## Motivation and Basics

Il-Chul Moon Dept. of Industrial and Systems Engineering KAIST

icmoon@kaist.ac.kr

# Weekly Objectives

- Motivate the study on
  - Machine learning, AI, Datamining....
  - Why? What?
  - Overview of the field
- Short questions and answers on a story
  - What consists of machine learning?
  - MLE
  - MAP
- Some basics
  - Probability
  - Distribution
  - And some rules...

#### **MOTIVATION**

## Keywords

- Many floating keywords
  - Data-mining, Knowledge discovery, Machine Learning, Artificial Intelligence...

AI in CS

- Comes from territory, perspectives, types of problems, researchers, etc
- We are going to focus on substance, not labeling.
- I am just going to call it "Machine Learning"
  - You can call it whatever you want



#### Abundance of Data

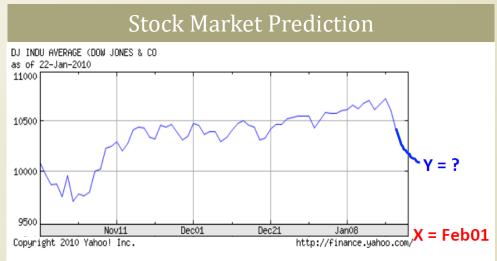


**Image Data** 

#### Examples of Machine Learning Applications

Machine Learning is everywhere...











# Spam Filtering and more



Table 2 Detailed evaluation results of SVMs with each representation scheme and varying training-set sizes. Macro-averaged MAE scores are provided with p-values, mulcating the statistical significances of performance improvement over that of BF (using basic features alone). Numbers in bold fond indicate the best method for each fixed training-set size. One star indicates the p-values in (0.01, 0.05]; two stars indicate the p-values equal or less than 1%.

	BF	BF+NC		BF+SI		BF+SIP		BF+SI+NC		BF+SI+NC+SIP	
# of tr	MAE	MAE	p-value	MAE	p-value	MAE	p-value	MAE	p-value	MAE	p-value
10	0.9666	0.9063	* 0.0382	0.8837	* 0.0106	0.8968	* 0.0311	0.9112	* 0.0211	0.8827	** 0.0087
20	0.9720	0.8969	0.0506	0.8596	* 0.0315	0.9095	* 0.0435	0.9071	0.0558	0.8659	* 0.0235

SVM?

- Spam filter
- More?
  - Importance vs. Urgency
- How to predict an important email?
  - Social networks
  - Contents
- Shinjae Yoo, Yiming Yang, Frank Lin, and Il-Chul Moon, Mining Social Networks for Personalized Email Prioritization, ACM SIGKDD Conference, Paris, France, Jun, 28, 2009

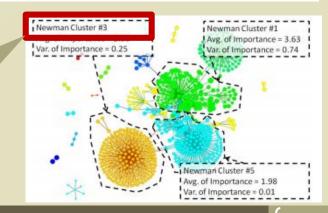
Features

Clusters?
Is this a
machine
learning
technique?

#### 5.3 Features

The basic features are the tokens in the sections of from, to, cc, title, and body text in email messages. Let us use a v-dimensional

is the vocabulary size. We call it the basic feature (BF) sub-vector.



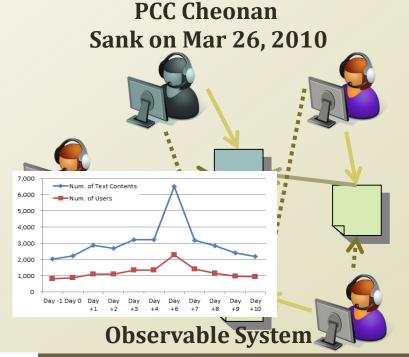
II-Chul Moon, Alice H. Oh, and Kathleen M. Carley, Analyzing Social Media in Escalating Crisis Situations, IEEE Conference on Intelligence and Security Informatics (ISI 2011), pp. 71-76, Beijing, China, Jul 10-12, 2011

