\infty}^{\infty} xp(x)dx & \text{continuous} \end{cases}$$

- **Variance:** the spread

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

Gaussian (Normal) density in 1D

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

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

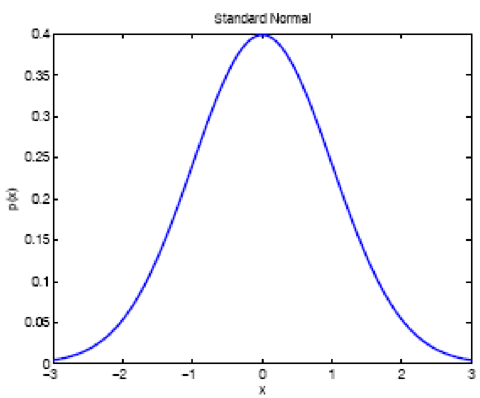
$$E(X) = \mu$$

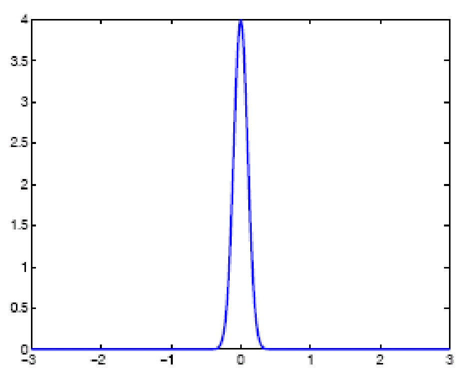
$$\mathrm{var}(X) = \sigma^2$$

  - Here is how we plot the pdf in matlab

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

Zero mean
Large variance





Zero mean
Small variance

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

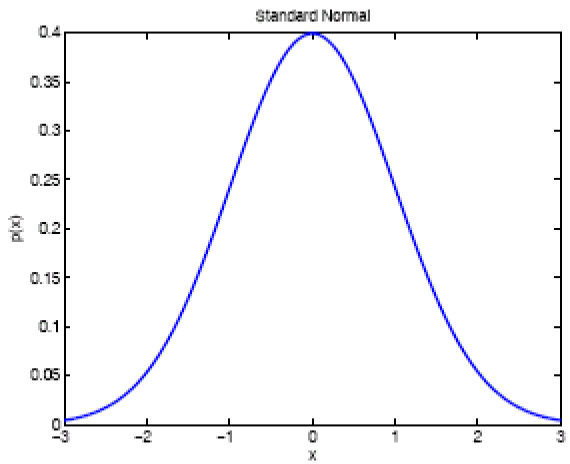
Gaussian CDF

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

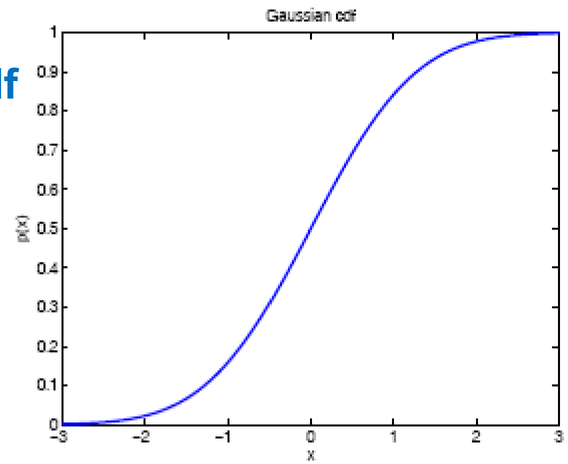
$$\Phi(x) = \int_{-\infty}^{x} p(z)dz$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-z^2/2} dz$$

