# CMSC 471: <br> Probability, and Reasoning and Learning with Uncertainty 

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## Topics

- Review probability theory
- Bayesian inference
- From the joint distribution
- Using independence/factoring
- From sources of evidence
- Representation and Learning
- Bayes nets (a type probabilistic graphical models)
- MLE (maximum likelihood estimation)
- Naïve Bayes algorithm for inference and classification tasks


## Many Sources of Uncertainty

- Uncertain inputs -- missing and/or noisy data
- Uncertain knowledge
- Multiple causes lead to multiple effects
- Incomplete enumeration of conditions or effects
- Incomplete knowledge of causality in the domain
- Probabilistic/stochastic effects
- Uncertain outputs
- Abduction and induction are inherently uncertain
- Default reasoning, even deductive, is uncertain
- Incomplete deductive inference may be uncertain
- Probabilistic reasoning only gives probabilistic results


## Decision making with uncertainty

Rational behavior: for each possible action:

- Identify possible outcomes and for each
- Compute probability of outcome
- Compute utility of outcome
- Compute probability-weighted (expected) utility over possible outcomes
- Select action with the highest expected utility (principle of Maximum Expected Utility)


## Consider

- Your house has an alarm system
- It should go off if a burglar breaks into the house
- It can go off if there is an earthquake
- How can we predict what's happened if the alarm goes off?
- Someone has broken in!
- It's a minor earthquake


## Probability theory 101

- Random variables
- Domain
- Atomic event:
complete specification of state
- Prior probability: degree of belief without any other evidence or info
- Joint probability: matrix of combined probabilities of set of variables
- Alarm, Burglary, Earthquake
- Boolean (like these), discrete, continuous
- Alarm=T^Burglary=T^Earthquake=F alarm $\wedge$ burglary $\wedge \neg$-earthquake
- $\mathrm{P}($ Burglary $)=0.1$
$\mathrm{P}($ Alarm $)=0.1$
$P($ earthquake $)=0.000003$
- $\mathrm{P}($ Alarm, Burglary $)=$

|  | alarm | -alarm |
| :---: | :---: | :---: |
| burglary | .09 | .01 |
| -burglary | .1 | .8 |


\section*{Probability theory 101 | burglary | .09 | .01 |
| :---: | :---: | :---: |
| -burglary | .1 | .8 |}

- Conditional probability: prob. - P(burglary | alarm) =. 47 of effect given causes

P(alarm | burglary) $=.9$

- Computing conditional probs:
$-P(a \mid b)=P(a \wedge b) / P(b)$
$-P(b)$ : normalizing constant
- Product rule:
$-P(a \wedge b)=P(a \mid b) * P(b)$
- Marginalizing:
- $P(B)=\Sigma_{a} P(B, a)$
- $P(B)=\Sigma_{a} P(B \mid a) P(a)$ (conditioning)
- $\mathrm{P}($ alarm $)=$
$\mathrm{P}($ alarm $\wedge$ burglary $)+$
P(alarm $\wedge \neg$ burglary)
= . 09+. 1 = . 19


## Example: Inference from the joint

|  | alarm |  | ᄀalarm |  |
| :---: | :---: | :---: | :---: | :---: |
|  | earthquake | ᄀearthquake | earthquake | ᄀearthquake |
| burglary | .01 | .08 | .001 | .009 |
| †burglary | .01 | .09 | .01 | .79 |

$P($ burglary | alarm $)=\alpha P($ burglary, alarm $)$
$=\alpha[P($ burglary, alarm, earthquake $)+P($ burglary, alarm, -earthquake $)$
$=\alpha[(.01, .01)+(.08, .09)]$
$=\alpha[(.09, .1)]$
Since $P($ burglary $\mid$ alarm $)+P(-b u r g l a r y \mid$ alarm $)=1, \alpha=1 /(.09+.1)=5.26$
(i.e., $\mathrm{P}($ alarm $)=1 / \alpha=.19-$ quizlet: how can you verify this?)
$\mathrm{P}($ burglary | alarm) $=.09 * 5.26=.474$
$\mathrm{P}(-$ burglary | alarm $)=.1 * 5.26=.526$

## Consider

- A student has to take an exam
- She might be smart
- She might have studied
- She may be prepared for the exam
- How are these related?


## Exercise: <br> Inference from the joint

| p(smart <br> study ^ prep) | smart |  | $\neg$ smart |  |
| :---: | :---: | :---: | :---: | :---: |
|  | study | $\neg$ study | study | $\neg$ study |
| prepared | .432 | .16 | .084 | .008 |
| $\neg$ prepared | .048 | .16 | .036 | .072 |

## Queries:

- What is the prior probability of smart?
- What is the prior probability of study?
- What is the conditional probability of prepared, given study and smart?


## Exercise: <br> Inference from the joint

| p(smart <br> study ^ prep) | smart |  | $\neg$ smart |  |
| :---: | :---: | :---: | :---: | :---: |
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## Queries:

- What is the prior probability of smart?
- What is the prior probability of study?
- What is the conditional probability of prepared, given study and smart?
$p($ smart $)=.432+.16+.048+.16=0.8$


## Exercise: <br> Inference from the joint

| p(smart <br> study ^ prep) | smart |  | $\neg$ smart |  |
| :---: | :---: | :---: | :---: | :---: |
|  | study | $\neg$ study | study | $\neg$ study |
| prepared | .432 | .16 | .084 | .008 |
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## Queries:

- What is the prior probability of smart?
- What is the prior probability of study?
- What is the conditional probability of prepared, given study and smart?


## Exercise: <br> Inference from the joint

| p(smart $\wedge$ <br> study $\wedge ~ p r e p) ~$ | smart |  | $\neg$ studyart |  |
| :---: | :---: | :---: | :---: | :---: |
|  | .432 | $\neg$ study | study | $\neg$ study |
| $\neg$ prepared | .048 | .16 | .084 | .008 |

## Queries:

- What is the prior probability of smart?
- What is the prior probability of study?
- What is the conditional probability of prepared, given study and smart?
$p($ study $)=.432+.048+.084+.036=0.6$


## Exercise: <br> Inference from the joint

| p(smart <br> study ^ prep) | smart |  | $\neg$ smart |  |
| :---: | :---: | :---: | :---: | :---: |
|  | study | $\neg$ study | study | $\neg$ study |
| prepared | .432 | .16 | .084 | .008 |
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## Queries:

- What is the prior probability of smart?
- What is the prior probability of study?
- What is the conditional probability of prepared, given study and smart?


## Exercise: <br> Inference from the joint

| p(smart ^ <br> study ^ prep) | smart |  | $\neg$ smart |  |
| :---: | :---: | :---: | :---: | :---: |
|  | study | $\neg$ study | study | $\neg$ study |
| prepared | .432 | .16 | .084 | .008 |
| $\neg$ prepared | .048 | .16 | .036 | .072 |

## Queries:

- What is the prior probability of smart?
- What is the prior probability of study?
- What is the conditional probability of prepared, given study and smart?
p(prepared|smart,study)= p(prepared,smart,study)/p(smart, study)
$=.432 /(.432+.048)$
$=0.9$


## Independence

- When variables don't affect each others' probabilities, they are independent; we can easily compute their joint \& conditional probability: Independent $(A, B) \rightarrow P(A \wedge B)=P(A) * P(B)$ or $P(A \mid B)=P(A)$
- \{moonPhase, lightLevel\} might be independent of \{burglary, alarm, earthquake\}
- Maybe not: burglars may be more active during a new moon because darkness hides their activity
- But if we know light level, moon phase doesn't affect whether we are burglarized
- If burglarized, light level doesn't affect if alarm goes off
- Need a more complex notion of independence and methods for reasoning about the relationships


## Exercise: Independence

| p(smart <br> study ^ prep) | smart |  | $\neg$ smart |  |
| :---: | :---: | :---: | :---: | :---: |
|  | study | $\neg$ study | study | $\neg$ study |
| prepared | .432 | .16 | .084 | .008 |
| $\neg$ prepared | .048 | .16 | .036 | .072 |

Queries:
-Q1: Is smart independent of study?
-Q2: Is prepared independent of study?
How can we tell?

## Exercise: Independence

| p(smart <br> study ^ prep) | smart |  | $\neg$ smart |  |
| :---: | :---: | :---: | :---: | :---: |
|  | study | $\neg$ study | study | $\neg$ study |
| prepared | .432 | .16 | .084 | .008 |
| $\neg$ prepared | .048 | .16 | .036 | .072 |

Q1: Is smart independent of study?

- You might have some intuitive beliefs based on your experience
- You can also check the data

Which way to answer this is better?

## Exercise: Independence

| p(smart $\wedge$ <br> study $\wedge ~ p r e p) ~$ | smart |  | $\neg$ smart |  |
| :---: | :---: | :---: | :---: | :---: |
|  | study | $\neg$ study | study | $\neg$ study |
| prepared | .432 | .16 | .084 | .008 |
| $\neg$ prepared | .048 | .16 | .036 | .072 |

Q1: Is smart independent of study?
Q1 true iff p(smart|study) == p(smart)
$p($ smart $\mid$ study $)=p($ smart, study $) / p(s t u d y)$
$=(.432+.048) / .6=0.8$
$0.8==0.8$, so smart is independent of study

## Exercise: Independence

| p(smart <br> study ^ prep) | smart |  | $\neg$ smart |  |
| :---: | :---: | :---: | :---: | :---: |
|  | study | $\neg$ study | study | $\neg$ study |
| prepared | .432 | .16 | .084 | .008 |
| $\neg$ prepared | .048 | .16 | .036 | .072 |

Q2: Is prepared independent of study?
-What is prepared?

