# Probabilistic Modeling and Reasoning

Traiko Dinev <traiko.dinev@gmail.com>

July 7, 2019

*NOTE: This partially follows Probabilistic Modeling and Reasoning, a masters level course at the University of Edinburgh.*

*NOTE: Note this "summary" is NOT a reproduction of the course materials nor is it copied from the corresponding courses. It was entirely written and typeset from scratch.*



## 1 Probability Identities

Non-exhaustive list of identities useful for the rest of this cheatsheet:

$$\mathrm{P}(A, B) = \mathrm{P}(A \mid B)\ \mathrm{P}(B) \qquad \text{product rule}$$

$$\mathrm{P}(A) = \sum_B \mathrm{P}(A \mid B)\ \mathrm{P}(B) = \sum_B \mathrm{P}(A, B) \qquad \text{sum rule}$$

$$x \perp\!\!\!\perp y \iff \mathrm{P}(x, y) = \mathrm{P}(x)\ \mathrm{P}(y)$$

$$x_1 \perp\!\!\!\perp x_2 \perp\!\!\!\perp, \ldots, x_N \iff \mathrm{P}(x1, \ldots, x_N) = \prod_i \mathrm{P}(x_i)$$

We can store discrete distributions as tables of data. Conditional independece allows us to save space. Consider the conditional independence rules first:

$$\mathrm{P}(x, y \mid z) = \mathrm{P}(x \mid z)\ \mathrm{P}(y \mid z) \iff x \perp\!\!\!\perp y \mid z$$

$$\mathrm{P}(x \mid y, z) = \mathrm{P}(x \mid z)$$

Then to store $\mathrm{P}(x, y, z) = \mathrm{P}(x)\mathrm{P}(y)\mathrm{P}(z)$ we would need $dim(x) \times dim(y) \times dim(z)$ space. If they are all equal this means $k^{3d} - 1$ entries. The factorization allows us to have $3(k^d - 1)$ entries instead.

## 2 Directed Graphical Models

From the chain rule, we can factorize any distribution as:

$$\mathrm{P}(\mathbf{x}) = \prod_i \mathrm{P}(x_i \mid \pi_i), \quad \pi_i = \{x_1, \ldots, x_{i-1}\}$$

We can prove that the following holds true by induction:

$$\mathrm{P}(\mathbf{x}) = \prod_i \mathrm{P}(x_i \mid \pi_i) \iff x_i \perp\!\!\!\perp (\mathrm{pre}_i \setminus \pi_i) \mid \pi_i,\ \forall i$$

where $\pi_i$ is some subset of elements. This is to say that the factorization implies independence and a set of independences implies a factorization.

Thus we can visualize a distribution by drawing a DAG (directed acyclic graph) where the parents are the above $\pi_i$'s. Thus if:

$$\mathrm{P}(\mathbf{x}) = \mathrm{P}(x_1)\ \mathrm{P}(x_2)\ \mathrm{P}(x_3 \mid x_1, x_2)\ \mathrm{P}(x_4 \mid x_3)\ \mathrm{P}(x_5 \mid x_2)$$

then the DAG is in Figure 1.

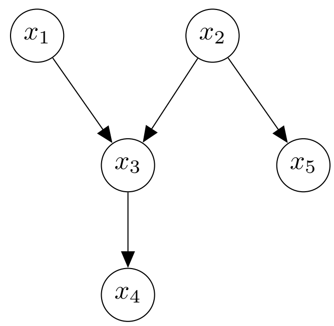



Figure 1: Simple DAG

A graph can be generated from a distribution and a (topological) ordering of the elements. A topological ordering is one where the parents come before the children. Note that different orderings may generate different graphs.

## 2.1 Examples

**Markov Models** (of order 1) or chains are a series of serial connections (Figure 2).

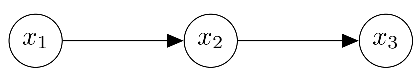



Figure 2: Markov Chain

**Hidden Markov Models** contain a markov chain that is not observed. Each hidden **h** influences an observable. **x**'s are often at different timesteps, making the chain represent a time series. Figure 3.

