Graphical Models

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Introduction

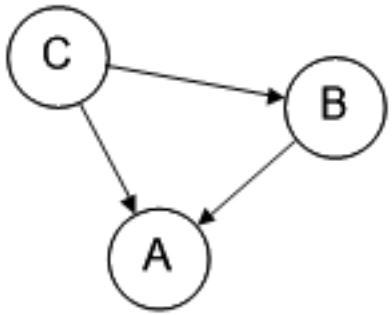
- In ***graphical models***, we model a problem using a graph where
  - Each node represents a random variable
  - Each link expresses a probabilistic relationship between two nodes
    - Directed link: conditional dependency (forming a ***Bayesian network***)
    - Undirected: correlation (forming a ***Markov random field***, or ***Markov network***)
- Graphical models offer the following advantages:
  - Visualization of the probabilistic models and motivating new models
  - Insight into the probabilistic properties (e.g., conditional independence between any two groups of nodes)
  - Complex computation (required to perform inference/learning) that can be carried along the graph

Outline

Outline

Definitions (1/3)

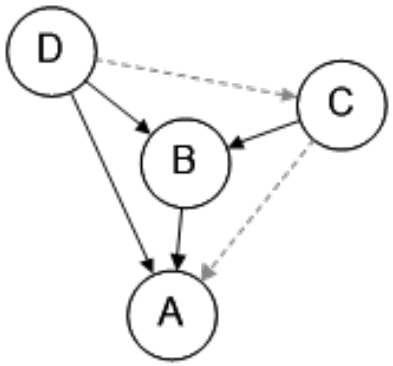
- Consider the joint probability $P(A = a, B = b, C = c)$ (or $P(A, B, C)$ ***for short***) of three random variables A, B, and C
- It can be factorized into, for example, $P(A|B, C)P(B|C)P(C)$
  - Holds for any distribution
- We can draw the factorization as a graph:



  - Each node is a random variable
  - A link denotes conditional dependency
- The graph must be a ***Directed Acyclic Graph*** (***DAG***) [Proof: by induction on the number of nodes]

Definitions (2/3)

- Given $P(X_1, X_2, \cdots, X_M)$ of M random variables, we have
  - Some factorization, e.g.,
    $P(X_1, X_2, \cdots, X_M) = P(X_1|X_2, \cdots, X_M) \cdots P(X_M)$
  - A fully connected graph
- It is the ***missing links*** that convey interesting information



  - A missing link from D to C implies independence between D and C
    - $P(C|D) = P(C)$, denoted by $\{C\} \perp\!\!\!\perp \{D\}$ or $\{C\} \perp\!\!\!\perp \{D\} \mid \emptyset$
  - A missing link from C to A implies ***conditional independence*** between C and A given B and D
    - $P(A|B, C, D) = P(A|B, D)$, denoted by $\{A\} \perp\!\!\!\perp \{C\} \mid \{B, D\}$

Definitions (3/3)

- A graph visualizes a factorization:

$$P(X_1, X_2, \cdots, X_M) = \prod_{i=1}^{M} P(X_i | parent(X_i)),$$

  where $parent(X_i)$ is the values of the parent nodes of X_i
- One graph for each factorization
  - Given a set of variables, we may construct different graphs based on different factorizations

Extensions (1/2)

- Values of some random variables may be observed in our problem
  - E.g., we may only care about $P(B, C, \cdots | A)$ given an observed variable $A = a$
  - Denoted as solid nodes in the graph
- There can be deterministic variables
  - E.g., we may assume parameters (e.g., $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ in classification, and $\boldsymbol{w}$ in regression) and hyperparameters (e.g., α and β in regression) to simplify calculation of a specific term in the factorization
  - Denoted by small dots in the graph
- Repeating subgraphs can be collapsed into a plate marked by multiplicity

Extensions (2/2)

- Observed variable $X = x$ vs deterministic variable α?

Extensions (2/2)

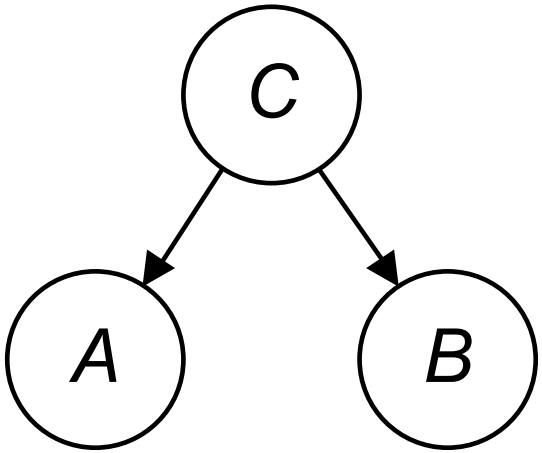
- Observed variable $X = x$ vs deterministic variable α?
- Even X is observed, $P(X = x) \neq 1$ if X has a nontrivial distribution
  - Can be in the consequent of a conditional probability
- $P(\alpha)$ is undefined
  - Can only be a parameter in a conditional probability
  - α cannot have parents
  - Must be observed
  - If α parametrizes $P(Y)$ (denoted by $P(Y) = P(Y; \alpha)$), then $P(X|Y; \alpha) = P(X|Y)$
    - Note, however, that $P(X; \alpha = c) \neq P(X; \alpha = c')$

Outline

Independence and Conditional Independence

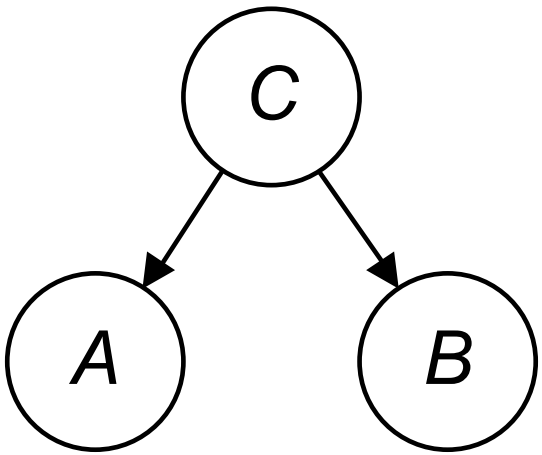
- $\{A\} \perp\!\!\!\perp \{B\} \mid \{C\}$ denotes conditional independence
  - $P(A|B,C) = P(A|C)$
  - Or equivalently, $P(A,B|C) = P(A|B,C)P(B|C) = P(A|C)P(B|C)$
- Many tasks are solved by the aid of conditional independence between nodes
- But checking conditional independence involving more than three nodes is usually cumbersome
- A graph visualizes the conditional independence and provides an easy way for checking
  - Given three sets of nodes P, Q, and R, you should be able to tell whether $P \perp\!\!\!\perp Q \mid R$ by directly looking at the graph

Canonical Cases (1/3)



- Consider a tail-to-tail path at C
- If C is not observed
  - $\{A\} \perp\!\!\!\perp \{B\} \mid \emptyset$?

Canonical Cases (1/3)



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- If C is not observed
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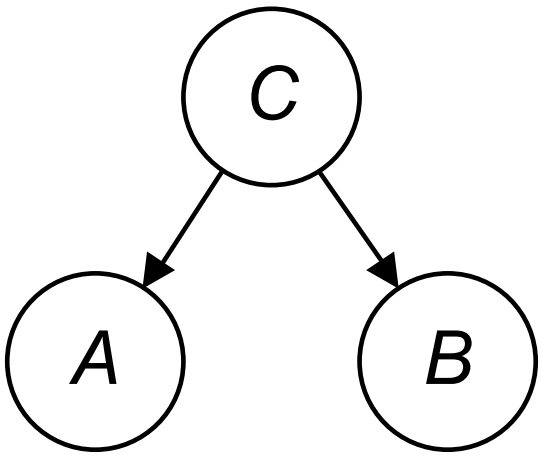

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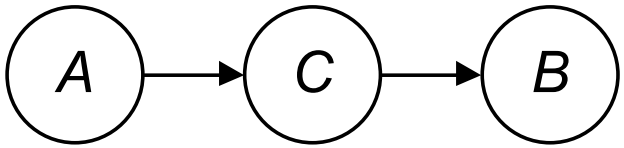
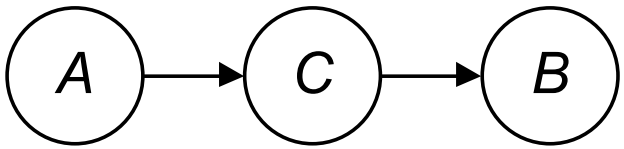
- If C is observed
  - $\{A\} \perp\!\!\!\perp \{B\} \mid \{C\}$? Yes
  - $p(A,B|C) = \frac{p(A,B,C)}{p(C)} = \frac{p(A|C)p(B|C)p(C)}{p(C)} = p(A|C)p(B|C)$
  - We say the path from A to B is ***blocked*** by C if C is observed

Canonical Cases (2/3)

- Consider a head-to-tail path at C
- If C is not observed
  - $\{A\} \perp\!\!\!\perp \{B\} \mid \emptyset$?