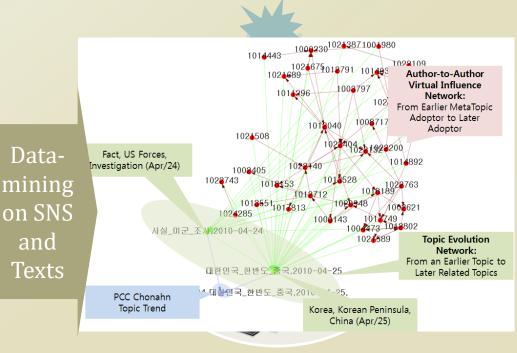
# pinion Mining and more



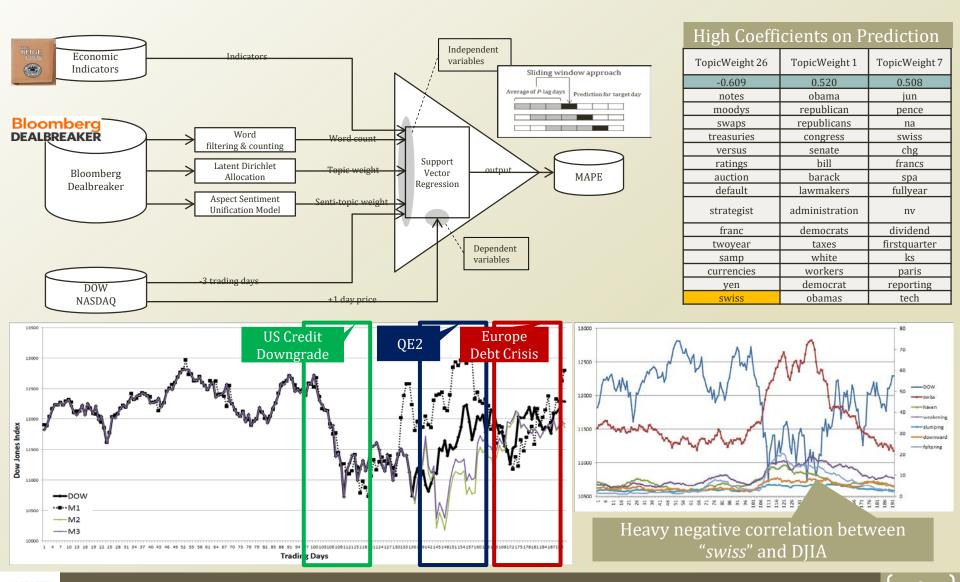
Finding out consensus of the population

- Mining population's perception of the event
- Mining key opinion buried in a data chunk
- Estimating future polarity of the population
- Strategy to maintain the unity of the population





#### Stock Market Prediction and more



# Types of Machine Learning

Machine Learning

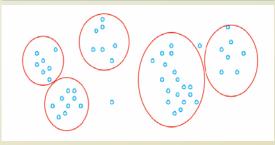
#### Supervised Learning

**You** know the true answers of some of instances



# Unsupervised Learning

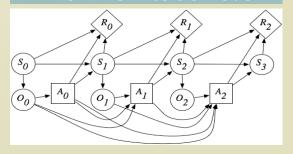
**You** do not know the true answers of instances



#### Reinforcement Learning

. . . . .

**You** do know the objective, but you do not know how to achieve



- You can
  - Machine learning
  - Dataset provider
  - Machine learning users
  - etc

- Various classifications by different professors
  - Purpose, data types, etc
- Other learning classifications also exist

# Supervised Learning

- You know the true value, and you can provide examples of the true value.
- Cases, such as
  - Spam filtering
  - Automatic grading
  - Automatic categorization
- Classification or Regression of
  - Hit or Miss: Something has either disease or not.
  - Ranking: Someone received either A+, B, C, or F.
  - Types: An article is either positive or negative.
  - Value prediction: The price of this artifact is X.
- Methodologies
  - Classification: estimating a discrete dependent value from observations
  - Regression: estimating a (continuous) dependent value from observations

#### Supervised Learning

**You** know the true answers of some of instances

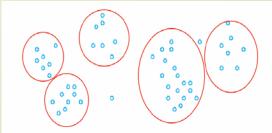


# Unsupervised Learning

- You don't know the true value, and you cannot provide examples of the true value.
- Cases, such as
  - Discovering clusters
  - Discovering latent factors
  - Discovering graph structures
- Clustering or filtering or completing of
  - Finding the representative topic words from text data
  - Finding the latent image from facial data
  - Completing the incomplete matrix of product-review scores
  - Filtering the noise from the trajectory data
- Methodologies
  - Clustering: estimating sets and affiliations of instances to the sets
  - Filtering: estimating underlying and fundamental signals from the mixture of signals and noises

#### Unsupervised Learning

**You** do not know the true answers of instances

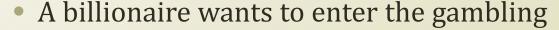




## WARMING UP A SHORT EPISODE

## Thumbtack Question

- There is a gambling site with a game of flipping a thumbtack
  - Nail is up, and you betted on nail's up you get your money in double
  - Same to the nail's down



- With scientific and engineering supports
  - He is paying you a big chunk of money
- He asks you
  - I have a thumbtack, if I flip it, what's the probability that it will fall with the nail's up?
- Your response?



