Chapter 6 Probability-based Learning Part B

Prof. Chang-Chieh Cheng

Dept. Computer Science

National Chiao Tung University, Taiwan

Continuous Features

- Categorical feature → Discrete random variable
 - $X = \{X_1, X_2, \dots, X_m\}$
 - $P(X_1) + P(X_2) + \dots + P(X_m) = 1.0$
- Continuous feature → Continuous random variable
 - $X \in \mathbf{R}$

$$P(a \le X \le b) = \int_a^b f(x) \, dx \le 1.0$$

$$P(X) = \int_{-\infty}^{\infty} f(x) \, dx = 1.0$$

Continuous Features

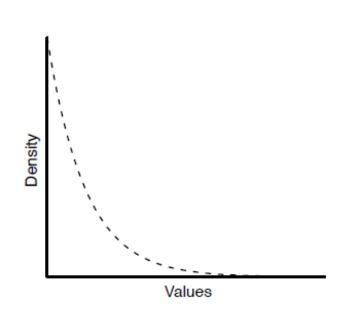
- Probability density function (PDF)
- If f is a PDF

$$\int_{-\infty}^{\infty} f(x) \, dx = 1.0$$

- A PDF can be used to represent the probability distribution of a continuous random variable.
- Using a PDF to fit a probability distribution
- Five standard PDFs
 - Exponential
 - Normal
 - Student-t
 - Mixture Gaussians
 - Gamma

Exponential

$$E(x,\lambda) = \lambda e^{-\lambda x}$$
 if $x > 0$, otherwise = 0

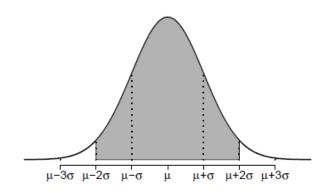


$$x \in \mathbf{R}$$

 $\lambda \in \mathbf{R} \text{ and } \lambda > 0$

- Normal distribution
 - Gaussian function

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



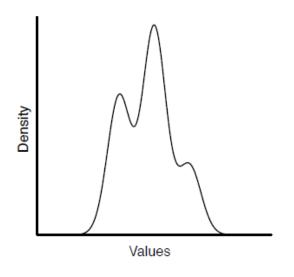
$$x \in \mathbf{R}$$

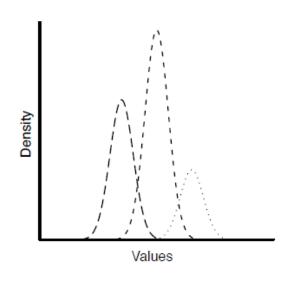
 $\mu \in \mathbf{R}$
 $\sigma \in \mathbf{R}$ and $\sigma > 0$

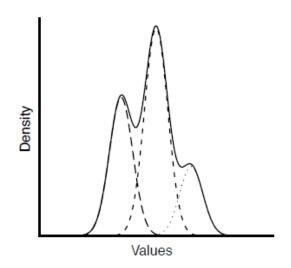
Mixture Gaussians

$$N(x, \mathbf{u}, \boldsymbol{\sigma}, \mathbf{w}) = \sum_{i=1}^{n} \frac{w_i}{\sigma_i \sqrt{2\pi}} e^{-\frac{(x-\mu_i)^2}{2\sigma_i^2}}$$

$$\begin{aligned} & x \in \mathbf{R} \\ & \mathbf{u} = \{\mu_1, \mu_2, ..., \mu_n | \mu_i \in \mathbf{R} \} \\ & \mathbf{\sigma} = \{\sigma_1, \sigma_2, ..., \sigma_n | \sigma_i \in \mathbf{R} > 0 \} \\ & \mathbf{w} = \{w_1, w_2, ..., w_n | w_i \in \mathbf{R} > 0 \} \end{aligned}$$







Student-t

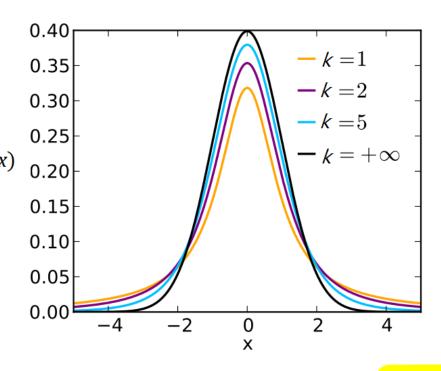
$$\tau(x,k) = \frac{\Gamma(\frac{k+1}{2})}{\sqrt{k\pi}\Gamma(\frac{k}{2})} (1 + \frac{x^2}{k})^{-\frac{k+1}{2}}$$

$$x \in \mathbf{R}$$

 $k \in \mathbf{N} \text{ and } k > 0$

$$\Gamma(n) = (n-1)!$$
 where $n \in \mathbb{N} > \mathbf{0}$

$$\Gamma(z) = \int_0^\infty x^{z-1} e^{-x} dx \qquad \tau(z)$$
where $z \in \mathbf{C} >$ and $\mathbf{real}(\mathbf{z}) > \mathbf{0}$