Canonical Cases (2/3)



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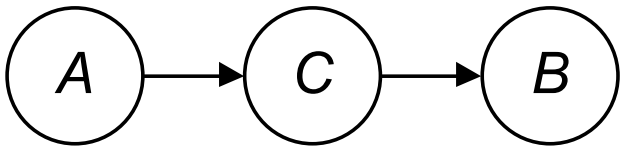
Canonical Cases (2/3)



- Consider a head-to-tail path at C
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- If C is observed
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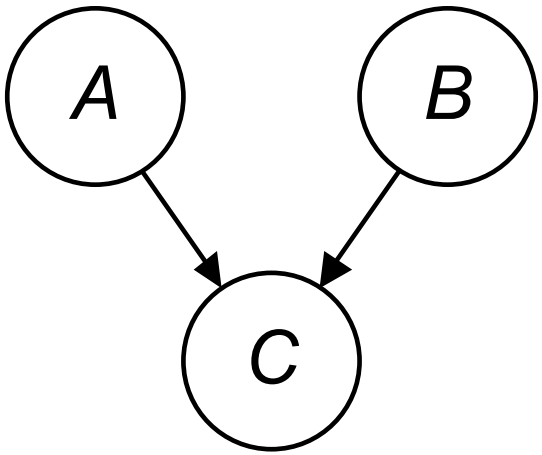
  - $p(A, B|C) = \frac{p(A,B,C)}{p(C)} = \frac{p(B|C)p(C|A)p(A)}{p(C)} = p(B|C)p(A|C)$
  - The path from A to B is blocked by C if C is observed

Canonical Cases (3/3)



- Consider a head-to-head path at C
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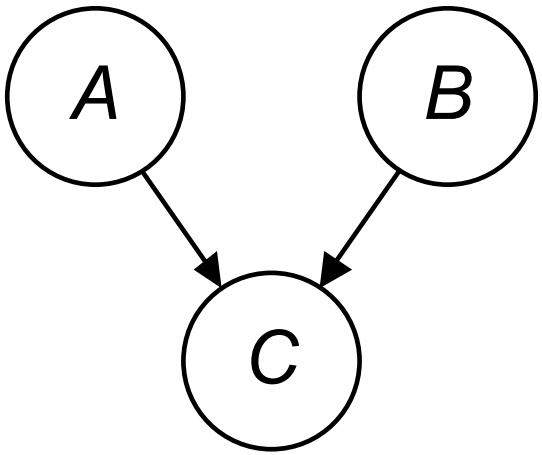
Canonical Cases (3/3)



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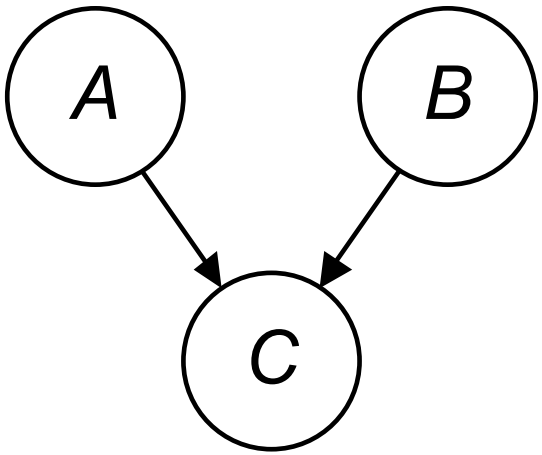

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- If C is not observed
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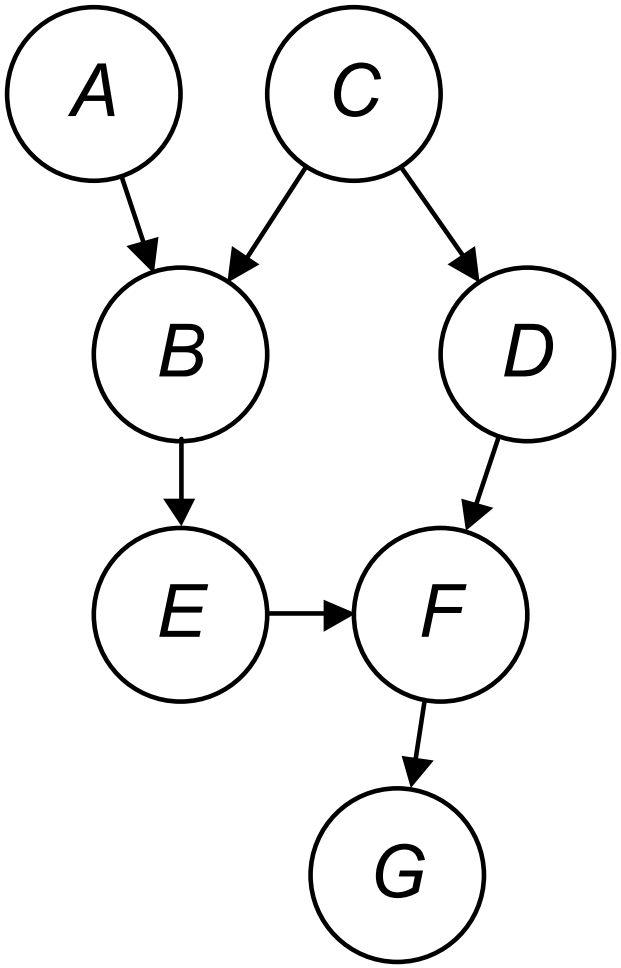
  - The path from A to B is blocked by C if C is not observed
- If C is observed
  - $\{A\} \perp\!\!\!\perp \{B\} \mid \{C\}$? ***No***
  - Actually, if C has descendents, A and B become dependent if any of the descendents is observed [Homework]

D-Separation (1/2)

- Given three sets of non-intersecting random variables P, Q, and R, we say P is ***d-separated*** ("d" means "direct") from Q given R, denoted as $P \perp\!\!\!\perp Q \mid R$, iff all paths from P to Q are blocked
- A path (of arbitrary length) is blocked if either
  - There are two links meet head-to-tail or tail-to-tail at a node, and that node is in R, or
  - There are two links meet head-to-head at a node, and neither the node, nor its descendents, is in R
- Deterministic parameters play no role in d-separation
  - A parameter α must be observed and have no parent
  - Path passing through α must be tail-to-tail, so is blocked

D-Separation (2/2)



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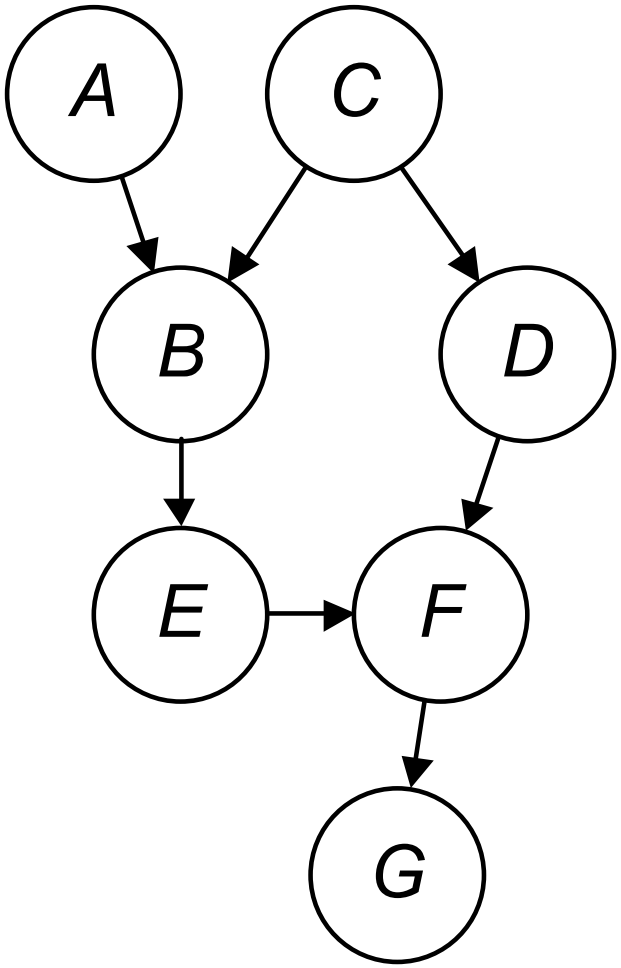

