CS 161 Intro. To Artificial Intelligence

Week 9, Discussion 1C

Li Cheng Lan

Today’s Topics

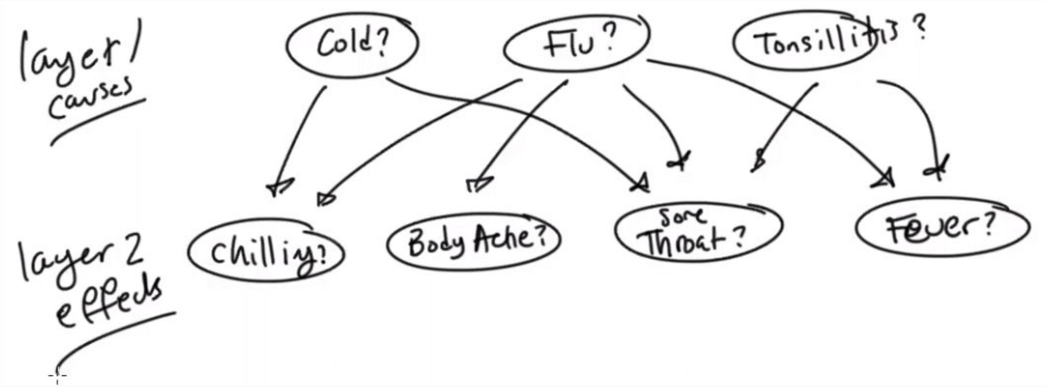
- **BN Learning and Inference**
  - Learning parameters
  - Learning BN structure
  - Model-oriented vs. Query-oriented learning
- Decision Tree and Random Forest
  - Entropy and Conditional Entropy
  - Classifier
  - BN Classifier

BN Learning - Example

Example

The flu is an acute disease characterized by fever, body aches and pains, and can be associated with chilling and a sore throat. The cold is a bodily disorder popularly associated with chilling and can cause a sore throat. Tonsillitis is inflammation of the tonsils which leads to a sore throat and can be associated with fever.

- Ways to learn parameters (probabilities) and construct CPTs (conditional probability table):
    - Problem statement
    - Subjective beliefs
    - **Learning from data**



BN Learning

CPTs can also be estimated from medical records of previous patients

Case	*Cold?*	*Flu?*	*Tonsillitis?*	*Chilling?*	*Bodyache?*	*Sorethroat?*	*Fever?*
1	true	false	?	true	false	false	false
2	false	true	false	true	true	false	true
3	?	?	true	false	?	true	false
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

CPT, → BN. → find prob. of all examples → score 1
→ score 2

- Complete data (e.g. 2nd case): if **every** row is complete, dataset is complete → efficient
- Incomplete data (e.g. 1st case): if **any** row is incomplete, dataset is incomplete
  - Use algorithm such as expectation maximization (EM) to find maximum likelihood parameters
- **BN structure + CPTs = BN**
  - May come out multiple BNs → The BN with **max score** (computed by multiplying prob. assigned to all cases based on each BN) is better
  - It's called maximum likelihood principle

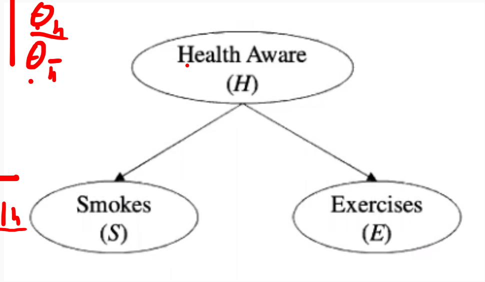
Learning Parameters

Goal: Estimate/Learn parameters in CPTs

- E.g. $\Theta_{s|h}$, $\Theta_{\neg s|h}$, $\Theta_{s|\neg h}$, $\Theta_{\neg s|\neg h}$ in the CPT of node S

H	
Yes	θ_h
No	$\theta_{\bar{h}}$

H	S	
T	T	$\theta_{s|h}$
T	F	
F	T	
F	F	



Case 1: using complete data

- Construct empirical distribution table from data
- Compute parameters using conditional probability based on empirical distribution
  - E.g. $\Theta_{s|h} = \Pr(s|h) = \frac{\Pr(s \wedge h)}{\Pr(h)}$ $\frac{2}{16}$ / $\frac{12}{16}$ $= \frac{1}{6}$

dataset:

Case	H	S	E
1	T	F	T
2	T	F	T
3	F	T	F
4	F	F	T
5	T	F	F
6	T	F	T
7	F	F	F
8	T	F	T
9	T	F	T
10	F	F	T
11	T	F	T
12	T	T	T
13	T	F	T
14	T	T	T
15	T	F	T
16	T	F	T

Empirical distribution

H	S	E	$\Pr_{\mathcal{D}}(.)$
T	T	T	2/16
T	T	F	0/16
T	F	T	9/16
T	F	F	1/16
F	T	T	0/16
F	T	F	1/16
F	F	T	2/16
F	F	F	1/16

Learning Parameters

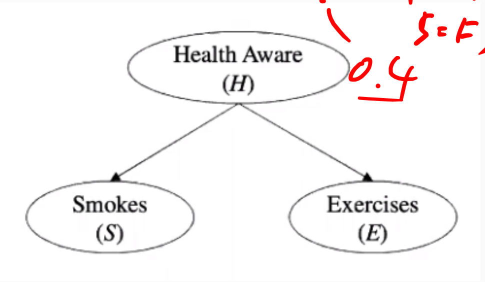
H	S	E
T	F	?