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

pdf



cdf



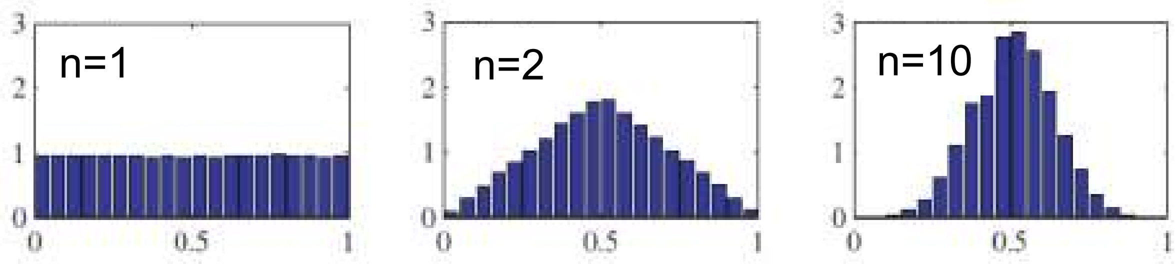
Central limit theorem

- If (X_1 ,X_2, … X_n) are i.i.d. (independent and identically distributed – to be covered next) random variables
- Then define

$$\overline{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$$

- As $n \rightarrow$ infinity,

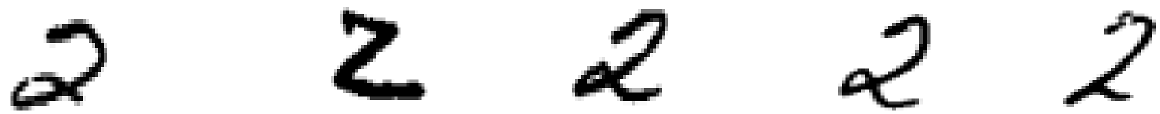
$p(\overline{X}) \rightarrow$ Gaussian with mean $E[X_i]$ and variance $Var[X_i]/n$



- Somewhat of a justification for assuming Gaussian distribution

Independence

Training and test samples typically assumed to be i.i.d. (independent and identically distributed)



A and B are independent events if

$$P(A \cap B) = P(A) * P(B)$$

Outcome of A has no effect on the outcome of B (and vice versa).

E.g. Roll of two die

$P(\{1\},\{3\}) = 1/6*1/6 = 1/36$

Independence

A, B and C are pairwise independent events if

$$P(A \cap B) = P(A) * P(B)$$
$$P(A \cap C) = P(A) * P(C)$$
$$P(B \cap C) = P(B) * P(C)$$

A, B and C are mutually independent events if, in addition to pairwise independence,

$$P(A \cap B \cap C) = P(A) * P(B) * P(C)$$

Conditional Probability

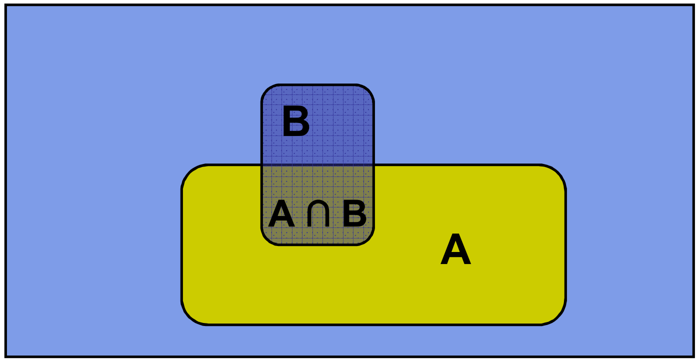
- P(A|B) = Probability of event A conditioned on event B having occurred

If P(B) > 0, then $$P(A|B) = \frac{P(A \cap B)}{P(B)}$$

E.g. H = "having a headache"

F = "coming down with Flu"

- P(H)=1/10
- P(F)=1/40
- P(H|F)=1/2 Fraction of people with flu that have a headache



Corollary: The Chain Rule

$$P(A \cap B) = P(A|B)\, P(B)$$

If A and B are independent, P(A|B) = P(A)

Conditional Independence

A and B are independent if

$$P(A \cap B) = P(A) * P(B) \quad \equiv \quad P(A|B) = P(A)$$

Outcome of B has no effect on the outcome of A (and vice versa).

A and B are conditionally independent given C if

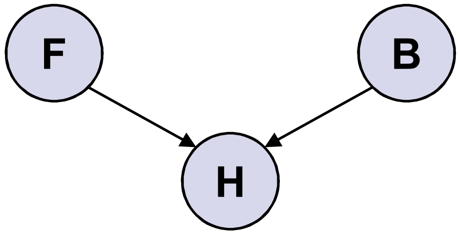
$$P(A \cap B|C) = P(A|C) * P(B|C) \quad \equiv \quad P(A|B,C) = P(A|C)$$

Outcome of B has no effect on the outcome of A (and vice versa) if C is true.