# Experience from trials

- My response is
  - Please flip it a few times
- Billionaire tried for five times
  - The nail's up case is three out of five trials
- My response is
  - You should invest
    - 3/5 to nail's up case
    - 2/5 to nail's down case
- The billionaire asks why?
- Then,
  - You answer.....



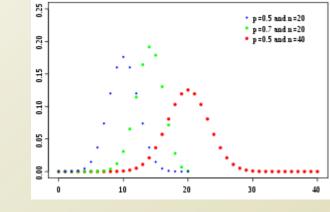








## Binomial Distribution



- Binomial distribution is
  - The discrete probability distribution
    - Of the number of successes in a sequence of n independent yes/no experiments, and each success has the probability of  $\theta$
  - Also called a Bernoulli experiment
- Flips are i.i.d
  - Independent events
  - Identically distributed according to binomial distribution
- $P(H) = \theta, P(T) = 1 \theta$
- P(HHTHT)=  $\theta\theta$  (1- $\theta$ )  $\theta$  (1- $\theta$ )= $\theta^3$ (1- $\theta$ )<sup>2</sup>
- Let's say
  - D as Data = H,H,T,H,T
    - n=5
    - $k=a_{H}=3$
    - p= θ

 $f(k; n, p) = P(K = k) = {n \choose k} p^k (1 - p)^{n-k}$ 

 $\boldsymbol{n}$  and  $\boldsymbol{p}$  are given as

parameters, and the value

is calculated by varying k

 $P(D|\theta) = \theta^{a_H} (1-\theta)^{a_T}$ 

Makes order insensitive

 $\binom{n}{k} = \frac{n!}{k! (n-k)!}$ 

## Maximum Likelihood Estimation

- $P(D|\theta) = \theta^{a_H}(1-\theta)^{a_T}$
- Data: We have observed the sequence data of D with a<sub>H</sub> and a<sub>T</sub>
- Our hypothesis
  - The gambling result of thumbtack follows the binomial distribution of  $\theta$
- How to make our hypothesis strong?
  - Finding out a better distribution of the observation
    - Can be done, but you need more rational.
  - Finding out the best candidate of  $\boldsymbol{\theta}$ 
    - What's the condition to **make**  $\theta$  *most plausible?*
- One candidate is the **Maximum Likelihood Estimation (MLE) of**  $\theta$ 
  - Choose θ that maximizes the probability of observed data

$$\widehat{\boldsymbol{\theta}} = argmax_{\boldsymbol{\theta}} P(\boldsymbol{D}|\boldsymbol{\theta})$$

#### **MLE Calculation**

• 
$$\hat{\theta} = argmax_{\theta}P(D|\theta) = argmax_{\theta}\theta^{a_H}(1-\theta)^{a_T}$$

- This is going nowhere, so you use a trick
  - Using the log function

• 
$$\hat{\theta} = argmax_{\theta} lnP(D|\theta) = argmax_{\theta} ln\{\theta^{a_H}(1-\theta)^{a_T}\}\$$
  
=  $argmax_{\theta}\{a_H ln\theta + a_T ln(1-\theta)\}\$ 

 Then, this is a maximization problem, so you use a derivative that is set to zero

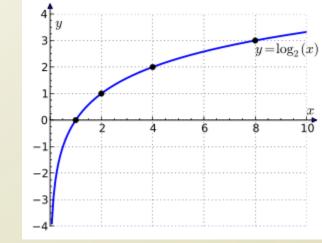
• 
$$\frac{d}{d\theta}(a_H \ln\theta + a_T \ln(1-\theta)) = 0$$

• 
$$\frac{a_H}{\theta} - \frac{a_T}{1-\theta} = 0$$

• 
$$\theta = \frac{a_H}{a_T + a_H}$$

• When  $\theta$  is  $\frac{a_H}{a_T + a_H}$ , the  $\theta$  becomes the best candidate from the MLE perspective

• 
$$\hat{\theta} = \frac{a_H}{a_H + a_T}$$



## Number of Trials

$$\widehat{\theta} = \frac{a_H}{a_H + a_T}$$











- You report your proof to the billionaire
  - From the observations of your trials, and from the MLE perspective, and by assuming the binomial distribution assumption.....
  - **0** is 0.6
  - So, you are more likely to win a bet if you choose the head
- He says okay.
  - Billionaire
    - While you were calculating, I was flipping more times.
    - It turns out that we have 30 heads and 20 tails.
    - Does this change anything?
  - Your response
    - No, nothing's changed. Same. 0.6
  - Billionaire
    - Then, I was just spending time for nothing????
- You say no
  - Your additional trials are valuable to ......

