10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Bayesian Networks

+

Reinforcement Learning

Matt Gormley
Lecture 22
Nov. 14, 2018

GRAPHICAL MODELS: DETERMINING CONDITIONAL INDEPENDENCIES

What Independencies does a Bayes Net Model?

- In order for a Bayesian network to model a probability distribution, the following must be true:

  Each variable is conditionally independent of all its non-descendants in the graph given the value of all its parents.

- This follows from

$$P(X_1 \ldots X_n) = \prod_{i=1}^{n} P(X_i \mid parents(X_i))$$

$$= \prod_{i=1}^{n} P(X_i \mid X_1 \ldots X_{i-1})$$

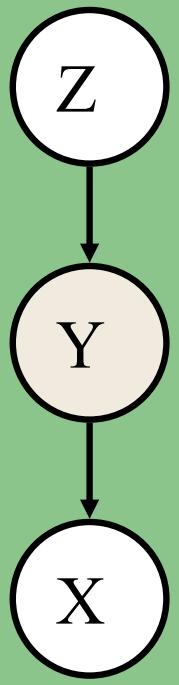
- But what else does it imply?

Slide from William Cohen

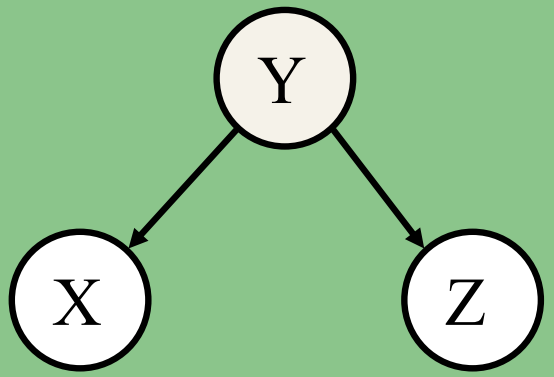
What Independencies does a Bayes Net Model?

Three cases of interest…

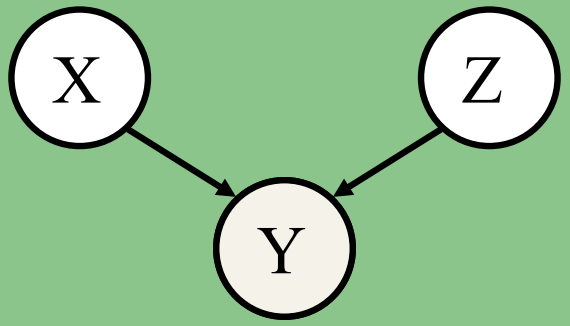
Cascade



Common Parent



V-Structure



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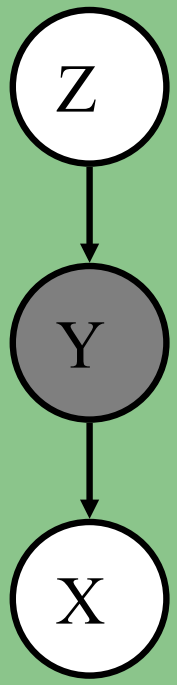

$X \perp\!\!\!\perp Z \mid Y$

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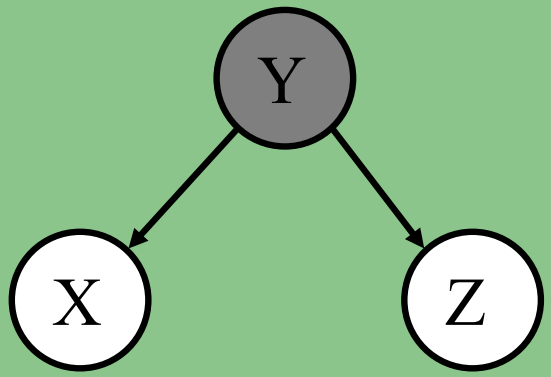

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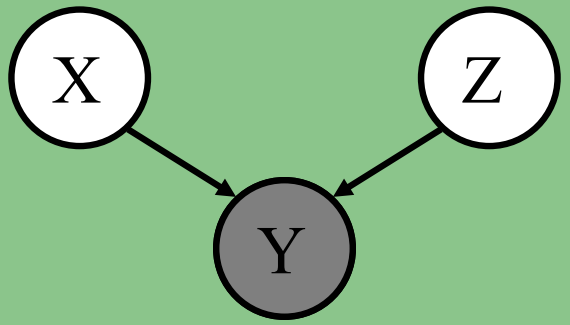


$X \not\perp\!\!\!\perp Z \mid Y$

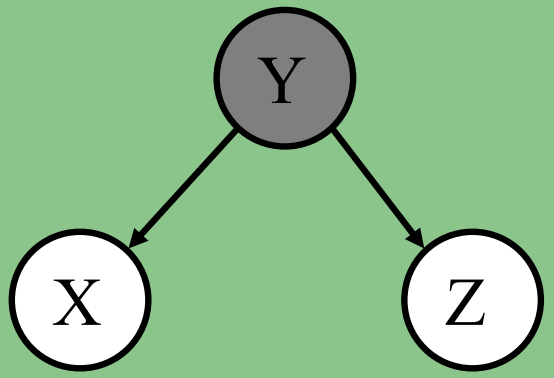
Knowing Y
decouples X and Z

Knowing Y
couples X and Z

Whiteboard

Proof of conditional independence

Common Parent

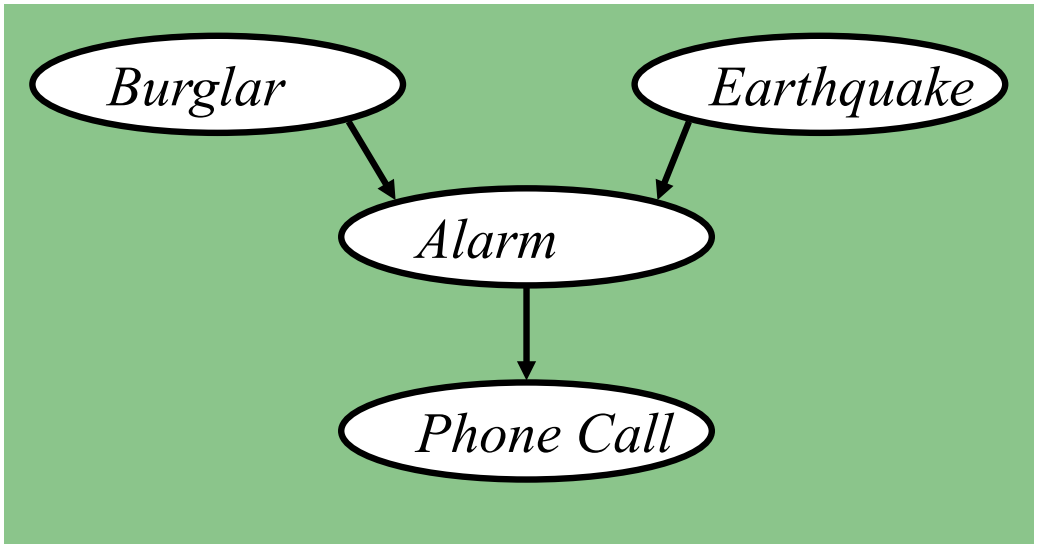


$$X \perp\!\!\!\perp Z \mid Y$$

(The other two cases can be shown just as easily.)

The "Burglar Alarm" example

- Your house has a twitchy burglar alarm that is also sometimes triggered by earthquakes.
- Earth arguably doesn't care whether your house is currently being burgled
- While you are on vacation, one of your neighbors calls and tells you your home's burglar alarm is ringing. Uh oh!