- $\{A\} \perp\!\!\!\perp \{C\} \mid \emptyset$? Yes
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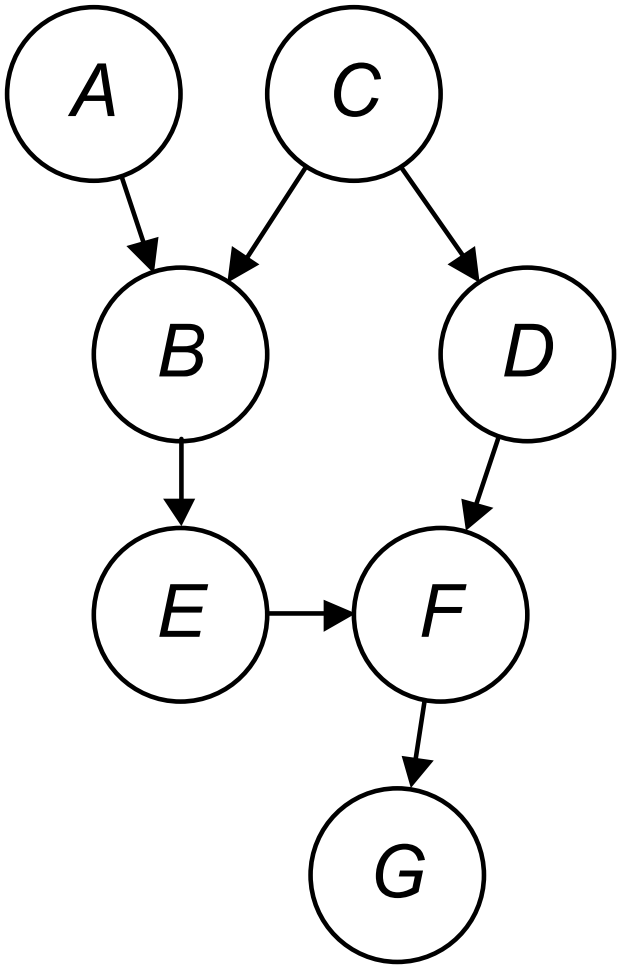
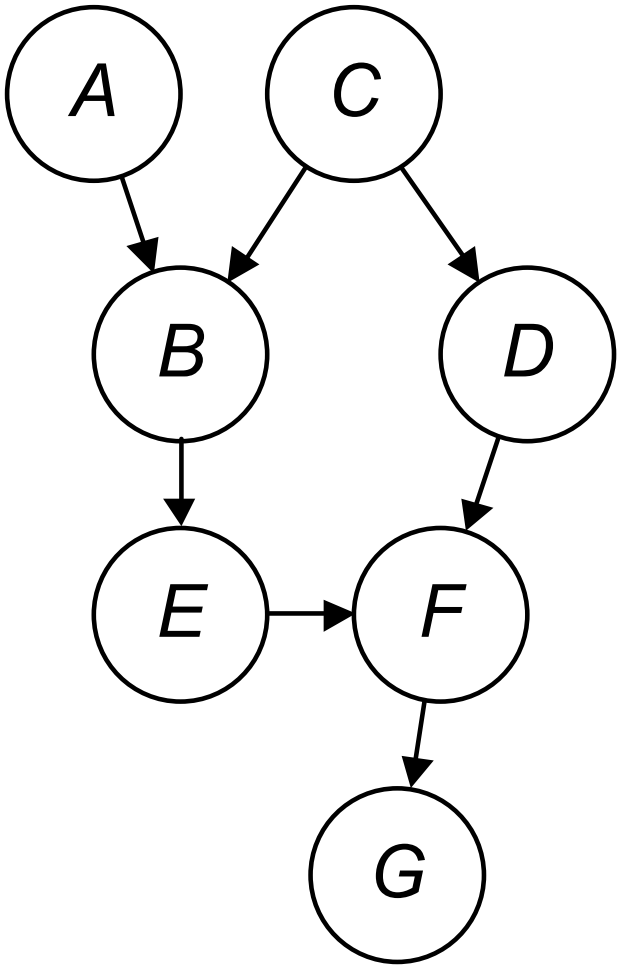
D-Separation (2/2)



- $\{A\} \perp\!\!\!\perp \{C\} \mid \emptyset$? Yes
- $\{B\} \perp\!\!\!\perp \{D\} \mid \{C\}$? Yes
- $\{B\} \perp\!\!\!\perp \{D, F\} \mid \{C, E\}$?

D-Separation (2/2)



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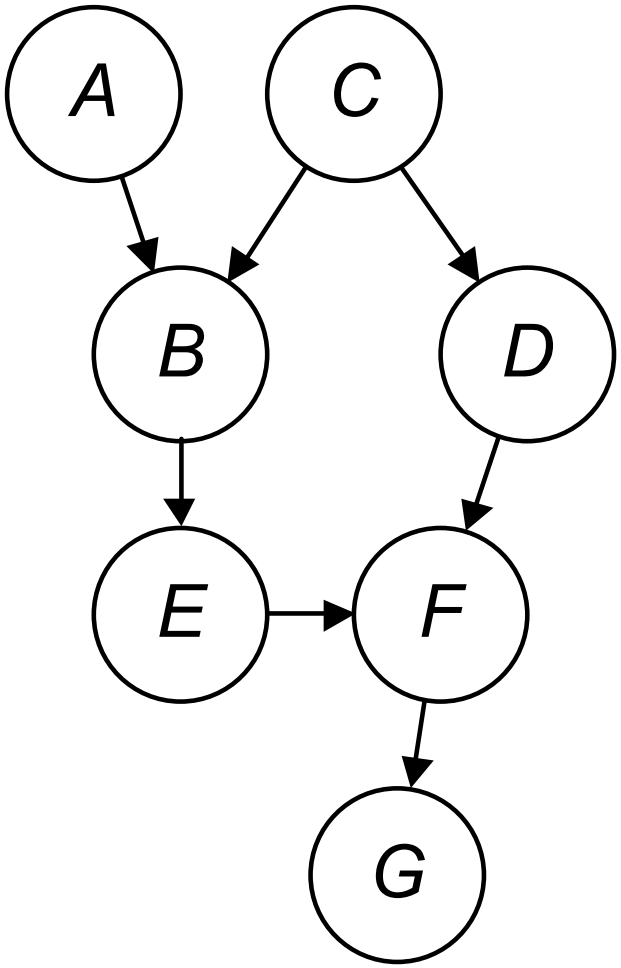
- $\{B\} \perp\!\!\!\perp \{D, F\} \mid \{C, E\}$? Yes
- $\{D\} \perp\!\!\!\perp \{E\} \mid \{C, G\}$?

D-Separation (2/2)



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Conditional Independence and Predictions

- Let's review how we make predictions

Outline

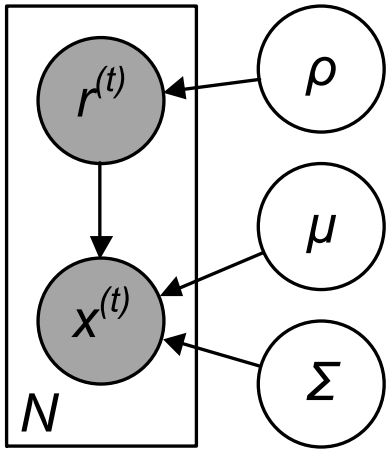
Modeling a Problem

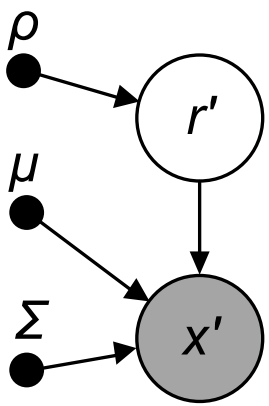
- How to model a problem as a graph right (or, how determine the right factorization)?

Modeling a Problem

- How to model a problem as a graph right (or, how determine the right factorization)?
  1. Identify nodes
  2. For each node X, draw links from others $Y_1, Y_2, \cdots$ to X if you know how to evaluate $P(X|Y_1, Y_2, \cdots)$ ***directly*** based on the problem definition and your assumptions
  3. Make sure
     - The network is connected
     - You did not add too many links that prevents the graph from being a DAG
- You ***should not*** invert the direction of a link just because you know how to use Bayes' rule

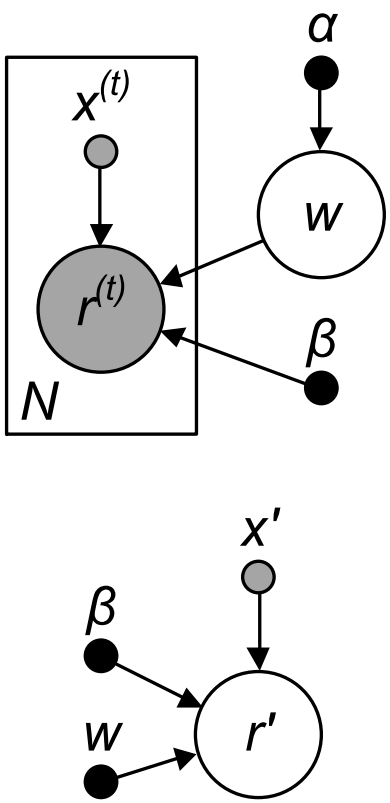
Example: Classification





- Model parameters $\boldsymbol{\rho} = \{\rho_i\}_{i=1}^K$, $\boldsymbol{\mu} = \{\boldsymbol{\mu}_i\}_{i=1}^K$, and $\boldsymbol{\Sigma} = \{\boldsymbol{\Sigma}_i\}_{i=1}^K$ are deterministic variables
- Here we assume a ***generative model*** where an observation ($\boldsymbol{x}$) is the cause of some reasons ($\boldsymbol{r}$) that may not be observable
- Training: $(\rho, \boldsymbol{\mu}, \boldsymbol{\Sigma})_{MAP} = \arg_{\rho,\boldsymbol{\mu},\boldsymbol{\Sigma}} \max p(\rho, \boldsymbol{\mu}, \boldsymbol{\Sigma} | \mathcal{X})$
- Prediction: $y' = \arg_y \max P(y | \boldsymbol{x}', \boldsymbol{\rho}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$

Example: Linear Regression (1/2)



- Why don't we draw links from $r^{(t)}/r'$ to $\boldsymbol{x}^{(t)}/\boldsymbol{x}'$?