- Student-t
 - if *k* is even

$$\frac{\Gamma(\frac{k+1}{2})}{\sqrt{k\pi}\Gamma(\frac{k}{2})} = \frac{(k-1)(k-3)\dots 5\cdot 3}{2\sqrt{k}(k-2)(k-4)\dots 4\cdot 2}$$

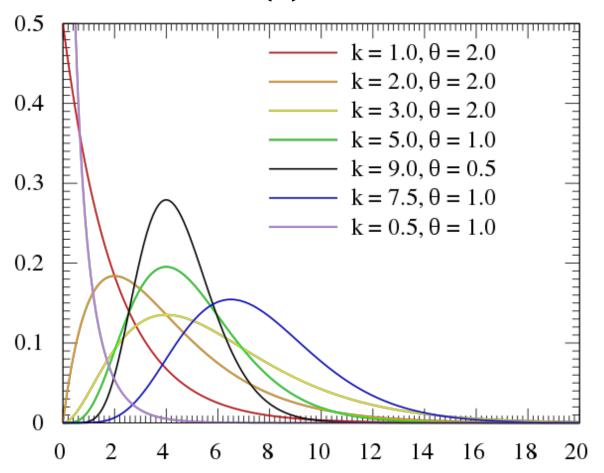
Otherwise

$$\frac{\Gamma(\frac{k+1}{2})}{\sqrt{k\pi}\Gamma(\frac{k}{2})} = \frac{(k-1)(k-3)\dots 4\cdot 2}{\pi\sqrt{k}(k-2)(k-4)\dots 5\cdot 3}$$

$$\Gamma\left(-\frac{3}{2}\right) = \frac{4}{3}\sqrt{\pi}$$
 $\Gamma\left(-\frac{1}{2}\right) = -2\sqrt{\pi}$
 $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$
 $\Gamma\left(\frac{3}{2}\right) = \frac{1}{2}\sqrt{\pi}$
 $\Gamma\left(\frac{5}{2}\right) = \frac{3}{4}\sqrt{\pi}$
 $\Gamma\left(\frac{7}{2}\right) = \frac{15}{8}\sqrt{\pi}$

Gamma distribution

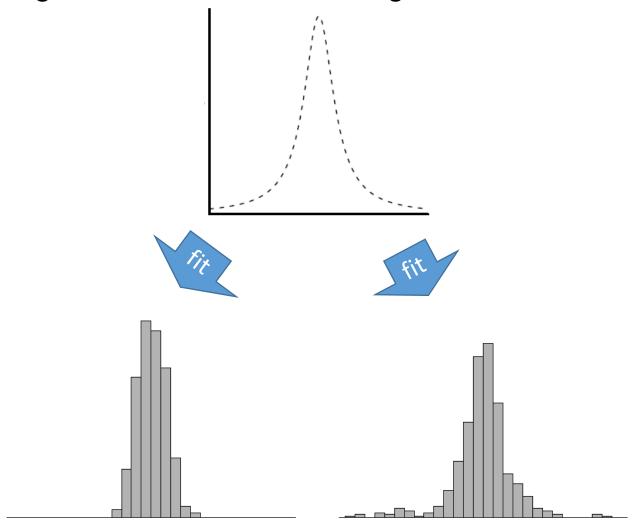
$$G(x, k, \theta) = \frac{1}{\Gamma(k)\theta^k} x^{k-1} e^{-\frac{x}{\theta}}$$



