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Exploiting Markov Equivalence for Fast Inference

MASTER THESIS

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MATHEMATICS

Author
Jenette SELLIN

Born December 22, 1995
in CALIFORNIA, USA

Advisor
Andreas GORAL

Supervisor
Prof. Dr. Joachim GIESEN

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Abstract

Zusammenfassung

Acknowledgements

Notation and Abbreviations

DAG	Directed Acyclic Graph
iff	If and only if
$G = (V, E)$	A graph G with vertices V and edges E
$[G]$	The Markov equivalence class of G
MEC	Markov Equivalence Class
G_*	essential graph of G
$G, G', G_1, G_2, ..., G_n$	directed graphs
$H, H', H_1, H_2, ..., H_n$	undirected and mixed graphs
$B, B', B_1, B_2, ..., B_n$	Bayesian networks
Capital letters e.g. X, Y, Z	random variables
Lowercase letters e.g. x, y, z	values attained by random variables
$\alpha(X)$	the set of ancestors of a vertex X in a graph G
$\prod_X^G$	the set of parents of a vertex X in a graph G

Contents

Chapter 1

Introduction

1.1 Motivation

Many fields rely on prediction and classification of new information using known data, processes which require encoding statistical relationships into analyzable structures. Conditional dependencies between random variables in probability distributions can be effectively modeled using Bayesian networks, giving us a reliable way to do inference on our model.

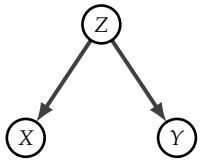
For instance, in the medical field, we may have information about a large number of patients (such as height, age, sex, blood type, etc.) and we may wish to use this information to predict whether a patient has a specific disease or not. In this scenario, we would need to model the known data and then query the model for the probability that, given these factors, a patient has the disease.

Naturally, it is in our best interest to create a model and a method for querying which allow us to do inference on our probabilistic models as efficiently as possible, in order to achieve results more quickly. This thesis explores a method for answering queries more efficiently in the context of graphical models.

1.2 Background

The family of models explored in this thesis are directed graphical models over discrete probability distributions. The purpose of graphical models is to encode information about vectors of random variables, namely the interdependencies satisfied by the vector's joint probability function. For example, consider a vector of three random binary variables (X, Y, Z). Suppose that the values of

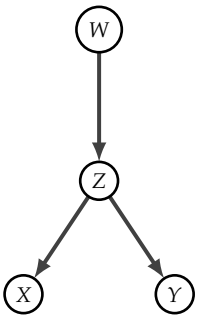
X and Y depend on Z, but X and Y are independent from one another given Z. These dependencies can be encoded in the following graph:



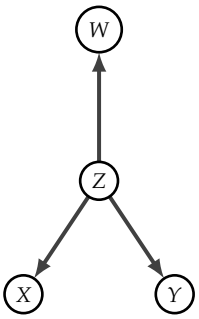
$$p(X,Y|Z) = p(X|Z) \cdot p(Y|Z)$$

Figure 1.2.1

In the case of directed models, which we explore in this thesis, there is not necessarily a unique graph which satisfies the dependency constraints of the joint probability function. A random vector and its constraints may be described by a variety of different graph structures which ultimately describe the same underlying probability distribution. This will be explored in more detail later. To understand how the complexity of answering a query depends on graph structure, consider the following two models:



G_1



G_2

$$p(X,Y,Z,W) = p(X|Z) \cdot p(Y|Z) \cdot p(Z|W) \cdot p(W)$$

$$p(X,Y,Z,W) = p(X|Z) \cdot p(Y|Z) \cdot p(W|Z) \cdot p(Z)$$

Figure 1.2.2

If we wish to answer a query about the random variable Y in G_1, for instance, we must also compute the probabilities of each vertex it depends on either directly or indirectly, that is, all of its **ancestors** (in this case Z and W in addition to Y itself). Alternatively, if we wish to answer a query about Y in graph G_2, we

need only to compute Z and Y. The number of variables which must be sampled is reduced when we consider G_2 instead of G_1.

In a context where answering queries about a single vertex may require us to sample arbitrarily many other vertices in the graph, we seek to find a graphical representation of our probability distribution which minimizes the number of vertices that must be sampled when answering a query.

1.3 Goal

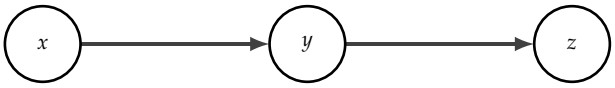
There are certain circumstances in which two Bayesian networks with different graphical structures can describe the same underlying probability distribution. This means that querying the graphs will produce statistically indistinguishable results. Such sets of graphs are called *Markov equivalent*.

The goal of this research is as follows: given a query and a Bayesian network B (which represents a single factorization of the probability distribution we wish to query), find a Markov equivalent Bayesian network B' which minimizes the number of variables that must be computed to answer the query. The purpose of the minimization is to reduce the cost of querying in order to achieve faster inference, as well as evaluate the gained speed-up versus the cost of transforming the graph structure.

To achieve this, we must first define the set of nodes which much be computed for a given query over a B. Then, we must search for a Markov equivalent Bayesian network B' such that the size of this set of necessary nodes is minimized for the same query over B'. Finally, we compare the costs of computing the query over B to the costs of computing the query over the minimized graph B' plus the costs of identifying B'.