Prior and Posterior Distribution

- Suppose that our propositions have a "causal flow"

  e.g.,



- Prior or unconditional probabilities of propositions

  e.g., P(Flu) = 0.025 and *P(DrinkBeer)* = 0.2

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

- Posterior or conditional probabilities of propositions

  e.g., P(Headache|Flu) = 0.5 and *P(Headache|Flu,DrinkBeer)* = 0.7

  correspond to updated belief after arrival of new evidence

  Not always useful: *P(Headache|Flu, Steelers win) = 0.5*

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”

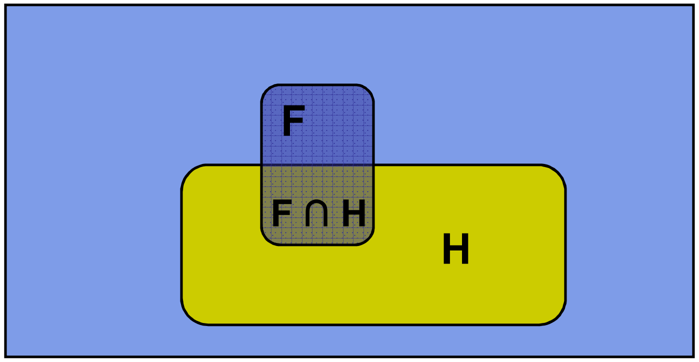
  Is this reasoning correct?

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) = ?



Probabilistic Inference

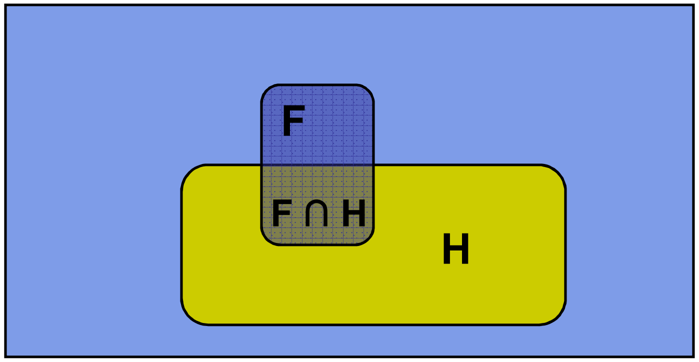
- H = "having a headache"
- F = "coming down with Flu"
  - P(H)=1/10
  - P(F)=1/40
  - P(H|F)=1/2

- The Problem:

$$P(F|H) = \frac{P(F \cap H)}{P(H)}$$

$$= \frac{P(H|F)\,P(F)}{P(H)}$$

$$= 1/8 \neq P(H|F)$$



The Bayes Rule

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

$$P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B)}$$

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**

Quiz

- $P(H)=1/10$
- $P(F)=1/40$
- $P(H|F)=1/2$
- $P(F|H) = 1/8$

- Which of the following statement is true?

$$P(F|\neg H) = 1 - P(F|H)$$

$$P(\neg F|H) = 1 - P(F|H)$$

$$P(F|\neg H) = \frac{P(\neg H|F)\,P(F)}{P(\neg H)} = \frac{(1 - P(H|F))\,P(F)}{1 - P(H)}$$

More General Forms of Bayes Rule

$$P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B)}$$

- Law of total probability

$P(B) = P(B \cap A) + P(B \cap \neg A)$
$= P(B|A)\, P(A) + P(B|\neg A)\, P(\neg A)$