Quiz: True or False?

$$Burglar \perp\!\!\!\perp Earthquake \mid PhoneCall$$

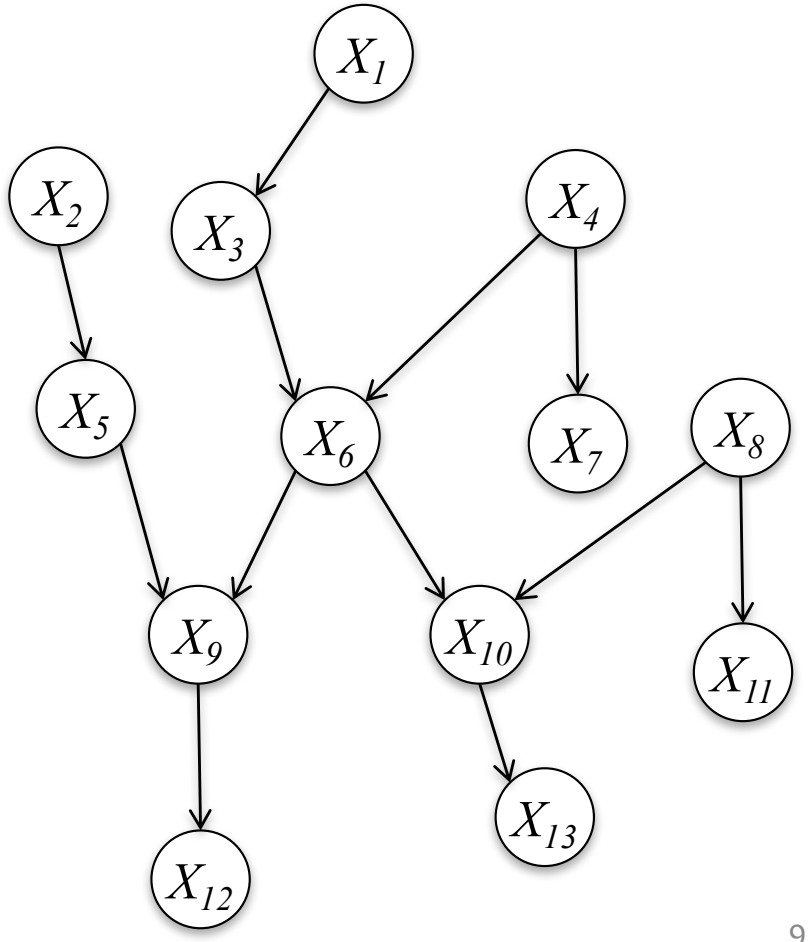
Slide from William Cohen

Markov Blanket

Def: the **co-parents** of a node are the parents of its children

Def: the **Markov Blanket** of a node is the set containing the node's parents, children, and co-parents.

Thm: a node is **conditionally independent** of every other node in the graph given its **Markov blanket**



Markov Blanket

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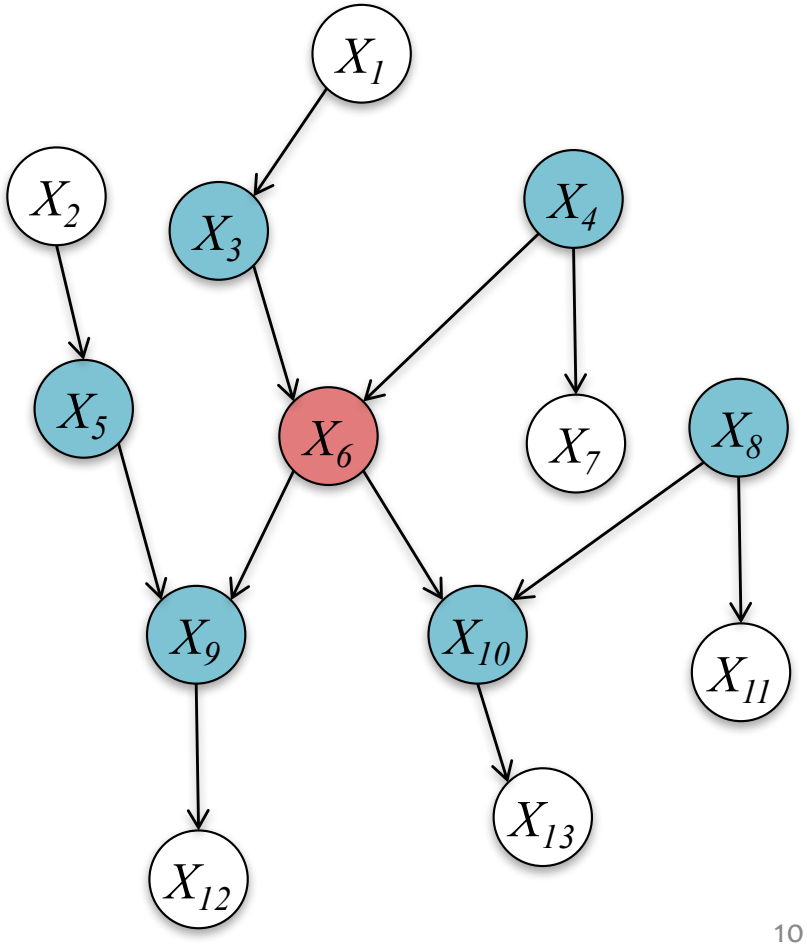
Theorem: a node is **conditionally independent** of every other node in the graph given its **Markov blanket**

Example: The Markov Blanket of X_6 is $\{X_3, X_4, X_5, X_8, X_9, X_{10}\}$



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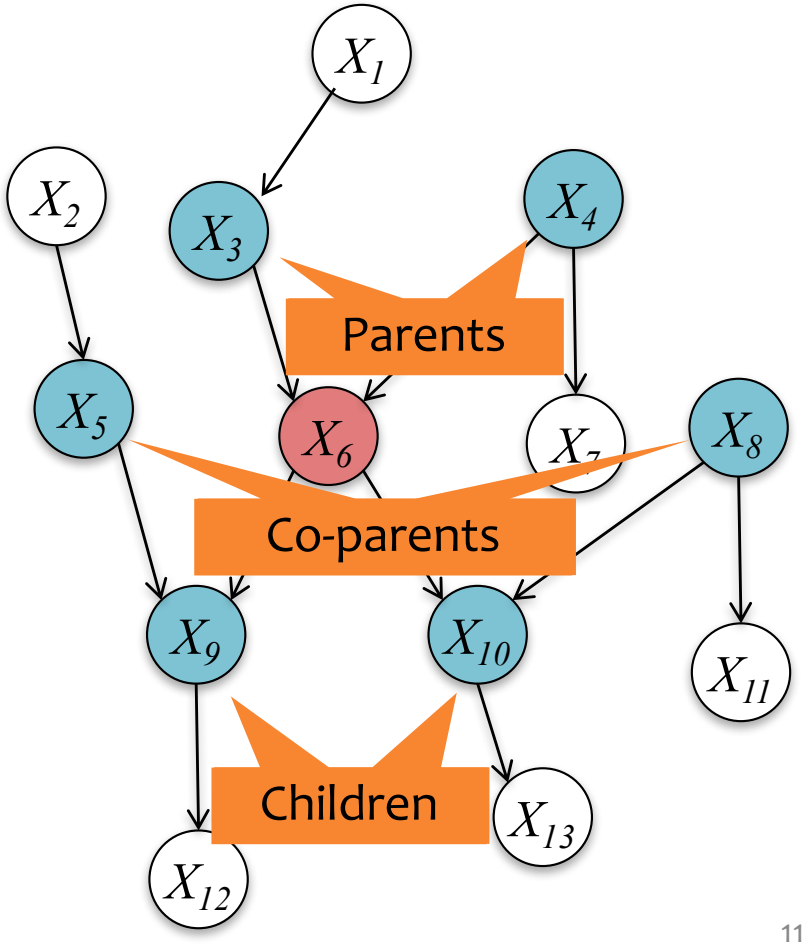


D-Separation

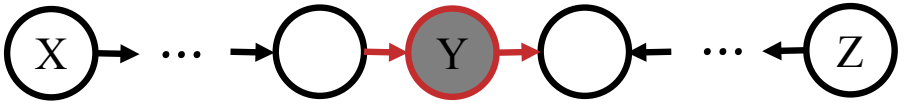
If variables X and Z are **d-separated** given a **set** of variables E
Then X and Z are **conditionally independent** given the **set** E

Definition #1:
Variables X and Z are **d-separated** given a **set** of evidence variables E iff every path from X to Z is "blocked".

