

CS 760: Machine Learning **Probability & Graphical Models**

Ilias Diakonikolas

University of Wisconsin-Madison

Nov. 8, 2022

Announcements

•Logistics:

•HW 5 released later this week

•Class roadmap:

Thursday, Nov. 10	Graphical Models I
Tuesday	Graphical Models II
Thursday	Less-than-full Supervision
Tuesday	Unsupervised Learning I

Outline

Review, SVMs, Kernels

Duality, feature maps, kernel trick

Probability Tutorial

·Basics, joint probability, conditional probabilities, etc

Bayesian Networks

Definition, examples, inference

Outline

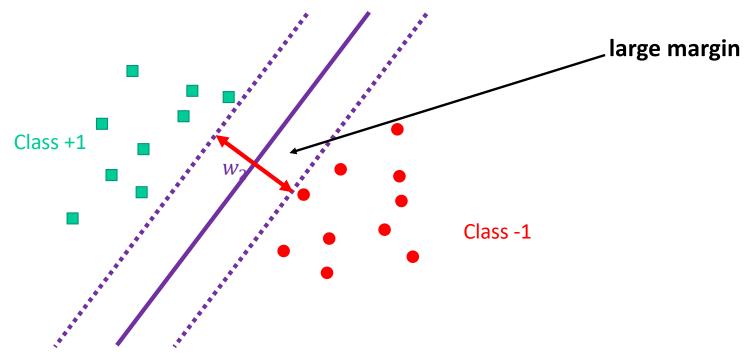
- Review, SVMs, Kernels
 - Duality, feature maps, kernel trick
- Probability Tutorial
 - Basics, joint probability, conditional probabilities, etc
- Bayesian Networks
 - Definition, examples, inference

Review: Constrained Optimization & Duality

- •Lagrangian: $\mathcal{L}(w, \boldsymbol{\alpha}, \boldsymbol{\beta}) = f(w) + \sum_i \alpha_i g_i(w) + \sum_j \beta_j h_j(w)$
- •Primal problem $p^* \coloneqq \min_{w} f(w) = \min_{w} \max_{\alpha, \beta: \alpha_i \ge 0} \mathcal{L}(w, \alpha, \beta)$
- •Dual problem $d^* \coloneqq \max_{\alpha, \beta: \alpha_i \ge 0} \min_{w} \mathcal{L}(w, \alpha, \beta)$
- •Always true: $d^* \le p^*$

Review: Apply to Training Linear Classifier

• Want: a large margin



Review: Support Vector Machines Goal

Define the margin to be

$$\gamma = \min_{i} \frac{y_i f_{w,b}(x_i)}{||w||} \quad \longleftarrow \text{We proved this}$$

- •If $f_{w,b}$ incorrect on some x_i , the margin is **negative**
- Fix scale: $y_{i^*}(w^Tx_{i^*} + b) = 1$. Then, margin overall is $\frac{1}{||w||}$

Primal problem:

$$\min_{w,b} \frac{1}{2} ||w||^2 \qquad \qquad \qquad \text{Objective:} \\ y_i(w^T x_i + b) \geq 1, \forall i \leftarrow \qquad \qquad \text{Constraints: Correct} \\ \text{on training data}$$

SVM: Dual Version

Reduces to dual problem:

$$\max_{\alpha} \mathcal{L}(w,b,\alpha) = \max_{\alpha} \sum_{i} \alpha_{i} - \frac{1}{2} \sum_{ij} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{T} x_{j}$$

$$\sum_{i} \alpha_{i} y_{i} = 0, \alpha_{i} \geq 0$$
 Note: only variables are primal

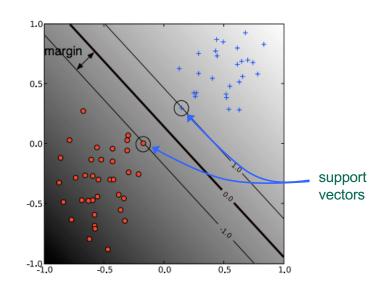
- •Since $w = \sum_i \alpha_i y_i x_i$, we have $w^T x + b = \sum_i \alpha_i y_i x_i^T x + b$
- Note: only deals with data via inner products $x_i^T x_j$

SVM: Support Vectors

Solution is a sparse linear combination of training instances

$$w = \sum_{i} \alpha_{i} y_{i} x_{i}$$

- Those instances with $\alpha_i > 0$ are called *support vectors*
 - Lie on the margin boundary
- Solution does not change if we delete instances with $\alpha_i = 0$



SVM: Soft Margin

What if our data isn't linearly separable?