 χ

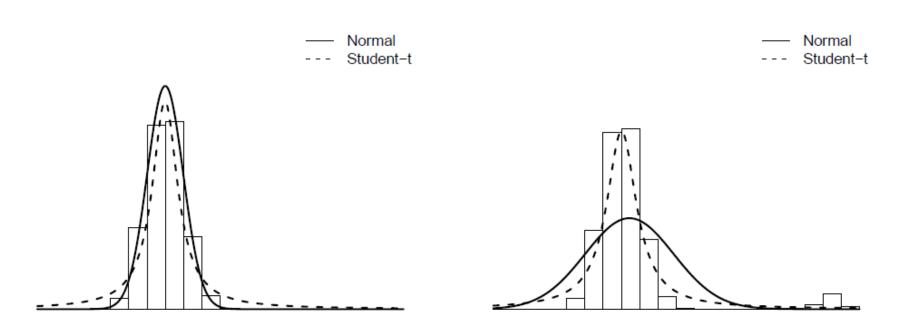
PDF Fitting

Fitting a PDF to different histograms



PDF Fitting

• Fitting different PDFs to a histogram



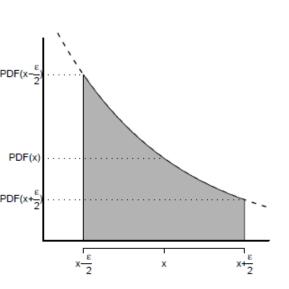
the same dataset

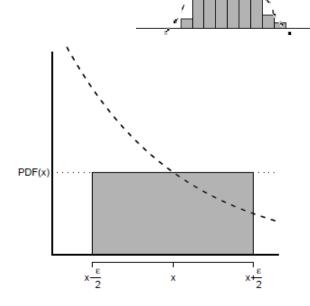
PDF Fitting

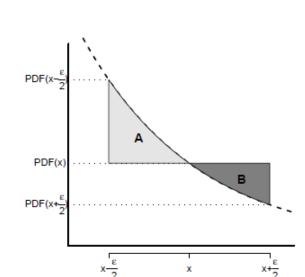
Interval error

- Errors produced by the interval size
- There is no hard and fast rule for deciding on interval size

By case







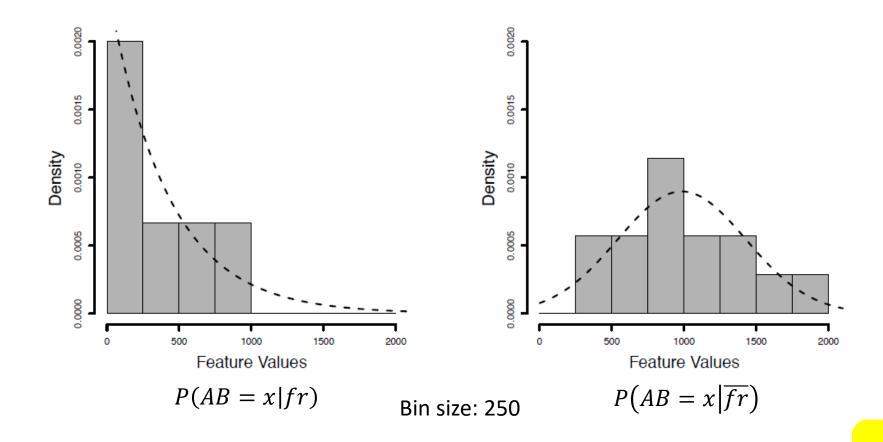
A: + error

B: - error

• An example of loan application fraud detection with account balance (AB)

	CREDIT	Guarantor/		ACCOUNT	
ID	HISTORY	CoApplicant	ACCOMMODATION	BALANCE	FRAUD
1	current	none	own	56.75	true
2	current	none	own	1,800.11	false
3	current	none	own	1,341.03	false
4	paid	guarantor	rent	749.50	true
5	arrears	none	own	1,150.00	false
6	arrears	none	own	928.30	true
7	current	none	own	250.90	false
8	arrears	none	own	806.15	false
9	current	none	rent	1,209.02	false
10	none	none	own	405.72	true
11	current	coapplicant	own	550.00	false
12	current	none	free	223.89	true
13	current	none	rent	103.23	true
14	paid	none	own	758.22	false
15	arrears	none	own	430.79	false
16	current	none	own	675.11	false
17	arrears	coapplicant	rent	1,657.20	false
18	arrears	none	free	1,405.18	false
19	arrears	none	own	760.51	false
20	current	none	own	985.41	false

- Binning for continuous data → Histogram
- Choose a PDF to fit each histogram



- A simple method to fit the exponential distribution
 - Compute the sample mean, μ , of the Account Balance where Fraudulent = 'True'
 - Let $\lambda = \frac{1}{\mu}$
 - Then,

$$E(x) = \frac{1}{\mu}e^{-\frac{x}{\mu}}$$

- A simple method to fit the normal distribution
 - Compute the sample mean, μ , and standard deviation, σ , of the Account Balance where Fraudulent = 'False'
 - Then,