1.4 Motivating Example

The following example demonstrates how answering a query can be sped up by querying a Markov equivalent graph with a different structure. Consider the following DAG:



G_1

Figure 1.4.1

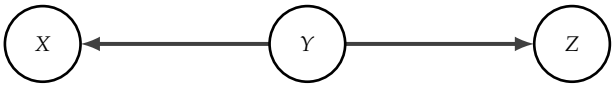
with conditional probabilities given by

$$p(X=1)=0.2$$
$$p(Y=1|X=0)=0.3 \qquad p(Y=1|X=1)=0.4$$
$$p(Z=1|Y=0)=0.1 \qquad p(Z=1|Y=1)=0.9$$

and the joint probability

$$p(X,Y,Z)=p(X)\cdot p(Y|X)\cdot p(Z|Y)$$

Here, if we wish to answer the query $p(Z|Y)$, our computation relies on all three random variables, since Z relies on Y and Y relies on X. However, we can find a Markov equivalent graph in which we can answer the same query while relying on fewer random variables. Consider the following DAG:



G_2

Figure 1.4.2

Here, we compute the conditional probabilities of G_2 to show that the model can equivalently describe our joint probability distribution from G_1, and therefore be used to answer the query $p(Z|Y)$. We then observe how the structure of the new model affects our computation of the query. By applying Bayes' Theorem, which states that $p(A|B)=\frac{p(B|A)p(A)}{p(B)}$, we can compute

$$p(X|Y)=\frac{p(Y|X)\cdot p(X)}{p(Y)}=\frac{p(Y|X)\cdot p(X)}{\sum_X p(Y|X)\cdot p(X)}$$

Using our pre-defined conditional probabilities,

$$\begin{aligned} p(Y=0) &= \sum_X p(Y=0|X) \cdot p(X) \\ &= 0.7 \cdot 0.8 + 0.6 \cdot 0.2 \\ &= 0.56 + 0.12 \\ &= 0.68 \end{aligned}$$

and

$$\begin{aligned} p(Y=1) &= \sum_X p(Y=1|X) \cdot p(X) \\ &= 0.3 \cdot 0.8 + 0.4 \cdot 0.2 \\ &= 0.24 + 0.08 \\ &= 0.32. \end{aligned}$$

which allow us to compute

$$p(X=1|Y=0) = \frac{p(Y=0|X=1) \cdot p(X=1)}{p(Y=0)} = \frac{0.6 \cdot 0.2}{0.68} = \frac{3}{17}$$

and

$$p(X=1|Y=1) = \frac{p(Y=1|X=1) \cdot p(X=1)}{p(Y=1)} = \frac{0.4 \cdot 0.2}{0.32} = \frac{1}{4}$$

Then, since X and Y do not depend on Z, the conditional probability of Z remains unchanged. Therefore, model G_2 is an equivalent model to G_1. If we answer the query $p(Z|Y)$ on model G_2, we do not need to consider X, since Y (and consequently Z) no longer depends on X.

Through this example, we see that it may be possible to find an equivalent graph to our original model, and to use the new graph structure to answer certain queries more efficiently. It is important to note that the efficiency of the new model for answering a query relies both on the conditional probabilites we are interested in, as well as the content of our query (as opposed to an arbitrary query).

1.5 Related work

Significant work has been done on individual aspects of the subject, though this thesis pioneers in using them together for fast inference. Verma and Pearl [1] give a framework for understanding how the same probability distribution can be encoded into two distinct graphs, as well as present a simplified criterion for when two graphs describe indistuingishable distributions. Flesch and Lucas [2] present a survey-style overview of Markov Equivalent graph structures, reduction of graph structures to simplified representations of equivalent distributions, as well as providing a strong background of relevant graph theory and probability preliminaries. Chickering [3] explores parameters of equivalent networks, presents a procedure for altering graphs without changing the described probability distribution, and quantifies the complexity of several such manipulations. Andersson et. al. [4] make similar headway by exploring reductions of graphs to representative form, as well as describing procedures by which one can alter the structure.

Adjacently, Schachter [5] confronts the same goal of faster inference of queries using a different method in a modified setting. His task focuses on eliminating unnecessary nodes from the computations directly, rather than by reversing edges.

1.6 Outline

In Chapter 2, we introduce preliminary concepts from Graph Theory and Bayesian statistics to robustly define our models, and to aid our understanding of graph manipulations and the process of querying over a graph. Chapter 3 details the problem and proposed querying method, then aims to quantify the computational costs of answering an arbitrary query over a graph by this method. Chapter 4 builds context for understanding Markov equivalence between graphs. In Chapter 5, we examine the circumstances under which a Markov equivalence can be utilized to answer a query more efficiently, and then quantify the computational costs of finding a suitable Markov equivalent graph for faster inference. Finally, in Chapter 6, we compare the quantities explored in Chapters 3 and 5 to determine whether our proposed algorithm indeed increases inference speed, and if so, where it is effective.

