# CPSC 540: Machine Learning

## Message Passing, Directed Acyclic Graphical Models

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# Admin

- Assignment 3:
  - 1 late day to hand in today, 2 for Monday.
- Assignment 4:
  - Due March 20.
- For graduate students planning to graduate in May:
  - Send me a private message on Piazza ASAP.

# Last Time: Monte Carlo Methods

- If we want to approximate expectations of random functions,

$$\mathbb{E}[g(X)] = \underbrace{\sum_{x \in \mathcal{X}} g(x)p(x)}_{\text{discrete } x} \quad \text{or} \quad \underbrace{\mathbb{E}[g(X)] = \int_{x \in \mathcal{X}} g(x)p(x)dx}_{\text{continuous } x},$$

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the Monte Carlo estimate is

$$\mathbb{E}[g(X)] \approx \frac{1}{n}\sum_{i=1}^{n} g(x^i),$$

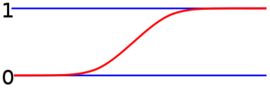
where the $x^i$ are independent samples from $p(x)$.

- We can use this to approximate marginals,

$$p(x_j = c) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{I}_{x_j^i = c}.$$

# Last Time: Inverse Transform Sampling Method

- The cumulative distribution function (CDF) $F$ is $p(X \leq x)$.
  - $F(x)$ is between $0$ and $1$ a gives proportion of times $X$ is below $x$.

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  - Given a number $u$ between $0$ and $1$, gives $x$ such that $p(X \leq x) = u$.

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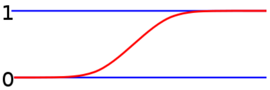


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- Inverse transfrom method for exact sampling in 1D:
  1. Sample $u \sim \mathcal{U}(0, 1)$.
  2. Compute $x = F^{-1}(u)$.

# Last Time: Markov Chains

- We can use Markov chains for density estimation,

$$p(x) = \underbrace{p(x_1)}_{\text{initial prob.}} \prod_{j=2}^{d} \underbrace{p(x_j | x_{j-1})}_{\text{transition prob.}},$$

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  - Gives more data to estimate transitions, allows examples of different sizes.
- Inhomogeneous chains allow different transitions at different times.

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- Ancestral sampling from a Markov chain:
  - Sample $x_1$, then $x_2$ given $x_1$, then $x_3$ given $x_2$, and so on.

# Last Time: Chapman-Kolmogorov Equations

- We can compute marginals like $p(x_j = c)$ recursively in a Markov chain,

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  which are called the Chapman-Kolmogorov equations.

- Yields closed-form solutions for marginals in discrete or Gaussian Markov chains.

# Outline

# Decoding: Maximizing Joint Probability

- The decoding problem in density models is finding most probable $x$:

$$\underset{x}{\operatorname{argmax}}\, p(x).$$

- For example, for binary $x$ we might have $\begin{bmatrix}1 & 0 & 0 & 1\end{bmatrix}$.

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- For independent models this is easy:
  - The log-likelihood is separable so we can optimize each $x_j$ independently.
  - For example, with three variables we have

$$\max_{x_1,x_2,x_3,x_4}\{p(x_1)p(x_2)p(x_3)p(x_4)\} = \left(\max_{x_1} p(x_1)\right)\left(\max_{x_2} p(x_2)\right)\left(\max_{x_3} p(x_3)\right)\left(\max_{x_4} p(x_4)\right).$$

- Can we also maximize the marginals to decode a Markov chain?

# Decoding vs. Maximizing Marginals

- Consider the "plane of doom" 2-variable Markov chain:
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$$x_2 = \begin{cases} \text{“alive”} & \text{If } x_1 = \text{“land”} \\ \text{“dead”} & \text{otherwise} \end{cases}$$

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  - The marginals for the different values of $x_2$ are given by

$$p(x_2 = \text{“alive”}) = 0.4, \quad p(x_2 = \text{“dead”}) = 0.6,$$

  so maximizing the marginals gives (“land”, “dead”) which has probability $0$.

# Distributing Max across Product

- Note that decoding can't be done forward in time as in CK equations.
  - Even if $p(x_0 = 2) = 0.99$, the most likely sequence could have $x_0 = 1$.
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where we're using that $\max_i \alpha a_i = \alpha \max_i a_i$ for non-negative $\alpha$.