- Q2 true iff


## Exercise: Independence

| p(smart <br> study ^ prep) | smart |  | $\neg$ smart |  |
| :---: | :---: | :---: | :---: | :---: |
|  | study | $\neg$ study | study | $\neg$ study |
| prepared | .432 | .16 | .084 | .008 |
| $\neg$ prepared | .048 | .16 | .036 | .072 |

Q2: Is prepared independent of study?
Q2 true iff $p$ (prepared|study) == p(prepared) p(prepared|study) $=$ p(prepared,study)/p(study)
$=(.432+.084) / .6=.86$
$0.86 \neq 0.8$, so prepared not independent of study

## Bayes' rule

Derived from the product rule:

$-P(A, B)=P(A \mid B) * P(B)$ \#from definition of conditional probability
$-P(B, A)=P(B \mid A) * P(A)$ \# from definition of conditional probability
$-P(A, B)=P(B, A) \quad$ \# since order is not important
So...

## $P(A \mid B)=P(B \mid A) * P(A)$ <br> P(B)

## Useful for diagnosis!

- $C$ is a cause, $E$ is an effect:

$-P(C \mid E)=P(E \mid C) * P(C) / P(E)$
- Useful for diagnosis:
-E are (observed) effects and C are (hidden) causes,
-Often have model for how causes lead to effects P(E|C)
-May also have info (based on experience) on frequency of causes (P(C))
-Which allows us to reason abductively from effects to causes (P(C|E))


## Ex: meningitis and stiff neck

- Meningitis (M) can cause stiff neck (S), though there are other causes too
- Use $S$ as a diagnostic symptom and estimate p(M|S)
- Studies can estimate $p(M), p(S) \& p(S \mid M)$, e.g. $p(M)=0.7, p(S)=0.01, p(M)=0.00002$
- Harder to directly gather data on $\mathrm{p}(\mathrm{M} \mid \mathrm{S})$
- Applying Bayes' Rule:

$$
p(M \mid S)=p(S \mid M) * p(M) / p(S)=0.0014
$$

## Reasoning from evidence to a cause

- In the setting of diagnostic/evidential reasoning

hypotheses
evidence/manifestations
- Know prior probability of hypothesis $\quad \boldsymbol{P}\left(\boldsymbol{H}_{\boldsymbol{i}}\right)$ conditional probability

$$
P\left(E_{j} \mid H_{i}\right)
$$

- Want to compute the posterior probability $\boldsymbol{P}\left(\boldsymbol{H}_{i} \mid \boldsymbol{E}_{j}\right)$
- Bayes' s theorem:

$$
P\left(H_{i} \mid E_{j}\right)=P\left(H_{i}\right) * P\left(E_{j} \mid H_{i}\right) / P\left(E_{j}\right)
$$

## Simple Bayesian diagnostic reasoning

- Naive Bayes classifier
- Knowledge base:
- Evidence / manifestations: $\mathrm{E}_{1}, \ldots \mathrm{E}_{\mathrm{m}}$
- Hypotheses / disorders: $\mathrm{H}_{1}, \ldots \mathrm{H}_{\mathrm{n}}$

Note: $\mathrm{E}_{\mathrm{j}}$ and $\mathrm{H}_{\mathrm{i}}$ are binary; hypotheses are mutually exclusive (non-overlapping) and exhaustive (cover all possible cases)

- Conditional probabilities: $\mathrm{P}\left(\mathrm{E}_{\mathrm{j}} \mid \mathrm{H}_{\mathrm{i}}\right), \mathrm{i}=1, \ldots \mathrm{n} ; \mathrm{j}=1, \ldots \mathrm{~m}$
- Cases (evidence for a particular instance): $\mathrm{E}_{1}, \ldots, \mathrm{E}_{1}$
- Goal: Find the hypothesis $\mathrm{H}_{\mathrm{i}}$ with highest posterior
- Max ${ }_{i} P\left(H_{i} \mid E_{1}, \ldots, E_{i}\right)$


## Simple Bayesian diagnostic reasoning

- Bayes' rule:

$$
P\left(H_{i} \mid E_{1} \ldots E_{m}\right)=P\left(E_{1} \ldots E_{m} \mid H_{i}\right) P\left(H_{i}\right) / P\left(E_{1} \ldots E_{m}\right)
$$

- Assume each evidence $E_{i}$ is conditionally independent of the others, given a hypothesis $\mathrm{H}_{\mathrm{i}}$, then:

$$
P\left(E_{1} \ldots E_{m} \mid H_{i}\right)=\prod_{j=1}^{m} P\left(E_{j} \mid H_{i}\right)
$$

- If only care about relative probabilities for $\mathrm{H}_{\mathrm{i}}$, then:

$$
P\left(H_{i} \mid E_{1} \ldots E_{m}\right)=\alpha P\left(H_{i}\right) \prod_{j=1}^{m_{j}} P\left(E_{j} \mid H_{i}\right)
$$

## Naïve Bayes

- Use Bayesian modeling
- Make the simplest possible independence assumption:
-Each attribute is independent of the values of the other attributes, given the class variable
- In our restaurant domain: Cuisine is independent of Patrons, given a decision to stay (or not)


## Bayesian Formulation

- $p\left(C \mid F_{1}, \ldots, F_{n}\right)=p(C) p\left(F_{1}, \ldots, F_{n} \mid C\right) / P\left(F_{1}, \ldots, F_{n}\right)$ $=\alpha p(C) p\left(F_{1}, \ldots, F_{n} \mid C\right)$
- Assume each feature $F_{i}$ is conditionally independent of others given the class $C$. Then:
$p\left(C \mid F_{1}, \ldots, F_{n}\right)=\alpha p(C) \Pi_{i} p\left(F_{i} \mid C\right)$
- Estimate each of these conditional probabilities from the observed counts in the training data:
$p\left(F_{i} \mid C\right)=N\left(F_{i} \wedge C\right) / N(C)$
- One subtlety of using the algorithm in practice: when your estimated probabilities are zero, ugly things happen
- Fix: Add one to every count (aka Laplace smoothing-they have a different name for everything!)


## Naive Bayes: Example

p (Wait | Cuisine, Patrons, Rainy?) =
$=\alpha \cdot p($ Wait $) \cdot p($ Cuisine $\mid$ Wait $) \cdot p($ Patrons $\mid$ Wait $) \cdot p($ Rainy ? $\mid$ Wait $)$
$=p($ Wait $) \cdot p($ Cuisine $\mid$ Wait $) \cdot p($ Patrons $\mid$ Wait $) \cdot p($ Rainy? $\mid$ Wait $)$ $p$ (Cuisine) • $p$ (Patrons) • $p$ (Rainy?)

We can estimate all of the parameters ( $p(F)$ and $p(C)$ just by counting from the training examples

## Naive Bayes: Analysis

- Naive Bayes is amazingly easy to implement (once you understand the math behind it)
- Naive Bayes can outperform many much more complex algorithms-it's a baseline that should be tried or used for comparison
- Naive Bayes can't capture interdependencies between variables (obviously)—for that, we need Bayes nets!


## Bag of Words Classifier



## Naïve Bayes (NB) Classifier



Start with Bayes Rule

## Naïve Bayes (NB) Classifier



Adopt naïve bag of words representation $X_{t}$

## Learning for a Naïve Bayes Classifier

Assuming V vocab types $w_{1}, \ldots, w_{V}$ and L classes $u_{1}, \ldots, u_{L}$ (and appropriate corpora)

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(values/weights) must
be learned?

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Assuming V vocab types $w_{1}, \ldots, w_{V}$ and L classes $u_{1}, \ldots, u_{L}$ (and appropriate corpora)

Q: What parameters (values/weights) must
$\mathrm{A}: p\left(w_{v} \mid u_{l}\right), p\left(u_{l}\right)$ be learned?

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$$
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$$

Q: How many
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## Learning for a Naïve Bayes Classifier

Assuming V vocab types $w_{1}, \ldots, w_{V}$ and L classes $u_{1}, \ldots, u_{L}$ (and appropriate corpora)

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Q: How many
parameters must be learned?

$$
\mathrm{A}: p\left(w_{v} \mid u_{l}\right), p\left(u_{l}\right)
$$

$$
\mathrm{A}: L K+L
$$

## Learning for a Naïve Bayes Classifier

Assuming V vocab types $w_{1}, \ldots, w_{V}$ and L classes $u_{1}, \ldots, u_{L}$ (and appropriate corpora)

Q: What parameters
(values/weights) must be learned?

Q: How many
parameters must be learned?

Q: What distributions need to sum to 1?
$\mathrm{A}: p\left(w_{v} \mid u_{l}\right), p\left(u_{l}\right)$

$$
\mathrm{A}: L K+L
$$

## Learning for a Naïve Bayes Classifier

Assuming V vocab types $w_{1}, \ldots, w_{V}$ and L classes $u_{1}, \ldots, u_{L}$ (and appropriate corpora)

Q: What parameters
(values/weights) must be learned?

Q: How many
parameters must be learned?

Q: What distributions need to sum to 1?