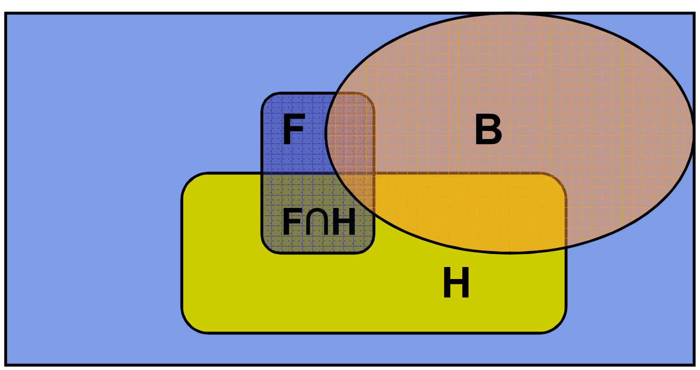
$$P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B \mid A)P(A) + P(B \mid \neg A)P(\neg A)}$$

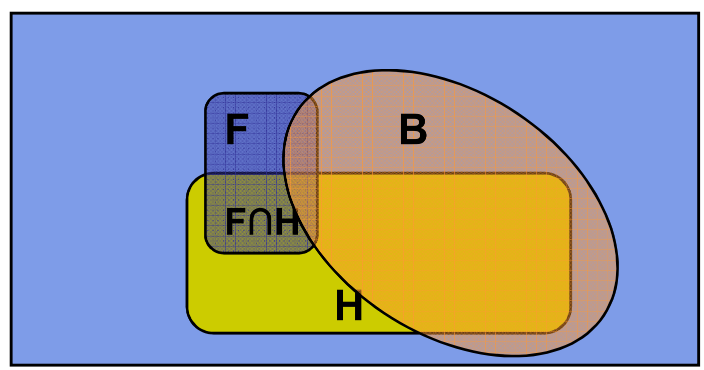
More General Forms of Bayes Rule

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

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

E.g. P(Flu | Headhead ∧ DrankBeer)





Joint and Marginal Probabilities

A joint probability distribution for a set of RVs (say X_1,X_2,X_3) gives the probability of every atomic event $P(X_1,X_2,X_3)$

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

	B	¬B
F	0.005	0.02
¬F	0.195	0.78

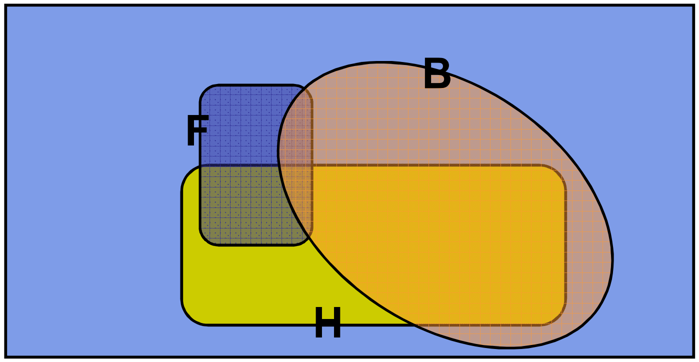
- **P**(*Flu,DrinkBeer, Headache*) = ?
- **Every question about a domain can be answered by the joint distribution**, as we will see later.

A marginal probability distribution is the probability of every value that a single RV can take $P(X_1)$ **P**(Flu) = ?