Chapter 2

Preliminaries

2.1 Foundations of Graph Theory

Definition 2.1.1 (Graph (directed, undirected, mixed)). *A **graph** is defined as a pair $G = (V, E)$ in which V is a finite set of vertices, and $E \subset V \times V$ is a finite set of edges. Vertices (also sometimes called **nodes**) will generally be denoted by capital letters, i.e. X, Y, Z. G is called **undirected** if every edge in G is undirected, meaning that for each edge $(X, Y) \in E$ (denoting an edge from vertex X to vertex Y), the edge (Y, X) is also in E, for $X \neq Y$. Otherwise, G is called **directed**. We denote such undirected edges by $\{X, Y\}$ or equivalently $\{Y, X\}$. A **mixed graph** (also called a hybrid graph) is a graph G which contains both directed and undirected edges.*

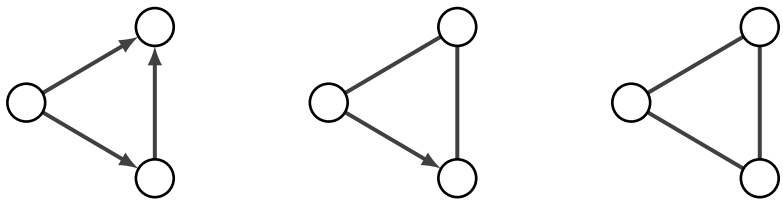


Figure 2.1.1

Definition 2.1.2 (Adjacent). *Two vertices $X, Y \in V$ in a graph $G = (V, E)$ are called adjacent if there is an edge between them, either (X, Y) or (Y, X).*

Definition 2.1.3 (Route). *A **route** in a graph $G = (V, E)$ is a sequence $X_1, X_2, ..., X_k$ of vertices in V such that there is an edge connecting X_i to X_{i+1} (independent of the*

direction of the edge), for $i = 1, ..., k-1, k \geq 1$. *The integer* k *is the length of the route.*

Definition 2.1.4 (Path, directed cycle). *A (directed)* ***path*** *in a directed graph* $G = (V, E)$ *is a route where vertices* X_i *and* X_{i+1} *are connected by a directed edge* (X_i, X_{i+1}). *A directed path which begins and ends at the same vertex is called a* ***directed cycle****.*

Definition 2.1.5 (Parent, ancestor). *Given two vertices* $X, Y \in V$ *in a directed graph* $G = (V, E)$, Y *is called a* ***parent*** *of* X *if the edge* $(Y, X) \in E$. *The set of parents of a vertex* X *in a graph* $G = (V, E)$ *is denoted* $\prod_X^G$. *Likewise,* X *is called a* ***child*** *of* Y. *The set of ancestors of* X, *denoted* $\alpha(X)$, *is the set of all vertices* Y *such that there exists a directed path from* Y *to* X, *but no path from* X *to* Y. *In the context of this thesis, this is the set of vertices upon which a vertex* X *depends, either directly or indirectly. Likewise, if* Y *is an ancestor of* X, *then* X *is a* ***descendant*** *of* Y.

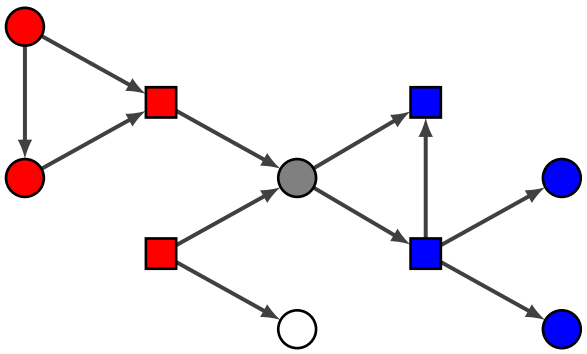


Figure 2.1.2: Red vertrices are ancestors of the gray vertex (squares denoting parents), and blue vertices are descendants of it (squares denoting children). The white vertex is neither an ancestor nor a descendent of the gray node, and therefore neither a parent nor child of it

Remark. $\prod_X^G \subseteq \alpha(X)$. Likewise, the set of children of X is a subset of the set of descendents of X.

Definition 2.1.6 (Chain graph, directed acyclic graph (DAG)). *A mixed graph* $G = (V, E)$ *is called a* ***chain graph*** *if it contains no directed cycles. A* ***directed acyclic graph*** *is a chain graph which is directed. This is abbreviated as DAG. The directed cycle is shown below in red.*

Remark. Every undirected graph is a chain graph.

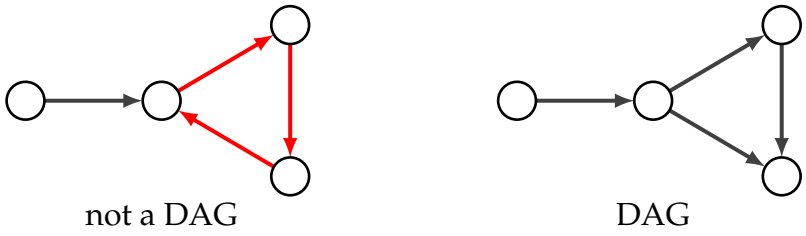


Figure 2.1.3

Definition 2.1.7 (Neighbor, adjacent). *Given two vertices $X, Y \in V$ in an undirected graph $G = (V, E)$, X is called a **neighbor** of Y if $\{X, Y\} \in E$. X and Y are also called **adjacent** in this scenario.*

2.2 Foundations of Bayesian Statistics

Definition 2.2.1 (Bayesian Network [6]). *A **Bayesian network** is a pair $B = (G, P)$ where $G = (V, E)$ is a DAG and P is a joint probability distribution defined on a set of random variables X. That is, it is a DAG and and associated joint probability distribution.*

Vertices in G have a one-to-one correspondence to the random variables X associated with P, meaning the set V indistinguishably represents both the vertices of G and the random variables of the joint probability distribution P of B.