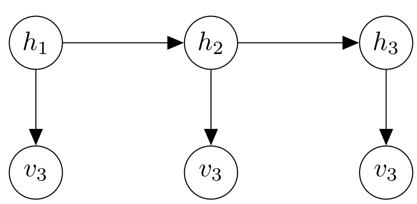



Figure 3: Hidden Markov Model

**Probabilistic PCA/ Independent Component Analysis** are methods that both use tha same graphical model. Here the latents (hiddens) variables are not connected. At the same time they influence all of the observables. Figure 4

## 2.2 D-Separation

The main reason for using graphical models is to more easily determinite independencies between variables. In a DAG a tool for using this is D-separation. We start by examining the three possible trail connections in a DAG.

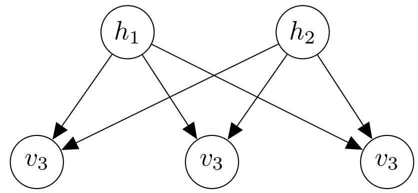



Figure 4: PPCA/ ICA graphical model

Note that these are not all possible connections between three elements, but rather *all possible connections when following a trail*.

**Serial Connections** are like Markov chains.

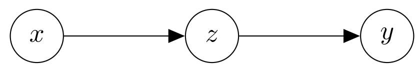



Figure 5: Serial Connecton

Importantly we have:

$$\mathrm{P}(x, z, y) = \mathrm{P}(x)\mathrm{P}(z \mid x)\mathrm{P}(y \mid z)$$
$$x \perp\!\!\!\perp y \mid z \qquad x \not\perp\!\!\!\perp y$$

This means that if we know the variable $z$, x and y, **and all their parents and children** that are not connected to $z$ are independent of each other.

**Diverging Connections**

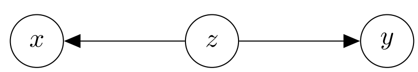



Figure 6: Diverging Connecton

The same property of independence holds true here:

$$\mathrm{P}(x, z, y) = \mathrm{P}(z)\mathrm{P}(x \mid z)\mathrm{P}(y \mid z)$$
$$x \perp\!\!\!\perp y \mid z \qquad x \not\perp\!\!\!\perp y$$

**Converging Connections (Colliders)**

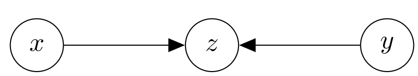



Figure 7: Collider

For colliders if we **do not know** $z$, $x$ and $y$ are independent:

$$\mathrm{P}(x, z, y) = \mathrm{P}(z)\mathrm{P}(x \mid z)\mathrm{P}(y \mid z)$$
$$x \perp\!\!\!\perp y \qquad x \not\perp\!\!\!\perp y \mid z$$

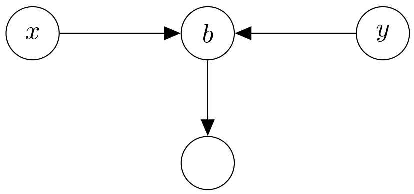
This is true since $\mathrm{P}(\cdot) =$...

**D-Separation** Sets $X$ and $Y$ are d-separated by $Z$ iff all trails are blocked by $Z$. One of the following needs to be true for a trail to be blocked:

**1)** Either $b$ is in a head-tail or tail-tail configuration


and $b$ is in $Z$.

**2)** $b$ is a part of a collider




and neither b or its descendents are in $z$. **Then** $X \perp\!\!\!\perp Y \mid Z$.

## 2.3 I-Maps

A graph is an I-map for a set of independencies $I$ iff all independencies asserted by the graph are part of $I$. A graph can thus have fewer independencies than the set. A fully-connected graph is a trivial I-map for all sets $I$.

## 2.4 Directed Local Markov Property

$$\mathbf{x}_i \perp\!\!\!\perp (\mathrm{pre}_i \setminus \mathrm{pa}_i) \mid \mathrm{pa}_i \leftrightarrow \mathbf{x}_i \perp\!\!\!\perp (\mathrm{nondesc}(\mathbf{x}_i) \setminus \mathrm{pa}_i) \mid \mathrm{pa}_i$$

This [todo] figure.

## 2.5 Gloabl directed Markov Property

All independencies asserted by D-separation.