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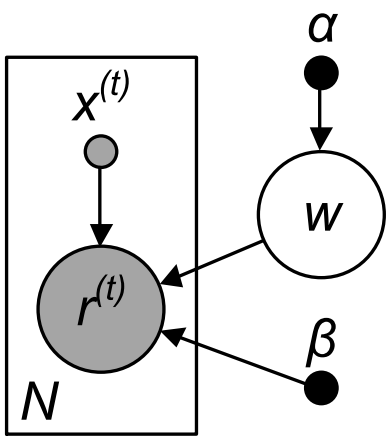
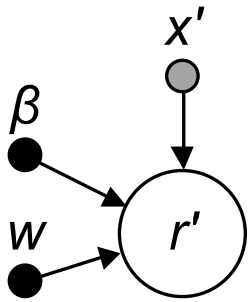
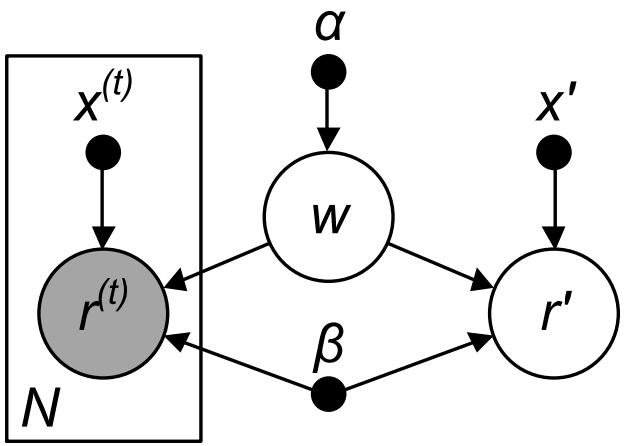




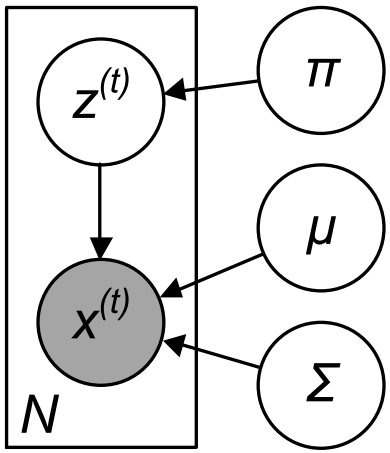
- Why don't we draw links from $r^{(t)}/r'$ to $\boldsymbol{x}^{(t)}/\boldsymbol{x}'$?
- Regression is ***not*** a generative model
  - We don't know how to evaluate $P(\boldsymbol{x}'|r', \cdots)$ given our assumptions
- Training: $\boldsymbol{w}_{MAP} = \arg_{\boldsymbol{w}} \max p(\boldsymbol{w}|\mathcal{X}, \alpha, \beta)$
  - Recall that we may assume $p(\boldsymbol{w}) \sim \mathcal{N}(\boldsymbol{0}, \alpha^{-1}\boldsymbol{I})$
- Prediction: $y' = \arg_y \max p(y|\boldsymbol{x}', \boldsymbol{w}, \beta)$

Example: Linear Regression (2/2)



- $\boldsymbol{w}$ is a random variable in Bayesian estimation for r'
- Prediction:
  $y' = \arg_y \max p(y|\boldsymbol{x}', \mathcal{X}, \alpha, \beta) =$
  $\arg_y \max \int p(y, \boldsymbol{w}|\boldsymbol{x}', \mathcal{X}) d\boldsymbol{w}$
- There is no separate training phase

Example: Clustering



- $\boldsymbol{\pi} = \{\pi_i\}_{i=1}^K$, $\boldsymbol{\mu} = \{\boldsymbol{\mu}_i\}_{i=1}^K$, $\boldsymbol{\Sigma} = \{\boldsymbol{\Sigma}_i\}_{i=1}^K$
- Target: $(\{z^{(t)}\}_t, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})_{MAP} =$ $\arg_{\{z^{(t)}\}_t, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}} \max p(\{z^{(t)}\}_t, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma} | \mathcal{X})$
  - $p(\{z^{(t)}\}_t, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma} | \mathcal{X}) =$ $p(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma} | \{z^{(t)}\}_t, \mathcal{X}) p(\{z^{(t)}\}_t | \mathcal{X})$ $\propto p(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma} | \{z^{(t)}\}_t, \mathcal{X}) p(\mathcal{X} | \{z^{(t)}\}_t) p(\{z^{(t)}\}_t)$
  - Can be simplified to $p(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma} | \{z^{(t)}\}_t, \mathcal{X}) p(\mathcal{X} | \{z^{(t)}\}_t)$ is we have no preference on a particular $\{z^{(t)}\}_t$ set
  - The problem is, we cannot evaluate $p(\mathcal{X} | \{z^{(t)}\}_t)$ without knowing $\boldsymbol{\pi}$, $\boldsymbol{\mu}$, and $\boldsymbol{\Sigma}$
- E-step: treat $\boldsymbol{\pi}$, $\boldsymbol{\mu}$, and $\boldsymbol{\Sigma}$ as parameters and estimate $\{z^{(t)}\}_t$
- M-step: treat $\{z^{(t)}\}_t$ as parameter and estimate $\boldsymbol{\pi}$, $\boldsymbol{\mu}$, and $\boldsymbol{\Sigma}$

Outline

Common Tasks

- Tasks given a graph, evidence E, and optionally parameters:
- Inference: solve $\arg_z \max P(Z = z|E)$
  - E.g., training a classifier/regressor, making predictions, clustering, etc.
- More?

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- Inference: solve $\arg_z \max P(Z = z|E)$
  - E.g., training a classifier/regressor, making predictions, clustering, etc.
- More?
- Sampling
- Evaluating the marginals: evaluate $P(Z|E)$
  - E.g., belief propagation, Latent Dirichlet Allocation (LDA), etc.
- Learning the structure of a graph
  - E.g., association rules, other advanced topics

Conjugate Prior of the Likelihood (1)

- In many cases, we want to write down $P(Z|E)$ in closed form
  - By Bayes' rule, we have $P(Z|E) = P(E|Z)P(E)$
- If we assume some distribution of the likelihood $P(E|Z)$, then we face a problem: how to pick the distribution of the prior $P(E)$ such that $P(Z|E)$ is tractable
- It is known that for certain likelihood distribution, some prior distribution will lead to the posterior distribution that is in the same family as prior distribution
  - Prior of such distribution is called the ***conjugate prior*** of the likelihood

Linear Gaussian Model

- For each node X_i, we assume $p(X_i|parent(X_i))$ follows some (parametrized) distribution
- A common choice is to form a ***linear Gaussian model***, where each node X_i resembles a linear combination of its parents $Y \in parent(X_i)$
  - $p(x_i|y_1, \cdots, y_p) = \mathcal{N}(x_i|\sum_{j=1}^{p} w_{i,j} y_j + b_i, \sigma_i^2)$, or
    $p(\boldsymbol{x}_i|\boldsymbol{y}_1, \cdots, \boldsymbol{y}_p) = \mathcal{N}(\boldsymbol{x}_i|\sum_{j=1}^{p} \boldsymbol{W}_{i,j} \boldsymbol{y}_j + \boldsymbol{b}_i, \boldsymbol{\Sigma}_i)$
  - And $p(\boldsymbol{y}_1, \cdots, \boldsymbol{y}_p)$ is Gaussian
- For two nodes X and Y, if $p(X_i|Y)$ and $p(Y)$ follow the linear Gaussian model, then $p(Y|X_i)$ and $p(X_i)$ are both normal distribution
  - $p(X_i)$ is called the ***conjugate prior*** of the likelihood $p(Y|X_i)$ of X_i

Space Complexity of Discrete Variables

- For each node X_i, we need to evaluate/store all possible values of $P(X_i|parent(X_i))$
- Suppose each node has K states and there are totally M nodes, what's the pace complexity?

Space Complexity of Discrete Variables

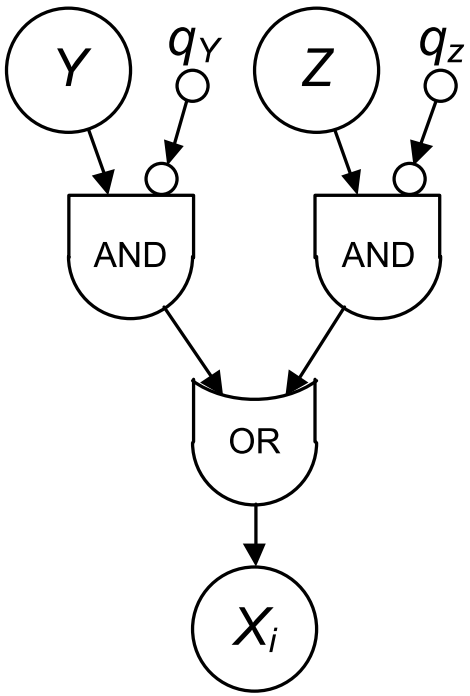
- For each node X_i, we need to evaluate/store all possible values of $P(X_i|parent(X_i))$
- Suppose each node has K states and there are totally M nodes, what's the pace complexity?
  - Chain: $(K-1)+(M-1)K(K-1) = O(M)$
  - Fully connected graph: $\sum_i (K-1)K^{|parent(X_i)|} = K^M - 1 = O(K^M)$

Reducing Space Complexity

- How to reduce the the space complexity?

Reducing Space Complexity

- How to reduce the the space complexity?
- Tying: sharing parameters between nodes
- ***Noisy OR gate*** for binary variables:



- Inhibitors are independent with each other and happens with probabilities q_i
- $P(X_i = 1 | Y = 1, Z = 0) = 1 - q_Y$
- $P(X_i | parent(X_i)) = 1 - \prod_{Y \in parent(X_i), Y=1} q_Y$
- Space complexity?