P factorizes on the sets $\{X \cup \prod_X^G | X \in G\}$. That is, for each $X \in G$ there is a factor in P that depends on X and $\prod_X^G$, namely $P_X(X|\prod_X^G)$.

Example 2.2.1 (Simple Bayesian Network). The DAG in Figure 2.2.1 paired with the joint probability distribution $p(X_1 = x_2, X_2 = x_2) = p(X_1 = x_1) \cdot p(X_2 = x_2 | X_1 = x_1)$ is a Bayesian network.

Figure 2.2.1

Remark. In the context of this paper, we only consider graphs G which are DAGs unless explicitly stated otherwise. Further, for our purposes, all such DAGS represent graphical models with associated probability distributions. Therefore we will refer to DAGS $G = (V, E)$ and Bayesian networks interchangably, with necessary details clarified in context.

Theorem 2.2.1 (Bayes' Theorem [7]). *Given two random variables X and Y with*

$p(Y) \neq 0$

$$p(X|Y) = \frac{p(Y|X) \cdot p(X)}{p(Y)}.$$

Definition 2.2.2 ((Statistical) independence [7]). *Let X and Y be random variables. Then X and Y are called **independent** whenever*

$$P(X,Y) = p(X)p(Y)$$

or equivalently if

$$p(X) = p(X|Y)$$

and vice versa.

Remark. 2.2.2 can be intuitively understood as follows: learning about B has no effect on our knowledge concerning A and vice versa.

Definition 2.2.3 (Conditional independence [7]). *Let X, Y, and Z be random variables. Then X is said to be **conditionally independent** of Y given Z whenever $p(X|Y,Z) = p(X|Z)$. Otherwise, they are said to be **conditionally dependent**.*

Remark. 2.2.3 can be intuitively understood as follows: learning about Y has no effect on our knowledge concerning X given our beliefs concerning Z and vice versa.

Example 2.2.2. Suppose Lisa and Evin each flip a biased coin which either results in heads (H) or tails (T). On first impression, we might assume that the probability of Lisa flipping heads is independent of the probability that Evin flips heads, that is,

$$p(Lisa = H|Evin = H) = p(Lisa = H),$$

which would mean that they are independent. However because the coin is weighted, if Lisa flips a heads, we learn that the coin is more likely biased toward heads. Let Z be the event that the coin is indeed weighted toward heads. Then

$$p(Lisa = H|Evin = H, Z) = p(Lisa = H|Z).$$

Therefore, given the information that the coin is biased toward heads (event Z), our knowledge about Evin's coin flip does not affect our knowledge about Lisa's

coin flip. That is, given Z, they are independent. This is conditional independence with respect to Z.

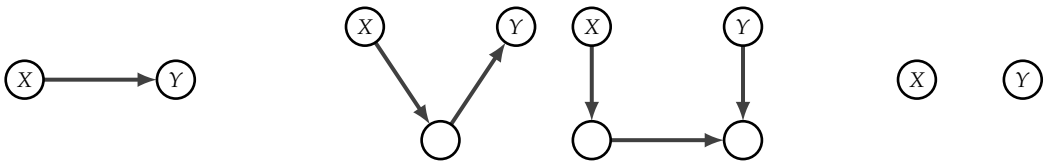
Remark. Definition 2.2.3 and Definition 2.2.2 also hold for disjoint sets A, B, and $C \subset V$ with p a joint probability distribution defined on V.

Remark. Dependence, independence, and conditional independence have an intuitive manifestation within graph structure.

Given a graph $G = (V, E)$ such as the graphs in Figure 2.2.2,if two nodes $X, Y \in V$ have an edge between them, either (X, Y) or (Y, X), then they are dependent variables by construction of our graphs.

If there exists a route between two nodes X and Y, but X and Y are not adjacent, then they are conditionally independent, where the conditions are the nodes on that route. This is because information about X can give us information about an intermediary node on the route, and allow us to gain information about Y (or vice versa).

Finally, if two nodes are not connected by a route (disconnected) then they are independent, since information about X cannot give us information about Y under any circumstances.



dependent X and Y conditionally independent independent

Figure 2.2.2

Definition 2.2.4 (Probabilistic query). *A probabilistic query q on a graph $G = (V, E)$ is an inference question of the form $p(X_1, ..., X_n | Y_1, ..., Y_m)$ where $X_i, i \in [0, n] \in V$ and $Y_j, j \in [0, m] \in V$. X_i are the **targets** of q while Y_j are the **conditions** or **observations**.*

Chapter 3

Querying

3.1 Outline of the Task

The first task outlined by our goal is to quantify the number of vertices representing random variables that must be considered for a given query over G. This will serve as our cost function for the minimization which occurs in later chapters; the minimization will therefore be to reduce the cost, that is, find an equivalent graph G' such that this number of vertices is minimized.

Naturally, before we consider the minimization itself, we begin by identifying such a set of vertices. This chapter will focus on identifying this set of vertices which must be computed for a given query.

3.2 Structure of a Query

An inference query is a question which askes the probability of one or multiple random variables in a probability distribution given some observations. Queries can take advantage of multiple observations and have multiple targets. For example, one can ask for the probability that the random variable X has takes on the value x given that we have observed $Y = y$. Let x be a value attained by the random variable X, and let y be a value attained by the variable Y. This is written $p(X = x|Y = y)$. The general form of a query is as follows:

Definition 3.2.1 (Query). *Given a graph $G = (V, E)$ with $X_1, ...X_n, Y_1, ...Y_n \in V$, the general form of a query q is $p(X_1, ..., X_n|Y_1, ...Y_n)$, meaning the probability of variables $X_1, ..., X_n$ given that we have conditioned on observed values attained by variables $Y_1, ..., Y_n$.*

Remark. Note that while a query on $G = (V, E)$ must have at least one target (otherwise there is nothing to compute), it does not necessarily need to include a condition. For example, $p(X = x)$ is a valid query for $X \in V$.