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- And defining $M_4(x_4) = \max_{x_3} p(x_4|x_3)M_2(x_3)$ the maximum value is given by

$$\max_{x_1,x_2,x_3,x_4} p(x) = \max_{x_4} M_4(x_4).$$

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$$M_2(\text{“alive”}) = 0.4, \quad M_2(\text{“dead”}) = 0.3.$$

  - This means the optimal decoding has probability $0.4$ and ends with "alive".
    - We now need need to backtrack to find the state that lead to "alive", giving "land".

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- Computing all $M_j(x_j)$ given all $M_{j-1}(x_{j-1})$ costs $O(k^2)$.
  - Total cost is only $O(dk^2)$ to search over all $k^d$ paths.

# Conditional Probabilities

- We often want to compute conditional probabilities in Markov chains.
  - We can ask "what lead to $x_{10} = 4$?" with queries like $p(x_1|x_{10})$.
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- Monte Carlo approach to estimating $p(x_j|x_{j'})$:
  1. Generate a large number of samples from the Markov chain, $x^i \sim p(x_1, x_2, \dots, x_d)$.
  2. Use Monte Carlo estimates of $p(x_j, x_{j'} = c)$ and $p(x_{j'} = c)$ to give

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$$p(x_j|x_{j'} = c) = \frac{p(x_j, x_{j'} = c)}{p(x_{j'} = c)}.$$

- This is a special case of rejection sampling (we'll see general case later).
  - Unfortunately, if $x_{j'} = c$ is rare then most samples are "rejected" (ignored).

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  1. We can generate exact samples from conditional distribution (bonus slide).
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     - Run Viterbi decoding with $M_{j'}(c) = 1$ and $M_{j'}(c') = 0$ for $c \neq c'$.

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  3. We can find univariate conditionals, $p(x_j|x_{j'})$.

# Conditional Probabilities

- For Gaussian/discrete Markov chains, we can do better than rejection sampling.
  1. We can generate exact samples from conditional distribution (bonus slide).
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- Example of computing $p(x_1 = c|x_3 = 1)$ in a length-4 discrete Markov chain:

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  where the normalizing constant is $p(x_3 = 1)$.

- This is a sum over $k^{d-2}$ possible assignments to other variables.

# Distributing Sum across Product

- Fortunately, the Markov property makes the sums simplify as before:

$$\sum_{x_4}\sum_{x_2} p(x_1 = c, x_2, x_3 = 1, x_4) = \sum_{x4}\sum_{x3=1}\sum_{x_2}\sum_{x_1=c} p(x_4|x_3)p(x_3|x_2)p(x_2|x_1)p(x_1)$$

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# Message-Passing Algorithms

- We've just discussed several algorithms with similar structure:
  - CK equations for computing univariate marginals in discrete Markov chains.
  - Recursive marginal updates for Gaussian Markov chains (Assignment 4).
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- In some cases we'll also need backwards message $V_j$ ("cost to go"):
  - $V_j$ summarizes all relevant information about the future at time $j$.

# Conditionals via Backwards Messages

- Performing our conditional calculation using backwards messages.

$$\sum_{x_4}\sum_{x_2} p(x_1 = c, x_2, x_3 = 1, x_4) = \sum_{x_1=c}\sum_{x_2}\sum_{x3=1}\sum_{x4} p(x_4|x_3)p(x_3|x_2)p(x_2|x_1)p(x_1)$$

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\end{aligned}
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# Forward-Backward Algorithm

- Generic forward and backward messages for discrete marginals have the form

$$M_j(x_j) = \sum_{x_{j-1}} p(x_j | x_{j-1}) M_{j-1}(x_{j-1}), \quad V_j(x_j) = \sum_{x_{j+1}} p(x_{j+1} | x_j) V_j(x_{j+1}).$$

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- We can compute $p(x_j = c|x_{j'} = c')$ using only forward messages:
    - Set $M_j(c) = 1$ and $M_{j'}(c') = 1$.
- Why we would need backward messages?

# Forward-Backward Algorithm

- We can compute $p(x_j = c | x_{j'} = c')$ for all $j$ in $O(nk^2)$ with both messages.