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



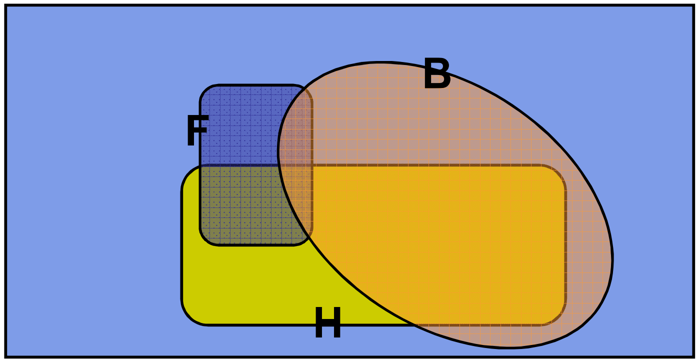
Inference with the Joint

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

$$P(E) = \sum_{i \in E} P(row_i)$$

¬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

E.g. E = {(¬F, ¬B,H),(¬F,B,H)}



Inference with the Joint

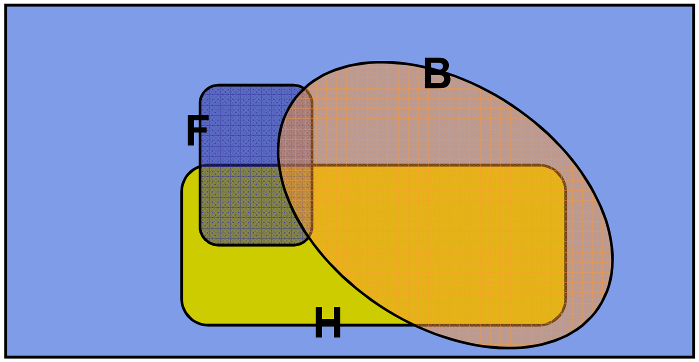
- Compute Marginals

$$P(Flu \wedge Headache)$$

$$= P(F \wedge H \wedge B) + P(F \wedge H \wedge \neg B)$$

¬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

Recall: Law of Total Probability



Inference with the Joint

- Compute Marginals

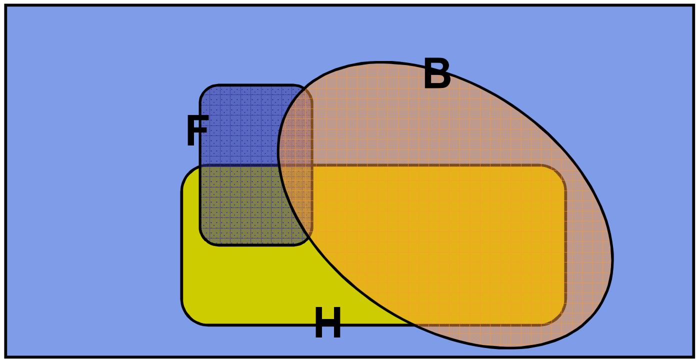
$$P(\text{Headache})$$

$$= P(H \wedge F) + P(H \wedge \neg F)$$

$$= P(H \wedge F \wedge B) + P(H \wedge F \wedge \neg B)$$

$$+ P(H \wedge \neg F \wedge B) + P(H \wedge \neg F \wedge \neg B)$$

¬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

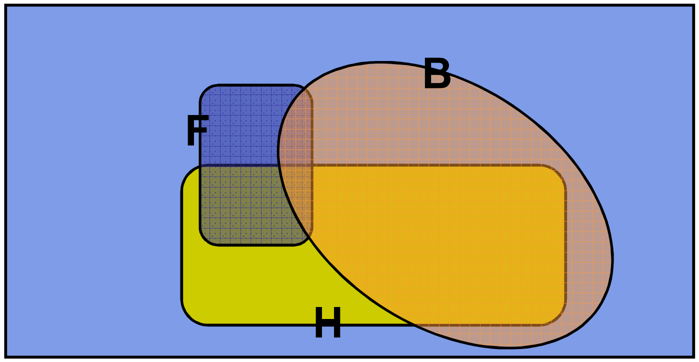


Inference with the Joint

- Compute Conditionals

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

¬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



Inference with the Joint

- Compute Conditionals

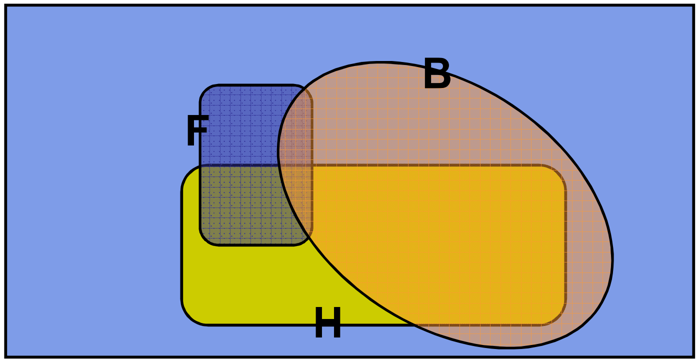
$$P(\text{Flu} \mid \text{Headache}) = \frac{P(\text{Flu} \wedge \text{Headache})}{P(\text{Headache})}$$

$$=$$

¬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**



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|¬F,B)

P(H|F,¬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

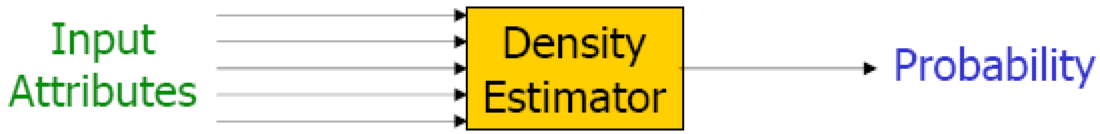
Use chain rule and independence assumptions to compute joint distribution

Where do probability distributions come from?