Reducing Space Complexity

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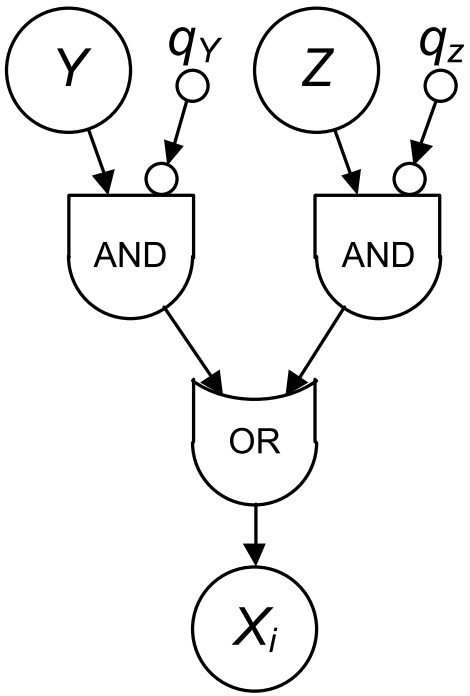

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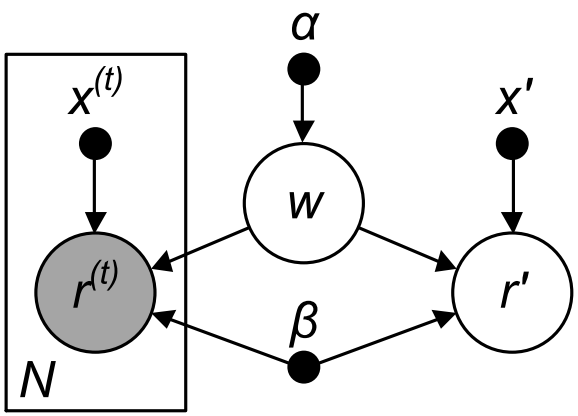
- Space complexity? $O(M^2)$

Bayesian Estimation for Linear Regression (1/3)



- Assuming hyperparameters α and β, we have
  $\int p(y, \boldsymbol{w}|\boldsymbol{x}', \mathcal{X}, \alpha, \beta) d\boldsymbol{w} =$
  $\int p(y|\boldsymbol{x}', \boldsymbol{w}, \mathcal{X}, \alpha, \beta) p(\boldsymbol{w}|\boldsymbol{x}', \mathcal{X}, \alpha, \beta) d\boldsymbol{w} =$
  $\int p(y|\boldsymbol{x}', \boldsymbol{w}, \mathcal{X}, \beta) p(\boldsymbol{w}|\boldsymbol{x}', \mathcal{X}, \alpha, \beta) d\boldsymbol{w} =$
  $\int p(y|\boldsymbol{x}', \boldsymbol{w}, \beta) p(\boldsymbol{w}|\mathcal{X}, \alpha, \beta) d\boldsymbol{w}$
  - $\{y\} \perp\!\!\!\perp \{\mathcal{X}\} \mid \{\boldsymbol{x}', \boldsymbol{w}, \beta\}$
    - $\{\boldsymbol{w}\} \perp\!\!\!\perp \{\boldsymbol{x}'\} \mid \{\mathcal{X}, \alpha, \beta\}$

Bayesian Estimation for Linear Regression (2/3)

- $y' = \arg_y \max \int p(y|\boldsymbol{x}', \boldsymbol{w}, \beta) p(\boldsymbol{w}|\mathcal{X}, \alpha, \beta) d\boldsymbol{w}$
  - $p(y|\boldsymbol{x}', \boldsymbol{w}, \beta) = \mathcal{N}(y|\boldsymbol{w}^\top \boldsymbol{x}', \beta^{-1})$
  - $p(\boldsymbol{w}|\mathcal{X}, \alpha, \beta) = p(\{r^{(t)}\}_t|\{\boldsymbol{x}^{(t)}\}_t, \boldsymbol{w}, \alpha, \beta) p(\boldsymbol{w}|\{\boldsymbol{x}^{(t)}\}_t, \alpha, \beta) = p(\{r^{(t)}\}_t|\{\boldsymbol{x}^{(t)}\}_t, \boldsymbol{w}, \beta) p(\boldsymbol{w}|\alpha)$
  - Let $\boldsymbol{r} = [r^{(1)}, \cdots, r^{(N)}]^\top$ and $\boldsymbol{X} = [\boldsymbol{x}^{(1)}, \cdots, \boldsymbol{x}^{(N)}]^\top \in \mathbb{R}^{N \times d}$, we have
    - $p(\{r^{(t)}\}_t|\{\boldsymbol{x}^{(t)}\}_t, \boldsymbol{w}, \beta) = p(\boldsymbol{r}|\boldsymbol{X}, \boldsymbol{w}, \beta) = \mathcal{N}(\boldsymbol{r}|\boldsymbol{X}\boldsymbol{w}, \beta^{-1}\boldsymbol{I})$
    - $p(\boldsymbol{w}|\alpha) = \mathcal{N}(\boldsymbol{w}|\boldsymbol{0}, \alpha^{-1}\boldsymbol{I})$
  - Notice that $p(\boldsymbol{r}|\boldsymbol{X}, \boldsymbol{w}, \beta)$ and $p(\boldsymbol{w}|\alpha)$ form a linear Gaussian model
    - $\boldsymbol{w}$ is the parent of $\boldsymbol{r}$ and the mean of $p(\boldsymbol{r}|\boldsymbol{X}, \boldsymbol{w}, \beta)$ is a linear combination of $\boldsymbol{w}$
  - Therefore, $p(\boldsymbol{w}|\mathcal{X}, \alpha, \beta) = p(\boldsymbol{w}|\boldsymbol{r}, \boldsymbol{X}, \alpha, \beta) = \mathcal{N}(\boldsymbol{w}|\beta\boldsymbol{\Sigma}\boldsymbol{X}^\top \boldsymbol{r}, \boldsymbol{\Sigma})$, where $\boldsymbol{\Sigma} = (\alpha\boldsymbol{I} + \beta\boldsymbol{X}^\top \boldsymbol{X})^{-1}$

Bayesian Estimation for Linear Regression (3/3)

- $y' = \arg_y \max \int p(y|\boldsymbol{x}', \boldsymbol{w}, \beta) p(\boldsymbol{w}|\mathcal{X}, \alpha, \beta) d\boldsymbol{w}$, where
  $p(y|\boldsymbol{x}', \boldsymbol{w}, \beta) = \mathcal{N}(y|(\boldsymbol{x}')^\top \boldsymbol{w}, \beta^{-1})$ and
  $p(\boldsymbol{w}|\mathcal{X}, \alpha, \beta) = \mathcal{N}(\boldsymbol{w}|\beta \boldsymbol{\Sigma} \boldsymbol{X}^\top \boldsymbol{r}, \boldsymbol{\Sigma})$
  - Again, $p(y|\boldsymbol{x}', \boldsymbol{w}, \beta)$ and $p(\boldsymbol{w}|\mathcal{X}, \alpha, \beta)$ form a linear Gaussian model
    - $\boldsymbol{w}$ is the parent of y and the mean of $p(y|\boldsymbol{x}', \boldsymbol{w}, \beta)$ is a linear combination of $\boldsymbol{w}$
  - We have
    $\int p(y|\boldsymbol{x}', \boldsymbol{w}, \beta) p(\boldsymbol{w}|\mathcal{X}, \alpha, \beta) d\boldsymbol{w} = \mathcal{N}(y|\beta (\boldsymbol{x}')^\top \boldsymbol{\Sigma} \boldsymbol{X}^\top \boldsymbol{r}, \frac{1}{\beta} + (\boldsymbol{x}')^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{x}')$
  - Finally, $y' = \beta (\boldsymbol{x}')^\top \boldsymbol{\Sigma} \boldsymbol{X}^\top \boldsymbol{r} = (\beta \boldsymbol{\Sigma} \boldsymbol{X}^\top \boldsymbol{r})^\top \boldsymbol{x}'$, where
    $\boldsymbol{\Sigma} = (\alpha \boldsymbol{I} + \beta \boldsymbol{X}^\top \boldsymbol{X})^{-1}$

Ancestral Sampling

- Given M random variables $X_1, X_2, \cdots, X_M$, we want to samples of these variables following their joint distribution $P(X_1, X_2, \cdots, X_M)$
  - How?

Ancestral Sampling

- Given M random variables $X_1, X_2, \cdots, X_M$, we want to samples of these variables following their joint distribution $P(X_1, X_2, \cdots, X_M)$
  - How?
- If we have a graph, we can draw sets of samples $\{x_1, x_2, \cdots, x_M\}$ one-by-one, each by:
  1. Sample nodes X's having no parent by following the corresponding $P(X)$
  2. Repeat: sample each child node X whose parents are all sampled by following $P(X|parent(X))$ with parents set to their sampled values
- We call this ***ancestral sampling***

Evidence

Gibbs Sampling (1/2)

- In statistics, *Gibbs sampling* is a *Markov chain Monte Carlo* (MCMC) algorithm for obtaining a sequence of observations which are approximately from a specified multivariate probability distribution (i.e. from the joint probability distribution of two or more random variables), when direct sampling is difficult.
- Suppose we want to obtain M samples of $\mathbf{X} = \{X_1, \ldots, X_N\}$ from a joint distribution $P(X_1, \ldots, X_N)$. Denote the ith sample by $\mathbf{X}^{(i)} = \left\{X_1^{(i)}, \ldots, X_N^{(i)}\right\}$. The sampling process is:
  1. Begin with some initial value $\mathbf{X}^{(0)}$ for each variable.
     1. For each sample $i = \{1, \ldots, M\}$, sample each variable $X_n^{(i)}$ from the conditional distribution $P\left(X_n | X_1^{(i)}, \ldots, X_{n-1}^{(i)}, X_{n+1}^{(i-1)}, \ldots, X_N^{(i-1)}\right)$.
        - That is, sample each variable from the distribution of that variable conditioned on all other variables, making use of the most recent values and updating the variable with its new value as soon as it has been sampled.
     1. The samples then approximate the joint distribution of all variables.