A: $p\left(w_{v} \mid u_{l}\right), p\left(u_{l}\right)$

$$
\mathrm{A}: L K+L
$$

A: Each $p\left(\cdot \mid u_{l}\right)$, and the prior

## Multinomial Naïve Bayes: Learning

From training corpus, extract Vocabulary

Calculate $P\left(c_{j}\right)$ terms
For each $c_{j}$ in $C$ do
docs $_{j}=$ all docs with class $=c_{j}$

$$
p\left(c_{j}\right)=\frac{\left|\operatorname{docs}_{j}\right|}{\# \text { docs }}
$$

Calculate $P\left(w_{k} \mid c_{j}\right)$ terms
Text $_{j}=$ single doc containing all docs $_{j}$
For each word $w_{k}$ in Vocabulary $n_{k}=\#$ of occurrences of $w_{k}$ in $^{\text {Text }}{ }_{j}$

$$
\begin{gathered}
p\left(w_{k} \mid c_{j}\right)=\text { class (unigram) LM } \\
\propto \text { count }\left(\text { word } w_{k}\right. \text { in doc } \\
\text { labeled with } \left.c_{j}\right)
\end{gathered}
$$

## Naive Bayes: Analysis

- Naive Bayes is amazingly easy to implement (once you understand the math behind it)
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With enough data, the classifier may not matter

## Naive Bayes: Analysis

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## Limitations



- Can't easily handle multi-fault situations or cases where intermediate (hidden) causes exist:
- Disease D causes syndrome S, which causes correlated manifestations $\mathrm{M}_{1}$ and $\mathrm{M}_{2}$
- Consider composite hypothesis $\mathrm{H}_{1} \wedge \mathrm{H}_{2}$, where $\mathrm{H}_{1}$ \& $\mathrm{H}_{2}$ independent. What's relative posterior?
$P\left(H_{1} \wedge H_{2} \mid E_{1}, \ldots, E_{1}\right)=\alpha P\left(E_{1}, \ldots, E_{1} \mid H_{1} \wedge H_{2}\right) P\left(H_{1} \wedge\right.$ $\mathrm{H}_{2}$ )

$$
\begin{aligned}
& =\alpha P\left(E_{1}, \ldots, E_{1} \mid H_{1} \wedge H_{2}\right) P\left(H_{1}\right) P\left(H_{2}\right) \\
& =\alpha \prod_{j=1}^{1} P\left(E_{j} \mid H_{1} \wedge H_{2}\right) P\left(H_{1}\right) P\left(H_{2}\right)
\end{aligned}
$$

- How do we compute $P\left(\mathrm{E}_{\mathrm{j}} \mid \mathrm{H}_{1} \wedge \mathrm{H}_{2}\right)$ ?


## Summary

- Probability a rigorous formalism for uncertain knowledge
- Joint probability distribution specifies probability of every atomic event
- Answer queries by summing over atomic events
- Must reduce joint size for non-trivial domains
- Bayes rule: compute from known conditional probabilities, usually in causal direction
- Independence \& conditional independence provide tools
- Next: Bayesian belief networks


## Overview

- Bayesian Belief Networks (BBNs) can reason with networks of propositions and associated probabilities
- Useful for many AI problems
- Diagnosis
- Expert systems
- Planning
- Learning


## Probabilistic Graphical Models

A graph G that represents a probability distribution over random variables $X_{1}, \ldots, X_{N}$

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Distribution $p\left(X_{1}, \ldots, X_{N}\right)$

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> Graph $\mathrm{G}=($ vertices V, edges E$)$
> Distribution $p\left(X_{1}, \ldots, X_{N}\right)$

Vertices $\leftrightarrow$ random variables
Edges show dependencies among random variables

## Probabilistic Graphical Models

A graph $G$ that represents a probability distribution over random variables $X_{1}, \ldots, X_{N}$

Graph G = (vertices V, edges E)
Distribution $p\left(X_{1}, \ldots, X_{N}\right)$

Vertices $\leftrightarrow$ random variables
Edges show dependencies among random variables

Two main flavors: directed graphical models and undirected graphical models (come talk to me)

## Directed Graphical Models

A directed (acyclic) graph $\mathrm{G}=(\mathrm{V}, \mathrm{E})$ that represents a probability distribution over random variables

$$
X_{1}, \ldots, X_{N}
$$

Joint probability factorizes into factors of $X_{i}$ conditioned on the parents of $X_{i}$

## Directed Graphical Models

A directed (acyclic) graph $\mathrm{G}=(\mathrm{V}, \mathrm{E})$ that represents a probability distribution over random variables

$$
X_{1}, \ldots, X_{N}
$$

Joint probability factorizes into factors of $X_{i}$ conditioned on the parents of $X_{i}$

## Benefit: the independence <br> properties are transparent

## Directed Graphical Models

A directed (acyclic) graph $\mathrm{G}=(\mathrm{V}, \mathrm{E})$ that represents a probability distribution over random variables

$$
X_{1}, \ldots, X_{N}
$$

Joint probability factorizes into factors of $X_{i}$ conditioned on the parents of $X_{i}$

A graph/joint distribution that follows this is a Bayesian network

## BBN Definition

- AKA Bayesian Network, Bayes Net
- A graphical model (as a DAG) of probabilistic relationships among a set of random variables
- Nodes are variables, links represent direct influence of one variable on another
- Nodes have associated prior probabilities or Conditional Proability Tables (CPTs)


## Why? Three (Four) kinds of reasoning

BBNs support three main kinds of reasoning:

- Predicting conditions given predispositions
- Diagnosing conditions given symptoms (and predisposing)
- Explaining a condition by one or more predispositions
To which we can add a fourth:
- Deciding on an action based on probabilities of the conditions


## Recall Bayes Rule

$$
P(H, E)=P(H \mid E) P(E)=P(E \mid H) P(H)
$$

$$
P(H \mid E)=\frac{P(E \mid H) P(H)}{P(E)}
$$

Note symmetry: can compute probability of a hypothesis given its evidence as well as probability of evidence given hypothesis

## Simple Bayesian Network

$$
S \in\{\text { no, light, heavy }\} \text { Smoking } \longrightarrow \xrightarrow[C \in\{\text { none, benign, malignant }\}]{\longrightarrow}
$$

## Simple Bayesian Network



## Simple Bayesian Network



Prior probability of $S$

| $P(S=$ no $)$ | 0.80 | Nodes with no in-links |
| :--- | :--- | :--- |
| $P(S=$ light $)$ | 0.15 |  |
| have prior probabilities |  |  |

Conditional distribution of S and $\mathbf{C}$

| Nodes with in-links have joint probability distributions | Smoking= | no | light | heavy |
| :---: | :---: | :---: | :---: | :---: |
|  | C=none | 0.96 | 0.88 | 0.60 |
|  | C=benign | 0.03 | 0.08 | 0.25 |
|  | C=malignant | 0.01 | 0.04 | $0.15^{54}$ |

## Bayesian Networks: <br> Directed Acyclic Graphs



$$
p\left(x_{1}, x_{2}, x_{3}, \ldots, x_{N}\right)=\prod_{\substack{i \\ \text { topological } \\ \text { sort }}} p\left(x_{i} \mid \pi\left(x_{i}\right)\right)
$$

## Bayesian Networks: <br> Directed Acyclic Graphs



$$
\begin{aligned}
& p\left(x_{1}, x_{2}, x_{3}, \ldots, x_{N}\right)=\prod_{i} p\left(x_{i} \mid \pi\left(x_{i}\right)\right) \\
& p\left(x_{1}, x_{2}, x_{3}, x_{4}, x_{5}\right)=? ? ?
\end{aligned}
$$

## Bayesian Networks: <br> Directed Acyclic Graphs



$$
p\left(x_{1}, x_{2}, x_{3}, x_{4}, x_{5}\right)=
$$

$$
p\left(x_{1}\right) p\left(x_{3}\right) p\left(x_{2} \mid x_{1}, x_{3}\right) p\left(x_{4} \mid x_{2}, x_{3}\right) p\left(x_{5} \mid x_{2}, x_{4}\right)
$$

## Bayesian Networks: <br> Directed Acyclic Graphs



$$
p\left(x_{1}, x_{2}, x_{3}, \ldots, x_{N}\right)=\prod_{i} p\left(x_{i} \mid \pi\left(x_{i}\right)\right)
$$

exact inference in general DAGs is NP-hard inference in trees can be exact

## More Complex Bayesian Network



## More Complex Bayesian Network

Nodes represent variables

- Does gender cause smoking?
- Influence might be a better term



## More Complex Bayesian Network



## More Complex Bayesian Network


predispositions

## More Complex Bayesian Network



## More Complex Bayesian Network

Can we predict likelihood of lung tumor given values of other 6 variables?


- Model has 7 variables
- Complete joint probability distribution will have 7 dimensions!
- Too much data required $:$ :
- BBN simplifies: a node has a CPT with data on itself \& parents in graph


## Independence \& Conditional Independence in BBNs

Read these independence relationships right from the graph!