Scenario	Query	Interpretation	Example
Query a single target, single observation	$p(X = x \mid Z = z)$	Probability that $X = x$ given that we have observed $Z = z$.	Probability that a patient has lung cancer given that they are a tobacco smoker.
Query with multiple targets, single observation	$p(X = x, Y = y \mid Z = z)$	Probability that $X = x$ and $Y = y$ given that we have observed $Z = z$.	Probability that a patient has lung cancer and high blood pressure given that they are a tobacco smoker.
Query with a single target, multiple observations	$p(X = x \mid W = w, Z = z)$	Probability that $X = x$ given that we have observed $W = w$ and $Z = z$.	Probability that a patient has lung cancer given that they are over 50 years of age and a tobacco smoker
Query with multiple targets, multiple observations	$p(X = x, Y = y \mid W = w, Z = z)$	Probability that $X = x$ and $Y = y$ given that we have observed $W = w$ and $Z = z$.	Probability that a patient has lung cancer and high blood pressure given that they are over 50 years of age and a tobacco smoker.

Let G be a DAG and q a query. Define $\Delta(G, q)$ to be the number of nodes involved in the computation of q on G. The goal of this chapter is to find this value. Ultimately, we intend to find $\arg\min_{G' \in [G]}(\Delta(G, q))$.

3.3 Cost of a Query

Corollary 1. *The definition of conditional independence can be written*

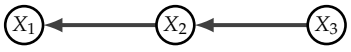
$$P(A|B) = \frac{P(A, B)}{P(B)}.$$

Lemma 3.3.1. *Computing a conditionless query $q = p(X_0, X_1, ..., X_n)$ over a DAG G depends on vertices $X_0, X_1, ..., X_n$ and all of their ancestors: $\alpha(X_0), \alpha(X_1), ..., \alpha(X_n)$.*

Proof. Let $q = p(X_0, X_1, ..., X_n)$ on a DAG G. Using the construction G, we have that the joint probability distribution $p(X_0, X_1, ...X_n) = \prod_{i=0}^{n} p(X_i | \prod_{X_i}^{G})$. Therefore q indeed depends on all ancestors of the targets.

□

Example 3.3.1. Let $q = p(X_1 = x_1)$ be a query on $G = (V, E)$ in Figure 3.3.1. The computation of q is as follows.



G

Figure 3.3.1

$$p(X_1 = x_1) \;=\; \sum_{x_2}\sum_{x_3} p(X_1 = x_1 | X_2 = x_2) \cdot p(X_2 = x_2 | X_3 = x_3) \cdot p(X_3 = x_3)$$

and therefore requires considering the target vertex X_1 and its ancestors, namely X_2 and X_3.

Theorem 3.3.2. *Let $q = p(X_0, X_1, ..., X_m | Y_0, Y_1, ..., Y_n)$ be a query on a DAG G. Then the computation of q requires the following sets of vertices depending on the structure of G:*

1. ***Special case*** *If X_i is conditionally independent of all elements in $\alpha(Y_j)$ for $i \in [0,m], j \in [0,n]\}$ given nodes Y_j, then q depends on the sets $\{X_i \cup \alpha(X_i) | i \in [0,m]\}$ and all nodes on a route between X_i and Y_j for all $i \in [0,m], j \in [0,n]$.*

2. ***General case*** *Otherwise, q depends on the sets $\{X_i \cup \alpha(X_i) | i \in [0,m]\}$ and $\{Y_j \cup \alpha(Y_j) | j \in [0,n]\}$ and all nodes on a route between X_i and Y_j for all $i \in [0,m], j \in [0,n]$.*

That is, if the targets X_is are conditionally independent from the parents of the Y_js, then q depends on X_is, their parents $\alpha(X_i)$, and Y_js. If the X_is are not independent from the parents of Y_js, then q depends on the above vertices as well as the sets of parents $\alpha(Y_j)$.

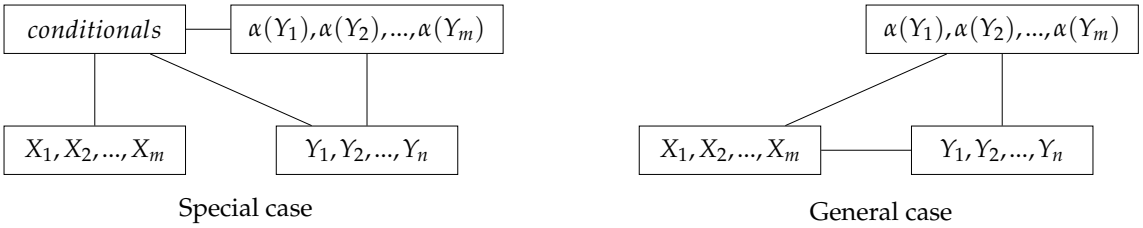
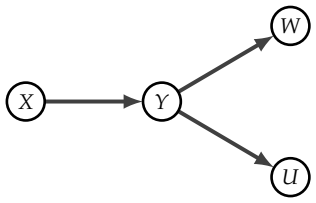


Figure 3.3.2

The following examples demonstrate the required vertices required in 3.3.2. First we present several computations in the general case, then computations in the special case. Finally, we show how two different queries over the same DAG G can fall into each case.