A path is "blocked" whenever:

1. $\exists$ Y on path s.t. Y $\in$ E and Y is a "common parent"

2. $\exists$ Y on path s.t. Y $\in$ E and Y is in a "cascade"



3. $\exists$ Y on path s.t. {Y, descendants(Y)} $\notin$ E and Y is in a "v-structure"

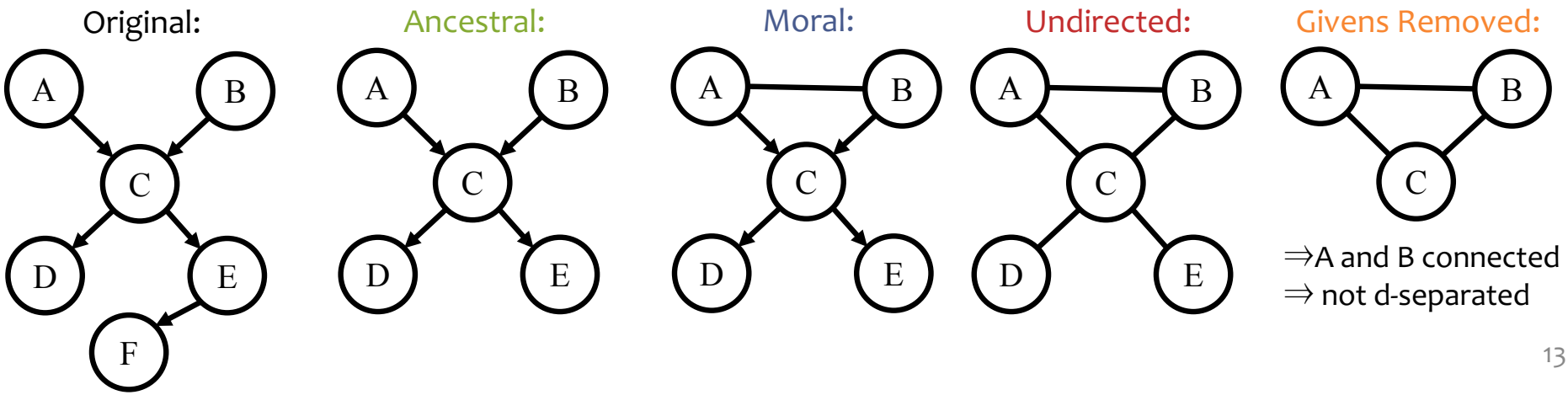
D-Separation

If variables X and Z are **d-separated** given a **set** of variables E
Then X and Z are **conditionally independent** given the **set** E

Definition #2:
Variables X and Z are **d-separated** given a **set** of evidence variables E iff there does **not** exist a path in the **undirected ancestral moral** graph **with E removed**.

1. **Ancestral graph**: keep only X, Z, E and their ancestors
2. **Moral graph**: add undirected edge between all pairs of each node's parents
3. **Undirected graph**: convert all directed edges to undirected
4. Givens Removed: delete any nodes in E

Example Query: $A \perp\!\!\!\perp B \mid \{D, E\}$

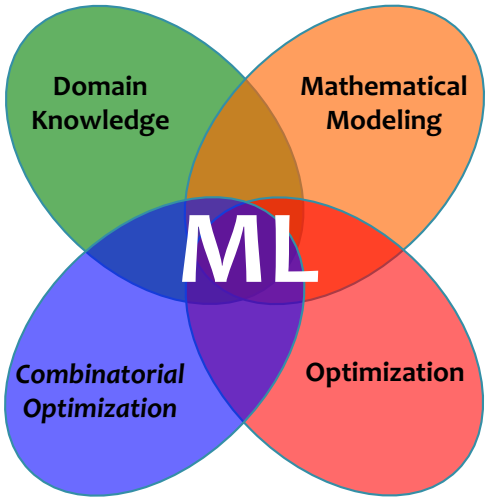


SUPERVISED LEARNING FOR BAYES NETS

Machine Learning

The **data** inspires the structures we want to predict

Our **model** defines a score for each structure



It also tells us what to optimize

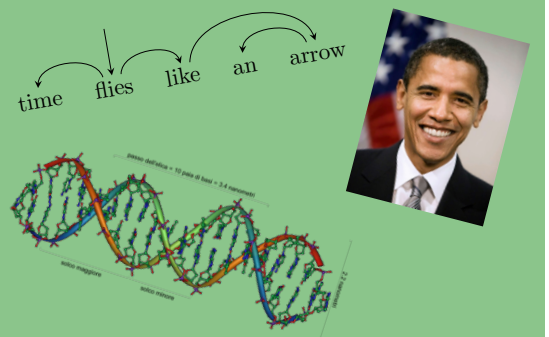
Inference finds {best structure, marginals, partition function} for a new observation

Learning tunes the parameters of the model

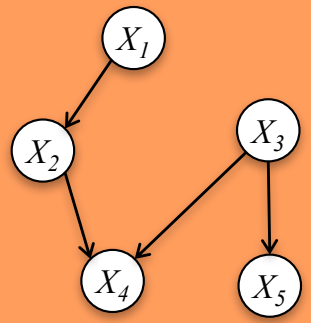
(**Inference** is usually called as a subroutine in learning)

Machine Learning

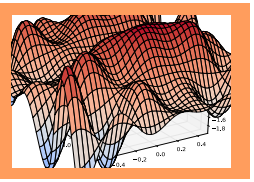
Data



Model



Objective



Inference

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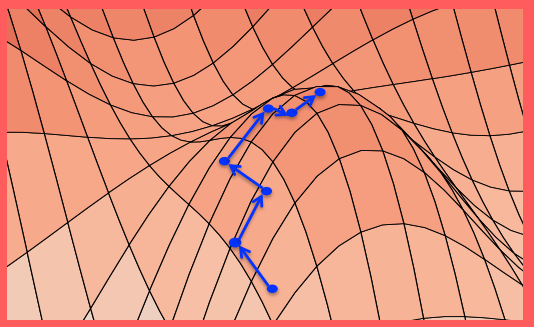
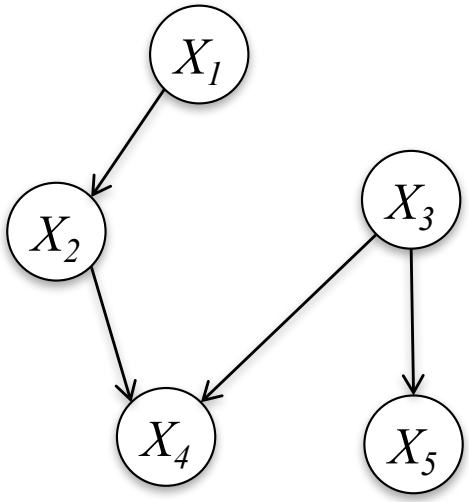
Learning

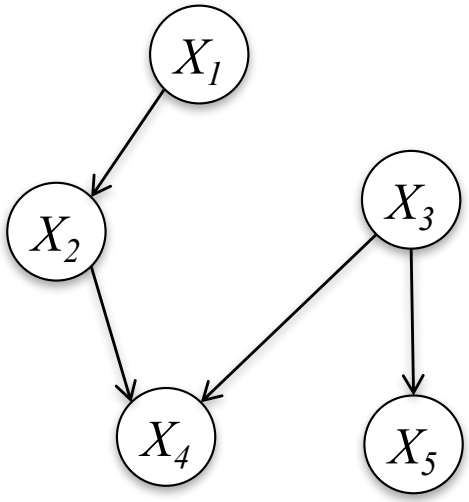


Learning Fully Observed BNs



$$p(X_1, X_2, X_3, X_4, X_5) =$$
$$p(X_5|X_3)p(X_4|X_2, X_3)$$
$$p(X_3)p(X_2|X_1)p(X_1)$$

Learning Fully Observed BNs



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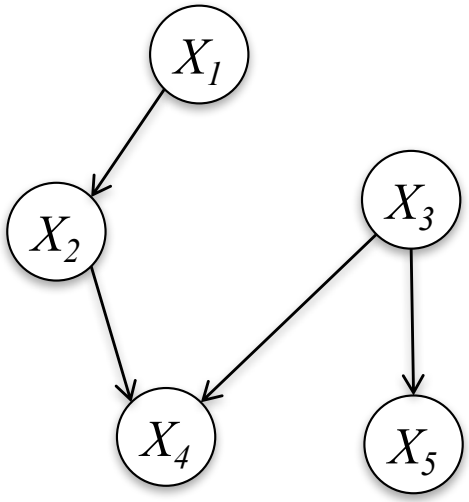