There are two common concepts that can help:

1. Markov blanket
2. D-separation (not covering)

## Markov Blanket

The Markov Blanket of a node $\mathrm{x}_{\mathrm{i}}$ the set of nodes needed to form the complete conditional for a variable $\mathrm{x}_{\mathrm{i}}$

## Markov Blanket



> Markov blanket of a node $x$ is its parents, children, and children's parents

The Markov Blanket of a node $\mathrm{x}_{\mathrm{i}}$ the set of nodes needed to form the complete conditional for a variable $\mathrm{x}_{\mathrm{i}}$


=


Given its Markov blanket, a node is conditionally independent of all other nodes in the BN

## Independence

Age
Age and Gender are independent.

$$
P(A, G)=P(G) * P(A)
$$

There is no path between them in the graph

$$
\begin{aligned}
& P(A \mid G)=P(A) \\
& P(G \mid A)=P(G) \\
& P(A, G)=P(G \mid A) P(A)=P(G) P(A) \\
& P(A, G)=P(A \mid G) P(G)=P(A) P(G)
\end{aligned}
$$

## Conditional Independence



## Conditional Independence



## Cancer is independent of Age and Gender given Smoking

- Instead of one big CPT with 4 variables, we have two smaller CPTs with 3 and 2 variables
- If all variables binary: 12 models $\left(2^{3}+2^{2}\right)$ rather than $16\left(2^{4}\right)$


## Conditional Independence: Naïve Bayes



Serum Calcium and Lung Tumor are dependent

Serum Calcium is independent of Lung Tumor, given Cancer

$$
\begin{aligned}
& P(L \mid S C, C)=P(L \mid C) \\
& P(S C \mid L, C)=P(S C \mid C)
\end{aligned}
$$

Naïve Bayes assumption: evidence (e.g., symptoms) independent given disease; easy to combine evidence

## Explaining Away



Exposure to Toxics and Smoking are independent

Exposure to Toxics is dependent on Smoking, given Cancer
$P(E=$ heavy | $C=$ malignant $)>P(E=$ heavy
| C=malignant, S=heavy)

- Explaining away: reasoning pattern where confirmation of one cause reduces need to invoke alternatives
- Essence of Occam's Razor (prefer hypothesis with fewest assumptions)
- Relies on independence of causes


## Conditional Independence



## Example from the Book: 8.15

## http://artint.info/2e/html/ArtInt2e.Ch8.S3.SS2.html



Some questions:

1. What's the joint factorization? That is, simplify the joint distribution

$$
p(F, T, A, S, L, R)
$$

2. Are A \& S independent?
3. Are there any nodes that make A \& S conditionally independent?
4. How many different conditional distributions do we need?


## D-Separation: Testing for Conditional Independence

## d-separation

$X \& Y$ are d-separated if for all paths $P$, one of the following is true:
$P$ has a chain with an observed middle node

$P$ has a fork with an observed parent node


P includes a " $v$-structure" or "collider" with all unobserved descendants



## D-Separation: Testing for Conditional Independence

Variables X \& Y are conditionally independent given $Z$ if all (undirected) paths from (any variable in) $X$ to (any variable in) $Y$ are d-separated by $Z$

## d-separation

$X \& Y$ are d-separated if for all paths $P$, one of the following is true:
$P$ has a chain with an observed middle node
observing Z blocks the path from $X$ to $Y$
observing Z blocks the path from $X$ to $Y$
not observing $Z$ blocks
the path from $X$ to $Y$

$P$ has a fork with an observed parent node


P includes a "v-structure" or "collider" with all unobserved descendants


## D-Separation: Testing for Conditional Independence

Variables X \& Y are conditionally independent given $Z$ if all (undirected) paths from (any variable in) $X$ to (any variable in) $Y$ are d-separated by $Z$

## d-separation

$X \& Y$ are d-separated if for all paths $P$, one of the following is true:
$P$ has a chain with an observed middle node
observing $Z$ blocks the path from $X$ to $Y$


P has a fork with an observed parent node
observing Z blocks the path from $X$ to $Y$


P includes a "v-structure" or "collider" with all unobserved descendants
not observing $Z$ blocks the path from $X$ to $Y$ $p(x, y, z)=p(x) p(y) p(z \mid x, y)$ $p(x, y)=\sum_{z} p(x) p(y) p(z \mid x, y)=p(x) p(y)$


## Probabilistic Graphical Models

A graph G that represents a probability distribution over random variables $X_{1}, \ldots, X_{N}$

> Graph $\mathrm{G}=($ vertices V , edges E$)$
> Distribution $p\left(X_{1}, \ldots, X_{N}\right)$

Vertices $\leftrightarrow$ random variables
Edges show dependencies among random variables

Two main flavors: directed graphical models and undirected graphical models (come talk to me)


## Maxent Models Make a Reappearance

- features $f(x, y)$ between x and y that are meaningful;
- weights $\theta$ (one per feature) to say how important each feature is; and
- a way to form probabilities from $f$ and $\theta$

$$
p(y \mid x) \propto \exp \left(\theta^{T} f(x, y)\right)
$$



## Markov Random Fields: Undirected Graphs

clique: subset of nodes, where nodes are pairwise connected
maximal clique: a clique that cannot add a node and remain a clique


$$
p\left(x_{1}, x_{2}, x_{3}, \ldots, x_{N}\right)=\frac{1}{7} \prod_{\substack{\text { global } \\ \text { normalization }}} \exp \left(-E_{C}\left(x_{C}\right)\right)
$$

## BBN Construction

The knowledge acquisition process for a BBN involves three steps

KA1: Choosing appropriate variables
KA2: Deciding on the network structure
KA3: Obtaining data for the conditional probability tables

## KA1: Choosing variables

- Variable values: integers, reals or enumerations
- Variable should have collectively exhaustive, mutually exclusive values

$$
\begin{aligned}
& x_{1} \vee x_{2} \vee x_{3} \vee x_{4} \\
& \neg\left(x_{i} \wedge x_{j}\right) \quad i \neq j
\end{aligned}
$$



## No Error

- They should be values, not probabilities


## Heuristic: Knowable in Principle

Example of good variables

- Weather: \{Sunny, Cloudy, Rain, Snow\}
- Gasoline: Cents per gallon $\{0,1,2 \ldots\}$
- Temperature: $\left\{\geq 100^{\circ} \mathrm{F},<100^{\circ} \mathrm{F}\right\}$
- User needs help on Excel Charts: \{Yes, No\}
- User's personality: \{dominant, submissive\}


## KA2: Structuring



Network structure corresponding to "causality" is usually good.

Initially this uses the designer's knowledge but can be checked with data

## KA3: The Numbers

- For each variable we have a table of probability of its value for values of its parents
- For variables w/o parents, we have prior probabilities

$$
\begin{aligned}
& S \in\{\text { no, light }, \text { heavy }\} \\
& C \in\{\text { none, benign,malignant }\}
\end{aligned}
$$



| smoking priors |  |
| :--- | :--- |
| no | 0.80 |
| light | 0.15 |
| heavy | 0.05 |


|  | smoking |  |  |
| :--- | :--- | :--- | :--- |
| cancer | no | light | heavy |
| none | 0.96 | 0.88 | 0.60 |
| benign | 0.03 | 0.08 | 0.25 |
| malignant | 0.01 | 0.04 | $0.15_{97}$ |

## Three (Four) kinds of reasoning

BBNs support three main kinds of reasoning:

- Predicting conditions given predispositions
- Diagnosing conditions given symptoms (and predisposing)
- Explaining a condition by one or more predispositions
To which we can add a fourth:
- Deciding on an action based on probabilities of the conditions


## Fundamental Inference \& Learning Question

- Compute posterior probability of a node given some other nodes

$$
p\left(Q \mid x_{1}, \ldots, x_{j}\right)
$$

- Some techniques
- MLE (maximum likelihood estimation)/MAP (maximum a posteriori) [covered $2^{\text {nd }}$ ]
- Variable Elimination [covered $1^{\text {st] }}$
- (Loopy) Belief Propagation ((Loopy) BP)
- Monte Carlo
- Variational methods


## Predictive Inference



## Predictive and diagnostic combined



How likely is an elderly male patient with high Serum Calcium to have malignant cancer?

## Explaining away



- If we see a lung tumor, the probability of heavy smoking and of exposure to toxics both go up
- If we then observe heavy smoking, the probability of exposure to toxics goes back down


## Decision making

- A decision is a medical domain might be a choice of treatment (e.g., radiation or chemotherapy)
- Decisions should be made to maximize expected utility
- View decision making in terms of
- Beliefs/Uncertainties
- Alternatives/Decisions
- Objectives/Utilities


## Decision Problem

Should I have my party inside or outside?


## Decision Making with BBNs

- Today's weather forecast might be either sunny, cloudy or rainy
- Should you take an umbrella when you leave?
- Your decision depends only on the forecast - The forecast "depends on" the actual weather
- Your satisfaction depends on your decision and the weather
- Assign a utility to each of four situations: (rain|no rain) $\times$ (umbrella, no umbrella)


## Decision Making with BBNs

- Extend BBN framework to include two new kinds of nodes: decision and utility
- Decision node computes the expected utility of a decision given its parent(s) (e.g., forecast) and a valuation
- Utility node computes utility value given its parents, e.g. a decision and weather
- Assign utility to each situations: (rain|no rain) x (umbrella, no umbrella)
- Utility value assigned to each is probably subjective


## Fundamental Inference \& Learning Question

- Compute posterior probability of a node given some other nodes

$$
p\left(Q \mid x_{1}, \ldots, x_{j}\right)
$$

- Some techniques
- MLE (maximum likelihood estimation)/MAP (maximum a posteriori) [covered 2 ${ }^{\text {nd }}$ ]
- Variable Elimination [covered $1^{\text {st] }}$
- (Loopy) Belief Propagation ((Loopy) BP)
- Monte Carlo
- Variational methods


## Variable Elimination

- Inference: Compute posterior probability of a node given some other nodes

$$
p\left(Q \mid x_{1}, \ldots, x_{j}\right)
$$

- Variable elimination: An algorithm for exact inference
- Uses dynamic programming
- Not necessarily polynomial time!