Example 3.3.2. General Case. Let $q = p(X_3 = x_3, X_4 = x_4)$ be a query on $G = (V, E)$ in Figure 3.3.3. The computation of q is as follows.



G

Figure 3.3.3

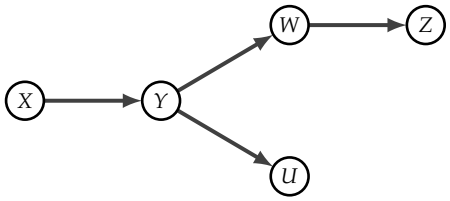
$$
\begin{aligned}
q &= p(X_3 = x_3, X_4 = x_4) \\
&= \sum_{x_2}\sum_{x_1} p(X_3 = x_3, X_4 = x_4 | X_2 = x_2) \cdot p(X_2 = x_2 | X_1 = x_1) \cdot p(X_1 = x_1) && [1] \\
&= \sum_{x_2}\sum_{x_1} p(X_3 = x_3 | X_2 = x_2) p(X_4 = x_4 | X_2 = x_2) \cdot p(X_2 = x_2 | X_1 = x_1) \cdot p(X_1 = x_1) && [2] \\
&= \sum_{x_2}\sum_{x_1} p(X_3 = x_3 | X_2 = x_2) \cdot p(X_4 = x_4 | X_2 = x_2) \cdot p(X_1 = x_1, X_2 = x_2) && [3]
\end{aligned}
$$

where [1] is by construction of the Bayesian network and [2] comes from Corollary 1 since X_3 and X_4 are conditionally independent. [3] comes from the following application of Corollary 1:

$$p(X_2 = x_2 | X_1 = x_1) \cdot p(X_1 = x_1) \;=\; p(X_1 = x_1, X_2 = x_2).$$

The query q depends on the targets X_4 and X_3 and their parents, X_2 and X_1.

Example 3.3.3. General case. The following example follows similar structure to Example 3.3.2 and uses real values for the conditional probabilities. Consider the graph $G = (V, E)$ from 3.3.4, where a vertex V takes a binary value $v \in [0, 1]$, and suppose we are given a query $q = p(Y = 1 | Z = 1)$.
Let the conditional probabilities be given by



G

Figure 3.3.4

$$
\begin{aligned}
&p(X=1)=0.2 \\
&p(Y=1|X=0)=0.6 \qquad\qquad p(Y=1|X=1)=0.4 \\
&p(W=1|Y=0)=0.4 \qquad\qquad p(W=1|Y=1)=0.3 \\
&p(Z=1|W=0)=0.7 \qquad\qquad p(Z=1|W=1)=0.3 \\
&p(U=1|Y=0)=0.8 \qquad\qquad p(U=1|Y=1)=0.4
\end{aligned}
$$

Then, the joint probability is given by

$$p(X,Y,W,U,Z) = p(X) \cdot p(Y|X) \cdot p(U|Y) \cdot p(W|Y) \cdot p(Z|W).$$

The aim of this example is to demonstrate that our query depends on the set of ancestors $\alpha(Y)$ and the nodes on route from Z to Y, in this case, the route $Y \to W \to Z$. For this computation, we set $Z=1$, and recall that since we are in a binary setting, for a vertex V we have $p(V=0) = 1 - p(V=1)$. Then, to determine $p(Y=1|Z=1)$, we first compute $p(Y=1)$:

$$
\begin{aligned}
p(Y=1) &= \sum_X p(Y=0|x) \cdot p(x) \\
&= 0.6 \cdot 0.8 + 0.4 \cdot 0.2 \\
&= 0.48 + 0.08 \\
&= 0.56 \\
P(Y=0) &= 1 - p(Y=1) = 0.44
\end{aligned}
$$

By similar calculation and plugging in the values $p(Y=1)$ and $p(Y=0)$, we ob-

tain that $p(W=0) = \sum_Y p(W=0|Y)p(Y) \approx 0.65$ and $P(W=1) \approx 0.34$. Likewise, we compute $p(Z=1) \approx 0.56$ and $p(Z=0) \approx 0,43$.

From here, we determine how the observation $Z=1$ affects the likelihood of values of W and consequently Y. Bayes' theorem allows us to do the calcultion using quantities specified in the conditional probabilities:

$$p(W=1|Z=1) \;=\; \frac{p(Z=1|W=1)\cdot p(W=1)}{p(Z=1)} \;\approx\; \frac{0.3\cdot 0.34}{0.56} \;\approx\; 0.18.$$

Subsequently $p(W=0|Z=1) \approx 0.81$. Now that we see how W is affected by the observation that $Z=1$, we can move upward in our route to determine who Y is affected by. Continuing with our condition that $Z=1$ and applying Bayes' theorem again,

$$p(Y=1|W=1) \;=\; \frac{p(W=1|Y=1)\cdot p(Y=1)}{p(W=1)} \;\approx\; \frac{0.18\cdot 0.44}{0.18} \;\approx\; 0.48.$$

Finally,

$$\begin{aligned} p(Y=1|Z=1) &= p(Y=1|W=0)\cdot p(W=0) + p(Y=1|W=1)\cdot p(W=1) \\ &\approx (0.59\cdot 0.81) + (0.48\cdot 0.18) \\ &\approx 0.17. \end{aligned}$$

Thus, by tracing the effects of the observation $Z=1$ on a route to $Y=1$ and using the ancestors $\alpha(Y)$, we have answered the query $q = p(Y=1|Z=1)$. Notice that this computation did not involve the vertex U, which is neither an ancestor of Y nor along the route between Y and Z.