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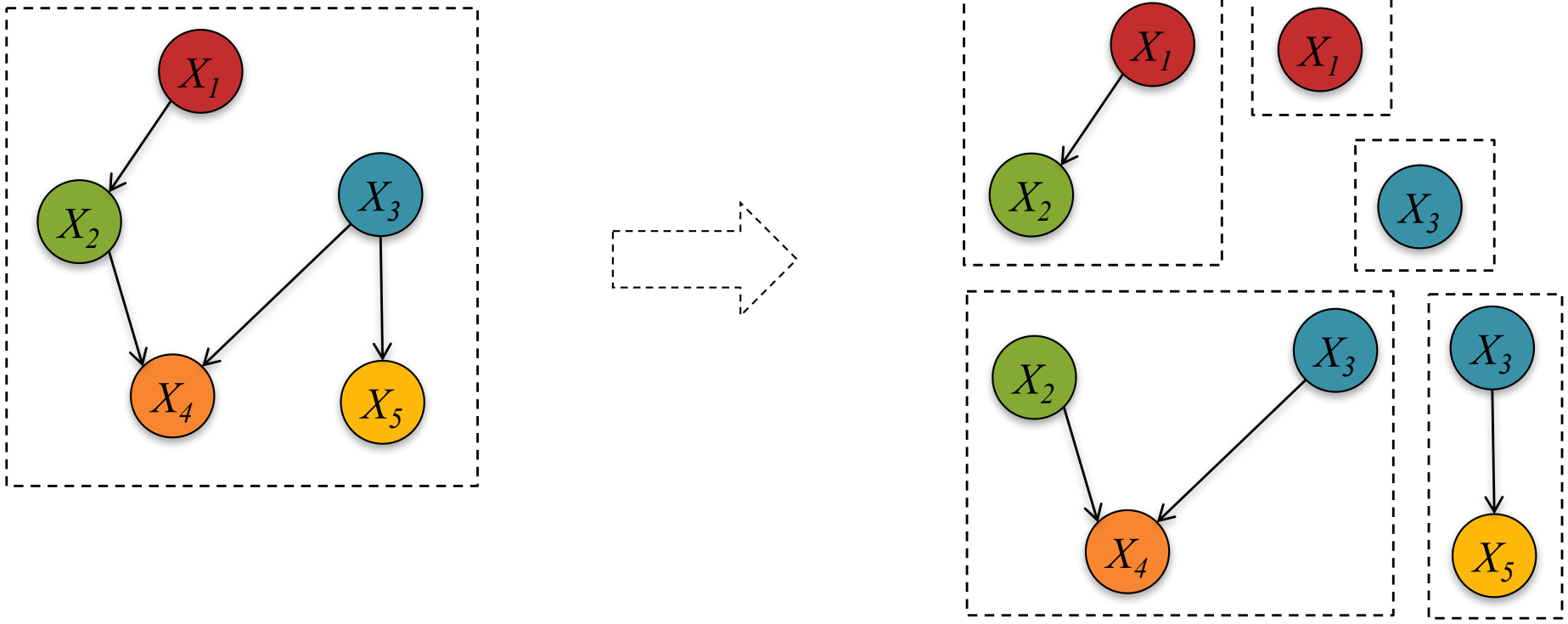
How do we learn these conditional and marginal distributions for a Bayes Net?

Learning Fully Observed BNs

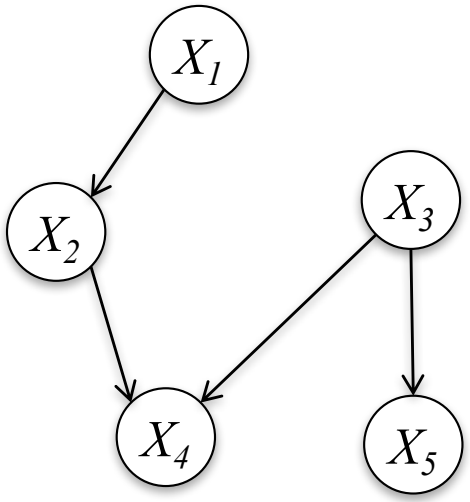
Learning this fully observed Bayesian Network is **equivalent** to learning five (small / simple) independent networks from the same data

$$p(X_1, X_2, X_3, X_4, X_5) = p(X_5|X_3)p(X_4|X_2, X_3) p(X_3)p(X_2|X_1)p(X_1)$$



Learning Fully Observed BNs

How do we **learn** these conditional and marginal distributions for a Bayes Net?



$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \log p(X_1, X_2, X_3, X_4, X_5)$$

$$= \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \log p(X_5|X_3, \theta_5) + \log p(X_4|X_2, X_3, \theta_4)$$
$$+ \log p(X_3|\theta_3) + \log p(X_2|X_1, \theta_2)$$
$$+ \log p(X_1|\theta_1)$$

$$\theta_1^* = \underset{\theta_1}{\operatorname{argmax}} \log p(X_1|\theta_1)$$

$$\theta_2^* = \underset{\theta_2}{\operatorname{argmax}} \log p(X_2|X_1, \theta_2)$$

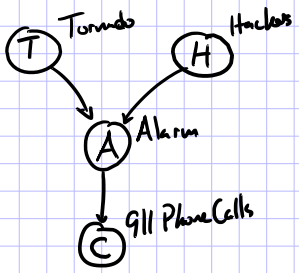
$$\theta_3^* = \underset{\theta_3}{\operatorname{argmax}} \log p(X_3|\theta_3)$$

$$\theta_4^* = \underset{\theta_4}{\operatorname{argmax}} \log p(X_4|X_2, X_3, \theta_4)$$

$$\theta_5^* = \underset{\theta_5}{\operatorname{argmax}} \log p(X_5|X_3, \theta_5)$$

Learning Fully Observed BNs

Ex: Tornado Alarms



$H \sim \text{Bernoulli}(\eta)$ — parameters

$T \sim \text{Bernoulli}(\tau)$ — parameters

$A \sim \text{Bernoulli}(\alpha_{H,T})$ — parameters

$C \sim \text{Uniform}(\{1,\dots,63\}) + A * \text{Uniform}(\{1,\dots,63\})$ — no parameters

C: integer

Dataset

i	T	H	A	C
1	0	0	0	2
2	0	0	0	6
3	0	0	0	4
:	1	0	0	3
	1	0	0	1
	1	0	1	10
	1	0	1	7
	0	1	0	2
	0	1	1	12
	0	1	0	5
:	1	1	1	10
12	1	0	0	2

What are the MLEs?

$\hat{\eta} = 1/3$

$\hat{\tau} = 1/2$

$\hat{\alpha}$ =

	H=0	H=1
T=0	0	1/3
T=1	2/3	1

MLE's in Closed Form

$$\ell(\eta, \tau, \alpha) = \log \prod_{i=1}^{12} p(t^{(i)}, h^{(i)}, a^{(i)}, c^{(i)} \mid \eta, \tau, \alpha)$$

$$= \sum_{i=1}^{12} \log p(t^{(i)} \mid \tau) + \log p(h^{(i)} \mid \eta) + \log p(a^{(i)} \mid t^{(i)}, h^{(i)}, \alpha) + \log p(c^{(i)} \mid a^{(i)})$$

$$\hat{\eta}, \hat{\tau}, \hat{\alpha} = \operatorname{argmax} \ell(\eta, \tau, \alpha)$$

$$\hat{\eta} = \operatorname*{argmax}_{\eta} \sum_{i=1}^{12} \log p(h^{(i)} \mid \eta) = \#(T=1)/N$$

$$\hat{\tau} = \operatorname*{argmax}_{\tau} \sum_{i=1}^{12} \log p(t^{(i)} \mid \tau) = \#(H=1)/N$$

$$\hat{\alpha} = \operatorname*{argmax}_{\alpha} \sum_{i=1}^{12} \log p(a^{(i)} \mid t^{(i)}, h^{(i)}, \alpha)$$

$$\hat{\alpha}_{t,h} = \frac{\#(A=1, T=t, H=h)}{\#(T=t, H=h)}$$

INFERENCE FOR BAYESIAN NETWORKS

A Few Problems for Bayes Nets

Suppose we already have the parameters of a Bayesian Network…

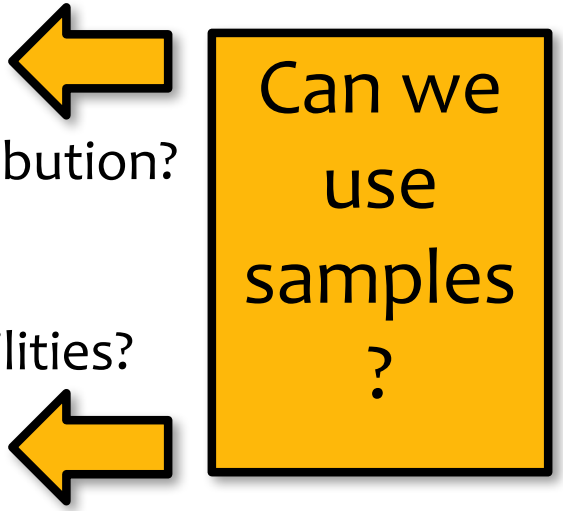
1. How do we compute the probability of a specific assignment to the variables?
   $P(T=t, H=h, A=a, C=c)$