•Can adjust our approach by using slack variables (denoted by ζ_i) to tolerate errors

$$\min_{w,b,\zeta_i} \frac{1}{2} ||w||^2 + C \sum_i \zeta_i$$
$$y_i(w^T x_i + b) \ge 1 - \zeta_i, \zeta_i \ge 0, \forall i$$

• C determines the relative importance of maximizing margin vs. minimizing slack

SVM: Soft Margin

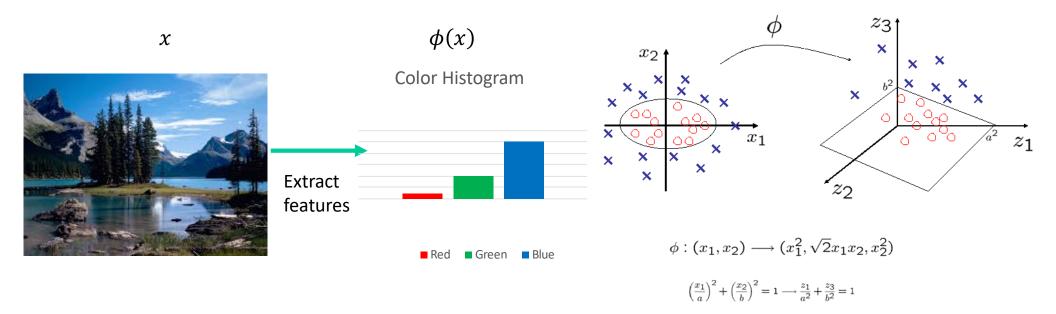
$$\min_{w,b,\zeta_i} \frac{1}{2} ||w||^2 + C \sum_{i} \zeta_i$$

$$y_i(w^T x_i + b) \ge 1 - \zeta_i, \zeta_i \ge 0, \forall i$$

Ben-Hur & Weston, Methods in Molecular Biology 2010

Feature Maps

- Can take a set of features and map them into another
 - Can also construct non-linear features
 - Use these inside a linear classifier?



Feature Maps and SVMs

Want to use feature space $\{\phi(x_i)\}$ in linear classifier...

- Downside: dimension might be high (even infinite!)
- So we don't want to write down $\phi(x_i) = [0.2, 0.3, ...]$

Recall our SVM dual form:

• Only relies on inner products $x_i^T x_j$ $\mathcal{L}(w,b,\pmb{\alpha}) = \sum_i \alpha_i - \frac{1}{2} \sum_{ij} \alpha_i \alpha_j y_i y_j x_i^T x_j$ $\sum_i \alpha_i y_i = 0, \alpha_i \geq 0$

Kernel Trick

- •Using SVM on the feature space $\{\phi(x_i)\}$: only need $\phi(x_i)^T\phi(x_i)$
- •Conclusion: no need to design $\phi(\cdot)$, only need to design

$$k(x_i, x_j) = \phi(x_i)^T \phi(x_j)$$

Kernel Matrix Feature Maps

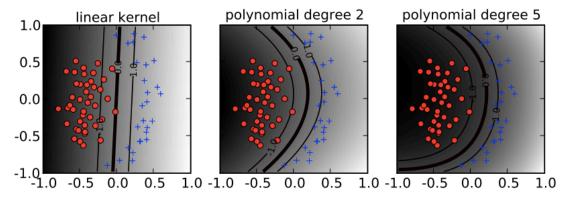
Kernel Types: Polynomial

• Fix degree d and constant c:

$$k(x, x') = (x^T x' + c)^d$$

- •What are $\phi(x)$?
- Expand the expression to get $\phi(x)$

$$\forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^2, \quad K(\mathbf{x}, \mathbf{x}') = (x_1 x_1' + x_2 x_2' + c)^2 =$$



xpression to get $\phi(x)$ $\forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^2, \quad K(\mathbf{x}, \mathbf{x}') = (x_1 x_1' + x_2 x_2' + c)^2 = \begin{bmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2} x_1 x_2 \\ \sqrt{2c} x_1 \end{bmatrix} \cdot \begin{bmatrix} x'_1^2 \\ x'_2^2 \\ \sqrt{2c} x_1' x_2' \\ \sqrt{2c} x_1' \end{bmatrix}$ ear kernel polynomial degree 2 polynomial degree 5

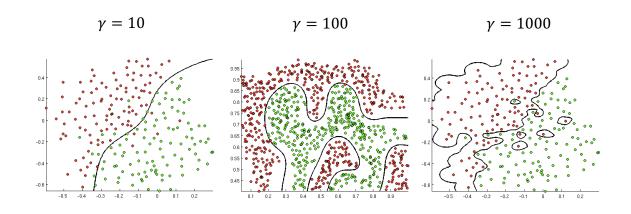
Ben-Hur & Weston, Methods in Molecular Biology 2010