G

Figure 3.3.5

Example 3.3.4. Special Case. Let $q = p(X_4 = x_4|X_2 = x_2)$ be a query on G in Figure 3.3.5. Then the query only involves vertices X_4, X_3, and X_2, so there is no need to consider vertex X_1. This is because X_4 is conditionally dependent on

$\alpha(X_2) = X_1$.

$$p(X_4 = x_4 | X_2 = x_2) = \sum_{x_3} p(X_4 = x_4 | X_3 = x_3) \cdot p(X_3 = x_3 | X_2 = x_2).$$

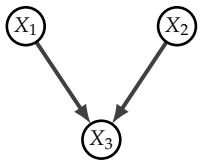


Figure 3.3.6

Example 3.3.5. This example compares two queries over the same graph G in Figure 3.3.6. Let $q_1 = p(X_2 = x_2 | X_3 = x_3)$ and let $q_2 = p(X_3 = x_3 | X_2 = x_2)$.

Note that X_2 is an ancestor of X_3, and trivially X_2 is not conditionally independent from X_2. Therefore q_1 is in the general case of Theorem 3.3.2, since the target of q_1 (namely X_2) is not disjoint from the ancestors of the condition, $\alpha(X_3)$.The computation of q_1 therefore requires the target X_2, the ancestors $\alpha(X_2)$, the condition X_3, and $\alpha(X_3)$. These sets together involve X_1, X_2, and X_3. This dependence is verified:

$$\begin{aligned} q_1 &= p(X_2 = x_2 | X_3 = x_3) \\ &= \frac{p(X_2 = x_2, X_3 = x_3)}{p(X_3 = x_3)} \\ &= \frac{\sum_{x_1} p(X_1 = x_1) \cdot p(X_2 = x_2) \cdot p(X_3 = x_3 | X_1 = x_1, X_2 = x_2)}{\sum_{x_1} \sum_{x_2} p(X_1 = x_1) \cdot p(X_2 = x_2) \cdot p(X_3 = x_3 | X_1 = x_1, X_2 = x_2).} \end{aligned}$$

Now we consider q_2. In this case, the conditional variable X_2 has no ancestors, and therefore we do not need to consider its distribution, since we are in the special case of Theorem 3.3.2. We show below that q_2 only relies only on X_3 and X_1.

Intuitively, setting $X_2 = x_2$ effectively removed the variable from the model, since we are conditioning other variables on this observation. Once the other variables are adjusted, X_2 no longer plays a role since it already has an established value and does not have parents that must be considered. That is, we are setting $p(X_3 = x_3 | X_1 = x_1) = p(X_3 = x_3' | X_1 = x_1', X_2 = x_2)$ for all x_1', x_2'. Thus:

Figure 3.3.7: X_2 effectively removed from the model.

$$\begin{aligned} q_2 &= p(X_3 = x_3 | X_2 = x_2) \\ &= \frac{p(X_3 = x_3, X_2 = x_2)}{p(X_2 = x_2)} \\ &= p(X_3 = x_3) \\ &= \sum_{x_1} p(X_3 = x_3 | X_1 = x_1, X_2 = x_2) \cdot p(X_1 = x_1) \\ &= \sum_{x_1} p(X_3 = x_3 | X_1 = x_1) \cdot p(X_1 = x_1). \end{aligned}$$

Therefore, q_2 relies only on X_3 and X_1 as described in the special case, whereas q_2 relies on X_2 as well, as described in the general case.

3.4 Notes from 9/5/2020

I've been trying to write up a short script which takes a graph G, a set of targets $[X_1, X_2, ..., X_m]$ and a set of targets $[Y_1, Y_2, ..., Y_n]$, and returns the case, either Special case or General case. Additionally, it should return the set of nodes the query $p(X_1, ...X_m | Y_1, ...Yn)$ depends on.

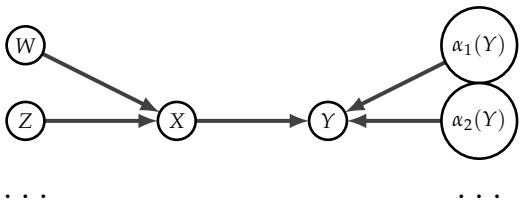
I had some trouble with this and decided to try to do the simple version, find_case(G, X, Y), which only takes one target X and one condition Y, but also had some trouble with this. Here are a few questions I ran into and problems I had solving them. These are in the context of the simpel case with one target X and one target Y:

The first check for me was whether an ancestor of Y, (I will write this $\alpha_i(Y)$, meaning the ith ancestor of Y) is a neighbor of X. If it is, then we immediately know that X is not conditionally independent of the set of ancestors of Y, $\alpha(Y)$. If it is a neighbor, we return General case.