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

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 …

- Some important issues:
  - Nature of the data (iid, correlated, …)
  - Objective function (MLE, MAP, …)
  - Algorithm (simple algebra, gradient methods, EM, …)
  - Evaluation scheme (likelihood on test data, predictability, consistency, …)

Parameter Learning from iid data

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

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

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

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

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

$$\hat{\theta}_{\mathrm{MLE}} = \arg\max_{\theta} L(\theta) = \arg\max_{\theta} \log L(\theta)$$

Example 1: Bernoulli model

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

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

- 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 $D = \{x_1, \ldots, x_N\}$:

$$L(\theta) = P(x_1, x_2, \ldots, x_N; \theta) = \prod_{i=1}^{N} P(x_i; \theta) = \prod_{i=1}^{N} \left(\theta^{x_i} (1-\theta)^{1-x_i} \right)$$

$$= \theta^{\sum_{i=1}^{N} x_i} (1-\theta)^{\sum_{i=1}^{N} 1-x_i} = \theta^{\#\text{head}} (1-\theta)^{\#\text{tails}}$$

MLE

- Objective function:

$$\ell(\theta) = \log L(\theta) = \log \theta^{n_h}(1-\theta)^{n_t} = n_h \log\theta + (N - n_h)\log(1-\theta)$$

- We need to maximize this w.r.t. θ

- Take derivatives wrt θ

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

Frequency as sample mean

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

Example 2: univariate normal

- Data:
  - We observed N ***iid*** real samples:

    D={-0.1, 10, 1, -5.2, …, 3}
- Model: $P(x) = \left(2\pi\sigma^2\right)^{-1/2} \exp\left\{-(x-\mu)^2 / 2\sigma^2\right\}$ $\quad \theta = (\mu,\sigma^2)$
- Log likelihood:

$$\ell(\theta) = \log L(\theta) = \prod_{i=1}^{N} P(x_i) = -\frac{N}{2}\log(2\pi\sigma^2) - \frac{1}{2}\sum_{i=1}^{N}\frac{(x_i-\mu)^2}{\sigma^2}$$

- MLE: take derivative and set to zero:

$$\frac{\partial \ell}{\partial \mu} = (1/\sigma^2)\sum_n (x_n - \mu)$$

$$\frac{\partial \ell}{\partial \sigma^2} = -\frac{N}{2\sigma^2} + \frac{1}{2\sigma^4}\sum_n (x_n-\mu)^2$$

$\Rightarrow$

$$\mu_{MLE} = \frac{1}{N}\sum_n x_n$$

$$\sigma^2_{MLE} = \frac{1}{N}\sum_n (x_n - \mu_{ML})^2$$

Overfitting

- Recall that for Bernoulli Distribution, we have

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

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

- The rescue "smoothing":
  - Where n' is know as the pseudo- (imaginary) count

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

  - But can we make this more formal?

Bayesian Learning

- The Bayesian Rule:

$$P(\theta \mid \mathcal{D}) = \frac{P(\mathcal{D} \mid \theta) P(\theta)}{P(\mathcal{D})}$$

Or equivalently,

$$\underbrace{P(\theta \mid \mathcal{D})}_{\text{posterior}} \propto \underbrace{P(\mathcal{D} \mid \theta)}_{\text{likelihood}} \underbrace{P(\theta)}_{\text{prior}}$$