## Variable Elimination (High-level)

Goal: $p\left(Q \mid x_{1}, \ldots, x_{j}\right)$
(The word "factor" is used for each CPT.)

1. Pick one of the non-conditioned, MB variables
2. Eliminate this variable by marginalizing (summing) it out from all factors (CPTs) that contain it
3. Go back to 1 until no (MB) variables remain
4. Multiply the remaining factors and normalize.

## Variable Elimination: Example

(The word "factor" is used for each CPT.)

1. Pick one of the nonconditioned, MB variables
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4. Multiply the remaining


Goal: P(Tampering | Smoke=true $\wedge$ Report=true)

| ConditionalProbability | Factor |
| :--- | :--- |
| $P($ Tampering $)$ | $f_{0}($ Tampering $)$ |
| $P($ Fire $)$ | $f_{1}($ Fire $)$ |
| $P($ Alarm $\mid$ Tampering, Fire $)$ | $f_{2}($ Tampering, Fire, Alarm $)$ |
| $P($ Smoke $=$ yes $\mid$ Fire $)$ | $f_{3}$ (Fire $)$ |
| $P($ Leaving $\mid$ Alarm $)$ | $f_{4}($ (larm, Leaving $)$ |
| $P($ Report $=$ yes $\mid$ Leaving $)$ | $f_{5}$ (Leaving $)$ | factors and normalize.

## Variable Elimination: Example

(The word "factor" is used for each CPT.)

1. Pick one of the nonconditioned, MB variables
2. Eliminate this variable by marginalizing (summing) it out from all factors (CPTs) that contain it

Goal: P(Tampering | Smoke=true $\wedge$ Report=true)

Task: Eliminate Fire
3. Go back to 1 until no (MB) variables remain
4. Multiply the remaining factors and normalize.

| ConditionalProbability | Factor |
| :--- | :--- |
| $P($ Tampering $)$ | $f_{0}($ Tampering $)$ |
| $P($ Fire $)$ | $f_{1}($ Fire $)$ |
| $P($ Alarm $\mid$ Tampering, Fire $)$ | $f_{2}($ Tampering, Fire, Alarm $)$ |
| $P($ Smoke $=$ yes $\mid$ Fire $)$ | $f_{3}($ Fire $)$ |
| $P($ Leaving $\mid$ Alarm $)$ | $f_{4}($ Alarm, Leaving $)$ |
| $P($ Report $=$ yes $\mid$ Leaving $)$ | $f_{5}($ Leaving $)$ |

## Variable Elimination: Example

(The word "factor" is used for each CPT.)

1. Pick one of the nonconditioned, MB variables
2. Eliminate this variable by marginalizing (summing) it out from all factors (CPTs) that contain it
3. Go back to 1 until no (MB) variables remain


Goal: P(Tampering | Smoke=true $\wedge$ Report=true)

> f1(Fire)
f2(Tampering, Fire, Alarm)
f3(Fire)

4. Multiply the remaining factors and normalize.

| ConditionalProbability | Factor |
| :--- | :--- |
| $P($ Tampering $)$ | $f_{0}($ Tampering $)$ |
| $P($ Fire $)$ | $f_{1}($ Fire $)$ |
| $P($ Alarm $\mid$ Tampering, Fire $)$ | $f_{2}($ Tampering, Fire, Alarm $)$ |
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| $P($ Leaving $\mid$ Alarm $)$ | $f_{4}($ Alarm, Leaving $)$ |
| $P($ Report $=$ yes $\mid$ Leaving $)$ | $f_{5}($ Leaving $)$ |

f6(Tampering, Alarm) $=$

$$
\begin{gathered}
=\sum_{u} f_{1}(\text { Fire }=u) f_{2}(T, F=u, A) f_{3}(F=u) \\
=\sum_{u} p(\text { Fire }=u) p(A \mid T, F=u) p(S=y \mid F=u)
\end{gathered}
$$

## Variable Elimination: Example

(The word "factor" is used for each CPT.)

1. Pick one of the nonconditioned, MB variables
2. Eliminate this variable by marginalizing (summing) it out from all factors (CPTs) that contain it
3. Go back to 1 until no (MB) variables remain


Goal: P(Tampering | Smoke=true $\wedge$ Report=true) f6 (Tampering, Alarm $)=$

$$
\begin{aligned}
= & \sum_{u} p(\text { Fire }=u) p(A \mid T, F=u) p(S=y \mid F=u) \\
= & p(\text { Fire }=y) p(A \mid T, F=y) p(S=y \mid F=y)+ \\
& p(\text { Fire }=n) p(A \mid T, F=n) p(S=y \mid F=n)
\end{aligned}
$$

4. Multiply the remaining factors and normalize.

| ConditionalProbability | Factor |
| :--- | :--- |
| $P($ Tampering $)$ | $f_{0}($ Tampering $)$ |
| $P($ Fire $)$ | $f_{1}($ Fire $)$ |
| $P($ Alarm $\mid$ Tampering, Fire $)$ | $f_{2}($ Tampering, Fire, Alarm $)$ |
| $P($ Smoke $=$ yes $\mid$ Fire $)$ | $f_{3}($ Fire $)$ |
| $P($ Leaving $\mid$ Alarm $)$ | $f_{4}($ Alarm, Leaving $)$ |
| $P($ Report $=$ yes $\mid$ Leaving $)$ | $f_{5}($ Leaving $)$ |

## Variable Elimination: Example

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| $P($ Report $=$ yes $\mid$ Leaving $)$ | $f_{5}($ Leaving $)$ |



Goal: P(Tampering | Smoke=true $\wedge$ Report=true)
f6(Tampering, Alarm) $=$
$=\sum_{u} p($ Fire $=u) p(A \mid T, F=u) p(S=y \mid F=u)$

| Tamp. | Alarm | $\mathbf{f 6}$ |
| :---: | :---: | :---: |
| Yes | Yes | $p($ Fire $=y) p(A=y \mid T=y, F=y) p(S=y \mid F=y)+$ <br> $p($ Fire $=n) p(A=y \mid T=y, F=n) p(S=y \mid F=n)$ |
| Yes | No | $\ldots$ |


| No |
| :---: |
| No |


| No |
| :---: |
| Yes |

## Variable Elimination: Example

(The word "factor" is used for each CPT.)

1. Pick one of the nonconditioned, MB variables
2. Eliminate this variable by marginalizing (summing) it out from all factors (CPTs) that contain it

Goal: P(Tampering | Smoke=true $\wedge$ Report=true)

Task: Eliminate Alarm
3. Go back to 1 until no (MB) variables remain
4. Multiply the remaining factors and normalize.

| ConditionalProbability | Factor |
| :--- | :--- |
| $P($ Tampering $)$ | $f_{0}$ (Tampering $)$ |
| $P($ Fire $)$ | $f_{1}$ (Fire $)$ |
| $P($ Alarm $\mid$ Tampering, Fire $)$ | $f_{2}$ (Tampering, Fire, Alarm $)$ |
| $P($ Smoke $=$ yes $\mid$ Fire $)$ | $f_{3}$ (Fire $)$ |
| $P($ Leaving $\mid$ Alarm $)$ | $f_{4}$ (Alarm, Leaving $)$ |
| $P($ Report $=$ yes $\mid$ Leaving $)$ | $f_{5}$ (Leaving $)$ |

## Variable Elimination: Example

(The word "factor" is used for each CPT.)

1. Pick one of the nonconditioned, MB variables
2. Eliminate this variable by marginalizing (summing) it out from all factors (CPTs) that contain it
3. Go back to 1 until no (MB) variables remain
...other computations not shown---see the book...
4. Multiply the remaining factors and normalize.

| ConditionalProbability | Factor |
| :--- | :--- |
| $P($ Tampering $)$ | $f_{0}($ Tampering $)$ |
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## Variable Elimination: Example

(The word "factor" is used for each CPT.)

1. Pick one of the nonconditioned, MB variables
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| ConditionalProbability | Factor |
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| $P($ Smoke $=$ yes $\mid$ Fire $)$ | $f_{3}$ (Fire $)$ |
| $P($ Leaving $\mid$ Alarm $)$ | $f_{4}$ (Alarm, Leaving $)$ |
| $P($ Report $=$ yes $\mid$ Leaving $)$ | $f_{5}$ (Leaving $)$ |

Goal: P(Tampering | Smoke=true $\wedge$ Report=true)

Task: Normalize in order to compute p(Tampering)

We'll have a single factor f9(Tampering):

$$
p(T=u)=\frac{f_{9}(T=u)}{\sum_{v} f_{9}(T=v)}
$$

## Variable Elimination: Example

(The word "factor" is used for each CPT.)