# Simple Error Bound

- Your response
  - Your additional trials reduce the error of our estimation
  - Right now, we have  $\hat{\theta} = \frac{a_H}{a_H + a_T}$ ,  $N = a_H + a_T$
  - Let's say  $\theta^*$  is the true parameter of the thumbtack flipping for any error,  $\epsilon > 0$
  - We have a simple upper bound on the probability provided by Hoeffding's inequality
  - $P(|\hat{\theta} \theta^*| \ge \varepsilon) \le 2e^{-2N\varepsilon^2}$

Coming from a friend in the math. dept.

- Billionaire asks you
  - Can you calculate the required number of trials, N?
    - To obtain  $\varepsilon = 0.1$  with 0.01% case
- Now, your professor jumps in and says
  - This is Probably Approximate Correct (PAC) learning
    - Probably? (0.01% case)
    - Approximately? ( $\varepsilon = 0.1$ )

# Probably Approximately Correct Learning

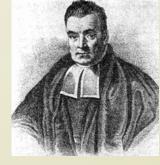


- The PAC learning theory from the machine learning community,
  - The learner
    - Receives sample data
    - Select a generalization function, hypothesis
      - From a certain class of possible functions
    - Such that the selected function
      - Has low generalization error
      - With high probability
- Definition of machine learning
  - Many views exist
  - Tom Mitchell
    - A computer program is said to
      - learn from experience E
      - With respect to some class of tasks T
      - And performance measure P, if its performance at tasks in T, as measured by P, improves with experience E
- Is PAC Learning machine learning?

Old, but good book, So called classic

#### **Machine Learning**

Given a dataset, we select a **generalized function** that provides **most probable and most approximate answers** 



# Wait!!!

A student whose name is Bayes raised his hand

# Incorporating Prior Knowledge

- Bayes says
  - Wait. Billionaire.
  - Is it really true that the thumbtack has 60% chance of head?
  - Don't you think it is 50 vs 50?
- Billionaire says
  - Well. I thought so...
  - But, how to merge the previous knowledge to my trials?
- Bayes says
  - So, I give you this theorem!

• 
$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$$

- You already dealt with  $P(D|\theta) = \theta^{a_H} (1-\theta)^{a_T}$
- $P(\theta)$  is the part of the prior knowledge
- Your response is
  - Then,  $P(\theta|D)$  is the conclusion influenced by the data and the prior knowledge?

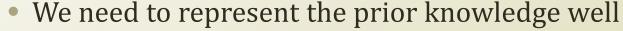
 $P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$ 

 $Posterior = \frac{Likelihood \times Prior \ Knowledge}{Normalizing \ Constant}$ 

- Bayes says
  - Yes, and it will be our future prior knowledge!

# More Formula from Bayes Viewpoint

- $P(\theta|D) \propto P(D|\theta)P(\theta)$ 
  - $P(D|\theta) = \theta^{a_H} (1-\theta)^{a_T}$
  - $P(\theta) = ????$



- Nice match to the range!
- So, the multiply goes smooth and does not complicate the formula

0.4

0.2

- Bayes says
  - Why not use the Beta distribution?

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

- Your response is
  - Wow convenient!

• 
$$P(\theta|D) \propto P(D|\theta)P(\theta) \propto \theta^{a_H}(1-\theta)^{a_T}\theta^{\alpha-1}(1-\theta)^{\beta-1}$$
  
=  $\theta^{a_H+\alpha-1}(1-\theta)^{a_T+\beta-1}$ 

Also, you notice one interesting face from the above formula...