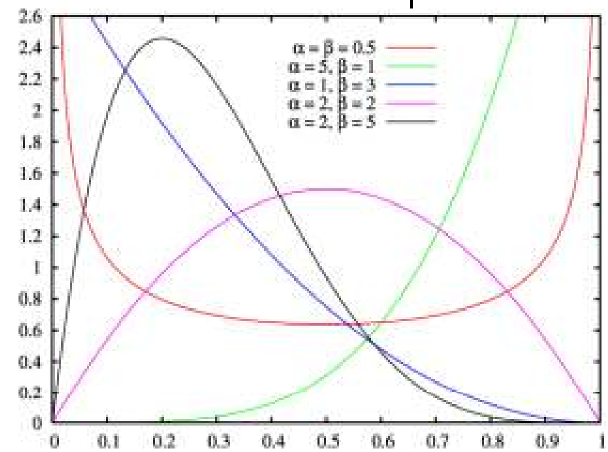
(Belief about coin toss probability)

MAP estimate: $\hat{\theta}_{MAP} = \arg\max_{\theta} P(\theta \mid D)$

If prior is uniform, MLE = MAP

Bayesian estimation for Bernoulli

- Beta(α,β) distribution:



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

- Posterior distribution of θ:

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

Beta($\alpha+n_h$,$\beta+n_t$)

  - Notice the isomorphism of the posterior to the prior,
  - such a prior is called a **conjugate prior**
  - *α and β* are hyperparameters (parameters of the prior) and correspond to the number of “virtual” heads/tails (pseudo counts)

MAP

- Posterior distribution of θ :

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

- Maximum *a posteriori* (MAP) estimation:

$$\hat{\theta}_{MAP} = \arg\max_{\theta} \log P(\theta \mid x_1,\ldots,x_N)$$

- Posterior mean estimation:

$$\hat{\theta}_{MAP} = \frac{n_h + \alpha}{N + \alpha + \beta}$$

Beta parameters can be understood as pseudo-counts

- With enough data, prior is forgotten

Dirichlet distribution

- number of heads in N flips of a two-sided coin
  - follows a binomial distribution
  - Beta is a good prior (conjugate prior for binomial)

- what it's not two-sided, but k-sided?
  - follows a multinomial distribution
  - Dirichlet distribution is the conjugate prior

$$P(\theta_1, \theta_2, \ldots \theta_K) = \frac{1}{B(\alpha)} \prod_{i}^{K} \theta_i^{(\alpha_1 - 1)}$$

Estimating the parameters of a distribution

- Maximum Likelihood estimation (MLE)

  Choose value that maximizes the probability of observed data

$$\hat{\theta}_{MLE} = \arg\max_{\theta} P(D \mid \theta)$$

- Maximum *a posteriori* (MAP) estimation

  Choose value that is most probable given observed data and prior belief

$$\hat{\theta}_{MAP} = \arg\max_{\theta} P(\theta \mid D) = \arg\max_{\theta} P(D \mid \theta) P(\theta)$$

MLE vs MAP (Frequentist vs Bayesian)

Frequentist/MLE approach:

θ is unknown constant, estimate from data

Bayesian/MAP approach:

θ is a random variable, assume a probability distribution

Drawbacks

MLE: Overfits if dataset is too small

MAP: Two people with different priors will end up with different estimates

Bayesian estimation for normal distribution

- Normal Prior:

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

- Joint probability:

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

- Posterior:

$$P(\mu \mid x) = \left(2\pi\tilde{\sigma}^2\right)^{-1/2} \exp\left\{-(\mu-\tilde{\mu})^2 / 2\tilde{\sigma}^2\right\}$$

where $\tilde{\mu} = \dfrac{N/\sigma^2}{N/\sigma^2+1/\tau^2}\bar{x} + \dfrac{1/\tau^2}{N/\sigma^2+1/\tau^2}\mu_0$, and $\tilde{\sigma}^2 = \left(\dfrac{N}{\sigma^2}+\dfrac{1}{\tau^2}\right)^{-1}$

Sample mean

Probability Review

What you should know:

- Probability basics
  - random variables, events, sample space, conditional probs, …
  - independence of random variables
  - Bayes rule
  - Joint probability distributions
  - calculating probabilities from the joint distribution
- Point estimation
  - maximum likelihood estimates
  - maximum a posteriori estimates
  - distributions – binomial, Beta, Dirichlet, …