T F T → P(E=T | H=T, S=F) — 0.6

T F F → P(E=F | H=T, S=F) — 0.4

Case 2: using **incomplete** data

- Apply **Expectation Maximization (EM)** algorithm
  1. Use estimate parameters to construct CPTs, BN and compute distribution. If for initialization, randomly choose parameters to get $\text{CPT}_1 \rightarrow \text{BN}_1 \rightarrow \text{Pr}_1(\cdot)$.
  2. Complete incomplete data cases/rows with all possible instances, and compute corresponding prob. using the current distribution
     - E.g. $\text{Pr}(E = T | H = T, S = F)$
  3. Build empirical distribution based on prob. in step 2
  4. Estimate parameters using empirical distribution to get updated CPTs, and **iteratively** perform steps 1-4 until the likelihood/score of parameters converge



Case	H	S	E
1	T	F	T
2	T	F	T
3	F	T	F
4	F	F	T
5	T	F	F
6	T	F	T
7	F	F	F
8	T	F	T
9	T	F	T
10	F	F	T
11	T	F	T
12	T	T	T
13	T	F	T
14	T	T	T
15	T	F	T
16	T	F	T

Empirical distribution

↓

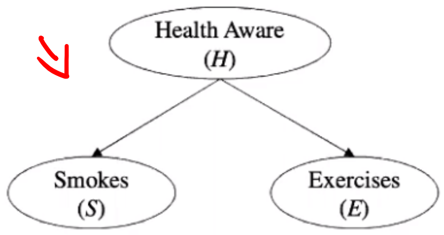
H	S	E	$\text{Pr}_{\mathcal{D}}(.)$	
T	T	T	2/16	
T	T	F	0/16	
T	F	T	9/16	9.6/16
T	F	F	1/16	1.4/16
F	T	T	0/16	
F	T	F	1/16	
F	F	T	2/16	
F	F	F	1/16	

Learning Parameters

Case 2: using **incomplete** data

- Apply **Expectation Maximization (EM)** algorithm
- It's guaranteed that the likelihood/score of parameters won't get worse through iterations
    - **Likelihood** is computed by multiplying probabilities of getting all cases
    - Likelihood will either be improved by iterations or converges to a number
- EM method is similar to local search algorithms in terms of initializing at random point and optimize through iterations
- Where EM converges to depends on where it started

→ may have multiple maximum likelihood parameters if data is incomplete



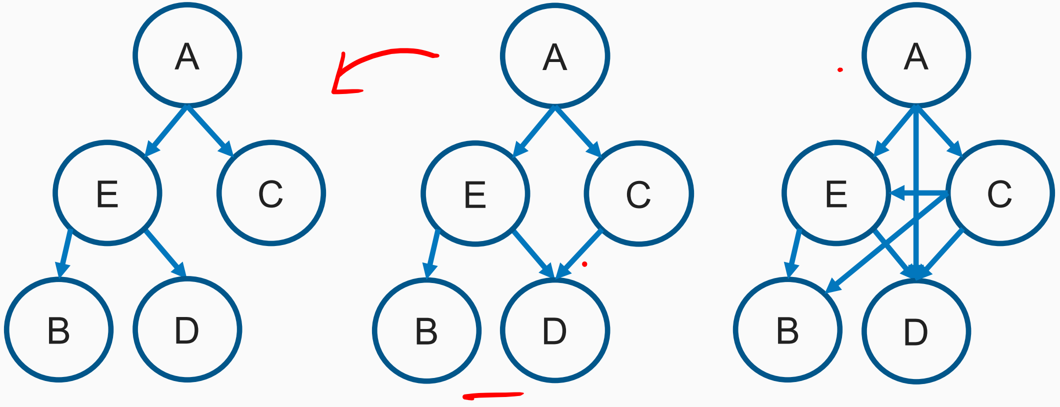
Case	H	S	E
1	T	F	T
2	T	F	T
3	F	T	F
4	F	F	T
5	T	F	F
6	T	F	T
7	F	F	F
8	T	F	T
9	T	F	T
10	F	F	T
11	T	F	T
12	T	T	T
13	T	F	T
14	T	T	T
15	T	F	T
16	T	F	T

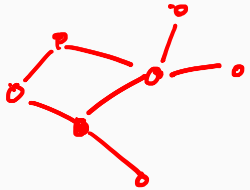
Empirical distribution

↓

H	S	E	$Pr_{\mathcal{D}}(.)$
T	T	T	2/16
T	T	F	0/16
T	F	T	9/16
T	F	F	1/16
F	T	T	0/16
F	T	F	1/16
F	F	T	2/16
F	F	F	1/16