2. How do we draw a sample from the joint distribution?
   $t,h,a,c \sim P(T, H, A, C)$

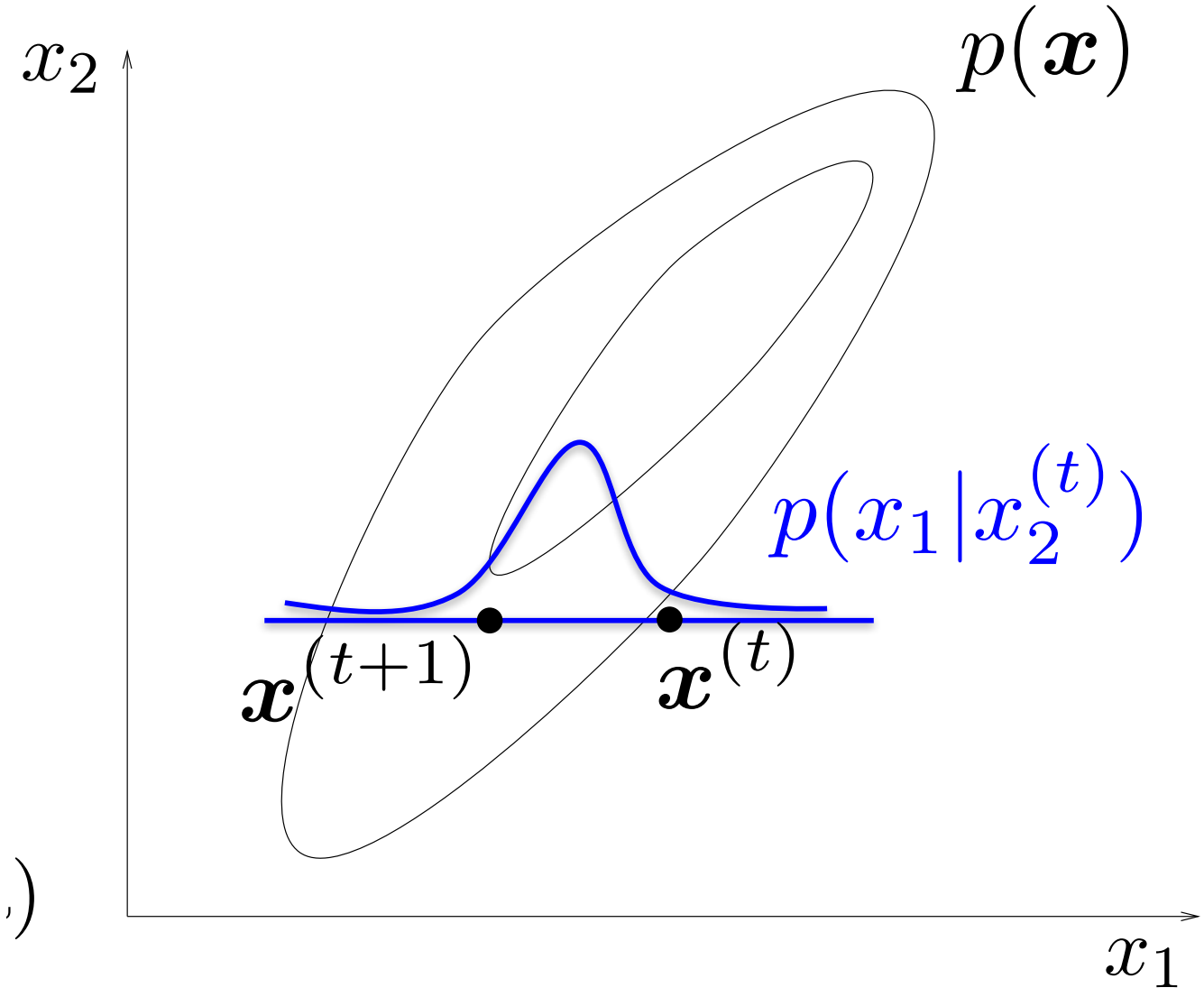
3. How do we compute marginal probabilities?
   $P(A) = \ldots$

4. How do we draw samples from a conditional distribution?
   $t,h,a \sim P(T, H, A \mid C = c)$

5. How do we compute conditional marginal probabilities?
   $P(H \mid C = c) = \ldots$



Gibbs Sampling



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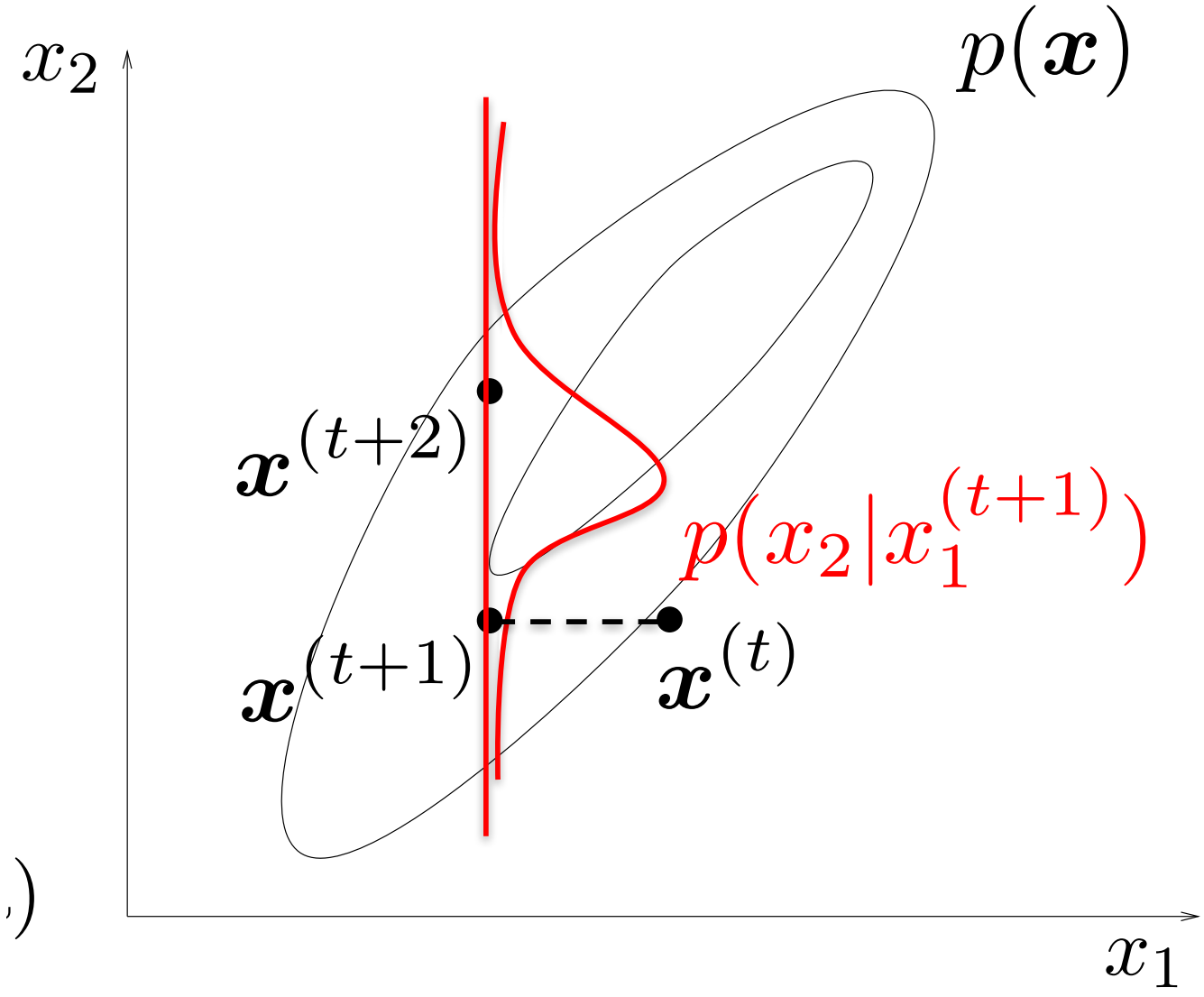