#### Maximum a Posteriori Estimation

- Billionaire says
  - Hey! Stop! I am here!
  - So, you are talking about the formula
  - I want the most probable and more approximate  $\theta$
- Your response is
  - We are there.
  - Previously in MLE, we found  $\theta$  from  $\hat{\theta} = argmax_{\theta}P(D|\theta)$ 
    - $P(D|\theta) = \theta^{a_H} (1-\theta)^{a_T}$
    - $\hat{\theta} = \frac{a_H}{a_H + a_T}$
  - Now in MAP, we find  $\theta$  from  $\hat{\theta} = argmax_{\theta}P(\theta|D)$ 
    - $P(\theta|D) \propto \theta^{a_H + \alpha 1} (1 \theta)^{a_T + \beta 1}$
    - $\hat{\theta} = \frac{a_H + \alpha 1}{a_H + \alpha + a_T + \beta 2}$
  - The calculation is same because anyhow it is the maximization

#### Conclusion from Anecdote

- Billionaire says
  - Wait you and Bayes!
  - Who is right? The numbers are different!
- Bayes says
  - Not really... if you give us enough money to replicate the game!
- You say
  - Yes! If  $a_H$  and  $a_T$  become big,  $\alpha$  and  $\beta$  becomes nothing...
- Billionaire says
  - Enough talking
  - Still,  $\alpha$  and  $\beta$  are important if I don't give you more trials
  - Who decides  $\alpha$  and  $\beta$ ?
- Bayes and you say
  - Well... maybe grad students? =)

#### MLE

$$\hat{\theta} = \frac{a_H}{a_H + a_T}$$

#### **MAP**

$$\hat{\theta} = \frac{a_H + \alpha - 1}{a_H + \alpha + a_T + \beta - 2}$$

#### **BASICS**

# What we just saw is...

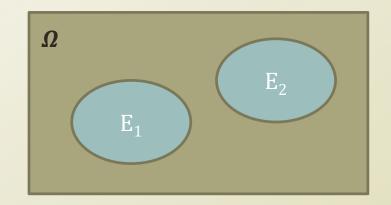
- A struggle
  - Billionaire
    - To earn money by analyzing a small dataset out of huge possibilities
  - You
    - To give the billionaire the best probable and approximate answers from the small dataset
  - Bayes
    - To convince you that the prior knowledge can be incorporated to the answers
- Eventually
  - Trying to find out the nature of the thumbtack game
  - The key is the probability of the thumbtack outcome, either head or tail
- Underlying knowledge to solve the problem
  - Probability
  - Distribution
  - Some mathematical tricks
- To go further, you need to know these

#### **Bayes says**

Why not use the Beta distribution?← From the knowledge of probability,

distribution, and statistics

# Probability



- Philosophically, Either of the two
  - Objectivists assign numbers to describe states of events, i.e. counting
  - Subjectivists assign numbers by your own belief to events, i.e. betting
- Mathematically
  - A function with the below characteristics

$$P(E) \in R$$
  $P(E) \ge 0$   $\forall E \in F$   $P(\Omega) = 1$  
$$P(E_1 \cup E_2 \cup \cdots) = \sum_{i=1}^{\infty} P(E_i) \text{ when a sequence of mutually exclusive}$$

Subsequent characteristics

if 
$$A \subseteq B$$
 then  $P(A) \le P(B)$   $P(\emptyset) = 0$   $0 \le P(E) \le 1$  
$$P(A \cup B) = P(A) + P(B) - P(A \cap B)$$
  $P(E^C) = 1 - P(E)$ 

# Conditional Probability

- Scope  $\approx$  Condition  $E_2$
- We often do not handle the universe,  $\Omega$
- Somehow, we always make conditions
  - Assuming that the parameters are X, Y, Z,....
  - Assuming that the events in the scope of X, Y, Z,....

• 
$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$

$$Posterior = \frac{Likelihood \times Prior \ Knowledge}{Normalizing \ Constant}$$

- The conditional probability of A given B
- Some handy formula

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

$$P(A) = \sum_{n} P(A|B_n)P(B_n)$$

Nice to see that we can switch the condition and the target event

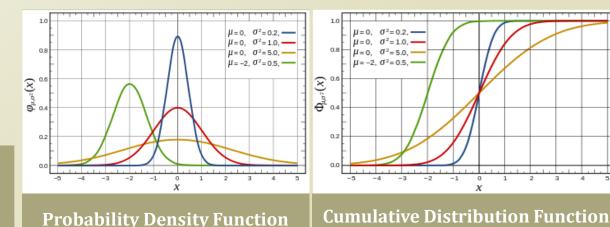
Nice to see that we can recover the target event by adding the whole conditional probs and priors