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- We then have that
  - $M_j(x_j)$ sums up all the paths that end in state $x_j$ (with $x_{j'} = c'$).
  - $V_j(x_j)$ sums up all the paths that start in state $x_j$ (wth $x_{j'} = c'$).
  - We can combine these values to get

$$p(x_j | x_{j'}) \propto M_j(x_j) V_j(x_j),$$

  - Special case of the forward-backward algorithm.

# Outline

# Higher-Order Markov Models

- Markov models use a density of the form

$$p(x) = p(x_1)p(x_2|x_1)p(x_3|x_2)p(x_4|x_3)\cdots p(x_d|x_{d-1}).$$

- They support efficient computation but Markov assumption is strong.

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- They support efficient computation but Markov assumption is strong.

- A more flexible model would be a second-order Markov model,

$$p(x) = p(x_1)p(x_2|x_1)p(x_3|x_2, x_1)p(x_4|x_3, x_2)\cdots p(x_d|x_{d-1}, x_{d-2}),$$

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or even a higher-order models.

- Directed acyclic graphical (DAG) models generalize Markov models:
  - They allow dependence on any subset of previous features.

# DAG Models

- DAG models use product rule, $p(a, b, c) = p(b, c|a)p(a)$, to write

$$p(x_1, x_2, \dots, x_d) = p(x_1)p(x_2, x_3, \dots, x_d|x_1)$$

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- This factorization holds for any distribution.
- But it has too many parameters:
  - For binary $x_i$, we need $2^d$ parameters for $p(x_j|x_1,x_2,\dots,x_{j-1})$ alone.

# DAG Models

- To reduce number of parameters, in DAG models we use

$$p(x_1, x_2, \dots, x_d) = \prod_{j=1}^{d} p(x_j | x_{\text{pa}(j)}),$$

where $\text{pa}(j)$ are the "parents" of node $j$.

  - If we have $k$ parents we only need $2^{k+1}$ parameters.
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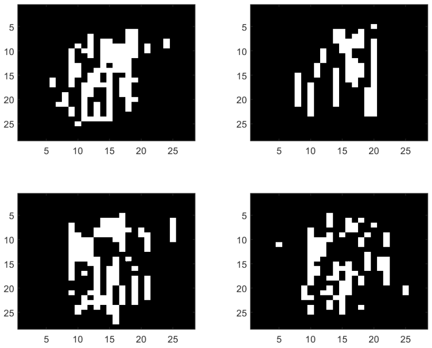
- This corresponds to a set of conditional independence assumptions,

$$p(x_j | x_{1:j-1}) = p(x_j | x_{\text{pa}(j)}),$$

  that we're independent of previous non-parents given the parents.

# MNIST DIgits with Markov Chains

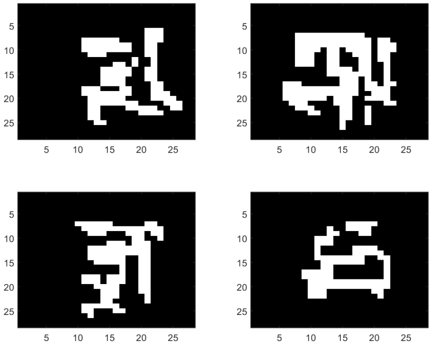
- Recall trying to model digits using an inhomogeneous Markov chain:




Only models dependence on pixel above, not on 2 pixels above nor across columns.

# MNIST Digits with DAG Model (Sparse Parents)

- Samples from a DAG model with 8 parents per feature:




Parents of $(i, j)$ are 8 other pixels in the neighbourhood $(i-2:i, j-2:j)$:

$$\{(i-2,j-2),(i-1,j-2),(i,j-2),(i-2,j-1),(i-1,j-1),(i,j-1),(i-2,j),(i-1,j)\}.$$

# From Probability Factorizations to Graphs

- DAG models are also known as "Bayesian networks" and "belief networks".
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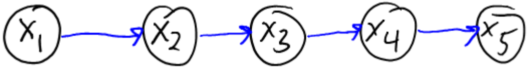

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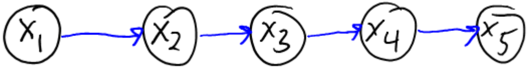
  - We place an edge into $j$ from each of its parents.
- The graph for Markov chains is:




- This graph is not just a visualization tool:
  - Can be used to test arbitrary conditional independences ("d-separation").
  - Graph structure tells us whether message passing is efficient ("treewidth").