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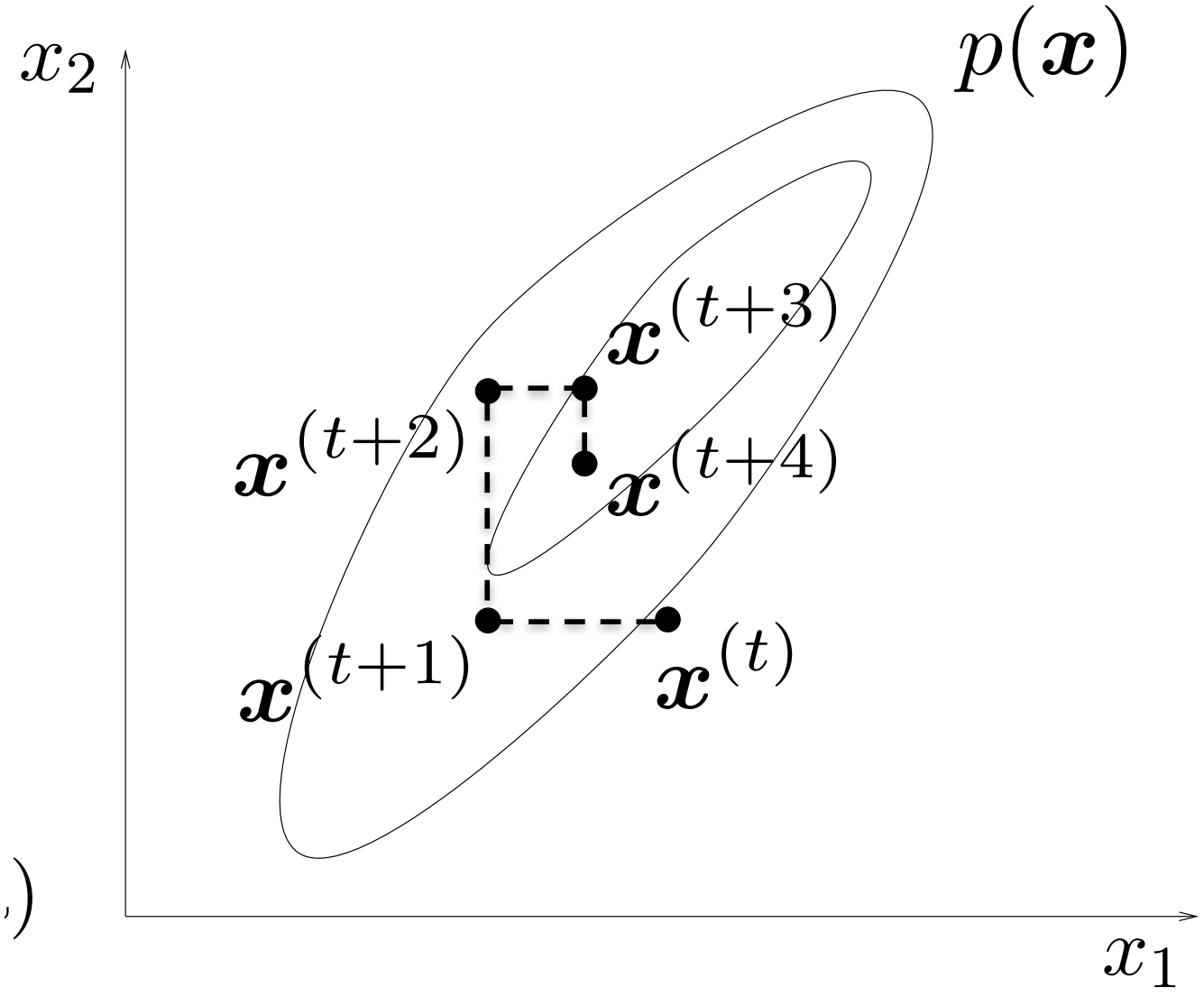


Gibbs Sampling

Question:
How do we draw samples from a conditional distribution?
$y_1, y_2, \ldots, y_J \sim p(y_1, y_2, \ldots, y_J \mid x_1, x_2, \ldots, x_J)$

(Approximate) Solution:

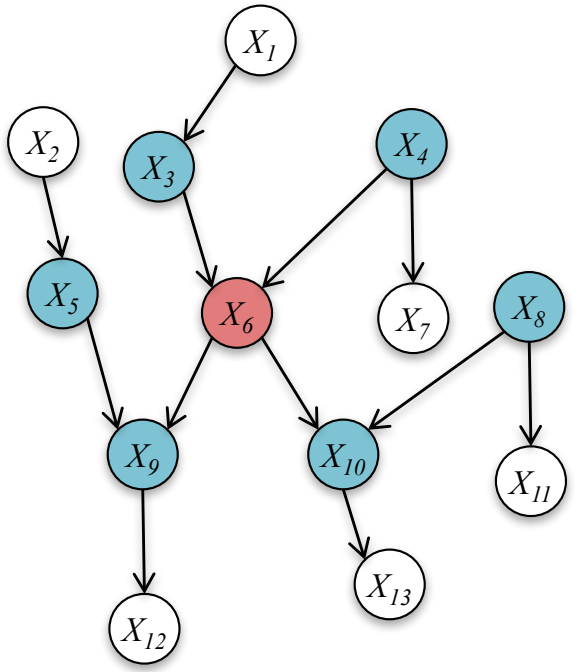
- Initialize $y_1^{(0)}, y_2^{(0)}, \ldots, y_J^{(0)}$ to arbitrary values
- For t = 1, 2, …:
  - $y_1^{(t+1)} \sim p(y_1 \mid y_2^{(t)}, \ldots, y_J^{(t)}, x_1, x_2, \ldots, x_J)$
  - $y_2^{(t+1)} \sim p(y_2 \mid y_1^{(t+1)}, y_3^{(t)}, \ldots, y_J^{(t)}, x_1, x_2, \ldots, x_J)$
  - $y_3^{(t+1)} \sim p(y_3 \mid y_1^{(t+1)}, y_2^{(t+1)}, y_4^{(t)}, \ldots, y_J^{(t)}, x_1, x_2, \ldots, x_J)$
  - …
  - $y_J^{(t+1)} \sim p(y_J \mid y_1^{(t+1)}, y_2^{(t+1)}, \ldots, y_{J-1}^{(t+1)}, x_1, x_2, \ldots, x_J)$

Properties:

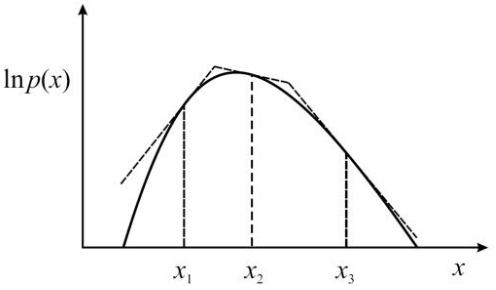
- This will eventually yield samples from $p(y_1, y_2, \ldots, y_J \mid x_1, x_2, \ldots, x_J)$
- But it might take a long time -- just like other Markov Chain Monte Carlo methods

Gibbs Sampling

Full conditionals only need to condition on the **Markov Blanket**



- Must be "easy" to sample from conditionals
- Many conditionals are log-concave and are amenable to adaptive rejection sampling



Learning Objectives

Bayesian Networks

You should be able to…

1. Identify the conditional independence assumptions given by a generative story or a specification of a joint distribution
2. Draw a Bayesian network given a set of conditional independence assumptions
3. Define the joint distribution specified by a Bayesian network
4. User domain knowledge to construct a (simple) Bayesian network for a real-world modeling problem
5. Depict familiar models as Bayesian networks
6. Use d-separation to prove the existence of conditional indenpendencies in a Bayesian network
7. Employ a Markov blanket to identify conditional independence assumptions of a graphical model
8. Develop a supervised learning algorithm for a Bayesian network
9. Use samples from a joint distribution to compute marginal probabilities
10. Sample from the joint distribution specified by a generative story
11. Implement a Gibbs sampler for a Bayesian network

Reminders

- **Homework 7: HMMs**
  - **Out: Wed, Nov 7**
  - **Due: Mon, Nov 19 at 11:59pm**
- **Schedule Changes**
  - **Lecture on Fri, Nov 16**
  - ~~**Recitation**~~ **Lecture on Mon, Nov 19**
  - **Recitation on Mon, Nov 26**

Q&A

LEARNING PARADIGMS

Learning Paradigms

Whiteboard

- Supervised
  - Regression
  - Classification
  - Binary Classification
  - Structured Prediction
- Unsupervised
- Semi-supervised
- Online
- Active Learning
- Reinforcement Learning

REINFORCEMENT LEARNING

Examples of Reinforcement Learning

- How should a robot behave so as to optimize its "performance"? (Robotics)

- How to automate the motion of a helicopter? (Control Theory)

- How to make a good chess-playing program? (Artificial Intelligence)

Autonomous Helicopter

Video:

https://www.youtube.com/watch?v=VCdxqn0fcnE

Robot in a room

actions: UP, DOWN, LEFT, RIGHT

UP

80% move UP
10% move LEFT
10% move RIGHT

- reward +1 at [4,3], -1 at [4,2]
- reward -0.04 for each step

- what's the strategy to achieve max reward?
- what if the actions were NOT deterministic?

History of Reinforcement Learning

- Roots in the psychology of animal learning (Thorndike,1911).
- Another independent thread was the problem of optimal control, and its solution using dynamic programming (Bellman, 1957).
- Idea of temporal difference learning (on-line method), e.g., playing board games (Samuel, 1959).
- A major breakthrough was the discovery of Q-learning (Watkins, 1989).