Learning BN Structure

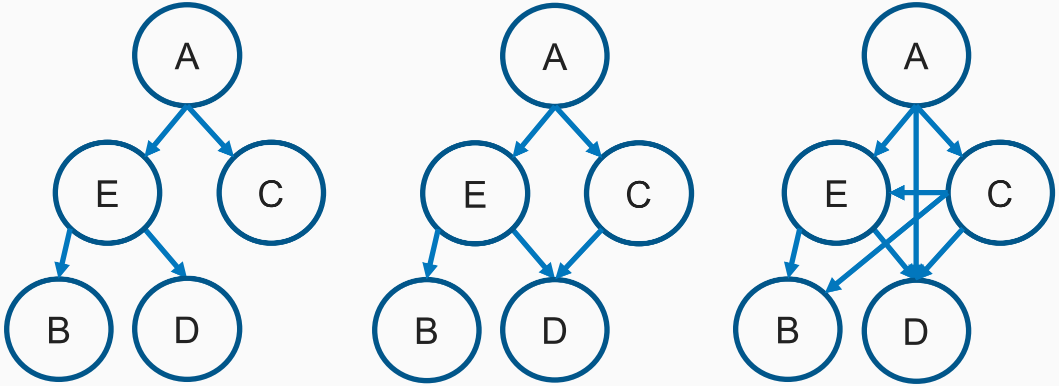


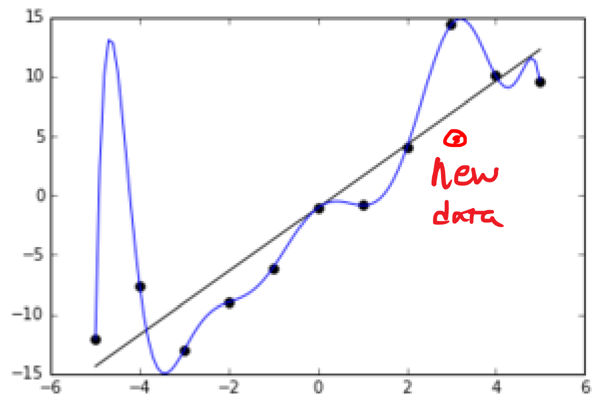


Goal: learn the BN structure given some scoring function

- Methods to find the structure with max. score:
    - Local search methods: add, remove, reverse an edge
        - Approximate method with no guarantee to find optimal structure, but efficient
    - Systematic search methods: A* search
        - Exact method to find optimal structure, but expensive

Learning BN Structure

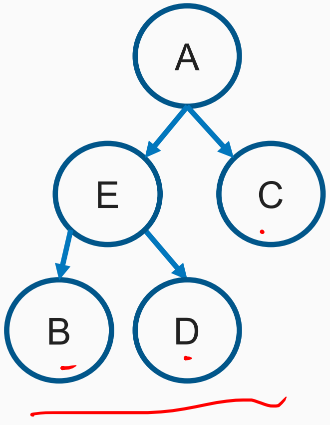




- Maximum likelihood is not enough due to **over-fitting problem**
  - Over-fitting: a statistical model is overfitting if it contains more parameters than can be justified by the data → very likely fail to fit additional data
  - A penalty term that penalizing the # of parameters in BN is needed to calculate scores
  - A good way is using MDL score, which uses both likelihood and penalty terms

Model-oriented vs. Query-oriented Learning

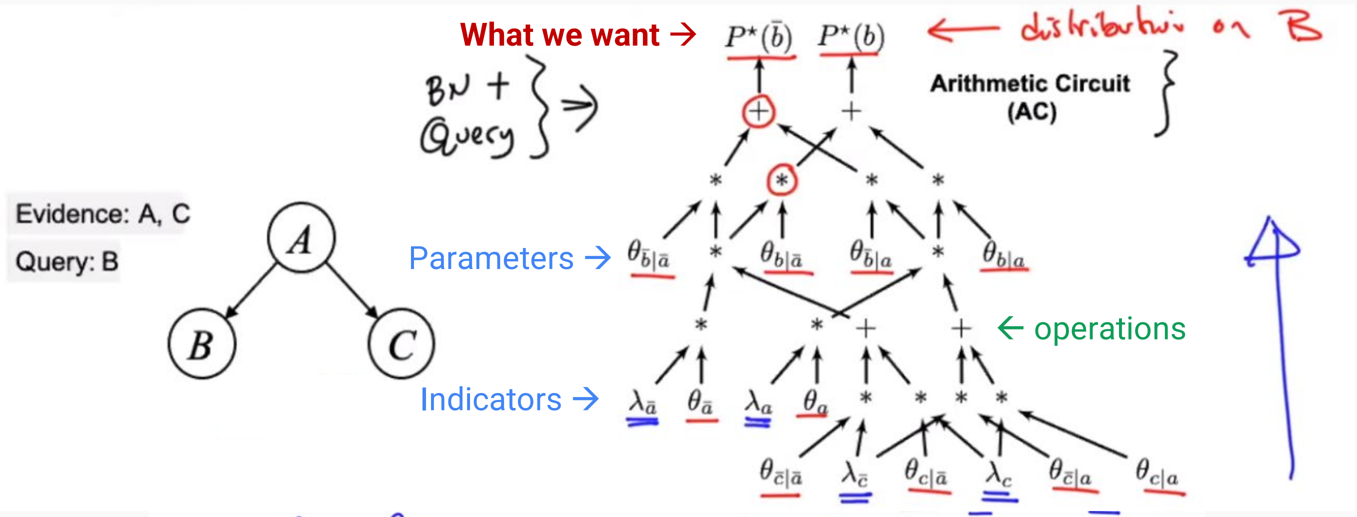
A.k.a. unsupervised vs. supervised learning, or un-labeled vs. labeled learning



Difference:

- Sometimes we want to learn the model to answer all kinds of queries
- Sometimes we only interest in one query, e.g. Pr(A | B, D, C), we need more focused learning → optimize performance while answering the query
  - We need different optimization score

Arithmetic Circuit



A	λ_a	$\lambda_{\bar{a}}$
T	1	0
F	0	1
?	1	1

C

→ evidence (input)