# Graph Structure Examples

With product of independent we have

$$p(x) = \prod_{j=1}^{d} p(x_j),$$

so $\text{pa}(j) = \varnothing$ and the graph is:

# Graph Structure Examples

With Markov chain we have

$$p(x) = p(x_1) \prod_{j=2}^{d} p(x_j | x_{j-1}),$$

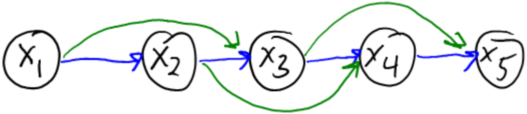
so $\text{pa}(j) = \{j - 1\}$ and the graph is:

# Graph Structure Examples

With second-order Markov chain we have

$$p(x) = p(x_1)p(x_2|x_1)\prod_{j=3}^{d} p(x_j|x_{j-1}, x_{j-2}),$$

so $\mathrm{pa}(j) = \{j-1, j-2\}$ and the graph is:

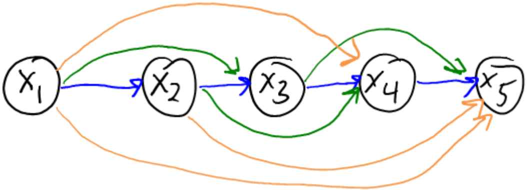


# Graph Structure Examples

With general distribution we have

$$p(x) = \prod_{j=1}^{d} p(x_j | x_{1:j-1}).$$

so $\text{pa}(j) = \{j-1, j-2, \dots, 1\}$ and the graph is:

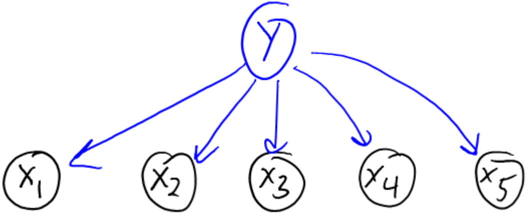


# Graph Structure Examples

In naive Bayes we add an extra variable $y$ and use

$$p(y, x) = p(y) \prod_{j=1}^{d} p(x_j | y),$$

which has $\text{pa}(y) = \emptyset$ and $\text{pa}(x_j) = y$ giving



# Graph Structure Examples

With mixture of independent models we have

$$p(z, x) = p(z) \prod_{j=1}^{d} p(x_j | z).$$

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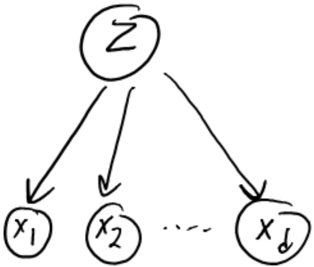

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Instead of factorizing by variables $j$, could factor into blocks $b$:

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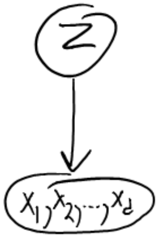
The corresponding graph structure is:



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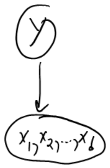

# Graph Structure Examples

With probabilistic PCA we have

$$p(z,x) = p(x|z)\prod_{c=1}^{k} p(z_c).$$

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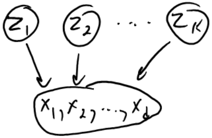

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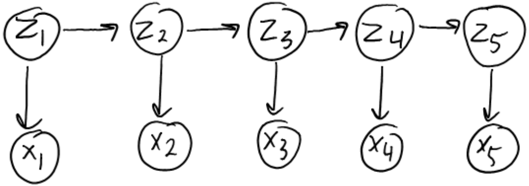
Sometimes it's easier to present a model using the graph.