Kernel Types: Gaussian/RBF

• Fix bandwidth σ :

$$k(x, x') = \exp(-||x - x'||^2/2\sigma^2)$$

Also called radial basis function (RBF) kernels



$$k(x, x') = \exp(-\gamma ||x - x'||^2)$$

Andrew Ng

Theory of Kernels

- Part of a deep mathematical theory
- With some conditions, any kernel yields a feature map:
 - Theorem: k(x, x') has expansion

$$k(x, x') = \sum_{i}^{+\infty} a_i \phi_i(x) \phi_i(x')$$
 Feature Maps

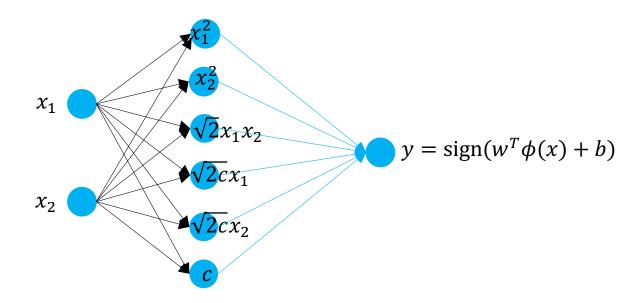
for nonnegative a_i 's, if and only if for any function c(x),

$$\int \int c(x)c(x')k(x,x')dxdx' \ge 0$$

 Given certain requirements/conditions, can construct a bunch of new kernels from existing ones

Kernel Methods VS Neural Networks

 Can think of our kernel SVM approach as fixing a layer of a neural network



SVM Review

- Can find globally optimal solutions: convex optimization
 - No local minima (unlike training general NNs)
- Can train primal or dual
 - Dual: relies on **support vectors**; enables use of **kernels**
- Variety of pre-existing optimization techniques
- Kernels: allow non-linear decision boundaries
 - And to represent all sorts of new data (strings, trees)
 - High-dimensional representations, but can use kernel trick to avoid explicitly computing feature maps
 - Good performance! Sometimes close to DNNs



Break & Quiz

- Q1-1: Are these statements true or false?
- (A) If we have multiple optimal solutions on a given training set, those solutions will also have the same test loss.
- (B) If a hyperplane only changes its bias term by 1, then the distance from some point x to the hyperplane will not change.
- 1. True, True
- 2. True, False
- 3. False, True
- 4. False, False

- Q1-1: Are these statements true or false?
- (A) If we have multiple optimal solutions on a given training set, those solutions will also have the same test loss.
- (B) If a hyperplane only changes its bias term by 1, then the distance from some point x to the hyperplane will not change.
- 1. True, True
- 2. True, False
- 3. False, True
- 4. False, False



- (A) Multiple optimal solutions on the training usually have different test loss. Please refer to the example given in the lecture.
- (B) Recall that the distance is given by $\frac{|f_{w,b}(x)|}{\|w\|}$. If only the bias term is changed, then $|f_{w,b}(x)|$ will change while $\|w\|$ remains same. So the distance will also be changed.

- Q1-2: Are these statements true or false?
- (A) Define the margin to be $\gamma = \min_{i} \frac{y_i f_{w,b}(x_i)}{\|w\|}$, if $f_{w,b}(x)$ predicts correctly on some x_i and incorrectly on others, then the margin will be positive. (B) If the training set can be correctly separated, then $\max_{w,b} \gamma$ can still be negative.
- 1. True, True
- 2. True, False
- 3. False, True
- 4. False, False

- Q1-2: Are these statements true or false?
- (A) Define the margin to be $\gamma = \min_{i} \frac{y_i f_{w,b}(x_i)}{\|w\|}$, if $f_{w,b}(x)$ predicts correctly on some x_i and incorrectly on others, then the margin will be positive. (B) If the training set can be correctly separated, then $\max_{w,b} \gamma$ can still be negative.
- 1. True, True
- 2. True, False
- 3. False, True
- 4. False, False



- (A) In this case, $\frac{y_i f_{w,b}(x_i)}{\|w\|}$ would be negative on those x_i with incorrect predictions. So take min on all training data, we will get the margin negative.
- (B) In this case, there exists at least one w and b such that all instances are correctly classified, so the corresponding margin is non-negative.

- Q1-3: Are these statements true or false?
- (A) The solution of SVM will always change if we remove some instances from the training set.
- (B) If we can only access the labels and the inner products of instances $\{x_i^T x_j\}_{i,j}$, we can NOT solve the learning problem in SVM.
- 1. True, True
- 2. True, False
- 3. False, True
- 4. False, False

- Q1-3: Are these statements true or false?
- (A) The solution of SVM will always change if we remove some instances from the training set.
- (B) If we can only access the labels and the inner products of instances $\{x_i^T x_j\}_{i,j}$, we can NOT solve the learning problem in SVM.
- 1. True, True
- 2. True, False
- 3. False, True
- 4. False, False



- (A) As is shown in the lecture, if we remove those instances with $\alpha_i=0$, it will not influence the SVM result.
- (B) We can see that the dual problem only depends on y_i and the inner products of training instances. So we can also solve the SVM problem in this case.