1. Pick one of the nonconditioned, MB variables
2. Eliminate this variable by marginalizing (summing) it out from all factors (CPTs) that contain it
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| ConditionalProbability | Factor |
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| $P($ Tampering $)$ | $f_{0}($ Tampering $)$ |
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Goal: P(Tampering | Smoke=true $\wedge$ Report=true)

> Task: Normalize in order to compute p(Tampering)

We'll have a single factor f9(Tampering):

$$
p(T=y)=\frac{f_{9}(T=y)}{f_{9}(T=y)+f_{9}(T=n)}
$$

## Learning Bayesian networks

- Given training set $\boldsymbol{D}=\{\boldsymbol{x}[1], \ldots, \boldsymbol{x}[\boldsymbol{M}]\}$
- Find graph that best matches $\boldsymbol{D}$
- model selection
- parameter estimation


Data D

## Learning Bayesian Networks

- Describe a BN by specifying its (1) structure and (2) conditional probability tables (CPTs)
- Both can be learned from data, but
-learning structure much harder than learning parameters
-learning when some nodes are hidden, or with missing data harder still
- Four cases:

| Structure | Observability Method |  |
| :--- | :--- | :--- |
| Known | Full | Maximum Likelihood Estimation |
| Known | Partial | EM (or gradient ascent) |
| Unknown | Full | Search through model space |
| Unknown | Partial | EM + search through model |
| space |  |  |

## Variations on a theme

- Known structure, fully observable: only need to do parameter estimation
- Unknown structure, fully observable: do heuristic search through structure space, then parameter estimation
- Known structure, missing values: use expectation maximization (EM) to estimate parameters
- Known structure, hidden variables: apply adaptive probabilistic network (APN) techniques
- Unknown structure, hidden variables: too hard to solve!


## Fundamental Inference Question

- Compute posterior probability of a node given some other nodes

$$
p\left(Q \mid x_{1}, \ldots, x_{j}\right)
$$

- Some techniques
- MLE (maximum likelihood estimation)/MAP (maximum a posteriori) [covered 2 ${ }^{\text {nd }}$ ]
- Variable Elimination [covered $1^{\text {st }}$ ]
- (Loopy) Belief Propagation ((Loopy) BP)
- Monte Carlo
- Variational methods
- ...


## Parameter estimation

- Assume known structure
- Goal: estimate BN parameters $\boldsymbol{\theta}$
- entries in local probability models, $\mathrm{P}(\mathrm{X} \mid$ Parents $(\mathrm{X})$ )
- A parameterization $\theta$ is good if it is likely to generate the observed data:

$$
L(\theta: D)=P(D \mid \theta)=\prod_{m} P(x[m] \mid \theta)
$$

- Maximum Likelihood Estimation (MLE) Principle: Choose $\theta^{*}$ so as to maximize $L$


## Parameter estimation II

- The likelihood decomposes according to the structure of the network
$\rightarrow$ we get a separate estimation task for each parameter
- The MLE (maximum likelihood estimate) solution for discrete data \& RV values:
- for each value $x$ of a node $X$
- and each instantiation $\boldsymbol{u}$ of Parents $(X)$

$$
\theta_{x \mid u}^{*}=\frac{\boldsymbol{N}(\boldsymbol{x}, \boldsymbol{u})}{\boldsymbol{N}(\boldsymbol{u})} \quad \text { sufficient statistics }
$$

- Just need to collect the counts for every combination of parents and children observed in the data
- MLE is equivalent to an assumption of a uniform prior over parameter values


## Learning:

## Maximum Likelihood Estimation (MLE)

Core concept in intro statistics:

- Observe some data $X$
- Compute some distribution $g(X)$ to \{predict, explain, generate\} $\mathcal{X}$
- Assume $g$ is controlled by parameters $\phi$, i.e., $g_{\phi}(\mathcal{X})$
- Sometimes written $g(X ; \phi)$
- Learning appropriate value(s) of $\phi$ allows you to generalize about $\mathcal{X}$


## Learning: <br> Maximum Likelihood Estimation (MLE)

## Central to machine learning:

- Observe some data $(\mathcal{X}, \mathcal{Y})$
- Compute some function $f(X)$ to $\{$ predict, explain, generate $\}$
- Assume $f$ is controlled by parameters $\theta$, i.e., $f_{\theta}(\mathcal{X})$
- Sometimes written $f(\mathcal{X} ; \theta)$


## Learning Parameters for the Die Model

$$
p\left(w_{1}, w_{2}, \ldots, w_{N}\right)=p\left(w_{1}\right) p\left(w_{2}\right) \cdots p\left(w_{N}\right)=\prod_{i} p\left(w_{i}\right)
$$

maximize (log-) likelihood to learn the probability parameters

Q: Why is maximizing loglikelihood a reasonable
thing to do?

## Learning Parameters for the Die Model

$$
p\left(w_{1}, w_{2}, \ldots, w_{N}\right)=p\left(w_{1}\right) p\left(w_{2}\right) \cdots p\left(w_{N}\right)=\prod_{i} p\left(w_{i}\right)
$$

maximize (log-) likelihood to learn the probability parameters

Q: Why is maximizing loglikelihood a reasonable thing to do?

## A: Develop a good model for what we observe

## Learning Parameters for the Die Model: <br> Maximum Likelihood (Intuition)

$$
p\left(w_{1}, w_{2}, \ldots, w_{N}\right)=p\left(w_{1}\right) p\left(w_{2}\right) \cdots p\left(w_{N}\right)=\prod_{i} p\left(w_{i}\right)
$$ maximize (log-) likelihood to learn the probability parameters

If you observe these 9 rolls...


...what are "reasonable" estimates for $p(w)$ ?

$$
\begin{array}{ll}
\mathrm{p}(1)=? & \mathrm{p}(2)=? \\
\mathrm{p}(3)=? & \mathrm{p}(4)=? \\
\mathrm{p}(5)=? & \mathrm{p}(6)=?
\end{array}
$$

## Learning Parameters for the Die Model: <br> Maximum Likelihood (Intuition)

$$
p\left(w_{1}, w_{2}, \ldots, w_{N}\right)=p\left(w_{1}\right) p\left(w_{2}\right) \cdots p\left(w_{N}\right)=\prod_{i} p\left(w_{i}\right)
$$ maximize (log-) likelihood to learn the probability parameters

If you observe these 9 rolls...

$p(3)=1 / 9$

$$
p(4)=3 / 9
$$

$$
p(5)=1 / 9
$$

$$
p(6)=1 / 9
$$

maximum
likelihood estimates

## Learning:

## Maximum Likelihood Estimation (MLE)

Core concept in intro statistics:

- Observe some data $X$
- Compute some distribution $g(X)$ to \{predict, explain, generate $\mathcal{X}$
- Assume $g$ is controlled by parameters $\phi$, i.e., $g_{\phi}(\mathcal{X})$
- Sometimes written $g(X ; \phi)$
- Learning appropriate value(s) of $\phi$ allows you to generalize about $\mathcal{X}$

How do we "learn appropriate value(s) of $\phi$ ?"
Many different options: a common one is maximum likelihood estimation (MLE)

- Find values $\phi$ s.t.
$g_{\phi}\left(\mathcal{X}=\left\{x_{1}, \ldots, x_{N}\right\}\right)$ is maximized
- Independence assumptions are very useful here!
- Logarithms are also useful!


## Learning:

## Maximum Likelihood Estimation (MLE)

Core concept in intro statistics:

- Observe some data $X$
- Compute some distribution $g(X)$ to \{predict, explain, generate\} $X$
- Assume $g$ is controlled by parameters $\phi$, i.e., $g_{\phi}(X)$
- Sometimes written $g(\mathcal{X} ; \phi)$
- MLE: Find values $\phi$ s.t.
$g_{\phi}\left(\mathcal{X}=\left\{x_{1}, \ldots, x_{N}\right\}\right)$ is maximized

Example: How much does it snow?

- $\mathcal{X}=\left\{x_{1}, x_{2}, \ldots, x_{N}\right\}$ are snowfall values from the previous N storms
- Goal: learn $\phi$ such that $g$ correctly models, as accurately as possible, the amount of snow likely


Learning:

## Maximum Likelihood

 Estimation (MLE)Core concept in intro statistics: Example: How much does it

- Observe some data $X$
- Compute some distribution $g(X)$ to \{predict, explain, generate $\mathcal{X}$
- Assume $g$ is controlled by parameters $\phi$, i.e., $g_{\phi}(X)$
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- MLE: Find values $\phi$ s.t. $g_{\phi}\left(\mathcal{X}=\left\{x_{1}, \ldots, x_{N}\right\}\right)$ is maximized
snow?
- $\mathcal{X}=\left\{x_{1}, x_{2}, \ldots, x_{N}\right\}$ are snowfall values from the previous N storms
- Goal: learn $\phi$ such that $g$ correctly models, as accurately as possible, the amount of snow likely
- Assumption: each $x_{i}$ is independent from all others

$$
\max _{\phi} \sum_{i=1}^{N} \log g_{\phi}\left(x_{i}\right)
$$

## Advanced

 topic
## MLE Snowfall Example

Example: How much does it snow?

- $\mathcal{X}=\left\{x_{1}, x_{2}, \ldots, x_{N}\right\}$ are snowfall values from the previous N storms
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Q: Why is taking logarithms okay?

Q : What other assumptions, or decisions, do we need to make?

## Advanced topic <br> MLE Snowfall Example

Example: How much does it snow?

- $\mathcal{X}=\left\{x_{1}, x_{2}, \ldots, x_{N}\right\}$ are snowfall values from the previous N storms
- Goal: learn $\phi$ such that $g$ correctly models, as accurately as possible, the amount of snow likely
- Assumption: each $x_{i}$ is independent from all others, but all from $g$

$$
\max _{\phi} \sum_{i=1}^{N} \log g_{\phi}\left(x_{i}\right)
$$

Q: Why is taking logarithms okay?

Q : What other assumptions, or decisions, do we need to make?
$x_{i}$ is positive, real-valued.
What's a faithful probability distribution for $x_{i}$ ?

- Normal?
- Gamma?
- Exponential?
- Bernoulli?
- Poisson?