$\boxed{A = T, C = F}$

$\lambda_a = 1$
$\lambda_{\bar{a}} = 0$
$\lambda_c = 0$
$\lambda_{\bar{c}} = 1$

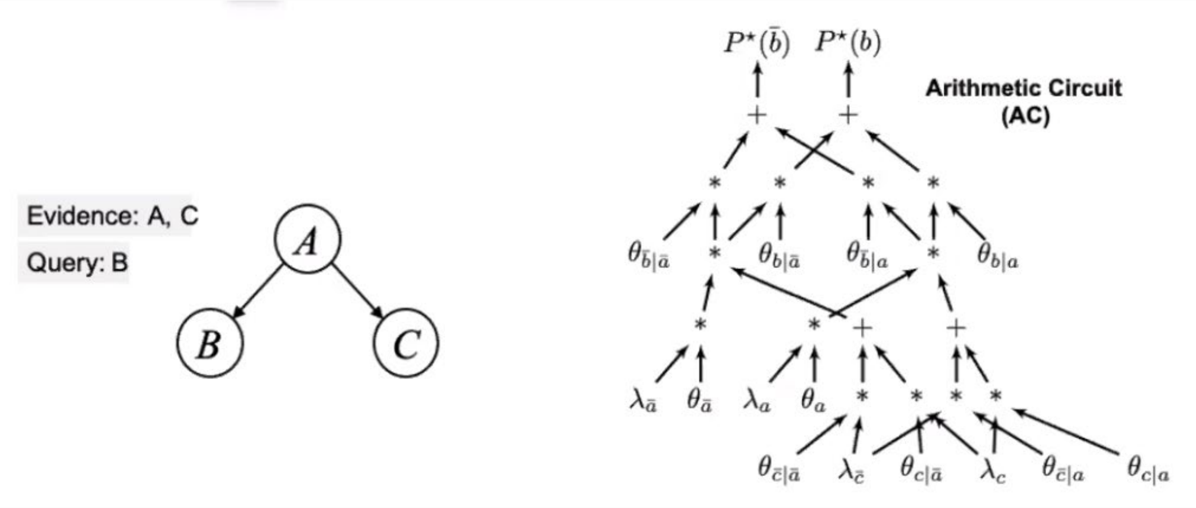
$\boxed{A = F}$

$\lambda_a = 0$
$\lambda_{\bar{a}} = 1$
$\lambda_c = 1$
$\lambda_{\bar{c}} = 1$

Supervised Learning in BN

- Arithmetic circuit (AC) can be compiled from a BN in $O(n \cdot d^w)$ time
  - N: # of variables, d: max # of values of each variable, w: treewidth

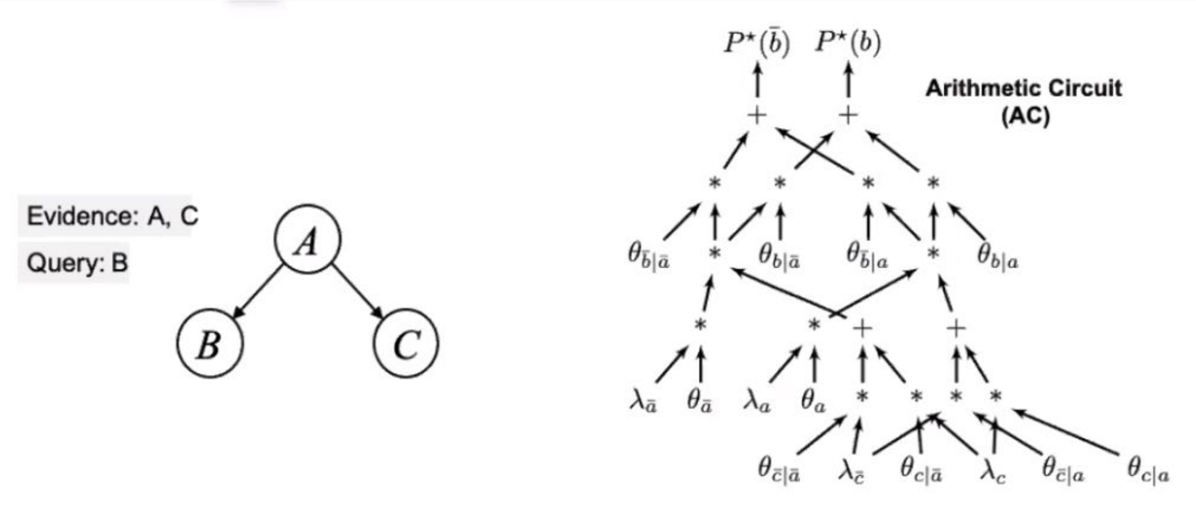
Q: If we don't know the parameters but has labeled data, what should we do?



Labeled Data

input		output
A	C	B
T	T	F
T	F	F
⋮	⋮	
T	T	F

Supervised Learning in BN



Labeled Data

	input		output
	A	C	B
case1	T	T	F
case 2	T	F	F
⋮	⋮	⋮	
	T	T	F

Use **loss function** to optimize parameters:

- Minimize the mean cross entropy between prediction in AC and one-hot distribution obtained from labeled data
    - **Cross entropy**: measures how close two distributions are, it takes P(x) and Q(x) and returns a number

A=T, C=T ⇒ Pr(B) ← prediction

A=T, C=T ⇒

B	
T	0
F	1.

← label, one-hot distribution

for each case

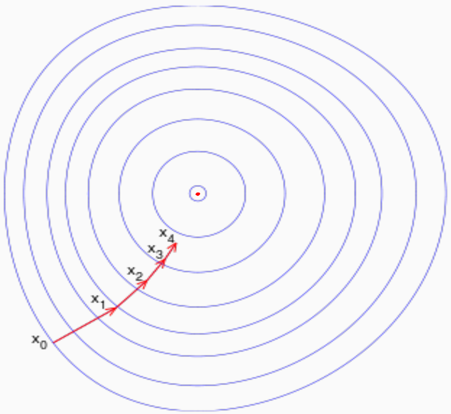
Supervised Learning in BN

Cross entropy (CE) calculation:

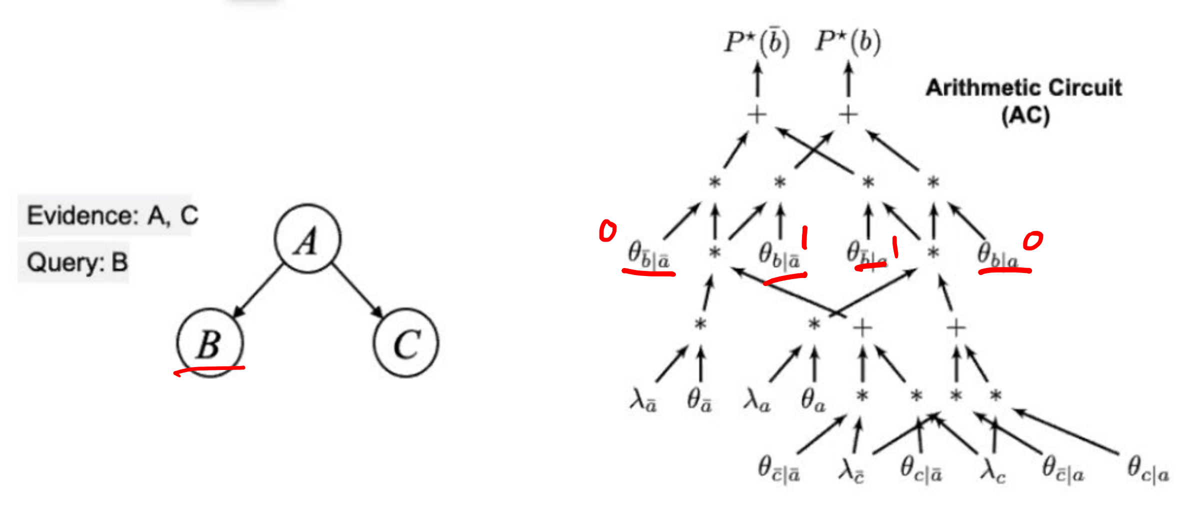
- Given two distributions: P(X) – prediction, Q(X) – label
- CE = $\sum_x Q(x)\log_2(P(x))$ → We try to minimize CE as a loss function using gradient descent

Gradient descent is often used to optimize loss function and find parameters together with neural network.

- It improves parameters by computing derivatives of loss function w.r.t those parameters, and move in the direction of the derivatives



Background Knowledge in BN



Assume we know "B = T iff A = F", we then have background knowledge:

A	B	
t	t	0
t	f	1
f	t	1
f	f	0

background knowledge

→ we can replace parameters in AC with numbers (no need to learn!)

- Background knowledge allows the model to achieve certain accuracy for prediction with less data
- Background knowledge makes the model more robust

Today’s Topics

- BN Learning and Inference
  - Learning parameters
  - Learning BN structure
  - Model-oriented vs. Query-oriented learning
- **Decision Tree and Random Forest**
  - Entropy and Conditional Entropy
  - Classifier
  - BN Classifier
- Hint of HW9

Entropy

Entropy can quantify uncertainty:

- Entropy is non-negative, higher entropy means more uncertainty
- **ENT(X)** = $-\sum_x Pr(x)\, log_2(Pr(x))$

E.g.

	Earthquake	Burglary	Alarm
True	$Pr(E=T)=$ 0.1	0.2	0.2442
False	$Pr(E=F)=$ 0.9	0.8	0.7558
E	0.469	0.722	0.802

$$ENT(E) = -0.1 \times \log_2(0.1) - 0.9 \times \log_2(0.9)$$
$$= 0.469$$

Conditional Entropy

We are interested in ENT(X) and we observe variable Y = y:

- **ENT(X | y)** = -$\sum_x Pr(x|y)\ log_2(Pr(x|y))$

If we want to know the entropy of X when we observe variable Y, but don't know the value of Y yet:

- **ENT(X | Y)** = $\sum_y Pr(y)\ ENT(x|y)$
- ENT(X | Y) ≤ ENT(X) → indicates that we never lose by observing a variable
- ENT(X | Y) = ENT(X) if X and Y are independent

Conditional Entropy - Example

	Burglary	Burglary | A=true	Burglary | A=false
True	0.2	0.741	0.025
False	0.8	0.259	0.975
E	0.722	0.825	0.169

- Unlike ENT(X | Y), ENT(X | y) can be higher or lower than ENT(X).

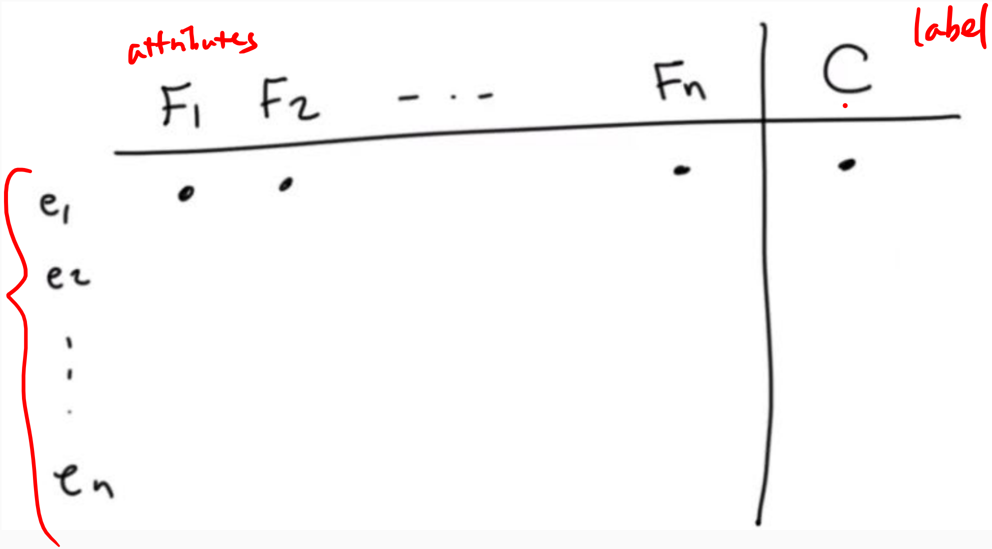
- ENT(Burglary | Alarm) = ENT(B | a) Pr(a) + ENT(B | ¬a) Pr(¬a)
  $= 0.329 \leq 0.722$