Gibbs Sampling (2/2)

- Why does it work?
  - Why does it update only a word-topic assignment at a time?

Why sample?

- Suppose the Bayesian network has variables $\mathbf{Y}$, whose values are observed, and variables $\mathbf{X}$, whose values are not known.
  - $\mathbf{X}$ include any parameters we want to estimate.
    - The goal is to compute the expected value of some function f:

$$\mathrm{E}[f|\mathbf{Y}=\mathbf{y}] = \sum_{\mathbf{x}} f(\mathbf{x},\mathbf{y}) P(\mathbf{X}=\mathbf{x}|\mathbf{Y}=\mathbf{y})$$

    - Suppose we can produce n samples $\mathbf{x}^{(t)}$, where $\mathbf{X}^{(t)} \sim P(\mathbf{X})$. Then we can estimate

$$\mathrm{E}[f|\mathbf{Y}=\mathbf{y}] = \frac{1}{n}\sum_{t=1}^{n} f\left(\mathbf{x}^{(t)},\mathbf{y}\right).$$

    - In what follows, everything is conditioned on $\mathbf{Y}=\mathbf{y}$, so we take $P(\mathbf{X})$ to mean $P(\mathbf{X}|\mathbf{Y}=\mathbf{y})$.

Markov Chains

- A (first-order) *Markov chain* is a distribution over random variables $\mathcal{S}^{(0)}, \ldots, \mathcal{S}^{(n)}$ all ranging over the same state space $\mathcal{S}$, where

$$P\left(\mathcal{S}^{(0)}, \ldots, \mathcal{S}^{(n)}\right) = P\left(\mathcal{S}^{(0)}\right) \prod_{t=0}^{n-1} P\left(\mathcal{S}^{(t+1)} | \mathcal{S}^{(t)}\right).$$

  - A Markov chain is homogeneous or time-invariant iff

$$P\left(\mathcal{S}^{(t+1)} = s' | \mathcal{S}^{(t)} = s\right) = \mathbf{P}_{s',s} \text{ for all } t, s, s'.$$

    - The matrix $\mathbf{P}$ is called the *transition probability matrix* (tpm) of the Markov chain.
    - If $P\left(\mathcal{S}^{(t)} = s\right) = \pi_s^{(t)}$ (i.e., $\boldsymbol{\pi}^{(t)}$ is a vector of state probabilities at time t), then
    - $\boldsymbol{\pi}^{(t+1)} = \mathbf{P}\boldsymbol{\pi}^{(t)}$
    - $\boldsymbol{\pi}^{(t)} = \mathbf{P}^t\boldsymbol{\pi}^{(0)}$

Ergodicity

- A Markov chain with tpm $\mathbf{P}$ is *ergodic* iff there is a positive integer m s.t. all elements of $\mathbf{P}^m$ are positive (i.e., there is an m-step path between any two states).

Theorem

For each homogeneous ergodic Markov chain with tpm $\mathbf{P}$, there is a unique limiting distribution $D_{\mathbf{P}}$, i.e., as N approaches infinity, the distribution converges on $D_{\mathbf{P}}$.

- *$D_{\mathbf{P}}$ is called the stationary distribution of the Markov chain.*

Use a Markov Chain for Inference of $P(\mathbf{X})$

1. Set the state space $\mathcal{S}$ of the Markov chain to the range of $\mathbf{X}$ ($\mathcal{S}$ may be astronomically large).
2. Find a tpm $\mathbf{P}$ such that $P(\mathbf{X}) \sim D_{\mathbf{P}}$.
    1. Run the Markov chain:
        1. Pick $\mathbf{x}^{(0)}$ somehow.
        2. For $t = 0, \ldots, N-1$, sample $\mathbf{x}^{(n+1)}$ from $P\left(\mathbf{X}^{(n+1)} | \mathbf{X}^{(n)} = \mathbf{x}^{(n)}\right)$.
        3. After discarding the first burn-in samples, use remaining samples to calculate statistics.

Why Does the Gibbs Sampling Work?

- The tpm of the Gibbs sampler for $P(\mathbf{X})$ where $\mathbf{X} = \{X_1, \ldots, X_N\}$ is $\mathbf{P} = \prod_{j=1}^{N} \mathbf{P}^{(j)}$,

$$\mathbf{P}^{(j)}_{\mathbf{x}',\mathbf{x}} = \begin{cases} 0 & \text{if } \mathbf{x}'_{-j} \neq \mathbf{x}_{-j} \\ P\left(X_j = x'_j | \mathbf{X}_{-j} = \mathbf{x}_{-j}\right) & \text{if } \mathbf{x}'_{-j} = \mathbf{x}_{-j} \end{cases}$$

  - The subscript $-j$ denotes all but the jth element.
    - Informally, the Gibbs sampler cycles through each of the variables X_j, replacing the current value x_j with a sample from $P\left(X_j | \mathbf{X}_{-j} = \mathbf{x}_{-j}\right)$.
    - If $\mathbf{x}$ is a sample from $P(\mathbf{X})$, then so is $\mathbf{x}'$, since $\mathbf{x}'$ differs from $\mathbf{x}$ only by replacing x_j with a sample from $P\left(X_j | \mathbf{X}_{-j} = \mathbf{x}_{-j}\right)$.
    - Since $\mathbf{P}^{(j)}$ maps samples from $P(\mathbf{X})$ to samples from $P(\mathbf{X})$, so does $\mathbf{P}$. Thus, $P(\mathbf{X})$ is a stationary distribution for $\mathbf{P}$.

Outline

Evaluating $P(X_i)$s in a Chain (1/2)

- Problem: to evaluate $P(X_i)$ of ***every*** node X_i in a chain:

  - We can evaluate $P(X_i)$ one-by-one
  - No problem if nodes are continuous and $p(X_i) = \int_{X_{j,j\neq i}} p(X_1, \cdots, X_i, \cdots, X_M)$ can be written as a closed form (e.g., by assuming a linear Gaussian model)
  - Time consuming for discrete variables though, since $P(X_i) = \sum_{\{X_j:,j\neq i\}} P(X_1)P(X_2|X_1), \cdots, P(X_i|X_{i-1}), P(X_{i+1}|X_i), \cdots, P(X_M|X_{M-1})$
    - Assuming that each node has K states, we have time complexity: $O(K^{M-1})$ for each node, $O(MK^{M-1})$ in total

Evaluating $P(X_i)$s in a Chain (2/2)

- Improvement for discrete variables?

Evaluating $P(X_i)$s in a Chain (2/2)

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  - Observer that when computing $P(X_i)$ and $P(X_j)$, $i \neq j$, most conditional probabilities $P(X_{k+1}|X_k)$, $1 \leqslant k \leqslant M-1$, are computed twice
    - It is plausible that we can "reuse" these conditional probabilities to reduce time complexity
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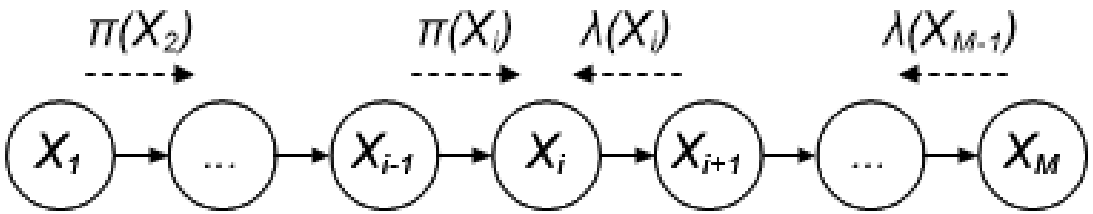
    - It is plausible that we can "reuse" these conditional probabilities to reduce time complexity
  - How?
  - One way is to precompute all $P(X_{k+1}|X_k)$s, $1 \leqslant k \leqslant M-1$, and then look up these results to obtain $P(X_i)$s
  - Still exponential to M in time complexity

Belief Propagation along a Chain (1/3)

- Notice that $P(X_i) = \sum_{X_1, X_M} P(X_1, X_i, X_M) = \sum_{X_1, X_M} P(X_1, X_M | X_i) P(X_i) = \sum_{X_1, X_M} P(X_1 | X_i) P(X_M | X_i) P(X_i) = \sum_{X_1, X_M} \frac{P(X_i | X_1) P(X_1)}{P(X_i)} P(X_M | X_i) P(X_i) = \sum_{X_1, X_M} \alpha(X_1) \pi(X_i) \lambda(X_i)$
  - $\pi(X_i) = P(X_i | X_1)$ if $i > 1$, and $\pi(X_1) = P(X_1)$
    - $\lambda(X_i) = P(X_M | X_i)$ if $i < M$, and $\lambda(X_M) = 1$
    - $\alpha(X_1) = P(X_1) = \pi(X_1)$ is independent with X_i
  - In addition, $\pi(X_i) = P(X_i | X_1) = \sum_{X_{i-1}} P(X_i, X_{i-1} | X_1) = \sum_{X_{i-1}} P(X_i | X_{i-1}, X_1) P(X_{i-1} | X_1) = \sum_{X_{i-1}} P(X_i | X_{i-1}) P(X_{i-1} | X_1) = \sum_{X_{i-1}} P(X_i | X_{i-1}) \pi(X_{i-1})$
- $\lambda(X_i) = P(X_M | X_i) = \sum_{X_{i+1}} P(X_M | X_{i+1}, X_i) P(X_{i+1} | X_i) = \sum_{X_{i+1}} P(X_M | X_{i+1}) P(X_{i+1} | X_i) = \sum_{X_{i+1}} P(X_{i+1} | X_i) \lambda(X_{i+1})$