Outline

- Review, SVMs, Kernels
 - Duality, feature maps, kernel trick
- Probability Tutorial
 - ·Basics, joint probability, conditional probabilities, etc
- Bayesian Networks
 - Definition, examples, inference

Probability Tutorial: Outcomes & Events

- Outcomes: possible results of an experiment
- •Events: subsets of outcomes we're interested in

Ex:

$$\Omega = \underbrace{\{1, 2, 3, 4, 5, 6\}}_{\text{outcomes}}$$

$$\mathcal{F} = \underbrace{\{\emptyset, \{1\}, \{2\}, \dots, \{1, 2\}, \dots, \Omega\}}_{\text{events}}$$



Probability Tutorial: Outcomes & Events

Event space can be smaller:

$$\mathcal{F} = \underbrace{\{\emptyset, \{1, 3, 5\}, \{2, 4, 6\}, \Omega\}}_{\text{events}}$$

•Two components always in it!

$$\emptyset, \Omega$$



Probability Tutorial: Sigma Fields

- F is a "sigma algebra".
 - Follows certain rules:
 - Everything in it (saw this already)
 - If A is in F, so is A^c
 - Closed under countable unions



Probability Tutorial: Probability Spaces

 Now we need a way to produce probabilities of events, so introduce a function

$$P: \mathcal{F} \to [0,1]$$

- Has certain properties, which we'll see in a second.
- Overall, we get a probability space

$$(\Omega, \mathcal{F}, P)$$

Probability Tutorial: Probability Spaces

- We have outcomes and events and probabilities
- •l.e.,

For
$$E \in \mathcal{F}$$
, $P(E) \in [0,1]$

Back to our example:

$$\mathcal{F} = \underbrace{\{\emptyset, \{1, 3, 5\}, \{2, 4, 6\}, \Omega\}}_{\text{events}}$$

$$P({1,3,5}) = 0.2, P({2,4,6}) = 0.8$$



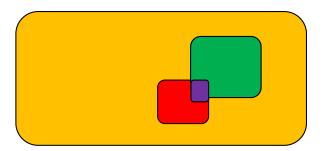
Basics: Axioms

- Rules for probability:
 - For all events $E \in \mathcal{F}, P(E) \ge 0$
 - •Always, $P(\emptyset) = 0, P(\Omega) = 1$
 - For disjoint events,

$$P(E_1 \cup E_2) = P(E_1) + P(E_2)$$

•Easy to derive other laws. Ex: non-disjoint events

$$P(E_1 \cup E_2) = P(E_1) + P(E_2) - P(E_1 \cap E_2)$$



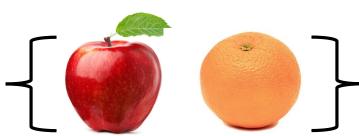
Basics: Random Variables

- Really, functions
- Map outcomes to real values

$$X:\Omega\to\mathbb{R}$$

- •Why?
 - •So far, everything is a set.
 - Hard to work with!
 - Real values are easy to work with
- •One requirement, "F measurable". For any c,

$$\{\omega: X(\omega) \le c\} \in \mathcal{F}$$



Basics: CDF & PDF

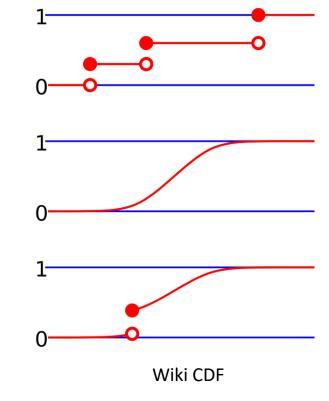
Can still work with probabilities:

$$P(X = 3) := P(\{\omega : X(\omega) = 3\})$$

Cumulative Distribution Func. (CDF)

$$F_X(x) := P(X \le x)$$

- •Density / mass function $p_X(x)$
 - •Doesn't always exist!



Basics: Expectation & Variance

- Another advantage of RVs are ``summaries''
- •Expectation:
 - •The "average" $E[X] = \sum_a a \times P(x=a)$
- •Variance: $Var[X] = E[(X E[X])^2]$
 - A measure of spread
- •Raw moments: $E[X], E[X^2], E[X^3], \dots$
- Note: also don't always exist...
 - •Ex: Cauchy distribution

Basics: **Expectation** Properties

- Expectation has very useful properties...
 - •Linearity: $E[\sum a_i X_i] = \sum a_i E[X_i]$
 - Independence ${\sf not}^i$ required!
 - Hat check problem:
 - There is a dinner party where n people check their hats. The hats are mixed up during dinner, so that afterward each man receives a random hat. In particular, each person gets their own hat with probability 1/n. What is the expected number of people who get their own hat?