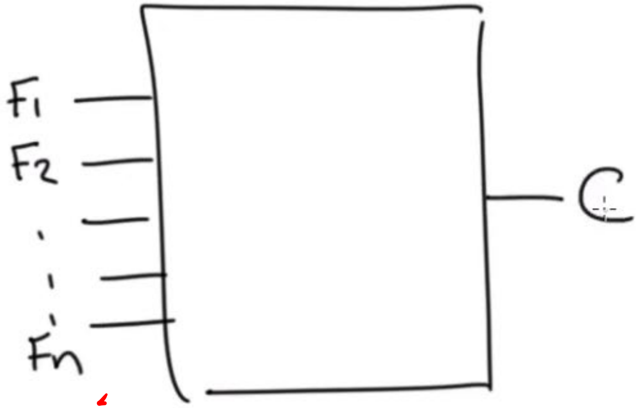
  E(Burglary)

Classifiers

Supervised learning with **labeled** data

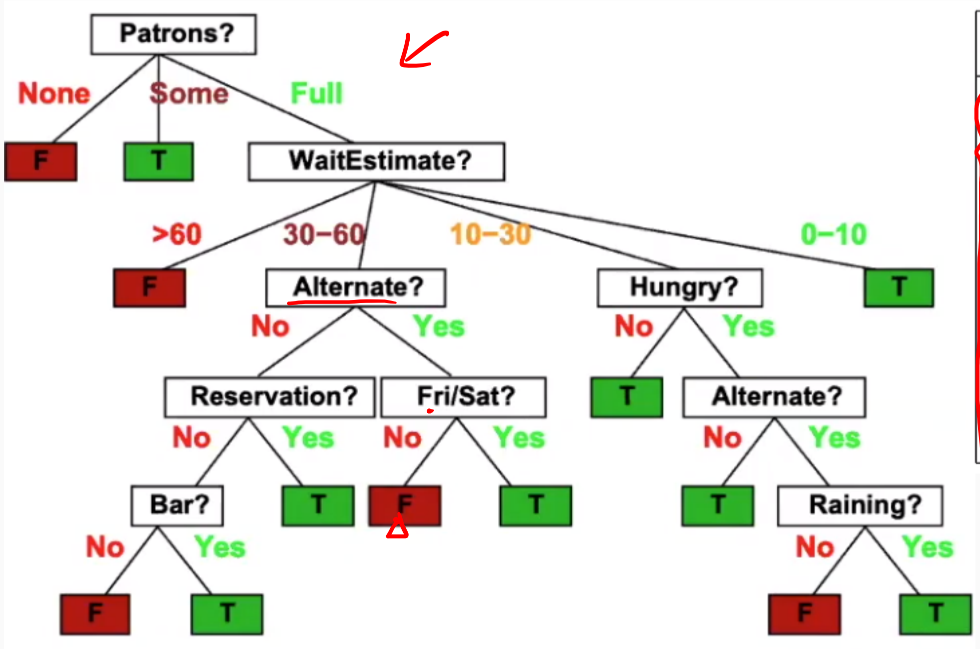
- Take features/attributes as input and output class labels
- A binary classifier has only two types of output





Inputs ↑ Output ↑

Decision Tree - Example



labeled data

label

Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

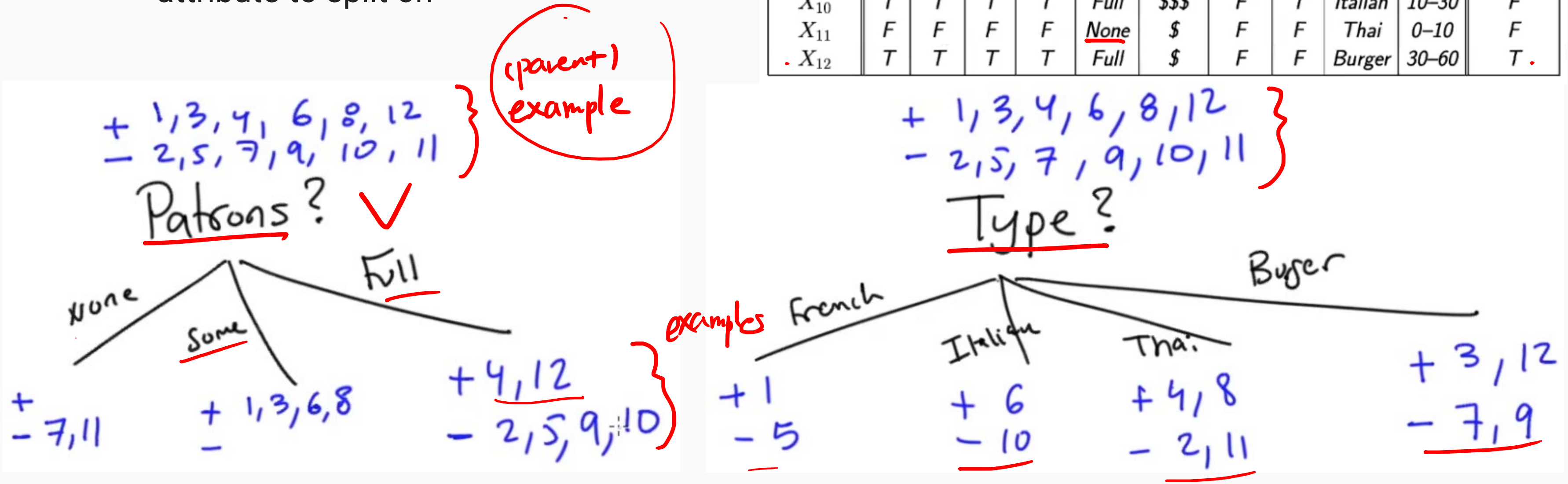
- This decision tree is interpretable
- Classification using decision tree is very simple (e.g. follow attributes to assign a missing label)

Build a Decision Tree

Key: decide which attribute to split on

- We want to split on the attribute with higher discriminating power
    - E.g. Patrons is better than Type as an attribute to split on