## Advanced

 topic
## MLE Snowfall Example

Example: How much does it snow?

- $\mathcal{X}=\left\{x_{1}, x_{2}, \ldots, x_{N}\right\}$ are snowfall values from the previous N storms
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$$

Q: Why is taking logarithms okay?

Q: What other assumptions, or decisions, do we need to make?
$x_{i}$ is positive, real-valued.
What's a faithful probability distribution for $x_{i}$ ?

- Normal? X $\quad$. Gamma? $\sqrt{ } p(X=x)=\frac{x^{k-1} \exp \left(\frac{-k}{\theta}\right)}{\theta^{k} \Gamma(k)}$
- Exponential?
- Bernoulli?
- Poisson?


## Advanced

## MLE Snowfall Example

Example: How much does it snow?

- $X=\left\{x_{1}, x_{2}, \ldots, x_{N}\right\}$ are snowfall values from the previous N storms
- Goal: learn $\phi$ such that $g$ correctly models, as accurately as possible, the amount of snow likely
- Assumption: each $x_{i}$ is independent from all others, but all from $g$

$$
\max _{\phi} \sum_{i=1}^{N} \log g_{\phi}\left(x_{i}\right)
$$

Q: Why is taking logarithms okay?
Q: What other assumptions, or decisions, do we need to make?
$x_{i}$ is positive, real-valued. What's a faithful/nice-to-compute-and-good-enough probability
distribution for $x_{i}$ ?

- Normal? $\times \sqrt{ } \longleftarrow p(X=x)=$
- Gamma? $\vee$ ? $\frac{1}{\sqrt{2 \pi} \sigma} \exp \left(\frac{-(x-\mu)^{2}}{2 \sigma^{2}}\right)$
- Exponential? $\sqrt{ }$ ?
- Bernoulli? $X \times$
- Poisson? X X


## Advanced

 topic
## MLE Snowfall Example

Example: How much does it snow?

- $\mathcal{X}=\left\{x_{1}, x_{2}, \ldots, x_{N}\right\}$ are snowfall values from the previous N storms
- Goal: learn $\phi$ such that $g$ correctly models, as accurately as possible, the amount of snow likely
- Assumption: each $x_{i}$ is independent from all others, but all from $g$

$$
\max _{\phi} \sum_{i=1}^{N} \log g_{\phi}\left(x_{i}\right)
$$

$$
x_{i} \sim \operatorname{Normal}\left(\mu, \sigma^{2}\right)
$$



## Advanced

 topic
## MLE Snowfall Example

Example: How much does it snow?

- $\mathcal{X}=\left\{x_{1}, x_{2}, \ldots, x_{N}\right\}$ are snowfall values from the previous N storms
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\max _{\phi} \sum_{i=1}^{N} \log g_{\phi}\left(x_{i}\right)
$$

$$
x_{i} \sim \operatorname{Normal}\left(\mu, \sigma^{2}\right)
$$

$$
\begin{gathered}
\max _{\left(\mu, \sigma^{2}\right)} \sum_{i=1}^{N} \log \operatorname{Normal}_{\mu, \sigma^{2}}\left(x_{i}\right)= \\
\max _{\left(\mu, \sigma^{2}\right)} \sum_{i=1}^{N}\left[\frac{-\left(x_{i}-\mu\right)^{2}}{\sigma^{2}}\right]-N \log \sigma=F
\end{gathered}
$$

## Advanced

 topic
## MLE Snowfall Example

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Q: How do we find $\mu, \sigma^{2}$ ?

## Advanced

 topic
## MLE Snowfall Example

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x_{i} \sim \operatorname{Normal}\left(\mu, \sigma^{2}\right)
$$

$$
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\max _{\left(\mu, \sigma^{2}\right)} \sum_{i=1}^{N}\left[\frac{-\left(x_{i}-\mu\right)^{2}}{\sigma^{2}}\right]-N \log \sigma=F
\end{gathered}
$$

Q: How do we find $\mu, \sigma^{2}$ ?
A: Differentiate and find that

$$
\begin{gathered}
\hat{\mu}=\frac{\sum_{i} x_{i}}{N} \\
\sigma^{2}=\frac{\sum_{i}\left(x_{i}-\hat{\mu}\right)^{2}}{N}
\end{gathered}
$$

## Learning: <br> Maximum Likelihood Estimation (MLE)

## Central to machine learning:

- Observe some data $(\mathcal{X}, \mathcal{Y})$
- Compute some function $f(X)$ to $\{$ predict, explain, generate $\}$
- Assume $f$ is controlled by parameters $\theta$, i.e., $f_{\theta}(\mathcal{X})$
- Sometimes written $f(\mathcal{X} ; \theta)$


## Learning: <br> Maximum Likelihood Estimation (MLE)

Central to machine learning:

- Observe some data $(X, Y)$
- Compute some function $f(X)$ to $\{$ predict, explain, generate\} $\mathcal{Y}$
- Assume $f$ is controlled by parameters $\theta$, i.e., $f_{\theta}(\mathcal{X})$
- Sometimes written $f(X ; \theta)$
- Parameters are learned to minimize error (loss) $\ell$


## Learning:

## Maximum Likelihood Estimation (MLE)

Example: Can I sleep in the next time it snows/is school canceled?

- $\mathcal{X}=\left\{x_{1}, x_{2}, \ldots, x_{N}\right\}$ are snowfall values from the previous N storms
- $\mathcal{Y}=\left\{y_{1}, y_{2}, \ldots, y_{N}\right\}$ are closure results from the previous N storms
- Goal: learn $\theta$ such that $f$ correctly predicts, as accurately as possible, if UMBC will close in the next storm:
- $y_{n+1}^{*}$ from $x_{n+1}$
- If we assume the output of $f$ is a probability distribution on $\mathcal{Y} \mid \mathcal{X}$...
$>f(X) \rightarrow$ $\{p(\mathrm{yes} \mid \mathcal{X}), p(\mathrm{no} \mid \mathcal{X})\}$
- Then re: $\theta$, \{predicting,
explaining, generating\}
Y means... what?


## Learning:

## Maximum Likelihood Estimation (MLE)

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- If we assume the output of $f$ is a probability distribution on $\mathcal{Y} \mid \mathcal{X}$...
- Then re: $\theta$, \{predicting,
explaining, generating\} Y means finding a value for $\theta$ that maximizes the probability of $\mathcal{Y}$ given $\mathcal{X}$


## Learning:

## Maximum Likelihood Estimation (MLE)

Example: Can I sleep in the next time it snows/is school canceled?

- $\mathcal{X}=\left\{x_{1}, x_{2}, \ldots, x_{N}\right\}$ are snowfall values from the previous N storms
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- $y_{n+1}^{*}$ from $x_{n+1}$
- If we assume the output of $f$ is a probability distribution on $\mathcal{Y} \mid \mathcal{X}$...
- Then re: $\theta$, \{predicting,
explaining, generating\} $\mathcal{Y}$ means finding a value for $\theta$ that maximizes the probability of $\mathcal{Y}$ given $\mathcal{X}$, according to $f$
- To model $\mathcal{X}$ : learn a distribution g, on $\mathcal{X}$

Extended examples of MLE


N different
(independent) rolls
$p\left(w_{1}, w_{2}, \ldots, w_{N}\right)=p\left(w_{1}\right) p\left(w_{2}\right) \cdots p\left(w_{N}\right)=\prod_{i} p\left(w_{i}\right)$

$$
\begin{aligned}
& \text { Generative Story } \\
& \text { for roll } i=1 \text { to } N: \\
& \quad w_{i} \sim \operatorname{Cat}(\theta) \\
& \text { Maximize Log-likelihood } \\
& \begin{aligned}
\mathcal{L}(\theta) & =\sum_{i} \log p_{\theta}\left(w_{i}\right) \\
& =\sum_{i} \log \theta_{w_{i}}
\end{aligned}
\end{aligned}
$$



N different
(independent) rolls
$p\left(w_{1}, w_{2}, \ldots, w_{N}\right)=p\left(w_{1}\right) p\left(w_{2}\right) \cdots p\left(w_{N}\right)=\prod_{i} p\left(w_{i}\right)$

Maximize Log-likelihood (with distribution constraints)

$$
\mathcal{L}(\theta)=\sum_{i} \log \theta_{w_{i}} \text { s.t. } \sum_{k=1}^{6} \theta_{k}=1 \quad \begin{gathered}
\text { (we can include the } \\
\text { inequality constraints } \\
0 \leq \theta_{k} \text {, but it complicates } \\
\text { the problem and, right } \\
\text { now, is not needed) }
\end{gathered}
$$

solve using Lagrange multipliers


N different
(independent) rolls
$p\left(w_{1}, w_{2}, \ldots, w_{N}\right)=p\left(w_{1}\right) p\left(w_{2}\right) \cdots p\left(w_{N}\right)=\prod_{i} p\left(w_{i}\right)$

Maximize Log-likelihood (with distribution constraints)

$$
\begin{aligned}
& \mathcal{F}(\theta)=\sum_{i} \log \theta_{w_{i}}-\lambda\left(\sum_{k=1}^{6} \theta_{k}-1\right) \\
& \frac{\partial \mathcal{F}(\theta)}{\partial \theta_{k}}=\sum_{i: w_{i}=k} \frac{1}{\theta_{w_{i}}}-\lambda \quad \frac{\partial \mathcal{F}(\theta)}{\partial \lambda}=-\sum_{k=1}^{6} \theta_{k}+1 \\
& \text { (we can include the } \\
& \text { inequality constraints } \\
& 0 \leq \theta_{k} \text {, but it } \\
& \text { problem and, right } \\
& \text { now, is not needed) }
\end{aligned}
$$