Belief Propagation along a Chain (2/3)

- $P(X_i) = \sum_{X_1, X_M} \alpha(X_1, X_M)\pi(X_i)\lambda(X_i)$
  - $\pi(X_{i+1}) = \sum_{X_i} P(X_{i+1}|X_i)\pi(X_i)$ for $1 \leqslant i \leqslant M-1$
    - $\lambda(X_{i-1}) = \sum_{X_i} P(X_i|X_{i-1})\lambda(X_i)$ for $2 \leqslant i \leqslant M$



- Starting from X_1 till X_{M-1}, each node X_i can forward all $\pi(X_{i+1})$s downward along to chain upon receiving $\pi(X_i)$s from its parent
- Starting from X_M till X_2, each node X_i forwards all its $\lambda(X_{i-1})$s upward along to chain upon upon receiving $\lambda(X_i)$s from its child
- After receiving both $\pi(X_i)$s and $\lambda(X_i)$s from its parent and child respectively, each node X_i can compute $P(X_i)$
  - Note that $\alpha(X_1)$s can be broadcasted to all nodes by X_1 parallel to the above propagations

Belief Propagation along a Chain (3/3)

- The task of evaluating all $P(X_i)$s is now divided into local computation of πs and λs and exchange of these local results
  - We call the inference using this message-passing style as ***belief propagation***
  - Time complexity?

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  - Time complexity?
    - $O(MK^2 + K^2)$ for each node ($O(MK^2)$ for message exchange and $O(K^2)$ for computing $P(X_i)$)
    - $O(MK^2 + MK^2)$ ***in total***, provided that each node X_i stores its intermediate messages (i.e., $\pi(X_i)$s and $\lambda(X_i)$s)
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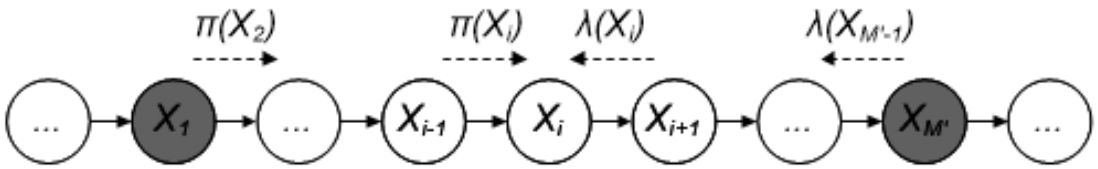
  - Space complexity?
    - $O(K^2)$ on each node X_i (for $P(X_{i+1}|X_i)$s, $P(X_i|X_{i-1})$s, $\pi(X_i)$s, and $\lambda(X_i)$s)
    - $O(MK^2)$ totally

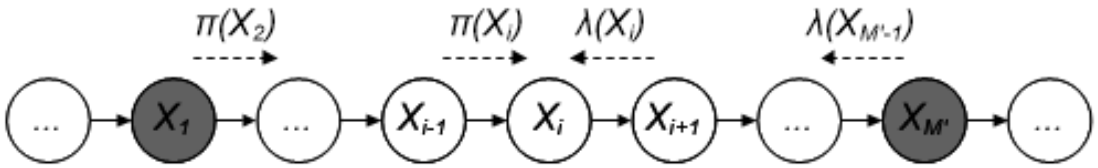
Evidences (1/2)

- What if we are given an evidence E?
  - Without loss of generality, let's consider a chain from X_1 to $X_{M'}$, where $\{X_1, X_{M'}\} \subseteq E$, as below:



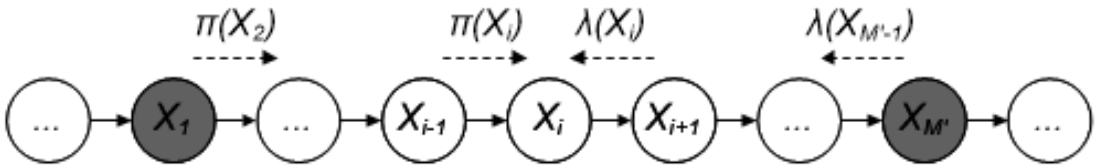
  - Problem: to evaluate $P(X_i)$ for $2 \leqslant i \leqslant M' - 1$
  - $P(X_i|E) = P(X_i|X_1, X_{M'}) = \frac{P(X_i, X_1, X_{M'})}{P(X_1, X_{M'})} = \alpha(X_1, X_{M'})\pi(X_i)\lambda(X_i)$
    [Proof]
    - $\pi(X_i) = P(X_i|X_1)$ if $i > 1$, and $\pi(X_1) = P(X_1)$
    - $\lambda(X_i) = P(X_{M'}|X_i)$ if $i < M'$, and $\lambda(X_{M'}) = 1$
    - $\alpha(X_1, X_{M'}) = \frac{P(X_1)}{P(X_1, X_{M'})} = \frac{P(X_1)}{P(X_{M'}|X_1)P(X_1)} = \frac{1}{\pi(X_{M'})} = \frac{1}{\lambda(X_1)}$ is independent with X_i

Evidences (2/2)



- Belief propagation is still applicable except that there is only one $\pi(X_{M'})$ and one $\lambda(X_1)$
  - $\alpha(X_1, X_{M'})$ can be broadcasted to all nodes by $X_{M'-1}$ once it computes $\pi(X_{M'})$ (or by X_2 once it computes $\lambda(X_1)$)
  - Time/space complexity?

Evidences (2/2)

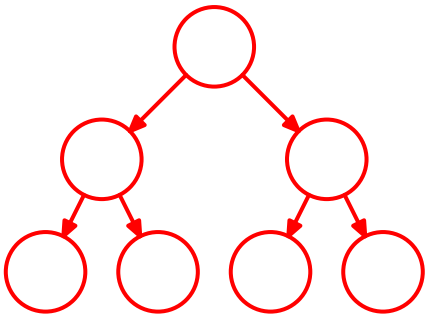


- Belief propagation is still applicable except that there is only one $\pi(X_{M'})$ and one $\lambda(X_1)$
  - $\alpha(X_1, X_{M'})$ can be broadcasted to all nodes by $X_{M'-1}$ once it computes $\pi(X_{M'})$ (or by X_2 once it computes $\lambda(X_1)$)
  - Time/space complexity? Still $O(M'K^2)$ in both time and space
  - If either X_1 or $X_{M'}$ is unobserved, we have either K $\lambda(X_1)$ or K $\pi(X_{M'})$ messages respectively

Outline

Trees

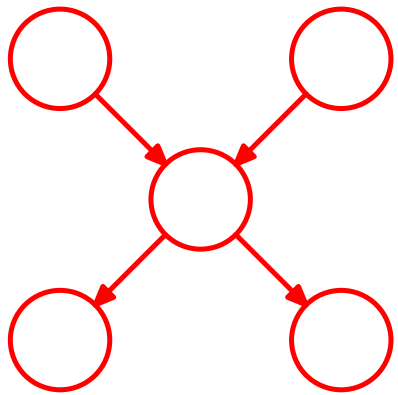
- We have seen that exact inference on a chain of nodes can be performed efficiently.
  - More generally, inference can be performed efficiently using local message passing on a broader class of graphs called *trees*.



- In an undirected graph, a tree is defined as a graph in which there is one, and only one, path between any pair of nodes.
- In the case of directed graphs, a tree is defined such that there is a single node, called the *root*, which has no parents, and all other nodes have one parent.
  - Note that the moralization step will not add any links as all nodes have at most one parent.

Polytree

- If there are nodes in a directed graph that have more than one parent, but there is still only one path between any two nodes, then the graph is called a *polytree*.
  - Such a graph will have more than one node with the property of having no parents, and furthermore, the corresponding moralized undirected graph will have loops.



Topic Model

- Topic modeling is a method for analyzing large quantities of unlabeled data.
  - For our purposes, a *topic* is a probability distribution over a collection of words and a *topic model* is a formal statistical relationship between a group of observed and latent (unknown) random variables that specifies a probabilistic procedure to generate the topics—a generative model.
    - The central goal of a topic is to provide a "thematic summary" of a collection of documents.

An Example

- Given 2 documents D_1, D_2 with words
  - $D_1 = \{\text{cat, dog, bird, fish}\}$
    - $D_2 = \{\text{car, bike, bus}\}$
    - We can discover the "topics" (pet, vehicle, ...).
    - A document may have one or more topics in practice.

Latent Dirichlet Allocation

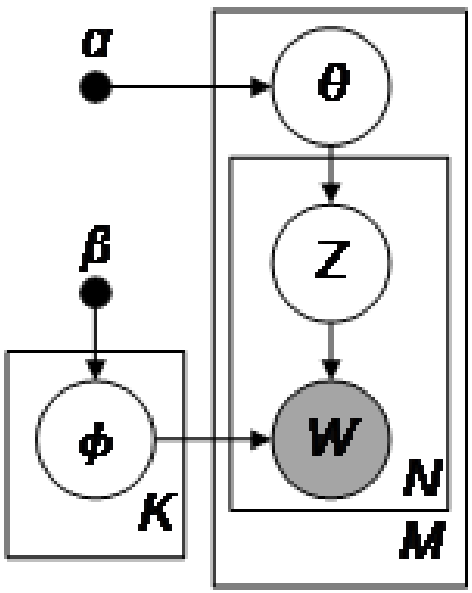
- *Latent Dirichlet allocation* (LDA) is the most common topic model currently in use, allowing documents to have a mixture of topics.
  - LDA provides a generative model that describes how the documents in a corpus were created.