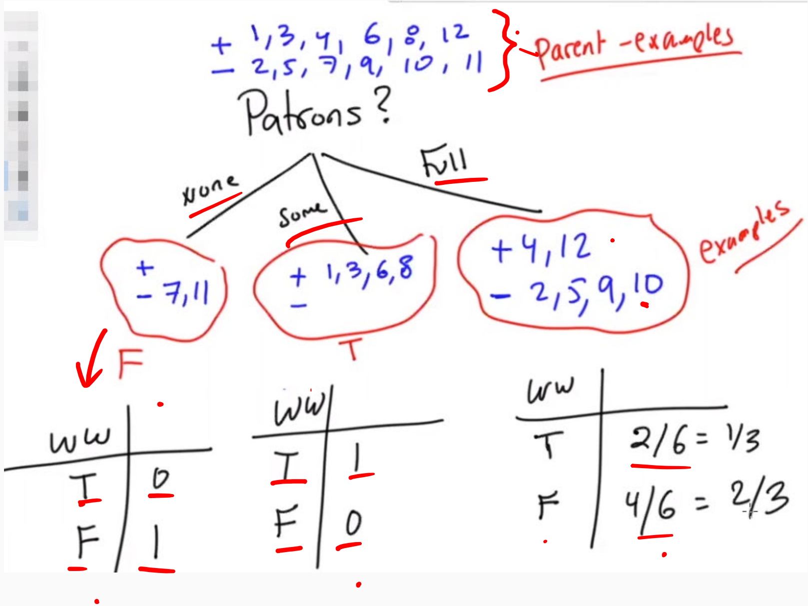
Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T



Build a Decision Tree

Steps:

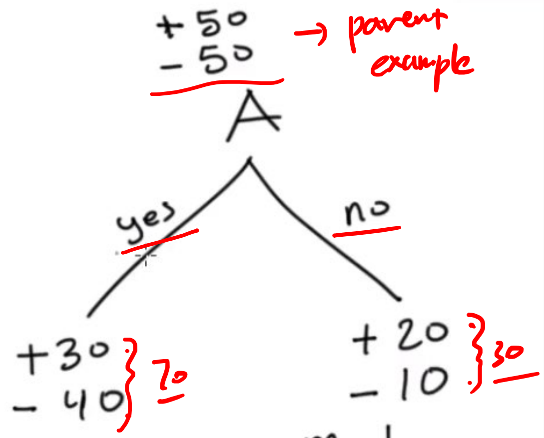
- Consider each of split case as a distribution
- Use **entropy** to quantify the distributions (how certain we are about the class label) after the split
- Compute **conditional entropy** of the output label given current attribute → score of attribute
    - Recall ENT(X | Y) = $\sum_y Pr(y)\ ENT(x|y)$
    - E.g. ENT(WillWait | Patrons)

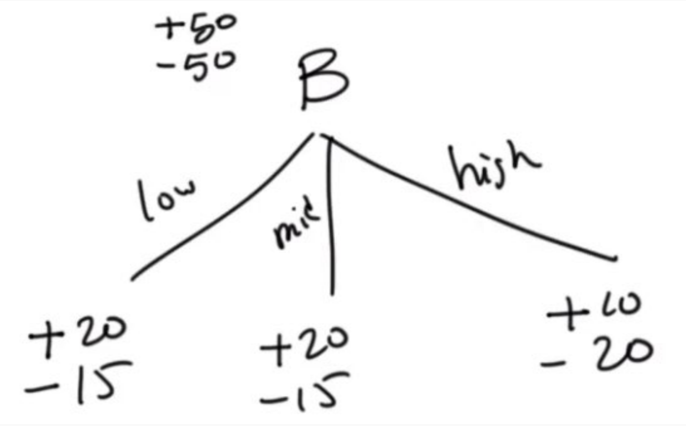


Build a Decision Tree – Example

Let's say we want to output labels of M = {low, high}   100 data examples

We have two attributes to choose – A and B





M	
+low	30/70
−high	40/70

m	
low	20/30
high	10/30

$\Rightarrow ENT(M|A=Yes) = -\frac{3}{7}\log_2\left(\frac{3}{7}\right) - \frac{4}{7}\log_2\left(\frac{4}{7}\right) \simeq 0.985$

$\Rightarrow ENT(M|A=No) = - - - \simeq 0.918$

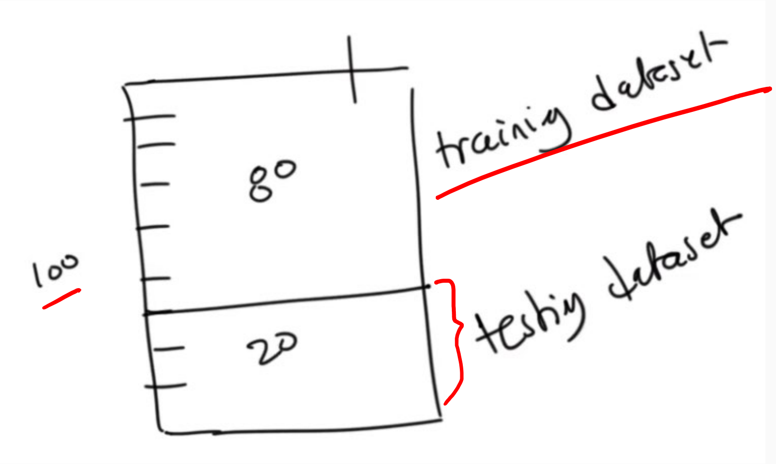
Score of A:

$\Rightarrow = ENT(M|A) = 0.7 \times 0.985 + 0.3 \times 0.918 \approx 0.965$

Cross Validation

Idea: split dataset to training and testing portions, build decision trees multiple times using different combinations of training and testing portions, take the average score

- Very useful to deal with over-fitting problem



5-fold CV
10-fold CV

Random Forests

Random Forests (RF) is an ensemble learning method that combine the results of multiple decision trees