# Probability Distribution

- Probability distribution assigns
  - A probability to a subset of the potential events of a random trial, experiment, survey, etc.
- A function mapping an event to a probability
  - Because we call it a probability, the probability should keep its own characteristics (or axioms)
  - An event can be
    - A continuous numeric value from surveys, trials, experiments...
    - A discrete categorical value from surveys, trials, experiments...
- For example,

$$f(x) = \frac{e^{-\frac{1}{2}x^2}}{\sqrt{2\pi}}$$

f: a probability distribution function x: a continuous value f(x): assigned probs



(CDF) =  $\int_{-\infty}^{x} f(x) dx$ 

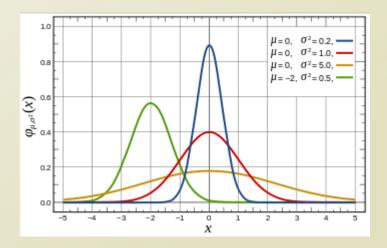
(PDF)=f(x)

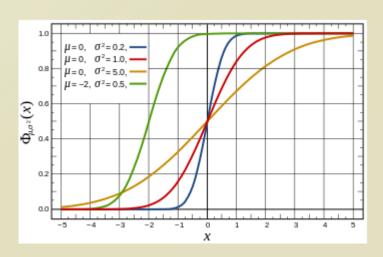
#### Normal Distribution

- Very commonly observed distribution
  - Continuous numerical value

• 
$$f(x; \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

- Notation:  $N(\mu, \sigma^2)$
- Mean: μ
- Variance:  $\sigma^2$





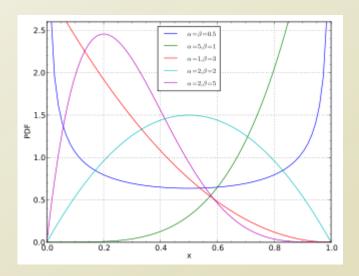
#### Beta Distribution

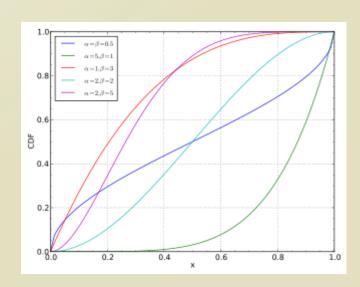
- Supports a closed interval
  - Continuous numerical value
  - [0,1]
  - Very nice characteristic
  - Why?
    - Matches up the characteristics of probs

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

$$\Gamma(\alpha) = (\alpha - 1)!$$

- Notation: Beta $(\alpha, \beta)$
- Mean:  $\frac{\alpha}{\alpha + \beta}$
- Variance:  $\frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$



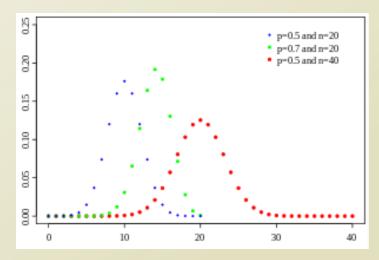


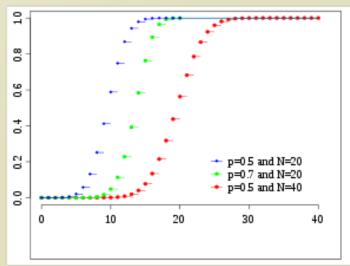
## Binomial Distribution

- Simplest distribution for discrete values
  - Bernoulli trial, yes or no
  - 0 or 1
  - Selection, switch....

• 
$$f(\theta; n, p) = \binom{n}{k} p^k (1-p)^{n-k}, \binom{n}{k} = \frac{n!}{k!(n-k)!}$$

- Notation: B(n, p)
- Mean: *np*
- Variance: np(1-p)





## Multinomial Distribution

- The generalization of the binomial distribution
  - Beyond yes/no
  - Choose A, B, C, D, E,...,Z
  - Word selection, cluster selection.....
- $f(x_1, ..., x_k; n, p_1, ..., p_k) = \frac{n!}{x_1!...x_k!} p_1^{x_1} ... p_k^{x_k}$
- Notation:  $Mult(P), P = \langle p_1, ..., p_k \rangle$
- Mean:  $E(x_i) = np_i$
- Variance:  $Var(x_i) = np_i(1 p_i)$

## Acknowledgement

- This slideset is greatly influenced
  - By Prof. Carlos Guestrin at CMU
  - By Prof. Eric P. Xing at CMU
- Some images are copied from the lecture slides made
  - By Prof. Carlos Guestrin at CMU
  - By Prof. Eric P. Xing at CMU

# Further Readings

Bishop Chapter 1 and 2