Later in the course we'll see hidden Markov models which have the structure



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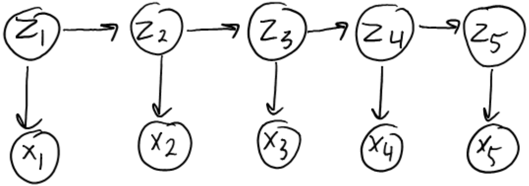



You should already be able to get an idea of what this model does:

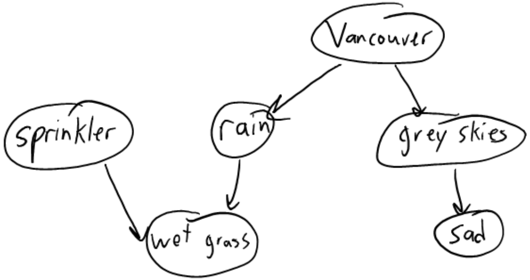
- We have hidden variables $z_j$ that follow a Markov chain.
- Each feature $x_j$ depends on corresponding feature $z_j$.

# Graph Structure Examples

We can consider less-structured examples,

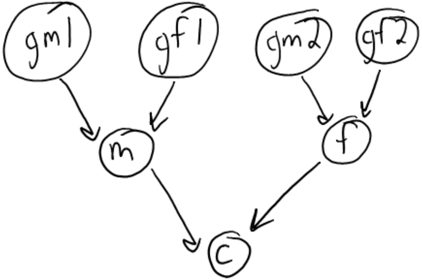
$$p(S, V, R, W, G, D) = p(S)p(V)p(R|V)p(W|S, R)p(G|V)p(D|G).$$

The corresponding graph structure is:



# Graph Structure Examples

We can consider phylogeny (family trees):



# Outline

# Review of Independence

- Let $A$ and $B$ are random variables taking values $a \in \mathcal{A}$ and $b \in \mathcal{B}$.
- We say that $A$ and $B$ are independent if we have

$$p(a, b) = p(a)p(b),$$

  for all $a$ and $b$.
- This is true iff $p(a, b) = f(a)g(b)$ for some functions $f$ and $g$.

# Review of Independence

- To denote independence of $x_i$ and $x_j$ we use the notation

$$x_i \perp x_j.$$

- For independent $a$ and $b$ we have

$$p(a|b) = \frac{p(a,b)}{p(b)} = \frac{p(a)p(b)}{p(b)} = p(a).$$

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- For independent $a$ and $b$ we have
$$p(a|b) = \frac{p(a,b)}{p(b)} = \frac{p(a)p(b)}{p(b)} = p(a).$$
- This gives us a more intuitive definition: $A$ and $B$ are independent if
$$p(a|b) = p(a)$$
for all $a$ and $b$.
  - In words: knowing $b$ tells us nothing about $a$ (and vice versa).

# Independence in "Independent Bernoulli" Model

- In a product of Bernoullis model we have

$$p(x) = \prod_{j=1}^{n} p(x_j).$$

From marginalization rule we have

$$p(x_i, x_j) = \sum_{x_{-ij}} p(x),$$

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because the sum is over a joint probability distribution.

# Independence in Product of Bernoullis Model

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$$p(x) = \prod_{j=1}^{n} p(x_j),$$

which we showed implies

$$p(x_i, x_j) = p(x_i)p(x_j),$$

so we have $x_i \perp x_j$ for all $i$ and $j$.

- In mixture of Bernoullis we have $x_i \not\perp x_j$:
  - Knowing $x_j$ tells you something about $x_i$.
  - But there are conditional independences in mixture of Bernoulli...

# Conditional Independence

- We say that $A$ is conditionally independent of $B$ given $C$ if

$$p(a, b|c) = p(a|c)p(b|c),$$

  for all $a$, $b$, and $c$.

- Equivalently, we have

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- Equivalently, we have

$$p(a|b, c) = p(a|c).$$

- "If you know $C$, then *also* knowing $B$ would tell you nothing about $A$"'.

- We often write this as

$$A \perp B \mid C.$$

# Conditional Indpendence in Mixture of Bernoulli

- In a mixture of Bernoulli model

$$p(x) = \sum_{c=1}^{k} p(z = c) \prod_{j=1}^{d} p(x_j | z = c),$$

we have that $x_i \perp x_j \mid z$ ("conditional independence given the cluster")

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- In particular, the same tedious notation-heavy cancellation gives that

$$p(x_i, x_j | z) = p(x_i | z) p(x_j | z).$$

- But we can also show [conditional] independencies using the graph...