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

- To implement a probability-based learning model, you have to do that
 - applying the Laplace smoothing for each categorical feature, and
 - fitting a PDF for each continuous feature

- For example, how about that FRAUDULENT (FR) = ? if
 - CREDIT HISTORY (CH) = paid
 - GUARANTOR/COAPPLICANT (GC) = guarantor
 - ACCOMODATION (ACC) = free
 - *ACCOUNT BALANCE* (*AB*) = 759.07

$$P(fr) = 0.3$$
 $P(\neg fr) = 0.7$ $P(CH = paid|fr) = 0.2222$ $P(CH = paid|\neg fr) = 0.2692$ $P(GC = guarantor|fr) = 0.2667$ $P(GC = guarantor|\neg fr) = 0.1304$ $P(ACC = free|fr) = 0.2$ $P(ACC = free|\neg fr) = 0.1739$ $P(AB = 759.07|fr)$ $P(AB = 759.07|\neg fr)$ $P(AB = 759.07, \ \lambda = 0.0024)$ $P(AB = 759.07, \ \mu = 984.26, \ \sigma = 460.94)$ $P(AB = 769.07, \ \mu = 984.26, \ \sigma = 460.94)$

 $(\prod_{k=1}^{m} P(\mathbf{q}[k]|\neg fr)) \times P(\neg fr) = 0.0000033$

Binning & Naive Bayes' Classifier

 The loan application fraud detection with a second continuous descriptive feature added: LOAN AMOUNT (LA)

	0	0		A	1	
	CREDIT	GUARANTOR/	-	ACCOUNT	Loan	
ID	HISTORY	CoApplicant	ACCOMMODATION	BALANCE	AMOUNT	FRAUD
1	current	none	own	56.75	900	true
2	current	none	own	1 800.11	150 000	false
3	current	none	own	1 341.03	48 000	false
4	paid	guarantor	rent	749.50	10 000	true
5	arrears	none	own	1 150.00	32 000	false
6	arrears	none	own	928.30	250 000	true
7	current	none	own	250.90	25 000	false
8	arrears	none	own	806.15	18 500	false
9	current	none	rent	1 209.02	20 000	false
10	none	none	own	405.72	9 500	true
11	current	coapplicant	own	550.00	16750	false
12	current	none	free	223.89	9850	true
13	current	none	rent	103.23	95 500	true
14	paid	none	own	758.22	65 000	false
15	arrears	none	own	430.79	500	false
16	current	none	own	675.11	16 000	false
17	arrears	coapplicant	rent	1 657.20	15 450	false
18	arrears	none	free	1 405.18	50 000	false
19	arrears	none	own	760.51	500	false
20	current	none	own	985.41	35 000	false

Binning & Naive Bayes' Classifier

• Bin size

Bin Thresholds					
	Bin1	≤ 9,925			
9,925 <	Bin2	\leq 19,250			
19,225 <	Bin3	\le 49,000			
49,000 <	Bin4				

		BINNED					BINNED	
	Loan	Loan				Loan	LOAN	
ID	A MOUNT	A MOUNT	FRAUD		ID	A MOUNT	A MOUNT	FRAUD
15	500	bin1	false	_	9	20,000	bin3	false
19	500	bin1	false		7	25,000	bin3	false
1	900	bin1	true		5	32,000	bin3	false
10	9,500	bin1	true		20	35,000	bin3	false
12	9,850	bin1	true		3	48,000	bin3	false
4	10,000	bin2	true		18	50,000	bin4	false
17	15,450	bin2	false		14	65,000	bin4	false
16	16,000	bin2	false		13	95,500	bin4	true
11	16,750	bin2	false		2	150,000	bin4	false
8	18,500	bin2	false		6	250,000	bin4	true

Binning & Naive Bayes' Classifier

- *FRAUDULENT (FR)* = ? if
 - CREDIT HISTORY (CH) = paid
 - GUARANTOR/COAPPLICANT (GC) = guarantor
 - ACCOMODATION (ACC) = free
 - ACCOUNT BALANCE (AB) = 759.07
 - LOAN AMOUNT(LA) = 8000