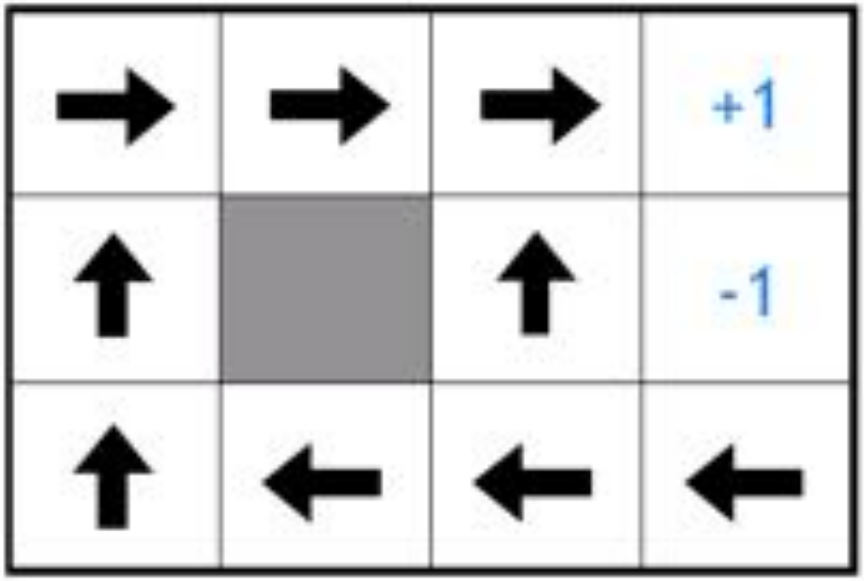
What is special about RL?

- RL is learning how to map states to actions, so as to maximize a numerical reward over time.
- Unlike other forms of learning, it is a multistage decision-making process (often Markovian).
- An RL agent must learn by trial-and-error. (Not entirely supervised, but interactive)
- Actions may affect not only the immediate reward but also subsequent rewards (Delayed effect).

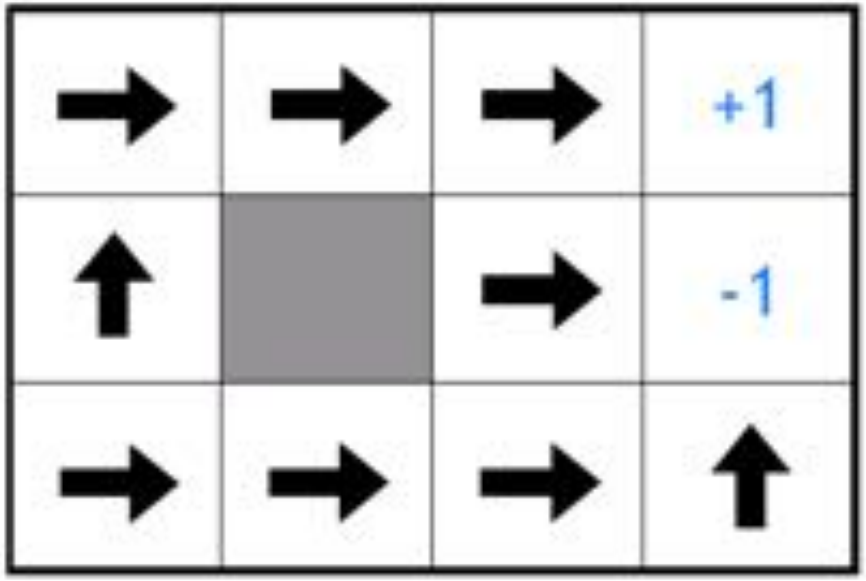
Elements of RL

- A policy
  - A map from state space to action space.
  - May be stochastic.
- A reward function
  - It maps each state (or, state-action pair) to a real number, called reward.
- A value function
  - Value of a state (or, state-action pair) is the total expected reward, starting from that state (or, state-action pair).

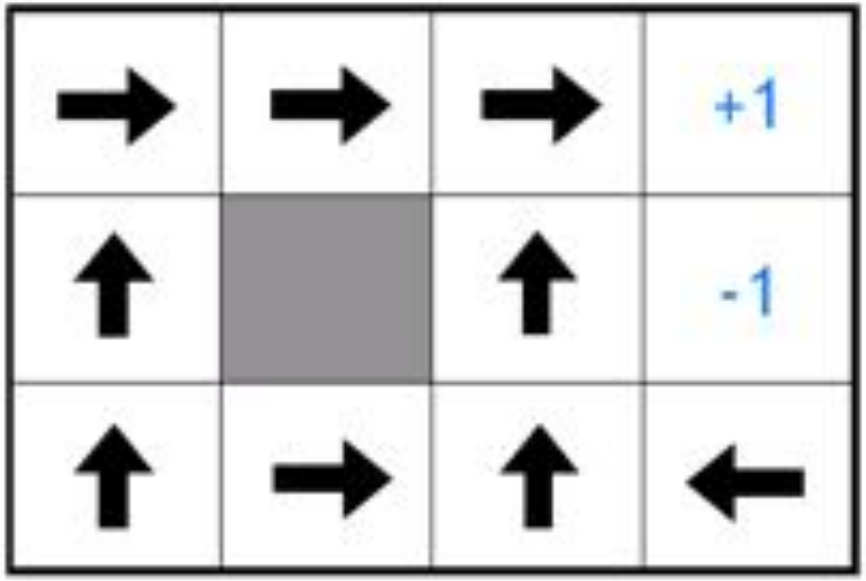
Policy



Reward for each step -2



Reward for each step: -0.1



The Precise Goal

- To find a policy that maximizes the Value function.
  - transitions and rewards usually not available
- There are different approaches to achieve this goal in various situations.
- Value iteration and Policy iteration are two more classic approaches to this problem. But essentially both are dynamic programming.
- Q-learning is a more recent approaches to this problem. Essentially it is a temporal-difference method.

MARKOV DECISION PROCESSES

Markov Decision Process

Whiteboard

- Components: states, actions, state transition probabilities, reward function
- Markovian assumption
- MDP Model
- MDP Goal: Infinite-horizon Discounted Reward
- deterministic vs. nondeterministic MDP
- deterministic vs. stochastic policy

Exploration vs. Exploitation

Whiteboard

- Explore vs. Exploit Tradeoff
- Ex: k-Armed Bandits
- Ex: Traversing a Maze

FIXED POINT ITERATION

Fixed Point Iteration for Optimization

- Fixed point iteration is a general tool for solving systems of equations
- It can also be applied to optimization.

$$J(\boldsymbol{\theta})$$

$$\frac{dJ(\boldsymbol{\theta})}{d\theta_i} = 0 = f(\boldsymbol{\theta})$$

$$0 = f(\boldsymbol{\theta}) \Rightarrow \theta_i = g(\boldsymbol{\theta})$$

$$\theta_i^{(t+1)} = g(\boldsymbol{\theta}^{(t)})$$

1. Given objective function:
2. Compute derivative, set to zero (call this function f).
3. Rearrange the equation s.t. one of parameters appears on the LHS.
4. Initialize the parameters.
5. For i in $\{1,\ldots,K\}$, update each parameter and increment t:
6. Repeat #5 until convergence

Fixed Point Iteration for Optimization

- Fixed point iteration is a general tool for solving systems of equations
- It can also be applied to optimization.

$$J(x) = \frac{x^3}{3} + \frac{3}{2}x^2 + 2x$$

$$\frac{dJ(x)}{dx} = f(x) = x^2 - 3x + 2 = 0$$

$$\Rightarrow x = \frac{x^2 + 2}{3} = g(x)$$

$$x \leftarrow \frac{x^2 + 2}{3}$$

1. Given objective function:
2. Compute derivative, set to zero (call this function f).
3. Rearrange the equation s.t. one of parameters appears on the LHS.
4. Initialize the parameters.
5. For i in $\{1,\ldots,K\}$, update each parameter and increment t:
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Fixed Point Iteration for Optimization

We can implement our example in a few lines of python.

$$J(x) = \frac{x^3}{3} + \frac{3}{2}x^2 + 2x$$

$$\frac{dJ(x)}{dx} = f(x) = x^2 - 3x + 2 = 0$$

$$\Rightarrow x = \frac{x^2 + 2}{3} = g(x)$$

$$x \leftarrow \frac{x^2 + 2}{3}$$

```
def f1(x):
    '''f(x) = x^2 - 3x + 2'''
    return x**2 - 3.*x + 2.

def g1(x):
    '''g(x) = \frac{x^2 + 2}{3}'''
    return (x**2 + 2.) / 3.

def fpi(g, x0, n, f):
    '''Optimizes the 1D function g by fixed point iteration
    starting at x0 and stopping after n iterations. Also
    includes an auxiliary function f to test at each value.'''
    x = x0
    for i in range(n):
        print("i=%2d x=%.4f f(x)=%.4f" % (i, x, f(x)))
        x = g(x)
    i += 1
    print("i=%2d x=%.4f f(x)=%.4f" % (i, x, f(x)))
    return x

if __name__ == "__main__":
    x = fpi(g1, 0, 20, f1)
```