(independent) rolls
$p\left(w_{1}, w_{2}, \ldots, w_{N}\right)=p\left(w_{1}\right) p\left(w_{2}\right) \cdots p\left(w_{N}\right)=\prod_{i} p\left(w_{i}\right)$

Maximize Log-likelihood (with distribution constraints)

$$
\begin{aligned}
& \mathcal{F}(\theta)=\sum_{i} \log \theta_{w_{i}}-\lambda\left(\sum_{k=1}^{6} \theta_{k}-1\right) \\
& \theta_{k}=\frac{\sum_{i: w_{i}=k} 1}{\lambda} \\
& \text { optimal } \lambda \text { when } \sum_{k=1}^{6} \theta_{k}=1 \\
& \text { we can include the }
\end{aligned}
$$



N different
(independent) rolls
$p\left(w_{1}, w_{2}, \ldots, w_{N}\right)=p\left(w_{1}\right) p\left(w_{2}\right) \cdots p\left(w_{N}\right)=\prod_{i} p\left(w_{i}\right)$

Maximize Log-likelihood (with distribution constraints)

$$
\begin{aligned}
& \mathcal{F}(\theta)=\sum_{i} \log \theta_{w_{i}}-\lambda\left(\sum_{k=1}^{6} \theta_{k}-1\right) \\
& \theta_{k}=\frac{\sum_{i: w_{i}=k} 1}{\sum_{k} \sum_{i: w_{i}=k} 1}=\frac{N_{k}}{N} \quad \text { optimal } \lambda \text { when } \sum_{k=1}^{6} \theta_{k}=1 \\
& \text { we can include the } \\
& \text { inequality constraints } \\
& 0 \leq \theta_{k} \text {, but it } \\
& \text { complicates the } \\
& \text { problem and, right } \\
& \text { now, is not needed) } \\
& \theta_{k}=\frac{\sum_{i: w_{i}=k} 1}{\sum_{k} \sum_{i: w_{i}=k} 1}=\frac{N_{k}}{N} \quad \text { optimal } \lambda \text { when } \sum_{k=1}^{6} \theta_{k}=1
\end{aligned}
$$

## Example: Conditionally Rolling a Die

$$
p\left(w_{1}, w_{2}, \ldots, w_{N}\right)=p\left(w_{1}\right) p\left(w_{2}\right) \cdots p\left(w_{N}\right)=\prod_{i} p\left(w_{i}\right)
$$

## add complexity to better

explain what we see

$$
\begin{gathered}
p\left(z_{1}, w_{1}, z_{2}, w_{2}, \ldots, z_{N}, w_{N}\right)=p\left(z_{1}\right) p\left(w_{1} \mid z_{1}\right) \cdots p\left(z_{N}\right) p\left(w_{N} \mid z_{N}\right) \\
=\prod_{i} p\left(w_{i} \mid z_{i}\right) p\left(z_{i}\right)
\end{gathered}
$$

## Example: Conditionally Rolling a Die

$$
p\left(w_{1}, w_{2}, \ldots, w_{N}\right)=p\left(w_{1}\right) p\left(w_{2}\right) \cdots p\left(w_{N}\right)=\prod_{i} p\left(w_{i}\right)
$$

$$
p\left(z_{1}, w_{1}, z_{2}, w_{2}, \ldots, z_{N}, w_{N}\right)=p\left(z_{1}\right) p\left(w_{1} \mid z_{1}\right) \cdots p\left(z_{N}\right) p\left(w_{N} \mid z_{N}\right)
$$

$$
=\prod_{i} p\left(w_{i} \mid z_{i}\right) p\left(z_{i}\right)
$$

First flip a coin...


## Example: Conditionally Rolling a Die

$$
p\left(w_{1}, w_{2}, \ldots, w_{N}\right)=p\left(w_{1}\right) p\left(w_{2}\right) \cdots p\left(w_{N}\right)=\prod_{i} p\left(w_{i}\right)
$$ add complexity to better

$$
p\left(z_{1}, w_{1}, z_{2}, w_{2}, \ldots, z_{N}, w_{N}\right)=p\left(z_{1}\right) p\left(w_{1} \mid z_{1}\right) \cdots p\left(z_{N}\right) p\left(w_{N} \mid z_{N}\right)
$$

$$
=\prod_{i} p\left(w_{i} \mid z_{i}\right) p\left(z_{i}\right)
$$

First flip a coin...
...then roll a different die


$$
\begin{array}{lll}
z_{1}=T & w_{1}=1 & \bullet \\
z_{2}=H & w_{2}=5 & \ddots \ddots
\end{array}
$$

## Learning in Conditional Die Roll Model: Maximize (Log-)Likelihood

$$
p\left(w_{1}, w_{2}, \ldots, w_{N}\right)=p\left(w_{1}\right) p\left(w_{2}\right) \cdots p\left(w_{N}\right)=\prod_{i} p\left(w_{i}\right)
$$

$$
p\left(z_{1}, w_{1}, z_{2}, w_{2}, \ldots, z_{N}, w_{N}\right)=p\left(z_{1}\right) p\left(w_{1} \mid z_{1}\right) \cdots p\left(z_{N}\right) p\left(w_{N} \mid z_{N}\right)
$$

$$
=\prod_{i} p\left(w_{i} \mid z_{i}\right) p\left(z_{i}\right)
$$

If you observe the $z_{i}$
values, this is easy!


First: Write the Generative Story
$\lambda=$ distribution over coin ( z )
$\gamma^{(H)}=$ distribution for die when coin comes up heads
$\gamma^{(T)}=$ distribution for die when coin comes up tails
for item $i=1$ to $N$ :

$$
\begin{aligned}
& z_{i} \sim \operatorname{Bernoulli}(\lambda) \\
& w_{i} \sim \operatorname{Cat}\left(\gamma^{\left(z_{i}\right)}\right)
\end{aligned}
$$



First: Write the Generative Story
$\lambda=$ distribution over coin (z) $\gamma^{(H)}=$ distribution for H die $\gamma^{(T)}=$ distribution for T die for item $i=1$ to $N$ :

$$
\begin{aligned}
& z_{i} \sim \operatorname{Bernoulli}(\lambda) \\
& w_{i} \sim \operatorname{Cat}\left(\gamma^{\left(z_{i}\right)}\right)
\end{aligned}
$$

Second: Generative Story $\rightarrow$ Objective

$$
\begin{gathered}
\mathcal{F}(\theta)=\sum_{i}^{n}\left(\log \lambda_{z_{i}}+\log \gamma_{w_{i}}^{\left(z_{i}\right)}\right) \\
-\quad \text { Lagrange multiplier } \\
\text { constraints }
\end{gathered}
$$



First: Write the Generative Story
$\lambda=$ distribution over coin (z) $\gamma^{(H)}=$ distribution for H die
$\gamma^{(T)}=$ distribution for T die for item $i=1$ to $N$ :
$z_{i} \sim \operatorname{Bernoulli}(\lambda)$
$w_{i} \sim \operatorname{Cat}\left(\gamma^{\left(z_{i}\right)}\right)$

Second: Generative Story $\rightarrow$ Objective

$$
\begin{aligned}
& \mathcal{F}(\theta)=\sum_{i}^{n}\left(\log \lambda_{z_{i}}+\log \gamma_{w_{i}}^{\left(z_{i}\right)}\right) \\
& -\eta\left(\sum_{k=1}^{2} \lambda_{k}-1\right)-\sum_{k=1}^{2} \delta_{k}\left(\sum_{j=1}^{6} \gamma_{j}^{(k)}-1\right)
\end{aligned}
$$

# Learning in Conditional Die Roll Model: Maximize <br> (Log-)Likelihood <br> $$
p\left(z_{1}, w_{1}, z_{2}, w_{2}, \ldots, z_{N}, w_{N}\right)=\prod_{i} p\left(w_{i} \mid z_{i}\right) p\left(z_{i}\right)
$$ <br> If you observe the $z_{i}$ <br> values, 

First: Write the Generative Story
$\lambda=$ distribution over coin (Z) $=$ distribution for H die $=$ distribution for T die

Second: Generative Story $\rightarrow$ Objective

$$
\begin{aligned}
& \mathcal{F}(\theta)=\sum_{i}^{n}\left(\log \lambda_{z_{i}}+\log \gamma_{w_{i}}^{\left(z_{i}\right)}\right) \\
& -\eta\left(\sum_{k=1}^{2} \lambda_{k}-1\right)-\sum_{k=1}^{2} \delta_{k}\left(\sum_{j=1}^{6} r_{j}^{(k)}-1\right)
\end{aligned}
$$

## Model selection

Goal: Select the best network structure, given the data

## Input:

- Training data
- Scoring function

Output:

- A network that maximizes the score


## Structure selection: Scoring

- Bayesian: prior over parameters and structure
- get balance between model complexity and fit to data as a byproduct

Marginal likelihood

- Score (G:D) $=\log P(G \mid D) \alpha \log [P(D \mid G) P(G)]$
- Marginal likelihood just comes from our parameter estimates
- Prior on structure can be any measure we want; typically a function of the network complexity


## Same key property: Decomposability

## Score(structure) $=\sum_{i}$ Score $\left(\right.$ family of $\left.X_{i}\right)$

## Heuristic search



## Exploiting decomposability