$$P(fr) = 0.3 \qquad P(\neg fr) = 0.7$$

$$P(CH = paid|fr) = 0.2222 \qquad P(CH = paid|\neg fr) = 0.2692$$

$$P(GC = guarantor|fr) = 0.2667 \qquad P(GC = guarantor|\neg fr) = 0.1304$$

$$P(ACC = free|fr) = 0.2 \qquad P(ACC = free|\neg fr) = 0.1739$$

$$P(AB = 759.07|fr) \qquad P(AB = 759.07|\neg fr)$$

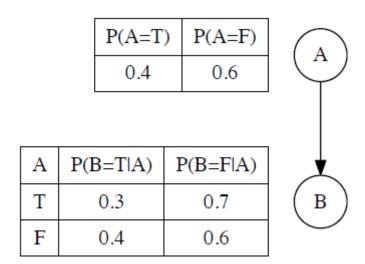
$$\approx E\left(\begin{array}{c} 759.07, \\ \lambda = 0.0024 \end{array}\right) = 0.00039 \qquad \approx N\left(\begin{array}{c} 759.07, \\ \mu = 984.26, \\ \sigma = 460.94 \end{array}\right) = 0.00077$$

$$P(BLA = bin1|fr) = 0.3333 \qquad P(BLA = bin1|\neg fr) = 0.1923$$

$$\left(\prod_{k=1}^{m} P(\mathbf{q}[k] \mid fr)\right) \times P(fr) = 0.000000462$$

$$\left(\prod_{k=1}^{n} P(\mathbf{q}[k] \mid \neg fr)\right) \times P(\neg fr) = 0.000000633$$

- A graph-based representation to encode the structural relationships
- It use a directed acyclic graph that is composed of thee basic elements:
 - Nodes
 - Edges
 - Conditional probability tables



 Recall the chain rule, the joint probability can be computed as follows

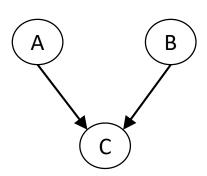
$$P(X_1, X_2, \dots, X_m) = P(X_1) \prod_{i=2}^m P(X_i | X_{i-1}, \dots, X_2, X_1)$$

In a Bayesian network

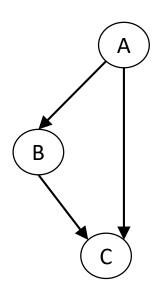
$$P(X_1, X_2, \dots, X_m) = \prod_{i=1}^m P(X_i | Parents(X_i))$$



$$P(A,B) = P(A)P(B \mid A)$$

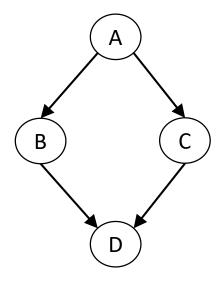


$$P(A, B, C) = P(A)P(B)P(C \mid A, B)$$



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

$$P(A,B,C) = P(A)P(B|A)P(C \mid A,B)$$



$$P(A, B, C) = P(A)P(B|A)P(C|A)$$

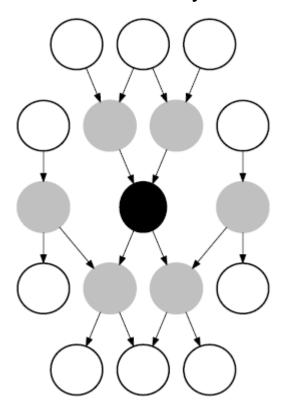
$$P(A, B, C, D) = P(A)P(B|A)P(C|A)P(D|B, C)$$

- Constructing a Bayesian network for m ordered variables, $\{X_1, X_2, ..., X_m\}$
 - For i = 1 to n
 - add X_i to the network
 - select parent from $\{X_1, X_2, ..., X_{i-1}\}$, the selected parent must guarantees

$$P(X_{1}, X_{2}, ..., X_{m}) = P(X_{1}) \prod_{i=2}^{m} P(X_{i} | X_{i-1}, ..., X_{2}, X_{1})$$

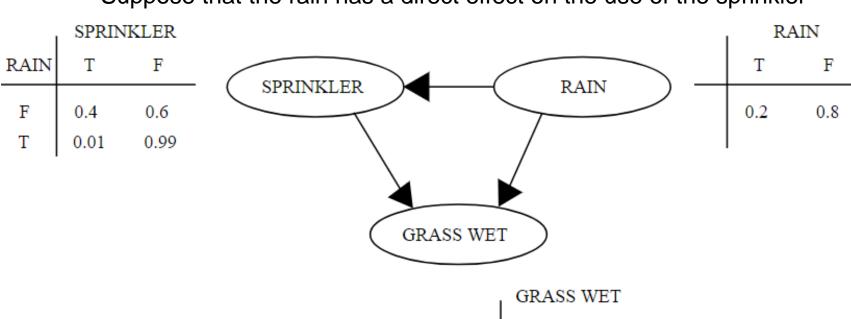
$$= \prod_{i=1}^{m} P(X_{i} | Parents(X_{i}))$$

- Markov blanket
 - The Markov blanket of a node is the set of nodes consisting of its parents, its children, and any other parents of its children.