Basics: Joint Distributions

- Move from one variable to several
- Joint distribution

$$P(X = a, Y = b)$$

•Or more variables.

$$P(X_1 = x_1, X_2 = x_2, \dots, X_k = x_k)$$

Basics: Marginal Probability

Given a joint distribution

$$P(X = a, Y = b)$$

•Get the distribution in just one variable:

$$P(X = a) = \sum_{b} P(X = a, Y = b)$$

•This is the "marginal" distribution.

Basics: Marginal Probability

$$P(X = a) = \sum_{b} P(X = a, Y = b)$$

	Sunny	Cloudy	Rainy
hot	150/365	40/365	5/365
cold	50/365	60/365	60/365

$$[P(\text{hot}), P(\text{cold})] = [\frac{195}{365}, \frac{170}{365}]$$







Independence

•Independence for a set of events A_1,\ldots,A_k

$$P(A_{i_1}A_{i_2}\cdots A_{i_j}) = P(A_{i_1})P(A_{i_2})\cdots P(A_{i_j})$$
 for all the i₁,...,i_i combinations

- Why useful? Dramatically reduces the complexity
- Collapses joint into product of marginals
 - Note sometimes we have only pair-wise, etc independence

Uncorrelatedness

•For random variables, uncorrelated means

$$E[XY] = E[X]E[Y]$$

Note: weaker than independence.

- Independence implies uncorrelated (easy to see)
- Other way around: usually false (but not always).
- •If X,Y independent, functions are not correlated:

$$E[f(X)f(Y)] = E[f(X)]E[f(Y)]$$

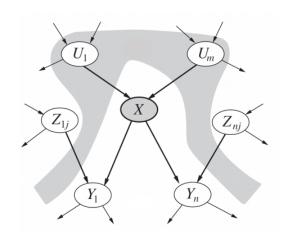
Conditional Probability

For when we know something,

$$P(X = a|Y = b) = \frac{P(X = a, Y = b)}{P(Y = b)}$$

Leads to conditional independence

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



Credit: Devin Soni

Chain Rule

Apply repeatedly,

$$P(A_1, A_2, \dots, A_n)$$

= $P(A_1)P(A_2|A_1)P(A_3|A_2, A_1)\dots P(A_n|A_{n-1}, \dots, A_1)$

- •Note: still big!
 - If some conditional independence, can factor!
 - Leads to probabilistic graphical models (this lecture)

Law of Total Probability

- •Partition the sample space into disjoint B_1 , ..., B_k
- Then,

$$P(A) = \sum_{i} P(A|B_i)P(B_i)$$

- Useful way to control A via conditional probabilities.
 - •Example: there are 5 red and 2 green balls in an urn. A random ball is selected and replaced by a ball of the other color; then a second ball is drawn. What is the probability the second ball is red?

Bayesian Inference

Conditional Prob. & Bayes:

$$P(H|E_1, E_2, \dots, E_n) = \frac{P(E_1, \dots, E_n|H)P(H)}{P(E_1, E_2, \dots, E_n)}$$

- Has more evidence.
 - Likelihood is hard---but conditional independence assumption

$$P(H|E_1, E_2, \dots, E_n) = \frac{P(E_1|H)P(E_2|H)\cdots, P(E_n|H)P(H)}{P(E_1, E_2, \dots, E_n)}$$

Random Vectors & Covariance

•Recall variance: $\mathbb{E}[(X - E[X])^2]$

$$\mathbb{E}[(X - E[X])^2]$$

- Now, for a random vector (same as joint of d RVs)
 - Note: size d x d. All variables are centered

$$\Sigma = \begin{bmatrix} \mathbb{E}[(X_1 - \mathbb{E}[X_1])^2] & \dots & [(X_1 - \mathbb{E}[X_1])((X_n - \mathbb{E}[X_n])] \\ \vdots & \vdots & \vdots \\ [(X_n - \mathbb{E}[X_n])((X_1 - \mathbb{E}[X_1])] & \dots & \mathbb{E}[(X_n - \mathbb{E}[X_n])^2] \end{bmatrix}$$

Cross-variance

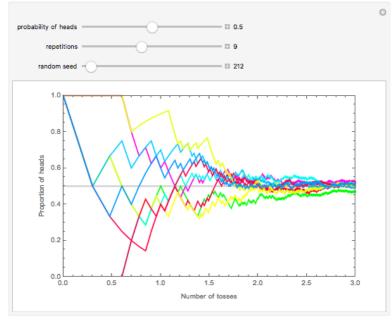
Diagonals: Scalar Variance

Estimation Theory

- •How do we know that the sample mean is a good estimate of the true mean?
 - Concentration inequalities

$$P(|\mathbb{E}[X] - \hat{\mathbb{E}}[X]| \ge t) \le \exp(-2nt^2)$$

- Law of large numbers
- Central limit theorems, etc.