Fixed Point Iteration for Optimization

$$J(x) = \frac{x^3}{3} + \frac{3}{2}x^2 + 2x$$

$$\frac{dJ(x)}{dx} = f(x) = x^2 - 3x + 2 = 0$$

$$\Rightarrow x = \frac{x^2 + 2}{3} = g(x)$$

$$x \leftarrow \frac{x^2 + 2}{3}$$

```
$ python fixed-point-iteration.py
i= 0 x=0.0000 f(x)=2.0000
i= 1 x=0.6667 f(x)=0.4444
i= 2 x=0.8148 f(x)=0.2195
i= 3 x=0.8880 f(x)=0.1246
i= 4 x=0.9295 f(x)=0.0755
i= 5 x=0.9547 f(x)=0.0474
i= 6 x=0.9705 f(x)=0.0304
i= 7 x=0.9806 f(x)=0.0198
i= 8 x=0.9872 f(x)=0.0130
i= 9 x=0.9915 f(x)=0.0086
i=10 x=0.9944 f(x)=0.0057
i=11 x=0.9963 f(x)=0.0038
i=12 x=0.9975 f(x)=0.0025
i=13 x=0.9983 f(x)=0.0017
i=14 x=0.9989 f(x)=0.0011
i=15 x=0.9993 f(x)=0.0007
i=16 x=0.9995 f(x)=0.0005
i=17 x=0.9997 f(x)=0.0003
i=18 x=0.9998 f(x)=0.0002
i=19 x=0.9999 f(x)=0.0001
i=20 x=0.9999 f(x)=0.0001
```

VALUE ITERATION

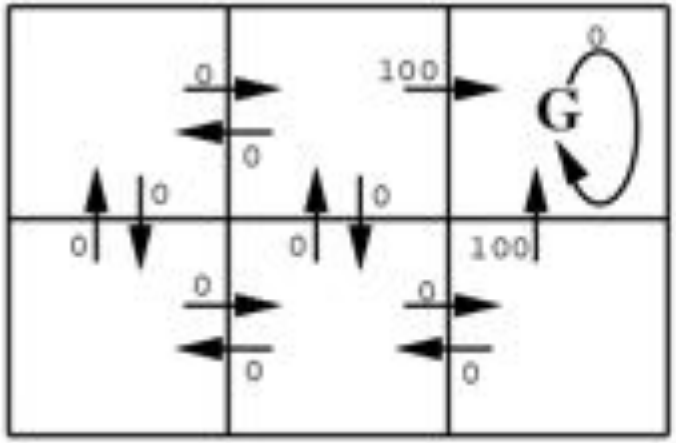
Definitions for Value Iteration

Whiteboard

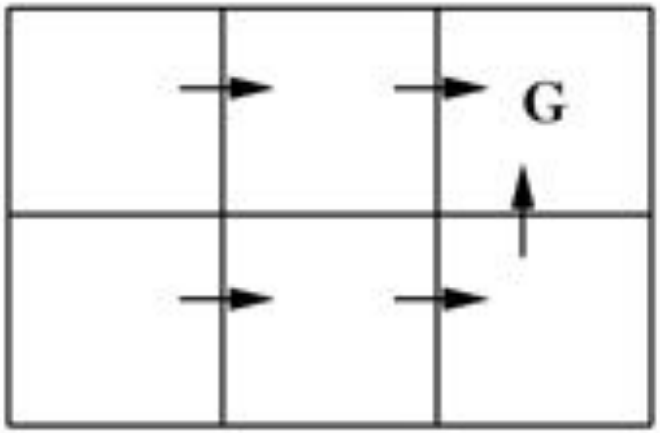
- State trajectory
- Value function
- Bellman equations
- Optimal policy
- Optimal value function
- Computing the optimal policy
- Ex: Path Planning

Example: Path Planning

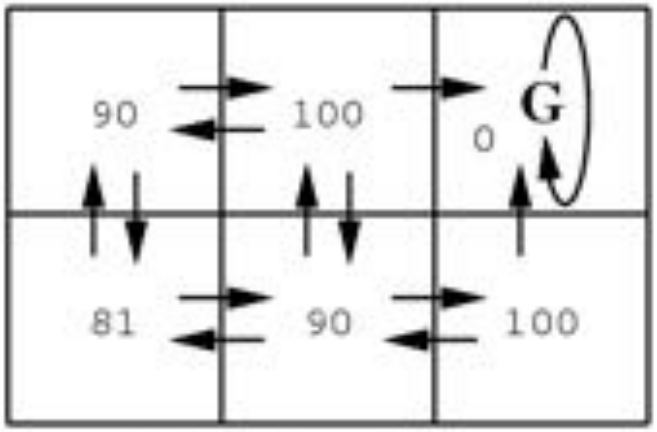
Example: Robot Localization



$r(s, a)$ (immediate reward) values



One optimal policy



$V^*(s)$ values

Figure from Tom Mitchell

Value Iteration

Whiteboard

- Value Iteration Algorithm
- Synchronous vs. Asychronous Updates
- Convergence Properties

Value Iteration

Algorithm 1 Value Iteration

procedure VALUEITERATION($R(s,a)$ reward function, $p(\cdot|s,a)$ transition probabilities)
  Initialize value function $V(s) = 0$ or randomly
  while not converged **do**
    for $s \in \mathcal{S}$ **do**
      for $a \in \mathcal{A}$ **do**
        $Q(s,a) = R(s,a) + \gamma \sum_{s' \in \mathcal{S}} p(s'|s,a) V(s')$
      $V(s) = \max_a Q(s,a)$
  Let $\pi(s) = \operatorname{argmax}_a Q(s,a), \ \forall s$
  return π

Policy Iteration

Whiteboard

- Policy Iteration Algorithm
- Solving the Bellman Equations for Fixed Policy
- Convergence Properties
- Value Iteration vs. Policy Iteration

Policy Iteration

Algorithm 1 Policy Iteration

1: **procedure** POLICYITERATION($R(s,a)$ reward function, $p(\cdot|s,a)$ transition probabilities)

2: Initialize policy π randomly

3: **while** not converged **do**

4: Solve Bellman equations for fixed policy π

$$V^{\pi}(s) = R(s,\pi(s)) + \gamma \sum_{s' \in \mathcal{S}} p(s'|s,\pi(s)) V^{\pi}(s'), \ \forall s$$

5: Improve policy π using new value function

$$\pi(s) = \operatorname*{argmax}_{a} R(s,a) + \gamma \sum_{s' \in \mathcal{S}} p(s'|s,a) V^{\pi}(s')$$

6: **return** π

Policy Iteration

Algorithm 1 Policy Iteration

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6: **return** π

Compute value function for fixed policy is easy

System of |S| equations and |S| variables

Greedy policy w.r.t. current value function

Greedy policy might **remain the same** for a particular state if there is no better action

Policy Iteration Convergence

In-Class Exercise:

How many policies are there for a finite sized state and action space?

In-Class Exercise:

Suppose policy iteration is shown to improve the policy at every iteration. Can you bound the number of iterations it will take to converge?

Value Iteration vs. Policy Iteration

- Value iteration requires $O(|A|\,|S|^2)$ computation per iteration
- Policy iteration requires $O(|A|\,|S|^2 + |S|^3)$ computation per iteration
- In practice, policy iteration converges in fewer iterations

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  Initialize policy π randomly
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    Improve policy π using new value function

$$\pi(s) = \operatorname*{argmax}_a R(s,a) + \gamma \sum_{s' \in \mathcal{S}} p(s'|s,a) V^\pi(s')$$

  return π

Learning Objectives

Reinforcement Learning: Value and Policy Iteration

You should be able to…

1. Compare the reinforcement learning paradigm to other learning paradigms
2. Cast a real-world problem as a Markov Decision Process
3. Depict the exploration vs. exploitation tradeoff via MDP examples
4. Explain how to solve a system of equations using fixed point iteration
5. Define the Bellman Equations
6. Show how to compute the optimal policy in terms of the optimal value function
7. Explain the relationship between a value function mapping states to expected rewards and a value function mapping state-action pairs to expected rewards
8. Implement value iteration
9. Implement policy iteration
10. Contrast the computational complexity and empirical convergence of value iteration vs. policy iteration
11. Identify the conditions under which the value iteration algorithm will converge to the true value function
12. Describe properties of the policy iteration algorithm