The black node is **conditionally independence** of the white nodes

- Example
 - There are two events which could cause grass to be wet (G): either the sprinkler (S) is on or it's raining (R).
 - Suppose that the rain has a direct effect on the use of the sprinkler



		GRASS WET		
SPRINKLER	RAIN	T	F	
F	F	0.0	1.0	
F	T	0.8	0.2	
T	F	0.9	0.1	
T	T	0.99	0.01	

- What is the probability that it is raining, given the grass is wet?
 - $P(R = true \mid G = true) = P(r \mid g) = ?$

$$P(r | g) = \frac{P(g,r)}{P(g)}$$

$$= \frac{P(g,s,r) + P(g,\bar{s},r)}{P(g,\bar{s},\bar{r}) + P(g,\bar{s},r) + P(g,s,r)}$$

$$P(G,S,R) = ?$$

The joint probability in Bayesian network:

$$P(G,S,R) = P(R) P(S|R)P(G|S,R)$$

- Check the Bayesian network, we have:
 - P(r) = 0.2
 - P(s|r) = 0.01
 - P(g|s,r) = 0.99
- Then,

$$P(g, s, r) = 0.2 \times 0.01 \times 0.99 = 0.00198$$

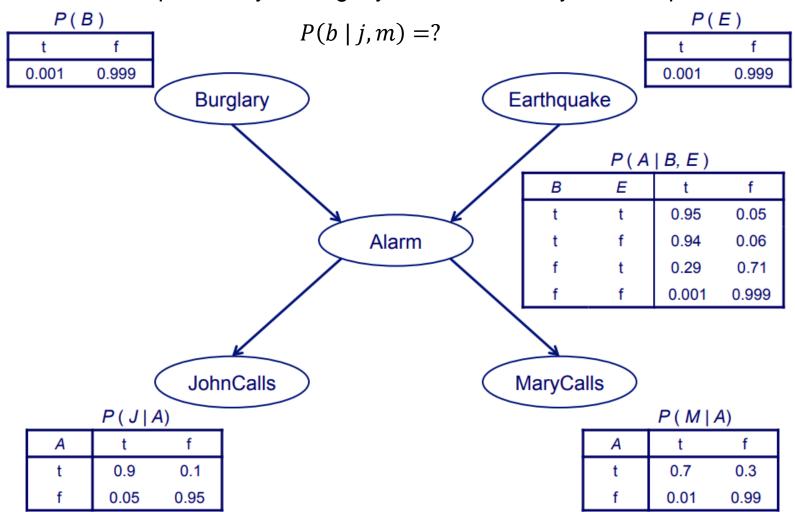
- Other joint probabilities
 - $P(g, \bar{s}, \bar{r}) = P(\bar{r})P(\bar{s}, |\bar{r})P(g|\bar{s}, \bar{r}) = 0.8 \times 0.6 \times 0.0 = 0.0$
 - $P(q, \bar{s}, r) = P(r)P(\bar{s}, |r)P(q|\bar{s}, r) = 0.2 \times 0.99 \times 0.8 = 0.1584$
 - $P(q, s, \bar{r}) = P(\bar{r})P(s, |\bar{r})P(q|s, \bar{r}) = 0.8 \times 0.4 \times 0.9 = 0.288$

• Therefore,

$$P(r \mid g) = \frac{0.00198 + 0.1584}{0.00198 + 0.288 + 0.1584 + 0.0} = 0.3577$$

Example

• What is the probability of burglary if John and Mary call to report the alarm



Because

$$P(b | j,m) = \frac{P(b,j,m)}{P(j,m)} = \frac{P(b,j,m)}{P(b,j,m) + P(\bar{b},j,m)}$$

And

$$P(b, e, a, j, m) = p(b)p(e)p(a|b, e)p(j|a)p(m|a)$$

Therefore,

$$P(b, e, j, m) = \sum_{A \in \{a, \bar{a}\}} P(b, e, A, j, m) = \sum_{A \in \{a, \bar{a}\}} p(b)p(e)p(A|b, e)p(j|A)p(m|A)$$

$$P(b,j,m) = \sum_{E \in \{e,\bar{e}\}} P(b,E,j,m) = \sum_{E \in \{e,\bar{e}\}} \sum_{A \in \{a,\bar{a}\}} p(b)p(E)p(A|b,E)p(j|A)p(m|A)$$

$$P(\bar{b},j,m) = \sum_{E \in \{e,\bar{e}\}} P(b,E,j,m) = \sum_{E \in \{e,\bar{e}\}} \sum_{A \in \{a,\bar{a}\}} p(b)p(E)p(A|b,E)p(j|A)p(m|A)$$