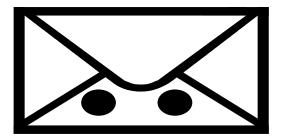
Wolfram Demo

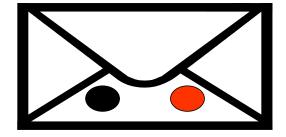


Break & Quiz

Two Envelopes Problem

- •We have two envelopes:
 - E₁ has two black balls, E₂ has one black, one red
 - •The red one is worth \$100. Others, zero
 - •Open an envelope, see one ball. Then, can switch (or not).
 - You see a black ball. Switch?





Two Envelopes Solution

•Let's solve it.

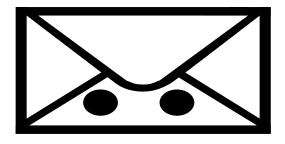
$$P(E_1|\text{Black ball}) = \frac{P(\text{Black ball}|E_1)P(E_1)}{P(\text{Black ball})}$$

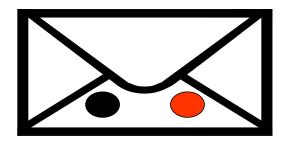
•Now plug in:

$$P(E_1|\text{Black ball}) = \frac{1 \times \frac{1}{2}}{P(\text{Black ball})}$$

So switch!

$$P(E_2|\text{Black ball}) = \frac{\frac{1}{2} \times \frac{1}{2}}{P(\text{Black ball})}$$





Break & Quiz

Q 3.1: 50% of emails are spam. Software has been applied to filter spam. A certain brand of software can detect 99% of spam emails, and the probability for a false positive (a nonspam email detected as spam) is 5%. Now if an email is detected as spam, then what is the probability that it is in fact a nonspam email?

- A. 5/104
- B. 95/100
- C. 1/100
- D. 1/2

Break & Quiz

Q 3.1: 50% of emails are spam. Software has been applied to filter spam. A certain brand of software claims that it can detect 99% of spam emails, and the probability for a false positive (a non-spam email detected as spam) is 5%. Now if an email is detected as spam, then what is the probability that it is in fact a nonspam email?

- A. 5/104
- B. 95/100
- C. 1/100
- D. 1/2

Outline

- Review, SVMs, Kernels
 - Duality, feature maps, kernel trick
- Probability Tutorial
 - Basics, joint probability, conditional probabilities, etc
- Bayesian Networks
 - Definition, examples, inference

Consider the following 5 binary random variables:

B = a burglary occurs at the house

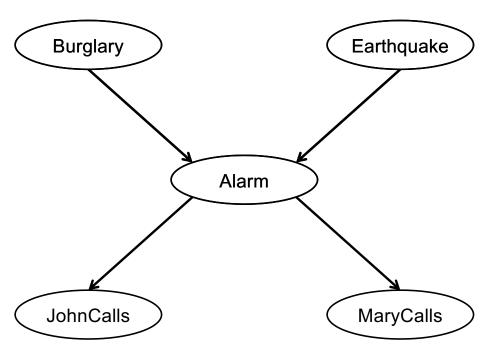
E = an earthquake occurs at the house

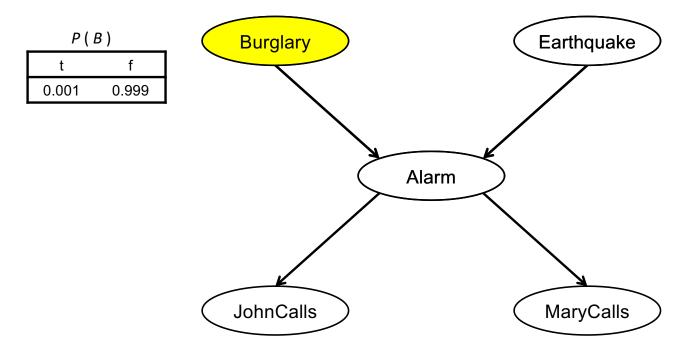
A = the alarm goes off

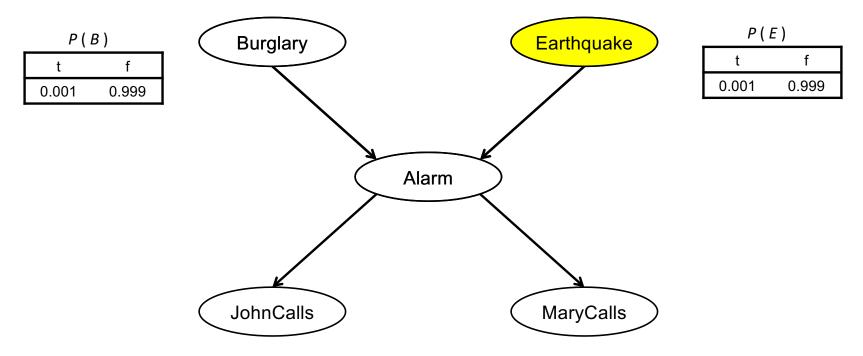
J = John calls to report the alarm

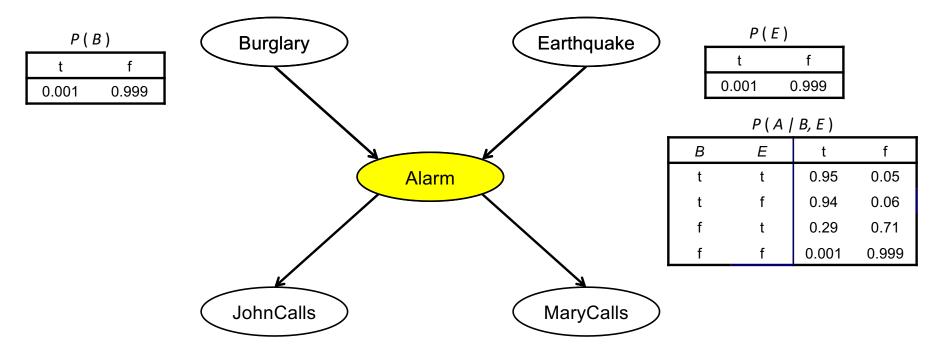
M = Mary calls to report the alarm

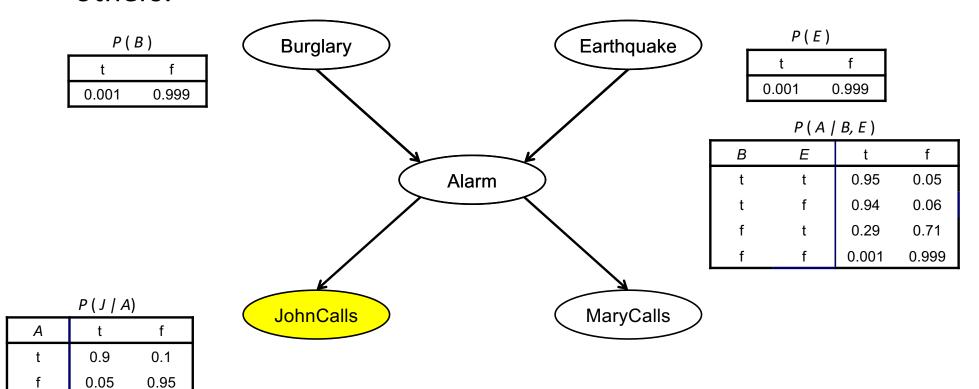
- Suppose Burglary or Earthquake can trigger Alarm, and Alarm can trigger John's call or Mary's call
- Now we want to answer queries like what is $P(B \mid M, J)$?