## 2.6 Markov Blanket

By definition:

$$x \perp\!\!\!\perp (\mathrm{all} \setminus \mathbf{x} \setminus \mathrm{MB}(\mathbf{x})) \mid \mathrm{MB}(\mathbf{x})$$

And for DAGs we get:

$$\mathrm{MB}(\mathbf{x}) = \mathrm{pa}(\mathbf{x}) \;\cup\; \mathrm{children}(\mathbf{x}) \;\cup\; \text{co-parents}(\mathbf{x})$$

# 3 Undirected Graphical Models

Firstly, we note the following. For non-negative functions $a$ and $b$:

$$x \perp\!\!\!\perp y \mid z \leftrightarrow \mathrm{P}(x,y,z) = a(x,z) \times b(y,z)$$
$$x \perp\!\!\!\perp y \leftrightarrow \mathrm{P}(x,y) = a(x) \times b(y)$$
$$\sum_{x,y,z} a(x,z)b(y,z) = 1$$
$$\textbf{if } p(x,y,z) = \frac{1}{Z}\phi_A(x,z)\phi_B(y,z), \quad Z = \sum_{x,y,z} \phi_A(x,z)\phi_B(y,z)$$

## 3.1 Gibbs Distribution

.. is a distribution that factorizes as:

$$\mathrm{P}(\mathbf{x}) = \frac{1}{Z}\prod_c \phi_C(\mathcal{X}_C), \qquad \mathcal{X}_C \subseteq \{x_1, \ldots, x_d\}$$

## 3.2 Energy-Based Model

If in the above $\phi_C(\mathcal{X}_C) = \exp(-\mathrm{E}_c(\mathcal{X}_c))$. Then:

$$\mathrm{P}(\mathbf{x}) = \frac{1}{Z} = \frac{1}{Z} exp\Big[-\sum_c \mathrm{E}_c(\mathcal{X}_c)\Big] = \frac{1}{Z}\prod_c \underbrace{\exp^{-\mathrm{E}_c(\mathcal{X}_c)}}_{\phi_c(\mathcal{X}_c)}$$

## 3.3 Undirected Graphs

Assuming a distribution (up to a constant) factorizes as:

$$\mathrm{P}(\mathbf{x}) \propto \phi_1(x_1,x_2,x_3)\phi_2(x_2,x_3,x_4)\phi_3(x_3,x_5)\phi_4(x_5,x_6)$$

then we visualize it as the following graph:

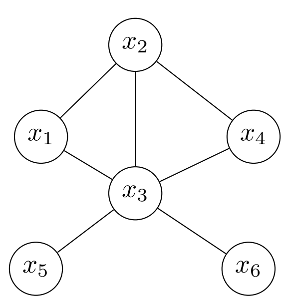



Figure 8: Undirected Graph

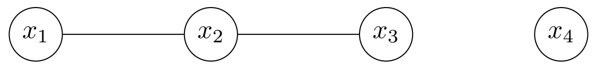
We form cliques for all variables in each factor $\phi_i$.

### 3.4 Independencies in Undirected Models

If

$$\mathrm{P}(\mathbf{x}) \propto \phi_1(x_1, x_2)\phi_2(x_2, x_3)\phi_3(x_4)$$

Then the corresponding graph is:




This directly implies that

$$x_4 \perp\!\!\!\perp x_1, x_2, x_3$$
$$x_1 \perp\!\!\!\perp x_3 \mid x_2$$

In other words, a trail is blocked if there are no paths between the two nodes. Thus D-separation is more easily done here.

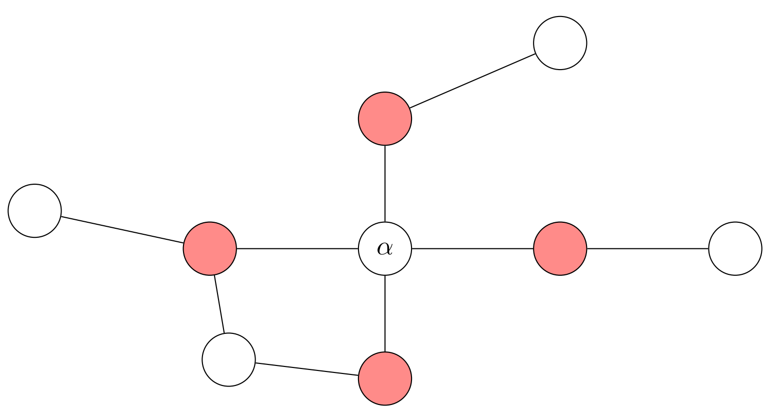
### 3.5 Graph → Distribution

Since we built undirected graphs by connecting cliques, it follows that given a graph we look at the maximum cliques to recover the distribution. **I-maps** are defined as before.