# D-Separation: From Graphs to Conditional Independence

- In DAGs we make the conditional independence assumption that

$$p(x_j|x_{j-1}, x_{j-2}, \ldots, x_1) = p(x_j|x_{\text{pa}}(j)).$$

- But these conditional independence assumptions imply other assumptions.

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and it implies that

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- All implied conditional independences can be read from the graph.
  - Variables $A$ and $B$ are conditionally independent given $C$ if:
    - "All paths from any variable in $A$ to any $B$ are blocked by d-separation by $C$".

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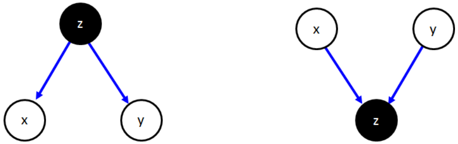
- E.g., consider three $\{X, Y, Z\}$ variables and the following graph structure:




- We use **black or shaded** nodes to denote observed values (we condition on $Z$).
- D-separation will tell us that $X \perp Y | Z$ on the left but $X \not\perp Y | Z$ on the right.

# D-Separation: From Graphs to Conditional Indpendence

- The rules of d-separation are intuitive in a simple model of gene inheritance:
  - Each person has single number, which we'll call a "gene".
  - If you have no parents, your gene is random.
  - If you have parents, your gene is a linear combination of your parents plus noise.

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- Genes of people can be conditionally independent given a third person:
  - Knowing your grandma's gene tells you something about your gene.
  - If you know you mom's gene, then grandma's gene isn't useful.
    - You are conditionally independent of grandma given mom.

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Are genes in person $x$ independent of the genes in person $y$?

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- Direct link: $x$ is the parent of $y$,


We have $x \not\perp y$: knowing $x$ tells you about $y$ (direct paths aren't blockable).

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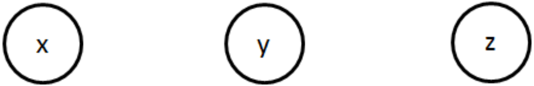


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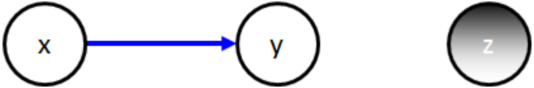


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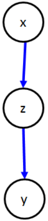

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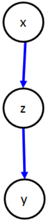


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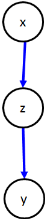
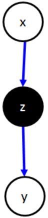



    We have $x \not\perp y$: knowing $x$ would give information about $y$ because of $z$
  - But if $z$ is *observed*:



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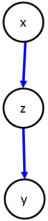


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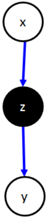


In this case $x \perp y \mid z$: knowing $z$ "breaks" dependence between $x$ and $y$.

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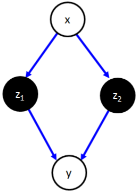


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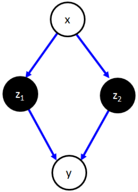


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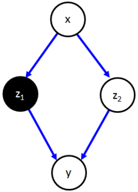
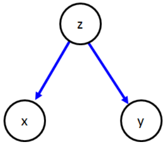
  - But if only $z_1$ is *observed*:




    We have $x \not\perp y \mid z_1$: dependence still "flows" through $z_2$.

# D-Separation Case 2: Common Parent

- Case 2: $x$ and $y$ are sibilings.
  - If $z$ is a common unobserved parent:



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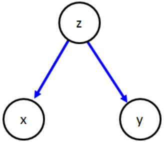


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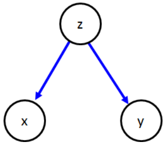


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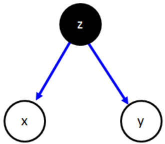

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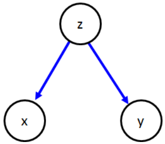
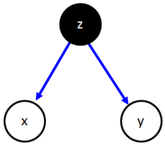



    We have $x \not\perp y$: knowing $x$ would give information about $y$.
  - But if $z$ is *observed*:




    In this case $x \perp y \mid z$: knowing $z$ "breaks" dependence between $x$ and $y$.