- Learning model using Bayesian network
- Given a query q with m features

•
$$\mathbf{q} = \{X_1, X_2, \dots, X_m\}$$

And there are n target levels

•
$$\mathbf{T} = \{Y_1, Y_2, ..., Y_n\}$$

Then,

•
$$M(\mathbf{q}) = \underset{Y \in \mathbf{T}}{\operatorname{argmax}} P(Y \mid X_1, X_2, ..., X_m)$$

Example:

•
$$M(\mathbf{q}) = \underset{B \in \{b, \bar{b}\}}{\operatorname{argmax}} P(B \mid j, m)$$

- The sequence of random variables such a process moves through.
- The next state of the process only depends on the previous state and not the sequence of states.
- Andrey Markov
 - 1856 1922
 - Russian mathematician



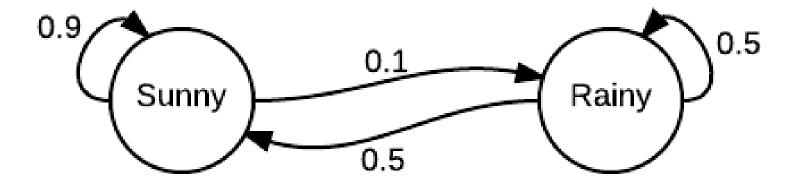
- Discrete-time Markov chain
 - a sequence of random variables $X_1, X_2, ..., X_n$ with the Markov property

$$P(X_n = x_n | X_{n-1} = x_{n-1}, X_{n-2} = x_{n-2}, \dots, X_1 = x_1)$$

$$= P(X_n = x_n | X_{n-1} = x_{n-1})$$

if
$$P(X_{n-1} = x_{n-1}, X_{n-2} = x_{n-2}, ..., X_1 = x_1) > 0$$

- A simple example: The probabilities of weather conditions
 - A sunny day is 90% likely to be followed by another sunny day.
 - A rainy day is 50% likely to be followed by another rainy day.



Trasition matrix:
$$P = \begin{bmatrix} 0.9 & 0.1 \\ 0.5 & 0.5 \end{bmatrix}$$

Initial state:
$$\mathbf{x}^0 = \begin{bmatrix} p_{sunny}^0 & p_{rainy}^0 \end{bmatrix}$$

$$\mathbf{x}^i = \mathbf{x}^{i-1}P = \mathbf{x}^0 p^i$$

A simple example: The probabilities of weather conditions

Given
$$\mathbf{x}^0 = [1.0 \quad 0.0]$$

The 1st day:
 $\mathbf{x}^1 = \mathbf{x}^0 P = [0.9 \quad 0.1]$
The 2nd day:
 $\mathbf{x}^2 = \mathbf{x}^1 P = [0.86 \quad 0.14]$
How about
 $\mathbf{q} = \lim_{i \to \infty} \mathbf{x}^i$

- A state t has period k if any return to state t must occur in multiples of k time steps.
- If k = 1, then the state is said to be **aperiodic**.
- A Markov chain is irreducible if its state space is a single communicating class; in other words,
 - if it is possible to get to any state from any state
 - all the states communicate with each other
 - all states are aperiodic.
- If the Markov chain is irreducible and aperiodic, then there is a unique stationary distribution **q**.

$$\mathbf{q} = \lim_{i \to \infty} \mathbf{x}^{i}$$
$$\mathbf{q}P = \mathbf{q}$$
$$\mathbf{q}(P - I) = 0$$

A simple example: The probabilities of weather conditions

$$P - I = \begin{bmatrix} -0.1 & 0.1 \\ 0.5 & -0.5 \end{bmatrix}$$

$$\mathbf{q}(P - I) = 0$$

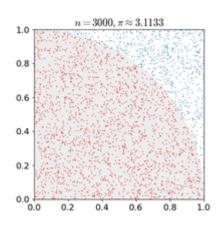
$$-0.1q_1 + 0.5q_2 = 0$$
and $q_1 + q_2 = 1.0$ (sum of probabilities)
$$\mathbf{q} = \begin{bmatrix} 0.833 & 0.166667 \end{bmatrix}$$

 In conclusion, in the long term, about 83.3% of days are sunny.