### 3.6 Local Markov Property

An edge is independent of all other edges given its neighbors. In the below graph the neighbors are colored in red. Formally, if $\mathrm{ne}(\alpha)$ are the neighbors of $\alpha$, then:

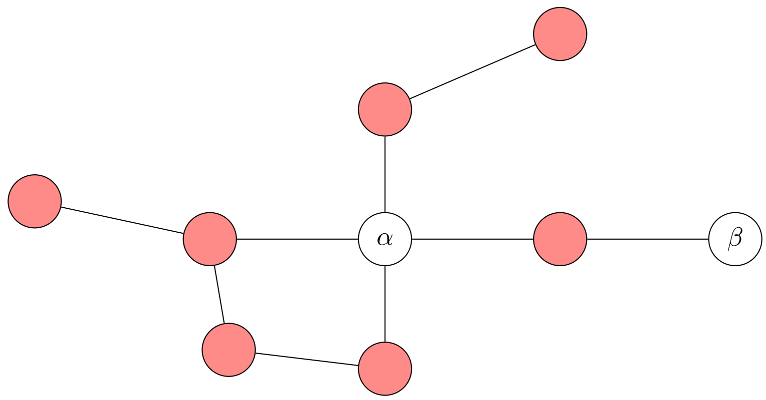
$$\alpha \perp\!\!\!\perp X \setminus (\alpha \ \cup \ \mathrm{ne}(\alpha)) \mid \mathrm{ne}(\alpha), \quad \forall \alpha \in X$$




### 3.7 Pairwise Markov Property

$$\alpha \perp\!\!\!\perp \beta \mid \underbrace{X}_{\text{all nodes}} \setminus \{\alpha, \beta\}$$

for all non-neighboring $\alpha, \beta \in X$.




### 3.8 Markov Blanket

For undirected graph, the markov blanket of $x$ is the neighbors of $x$.

| |
|---|
| N.B. All of the above properties (Markov properties) are equivalent for both directed and undirected graphical models. This means if one of them is true **for a distribution**, then all of them are true. |

**TODO: Add Bishop plots with repetition boxes.**

### 3.9 Minimal I-map

- If an edge is removed, it ceases to be an imap.
- A graph is an I-map if P($\cdot$) factorizes over the graph.

**Undirected Models**

- For all $\mathbf{x}_i$ find $MB(\mathbf{x}_i)$ and connect.

**Directed Models**

- For all $\mathbf{x}_i$ find $\pi_i \subseteq \text{pre}_i$ such that $\mathbf{x}_i \perp\!\!\!\perp \{\text{pre}_i \setminus \pi_i\} \mid \pi_i$
- Set $\text{pa}_i = \pi_i$

## 4 Equivalence and Conversion Between Models

Two directed graphs $G_1$ and $G_2$ are $I$-equivalent if they have the same set of immoralities and the same skeleton. An immorality is a collider without covering edge. **Look for colliders that don't match.** Since serial (head-tail) and diverging (tail-tail) connections imply the same independencies, we only need to look for converging (head-head) connections that don't match.

### 4.1 Directed $\to$ Undirected

We have:

$$\mathrm{P}(\cdot) = \prod_i \mathrm{P}(\mathbf{x}_i \mid \mathrm{pa}_i) = \prod_i \underbrace{\phi_i(\mathbf{x}_i, \mathrm{pa}_i)}_{\textit{cliques}}$$

- This is called **moralization** and we obtain a **moral graph**
- This it **NOT** an undirected I-map for the distribution. Most notably we can not represent collider independencies.