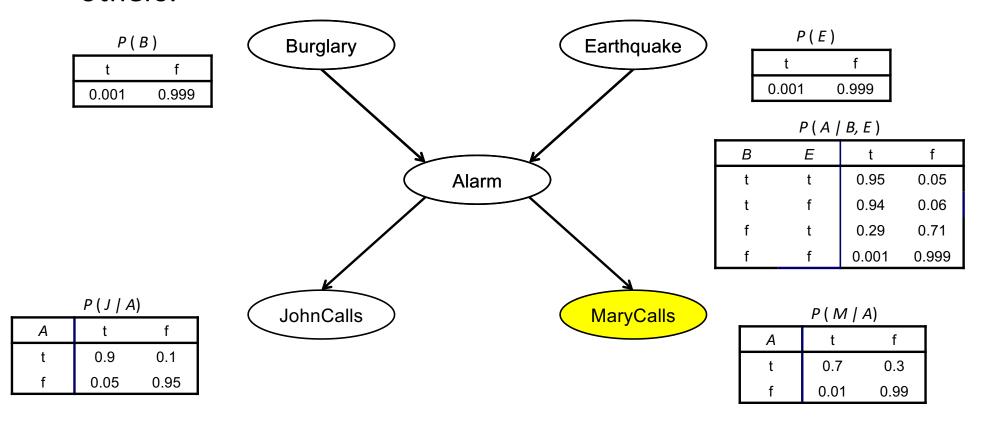












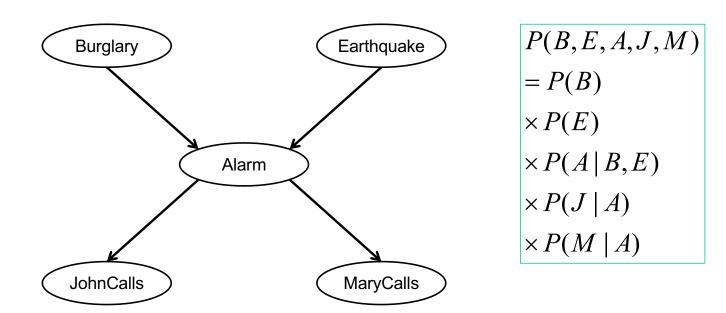
Bayesian Networks: Definition

- A BN consists of a Directed Acyclic Graph (DAG) and a set of conditional probability distributions
- The DAG:
 - each node denotes a random variable
 - each edge from X to Y represents that X directly influences Y
 - (formally: each variable X is independent of its non-descendants given its parents)
 - Each CPD: represents $P(X \mid Parents(X))$

$$p(x_1, \dots, x_d) = \prod_{v \in V} p(x_v | x_{\text{pa}(v)})$$

Bayesian Networks: Parameter Counting

- Parameter reduction: a standard representation of the joint distribution for the Alarm example has $2^5 = 32$ parameters
- the BN representation of this distribution has 20 parameters



Inference in Bayesian Networks

Given: values for some variables in the network (*evidence*), and a set of *query* variables

Do: compute the posterior distribution over the query variables

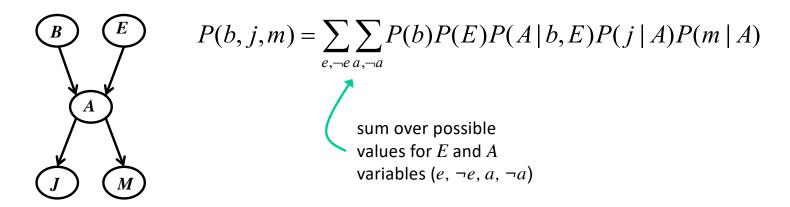
- variables that are neither evidence variables nor query variables are *hidden* variables
- •the BN representation is flexible enough that any set can be the evidence variables and any set can be the query variables

Inference by Enumeration

- •Let a denote A=true, and $\neg a$ denote A=false
- •Suppose we're given the query: $P(b \mid j, m)$

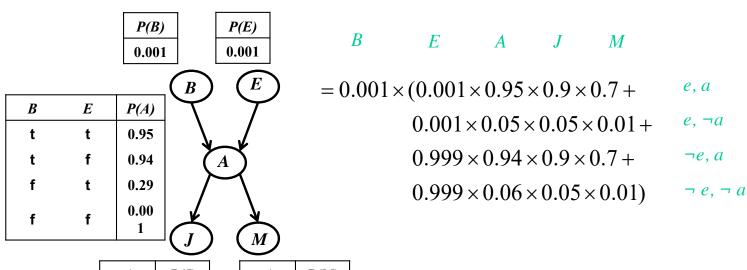
"probability the house is being burglarized given that John and Mary both called"

• From the graph structure we can first compute:



Inference by Enumeration

$$P(b, j, m) = \sum_{e, \neg e} \sum_{a, \neg a} P(b) P(E) P(A \mid b, E) P(j \mid A) P(m \mid A)$$
$$= P(b) \sum_{e, \neg e} \sum_{a, \neg a} P(E) P(A \mid b, E) P(j \mid A) P(m \mid A)$$



\boldsymbol{A}	P(J)
t	0.9
f	0.05

A	P(M)	
t	0.7	
f	0.01	

Inference by Enumeration

•Next do equivalent calculation for $P(\neg b, j, m)$ and determine $P(b \mid j, m)$

$$P(b \mid j, m) = \frac{P(b, j, m)}{P(j, m)} = \frac{P(b, j, m)}{P(b, j, m) + P(\neg b, j, m)}$$

So: exact method, but can be intractably hard.

- Some cases: efficient
- Approximate inference sometimes available



Thanks Everyone!

Some of the slides in these lectures have been adapted/borrowed from materials developed by Mark Craven, David Page, Jude Shavlik, Tom Mitchell, Nina Balcan, Elad Hazan, Tom Dietterich, Pedro Domingos, Jerry Zhu, Yingyu Liang, Volodymyr Kuleshov, Fei-Fei Li, Justin Johnson, Serena Yeung, Pieter Abbeel, Peter Chen, Jonathan Ho, Aravind Srinivas, Fred Sala