- It does **majority voting** to do classification

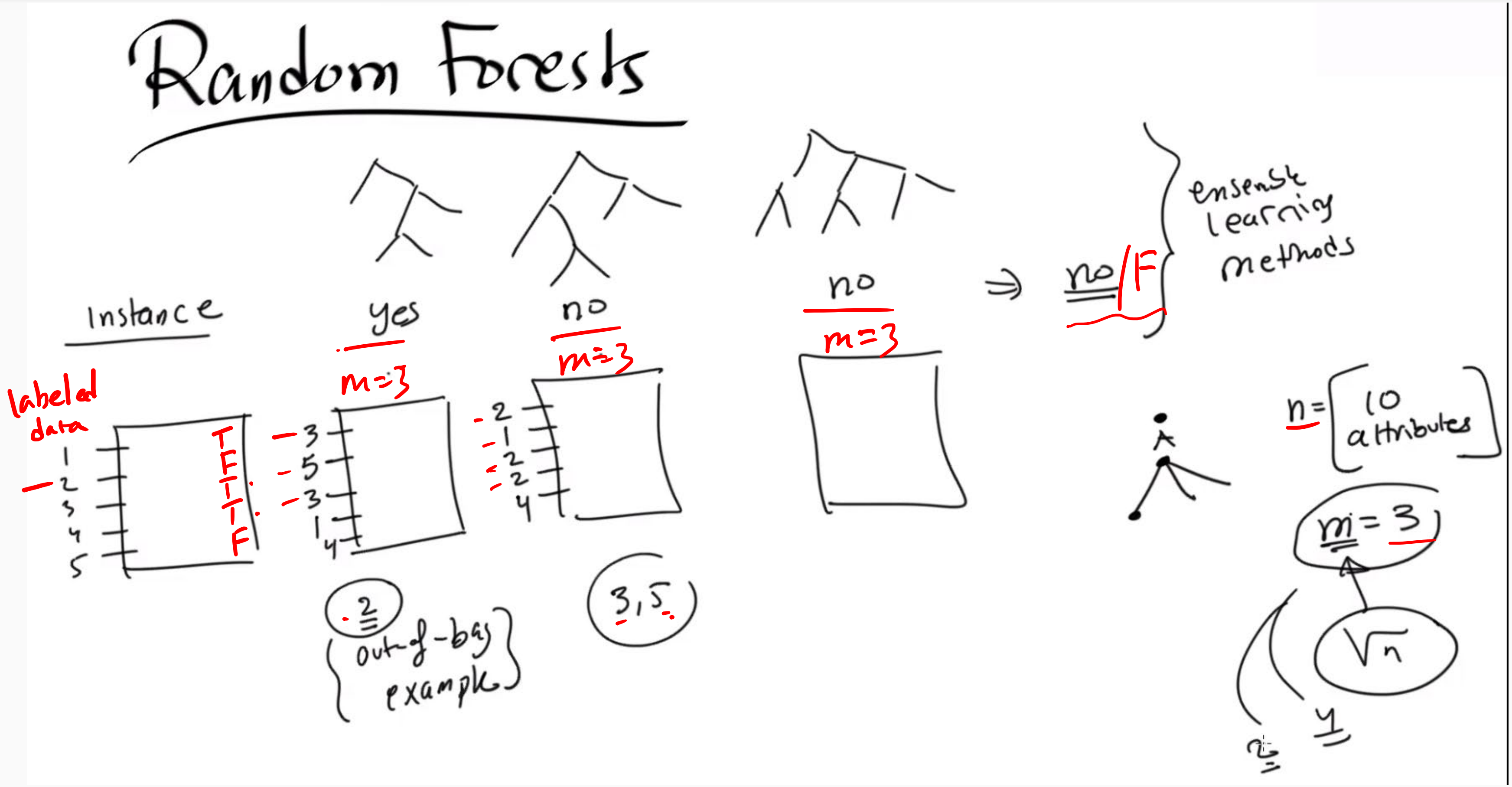
Techniques of construct individual decision trees in RF:

- **Bootstrapping dataset**: randomly sample (with replacement) from the dataset to construct each tree
  - Unselected examples are called out-of-bag examples
- Randomly choose a subset of attributes, then scoring and choose among them

Evaluate the RF:

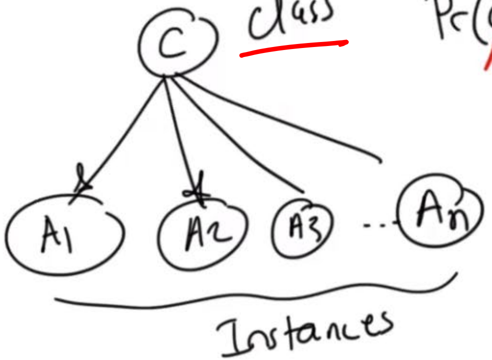
- Run the constructed RF on out-of-bag examples check how well it performs
- Change parameters (e.g. # of picked attributes) to improve performance

Random Forests – Example



BN Classifier

Bayesian Network Classifiers



$Pr(c \mid a_1 \dots a_n)$ $\qquad$ $Pr(\bar{c} \mid a_1 \dots a_n)$

Threshold (T)

c : $Pr(c \mid a_1 \dots a_n) \geq T$

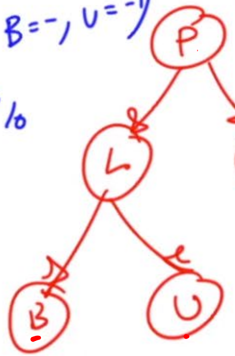
$\bar{c}$: " $< T$

$T = 90\%$

Example: $Pr(P \mid S=+, B=-, U=-1)$

$\geq 90\%$

not pregnant $\qquad$ pregnant



Instance

S, B, U

$+ \quad - \quad -$

Questions?

My slides take the following materials as references:

- Prof. Darwiche's lecture video

Thank you!