Notation and Terminology

- A *word* is the basic unit of discrete data, defined to be an item from a vocabulary $\{w^1, \ldots, w^V\}$.
  - A *document* D_i is a sequence of N words denoted by $\mathbf{w}_i = (w_{i,1}, w_{i,2}, \ldots, w_{i,N})$, where $w_{i,n}$ is the nth word in the sequence.
    - A *corpus* is a collection of M documents denoted by $D = \{\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_M\}$.

The Generative Process

- Assume we know K topic distributions for our corpus, meaning K categoricals containing V elements each.



1. Choose the topic distribution $\theta_i \sim \text{Dir}(\alpha)$ for each document D_i where $i \in \{1, \ldots, M\}$ (θ_i is a categorical of length K).
2. Choose the word distribution $\Phi_k \sim \text{Dirichlet}(\beta)$ for each topic where $k \in \{1, \ldots, K\}$ (Φ_k is a vector of length V).
   - β is a V-dimension vector of positive reals.
   a. For each of the words $w_{i,n}$ where $j \in \{1, \ldots, N_i\}$:
      1. Choose a topic $z_{i,n} \sim \text{Categorical}(\theta_i)$.
      2. Choose a word $w_{i,n} \sim \text{Categorical}(\Phi_{z_{i,n}})$.

Our Goal

- Given α, β, and document D_i with word sequence $\mathbf{w}_i$, what are the most probable values for $\mathbf{z}_i$ and θ_i?

Our Goal

- Given α, β, and document D_i with word sequence $\mathbf{w}_i$, what are the most probable values for $\mathbf{z}_i$ and θ_i?
  - A simple approach is to maximize the log likelihood. First we write

$$P(\theta_i, \mathbf{z}_i | \mathbf{w}_i, \alpha, \beta) = \frac{P(\theta_i, \mathbf{z}_i, \mathbf{w}_i | \alpha, \beta)}{P(\mathbf{w}_i | \alpha, \beta)}.$$

    - By definitions, we have

$$P(\mathbf{w}_i | \alpha, \beta) = \int P(\theta_i | \alpha) \left(\prod_{n=1}^{N} \sum_{z_{i,n}=1}^{K} P(z_{i,n} | \theta_i) P\left(\Phi_{z_{i,n}} | \beta\right) P\left(w_{i,n} | \Phi_{z_{i,n}}\right) \right)$$

$$= \int P(\theta_i | \alpha) \left(\prod_{n=1}^{N} \sum_{k=1}^{K} P(\Phi_k | \beta) \prod_{j=1}^{V} \left(\theta_{i,k} \phi_{k,w_{i,n}}\right) \right) d\theta$$

    - Maximizing the log likelihood is intractable due to the summation over latent topics.

Gibbs Sampling for LDA (1/3)

- In LDA, the distribution of the topics $\mathbf{Z}$ for words $\mathbf{W}$ is unknown and $\mathbf{Z}$ is multivariate.
  - Hence, the Gibbs sampling procedure boils down to estimate

$$P\left(Z_{i,n} = t | \mathbf{z}_{-i,n}, \mathbf{w}\right).$$

    - Here, θ, ϕ are integrated out. If we know the exact $\mathbf{Z}_i$ for each document D_i, it's trivial to estimate θ_i and ϕ_i.
    - We have

$$\begin{aligned} P\left(Z_{i,n} = t | \mathbf{z}_{-i,n}, \mathbf{w}, \alpha, \beta\right) & \\ \propto P\left(Z_{i,n} = t, \mathbf{z}_{-i,n}, \mathbf{w}, \alpha, \beta\right) & \\ = P\left(w_{i,n} | Z_{i,n} = t, \mathbf{z}_{-i,n}, \mathbf{w}_{-i,n}, \beta\right) P\left(Z_{i,n} = t | \mathbf{z}_{-i,n}, \mathbf{w}_{-i,n}, \alpha\right) & \\ = P\left(w_{i,n} | Z_{i,n} = t, \mathbf{z}_{-i,n}, \mathbf{w}_{-i,n}, \beta\right) P\left(Z_{i,n} = t | \mathbf{z}_{-i,n}, \alpha\right) & \end{aligned}$$

Gibbs Sampling for LDA (2/3)

- For the first term, we have

$$P(w_{i,n}|Z_{i,n}=t,\mathbf{z}_{-i,n},\mathbf{w}_{-i,n},\beta) = \int P(w_{i,n}|Z_{i,n}=t,\phi_t)\,P(\phi_t|\mathbf{z}_{-i,n},\mathbf{w}_{-i,n},\beta)\,d\phi_t$$

$$P(\phi_t|\mathbf{z}_{-i,n},\mathbf{w}_{-i,n},\beta) = \frac{P(\mathbf{w}_{-i,n}|\phi_t,\mathbf{z}_{-i,n})\,P(\phi_t|\beta)}{P(\mathbf{w}_{-i,n}|\mathbf{z}_{-i,n},\beta)} \sim \text{Dirichlet}\left(\beta+\mathbf{N}_t^{-i,n(w)}\right)$$

  - Here, $\mathbf{N}_t^{-i,n(w)}$ is a V-dimension vector and $\mathbf{N}_{t,v}^{-i,n(w)}$ is the number of instances of the v-th word in the vocabulary assigned to topic t in document D_i, excluding the instance $w_{i,n}$. Recall that the Dirichlet is the conjugate prior for the multinomial. Thus, the posterior is also Dirichlet.
    - Using the property of Dirichlet-multinomial distribution, we have

$$P(w_{i,n}|Z_{i,n}=t,\mathbf{z}_{-i,n},\mathbf{w}_{-i,n},\beta) = \frac{\Gamma\left(\sum_v\left(\beta_v+\mathbf{N}_{t,v}^{-i,n(w)}\right)\right)}{\Gamma\left(1+\sum_v\left(\beta_v+\mathbf{N}_{t,v}^{-i,n(w)}\right)\right)}\left(\frac{\Gamma\left(\mathbf{N}_{t,w_{i,n}}^{-i,n(w)}+\beta_{w_{i,n}}+1\right)}{\Gamma\left(\mathbf{N}_{t,w_{i,n}}^{-i,n(w)}+\beta_{w_{i,n}}\right)}\right) = \frac{\mathbf{N}_{t,w_{i,n}}^{-i,n(w)}+\beta_{w_{i,n}}}{\sum_v\left(\mathbf{N}_{t,v}^{-i,n(w)}+\beta_v\right)}.$$

Gibbs Sampling for LDA (3/3)

- Similarly, for the second term, we have

$$P(Z_{i,n} = t|\mathbf{z}_{-i,n}, \boldsymbol{\alpha}) = \int P(Z_{i,n} = t|\theta_i) P(\theta_i|\mathbf{z}_{-i,n}, \boldsymbol{\alpha}) d\theta_i$$

$$P(\theta_i|\mathbf{z}_{-i,n}, \boldsymbol{\alpha}) \propto P(\mathbf{z}_{-i,n}|\theta_i) P(\theta_i|\boldsymbol{\alpha})$$
$$\sim \text{Dirichlet}\left(\boldsymbol{\alpha} + \mathbf{N}^{-i,n(z)}\right)$$

where $\mathbf{N}^{-i,n(z)}$ is a K-dimension vector and $\mathbf{N}_k^{-i,n(z)}$ is the number of words assigned to topic k in document D_i, excluding the instance $z_{i,n}$.

- Then, we have

$$P(Z_{i,n} = t|\mathbf{z}_{-i,n}, \boldsymbol{\alpha}) = \frac{\mathbf{N}_t^{-i,n(z)} + \boldsymbol{\alpha}_t}{\sum_k \left(\mathbf{N}_k^{-i,n(z)} + \boldsymbol{\alpha}_k\right)}.$$

- Thus,

$$P(Z_{i,n} = t|\mathbf{z}_{-i,n}, \mathbf{w}, \boldsymbol{\alpha}, \boldsymbol{\beta}) \propto \frac{\mathbf{N}_{t,w_{i,n}}^{-i,n(w)} + \beta_{w_{i,n}}}{\sum_v \left(\mathbf{N}_{t,v}^{-i,n(w)} + \beta_v\right)} \times \frac{\mathbf{N}_t^{-i,n(z)} + \boldsymbol{\alpha}_t}{\sum_k \left(\mathbf{N}_k^{-i,n(z)} + \boldsymbol{\alpha}_k\right)}.$$

Estimate ϕ and θ

- To obtain ϕ and θ, we can simply calculate

$$\phi_{k,v} = \frac{n_v^{(k)} + \beta_v}{\sum_{j=1}^{V} \left(n_j^{(k)} + \beta_j \right)}$$

$$\theta_{i,k} = \frac{n_k^{(i)} + \alpha_k}{\sum_{t=1}^{K} \left(n_t^{(i)} + \alpha_t \right)}$$

where $n_j^{(k)}$ is the frequency of word w^j in the vocabulary assigned to topic k, and $n_t^{(i)}$ is the number of words assigned to topic t in document D_i.