- A big question of applying Markov chain to machine learning
 - The number of data instances in our training is pretty large.
 - The number of features is also large.
 - There are many choices to create a Markov chain for our training data.
 - How to create the best Markov chain for our training data?

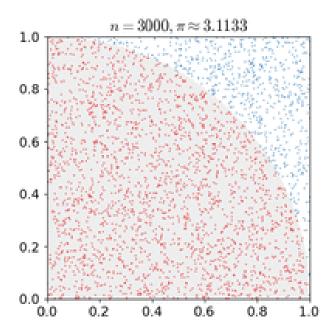
Monte Carlo Method

- Repeatedly, evenly, and randomly sample from a domain to obtain numerical results.
 - 1. Define a domain of possible inputs
 - 2. Generate inputs randomly from a probability distribution over the domain
 - 3. Perform a deterministic computation on the inputs
 - 4. Aggregate the results



Monte Carlo Method

- Example: $\pi = ?$
 - 1. Draw a square, then inscribe a circle within it
 - 2. Uniformly scatter objects of uniform size over the square
 - 3. Count the number of objects inside the circle and the total number of objects
 - 4. The ratio of the inside-count and the total-sample-count is an estimate of the ratio of the two areas, which is π /4. Multiply the result by 4 to estimate π



- MCMC methods are a class of algorithms for sampling from a probability distribution based on constructing a Markov chain that has the desired distribution as its equilibrium distribution.
- Finding a good state transition
- Two MCMC methods are commonly used in machine learning
 - Metropolis-Hastings method
 - Gibbs sampling

Metropolis-Hastings method

- 1. Initialize x_0
- 2. For i = 0 to n 1
- 3. Randomly generate a candidate state $x' \sim q(x'|x_i)$
- 4. Generate a uniform random number $u \sim U[0,1]$

5. If
$$u < A(x_i, x') = \min(1, \frac{p(x')q(x_i|x')}{p(x_i)q(x'|x_i)})$$

- 6. $x_{i+1} = x'$
- 7. else
- 8. $x_{i+1} = x_i$
- where q is called proposal density, which is an arbitrary probability density
 - q must satisfy q(x|y) = q(y|x)
 - Gaussian distribution is commonly used be q

Gibbs sampling

- 1. Initialize $\mathbf{x}^0 = [x_1^0, x_2^0, ..., x_m^0]$
- 2. For i = 0 to n 1
- 3. Crate the next sample $\mathbf{x}^{i+1} = [x_1^{i+1}, x_2^{i+1}, \dots, x_m^{i+1}]$
- 4. sample $x_1^{i+1} \sim p(x_1 | x_2^i, x_3^i, ... x_m^i)$
- 5. sample $x_2^{i+1} \sim p(x_2 | x_1^{i+1}, x_3^i, \dots x_m^i)$

. . .

- 6. sample $x_j^{i+1} \sim p(x_j | x_1^{i+1}, ..., x_{j-1}^{i+1}, x_{j+1}^i, ... x_m^i)$
- 7. sample $x_m^{i+1} \sim p(x_m | x_1^{i+1}, x_2^{i+1}, \dots, x_{m-1}^{i+1})$
- 8. Repeat step 2 7 k times ($\mathbf{x}^0 = \mathbf{x}^n$).

- An example of Gibbs sampling
 - Darren Wilkinson, "MCMC programming in R, Python, Java, and C", 2016
- Two variables: x and y

•
$$p(x|y) = \text{Gamma PDF with } k = 3, \theta = y^2 + 4$$

$$G(x, k, \theta) = \frac{1}{\Gamma(k)\theta^k} x^{k-1} e^{-\frac{x}{\theta}}$$

•
$$p(y|x) = \text{Gaussian PDF with } \mu = \frac{1}{x+1}, \sigma = \frac{1}{\sqrt{2(x+1)}}$$

$$N(y,\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(y-\mu)^2}{2\sigma^2}}$$

- 1. x = 0, y = 0
- 2. for i = 1 to N
- 3. for j = 1 to M
- 4. $x \sim G(x, k, \theta)$
- 5. $y \sim N(y, \mu, \sigma)$
- 6. Output[i] = (x, y)

- Advanced reading
 - C. Andrieu, et al. "An Introduction to MCMC for Machine Learning," *Kluwer Academic*, 2003
 - Paolo, et al. "Bayesian Function Learning Using MCMC Methods," IEEE Transactions on Pattern Analysis and Machine Intelligence, Vol. 20, No. 12, Dec. 1998.