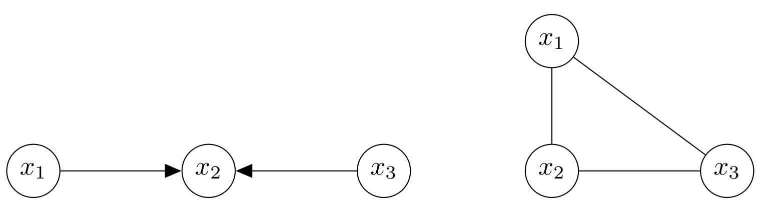
### 4.2 Undirected $\to$ Directed

(See example below)

- Choose an ordering.
- Read independencies off of the graph and find $\pi_i$ for each $i$.
- Connect $\pi_i \to \mathbf{x}_i$

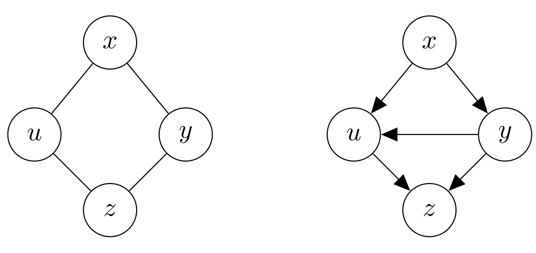
### 4.3 Non-equivalent Trails

**Colliders can not be represented by undirected graphs.**




In the moralized graph on the right the independence $\mathbf{x}_1 \perp\!\!\!\perp \mathbf{x}_3$ is lost.

**Closed loops can not be represented by directed graphs.**




Consider the left graph. Let's review the process of creating the directed graph:

- Choose an ordering: $x, y, u, z$.
- For each element, consider the parent set and read independencies off the directed graph.

- Start with $y \not\perp\!\!\!\perp x$, which implies the edge $x \to y$.
- Find the minimal set for which $u$ is independent of the parents $\pi_u$. This is $x, y$. Hence $x, y \to u$.
- For $z$ this set is $u, y$. Hence $u \to z$ and $y \to z$

**We no longer have the independence** $u \perp\!\!\!\perp y \mid x, z$.

# 5 Factor Graphs

$$\mathrm{P}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4) = \frac{1}{Z} \phi_1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) \phi_2(\mathbf{x}_3, \mathbf{x}_4) \phi_3(\mathbf{x}_4) \quad (1)$$

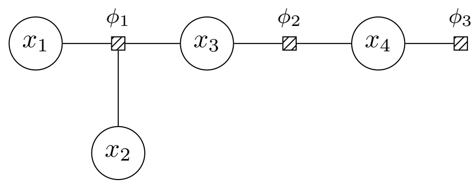



Figure 9: Factor Graph

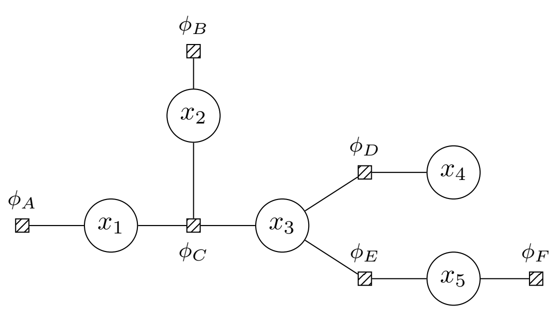
# 6 Exact Inference in Factor Graphs

Assume discrete variables. The task is to compute $\mathrm{P}(\mathbf{x}_k = k)$ for all $k$.

We can group terms in the leaves of the tree. Consider:

$$\mathrm{P}(\cdot) \propto \phi_A(\mathbf{x}_1) \phi_B(\mathbf{x}_2) \phi_C(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) \phi_D(\mathbf{x}_3, \mathbf{x}_4) \phi_E(\mathbf{x}_3, \mathbf{x}_5) \phi_F(\mathbf{x}_5) \quad (2)$$

which is:




We iteratively "eliminate" variables by summing or integrating them out. Firstly, we eliminate $\mathbf{x}_5$:

$$
\begin{aligned}
\mathrm{P}(\mathbf{x}_1,\dots,\mathbf{x}_4) &= \sum_{\mathbf{x}_5} \mathrm{P}(\mathbf{x}_1,\dots,\mathbf{x}_5) \\
&\propto \sum_{\mathbf{x}_5} \phi_A(\mathbf{x}_1)\phi_B(\mathbf{x}_2)\phi_C(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)\phi_D(\mathbf{x}_3,\mathbf{x}_4)\phi_E(\mathbf{x}_3,\mathbf{x}_5)\phi_F(\mathbf{x}_5) \\
&\propto \phi_A(\mathbf{x}_1)\phi_B(\mathbf{x}_2)\phi_C(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)\phi_D(\mathbf{x}_3,\mathbf{x}_4)\sum_{\mathbf{x}_5} \phi_E(\mathbf{x}_3,\mathbf{x}_5)\phi_F(\mathbf{x}_5) \\
&\propto \phi_A(\mathbf{x}_1)\phi_B(\mathbf{x}_2)\phi_C(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)\phi_D(\mathbf{x}_3,\mathbf{x}_4)\widetilde{\phi}_5(\mathbf{x}_3)
\end{aligned}
$$

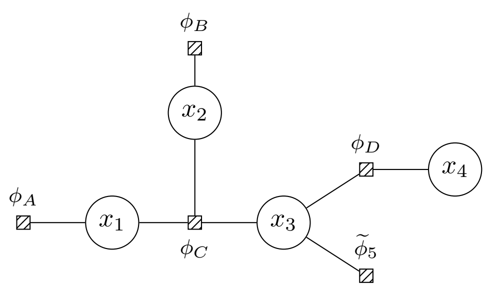
The idea is that we have reduced the factors above. Numerically, we would have the following:

$$
\widetilde{\phi}_5(\mathbf{x}_3) = \begin{cases} a & \mathbf{x}_3 = 1 \\ \dots & \\ z & \mathbf{x}_3 = N \end{cases}
$$

For each value of the factor. This is pre-computing all of the values, which in this case costs $O(N^2)$. For each value of $\mathbf{x}_3$ we need to sum over $\mathbf{x}_5$.

If we keep on doing this, the total cost will be greatly reduced from the $O(N^4)$ that is needed to sum over $\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_5$.

The above operation is represented by the following **reduced** factor graph:




## 6.1 Message Passing

**TODO: Graphs**

$$
\mu_{\phi\to\mathbf{x}}(\mathbf{x}) = \sum_{\mathbf{x}_1,\dots,\mathbf{x}_j} \phi(\mathbf{x}_1,\dots,\mathbf{x}_j,x)\prod_{i=1}^{j}\mu_{\mathbf{x}_i\to\phi}(\mathbf{x}_i)
$$

$$
\mu_{\mathbf{x}\to\phi}(\mathbf{x}) = \prod_{i=1}^{j}\mu_{\phi_i\to\mathbf{x}}
$$

$$
\mathrm{P}(\mathbf{x}) \propto \prod_{i=1}^{j}\mu_{\phi_i\to\mathbf{x}}(\mathbf{x})
$$

$$
\mathrm{P}(\mathbf{x}_1,\dots,\mathbf{x}_j) \propto \phi(\mathbf{x}_1,\dots,\mathbf{x}_j)\prod_{i=1}^{j}\mu_{\mathbf{x}_i\to\phi}(\mathbf{x}_i)
$$

# 7 Inference for Markov Chains

**TODO: Just scan this..**

## 7.1 $\alpha$-recursion

## 7.2 Smoothing

## 7.3 $\alpha$-$\beta$ Recursion

# 8 Model-Based Learning

- Probabilistic model: table for a distribution $\mathrm{P}(\mathbf{x})$
- Statistical model: set of probabilistic models: $\{\mathrm{P}(\mathbf{x};\theta)\}$
- Bayesian model: prior on theta, replace "parametrized by" with "conditioned on" $\mathrm{P}(\mathbf{x}) = \int \mathrm{P}(\mathbf{x} \mid \theta)\ \mathrm{P}(\theta)$. To get the probability distribution of $\mathbf{x}$ as above, we need to integrate over all possible values of $\theta$.

# 9 Moment Matching

# 10 Bayesian Inference

# 11 Factor Analysis

# 12 Independent Component Analysis (ICA)

# 13 Intractable Likelihood Functions

# 14 Score Matching

# 15 Sampling and Monte Carlo

# 16 Sampling from Continuous Distributions

## 16.1 Rejection Sampling

## 16.2 Ancestral Sampling

## 16.3 Gibbs Sampling

# 17 Variational Inference