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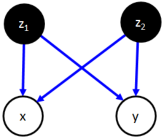
- Case 2: $x$ and $y$ are sibilings.
  - If $z_1$ and $z_2$ are common observed parents:



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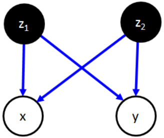


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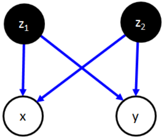


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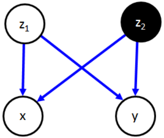


    Then we have $x \not\perp y \mid z_2$: dependence still "flows" through $z_1$.

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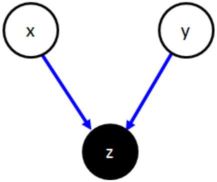

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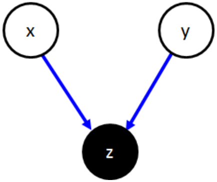


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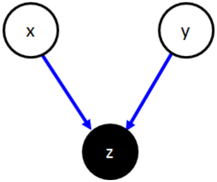


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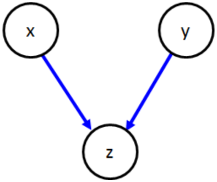

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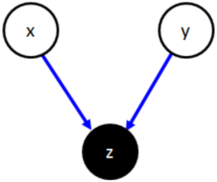


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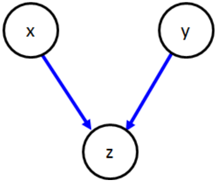


    We have $x \perp y$: if you don't observe $z$ then $x$ and $y$ are independent.
- Different from Case 1 and Case 2: not observing the child blocks path.

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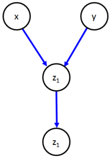

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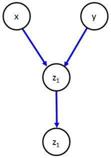


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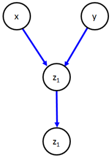


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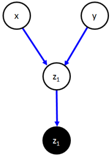

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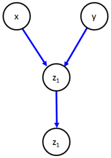


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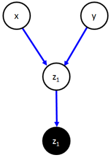


    We have $x \not\perp y \mid z_2$: grandchild creates dependence even with unobserved parent.
- Case 3 needs to consider descendants of child.

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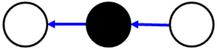

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     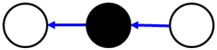

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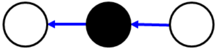
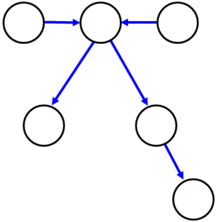
     
  2. $P$ includes a "fork" with an observed parent node:
     
  3. $P$ includes a "v-structure" or "collider":
     

     where child $C$ and all its descendants are unobserved.

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- D-separation allows us to test conditional independences based on graph.

- Next time: undirected graphical models and how we use graphical models.

# Bonus Slide: Conditional Samples from Gaussian/Discrete Markov Chain

Generating exact conditional samples from Gaussian/discrete Markov chains:

1. If we're only conditioning on first $j$ states, $x_{1:j}$, just fix these values and start ancestral sampling from time $(j+1)$.
2. If we have the marginals $p(x_j)$, we can get the "backwards" transition probabilities using Bayes rule,

$$p(x_j|x_{j+1}) = \frac{p(x_{j+1}|x_j)p(x_j)}{p_{j+1})},$$

   which lets us run ancestral sampling in reverse: sample $x_d$ from $p(x_d)$, then $x_{d-1}$ from $p(x_{d-1}|x_d)$, and so on.
3. If we're only conditioning on last $j$ states $x_{d-j:d}$, run CK equations to get marginals and then start ancestral sampling "backwards" starting from $(d-j-1)$ to sample the earlier states.

# Bonus Slide: Conditional Samples from Gaussian/Discrete Markov Chain

4. If we're conditioning on contiguous states in the middle, $x_{j:j'}$, run ancestral sampling forward starting from position $(j'+1)$ and backwards starting from position $(j-1)$.
5. If you condition on non-contiguous positions $j$ and $j'$ with $j < j'$, need to do (i) forward sampling starting from $(j'+1)$, (ii) backward sampling starting from $(j-1)$, and (iii) CK equations on the sequence $(j:j')$ to get marginals conditioned on value of $j$ then backwards sampling back to $j$ starting from $(j'-1)$.

The above are all special cases of conditioning in an undirected graphical model (UGM), followed by applying the "forward-filter backward-sampling" algorithm on each of the resulting chain-structured UGMs.