The next test brought me to the question of *exclusivity* of the conditions. Suppose we have the following graph:

The question is, does any aspect of this count as the Special case? X is independent of $\alpha(Y) = Z$ given Y **and** W. So far I've been interpreting this as the General case, since X isn't independent of $alpha(Y)$ given exclusively Y. In this case we would still need to see how W is affected, and still need to consider nodes on the path from X to Y until Y (in this case, just X and W). Seems like this case still allows us to remove Y and its ancestors, though, in my tiny calculation. My guess (that I am still exploring) is that this should count as the general case, but we need to be explicit that the query still depends on a route from X to Y not including Y. ***

The next question I have been considering is the following: Suppose we have the graph like this

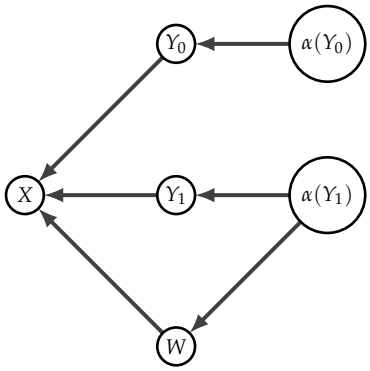


(The large nodes are just large to fit the label, no other reason). Clearly, to make sure that X is conditionally independent of $\alpha(Y)$ given Y, we have to check that there is not another path, for example, from W to $\alpha_1(W)$. To do so requires a search over the graph for simple paths* from X to $\alpha_i(Y)$ for all $i \in [0, n]$, not includng that path $X \to Y \leftarrow \alpha_i(Y)$.

*At first I used the networkx function nx.all_simple_paths, but then realized that this must be directionless routes. My current approach is to search for simple paths over the skeleton of G and check them over G itself, so that I can still use this function for routes, not paths. I think this works, overall, but hard to say because of other issues in my code.

Finally, my last observation is that the Special case seems to apply to individual observations Y instead of all at once. Say we have one target X. That is, if we have observations $Y_0, Y_1, ...Y_n$, then Y_0 can be in the special case while Y_1, for example, is not. This is possible if $\alpha(Y_0)$ is conditionally independent from

X given Y_0, but $\alpha(Y_1)$ is not conditionally independent of X given Y_1. Then the query should no longer rely on Y_0 and $\alpha(Y_0)$ but still relies on Y_1 and $\alpha(Y_1)$. So it seems as though, with multiple observations, a graph doesn't fall into one of two categories, either Special or General. It seems as though observations Y_j fall into those cases instead. Then we can only say the graph falls into one of the cases if it has only one observation, (or perhaps even that all observations evaluate to the same case).



In this graph, X is conditionally independent from $\alpha(Y_0)$ given Y_0, meaning Y_0 is in the Special case, and ensuring that the query shouldn't rely on Y_0 nor $\alpha(Y_0)$. However, X is not conditionally independent of $\alpha(Y_1)$ given only Y_1 since there exists a different route to $\alpha(Y_1)$ via W. Therefore the query *does* depend on Y_1 and $\alpha(Y_1)$. So the Special case only applies to a single observation and its ancestors here.

This gets even more confusing and awkward with multiple targets $X_0, X_1, ...X_m$ of course. Does X_0 have to be conditionally independent from $\alpha(Y)$ given Y, but X_1 doesn't? Do all targets X_i need this conditional independence? If so, that has implications about ***, where there could be a problem if X_0 is independent of $\alpha(Y)$ given Y **and** X_1.

Chapter 4

Markov Equivalence

4.1 Goal

In order to reduce the cost of a query on a graph G, we will exploit the observation that two graphs with distinguishable structures can model the same probability distribution. Such graphs are called *Markov equivalent*. Given a query on a graph G, we search for a Markov equivalent graph G' such that the cost of the query is minimized when considered on G' instead of G.

To do so, we must develop a robust understanding of Markov equivalence. This includes: how to identify whether two graphs are Markov equivalent, how a graph can be altered while remaining in the set of Markov equivalent graphs (called the *Markov equivalence class*), how computations of queries on a graph are altered when the graph structure is altered, and how to search for minimizing graphs.

In this chapter, we present definitions, theorems, and examples to establish a sufficient understanding of Markov equivalence for this purpose.

4.2 Basic Properties of Markov Equivalence

Definition 4.2.1 (Markov equivalence [1]). *Two directed acyclic graphs G and G' are **Markov equivalent** if for every Bayesian network $B = (G, \theta_G)$, there exists a Bayesian network $B' = (G', \theta_{G'})$ such that B and B' describe the same probability distribution, and vice versa. This is denoted $G \sim_M G'$.*

Definition 4.2.2 (Markov equivalence class [1]). *The set of all DAGs which are*

Markov equivalent to a DAG G is called the ***Markov equivalence class****(MEC) of G, denoted* $[G]$.

Significant research has been done to characterize Markov equivalence classes ([3], [1], [4]). This research has identified several key features of a graphs which allow us to more easily identify reversible edges and construct MECs. The following definitions outline several properties of graphs (and edges within them) which we will use to determine whether two graphs lie in the same MEC. Furthermore, it will help us build an understanding of how a graph can be manipulated without altering which MEC it belongs to.

Definition 4.2.3 (Covered Edge [3]). *Given a DAG* $G = (V, E)$*, an edge* $e = (X, Y) \in E$ *is called* ***covered*** *in* G *iff* $\prod_X^G = \prod_Y^G \cup Y$*. That is,* (X, Y) *is covered in* G *iff* X *and* Y *have identical parents in* G *with the exception that* X *is not a parent of itself.*

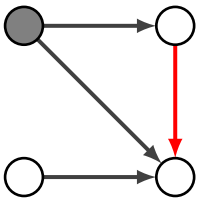
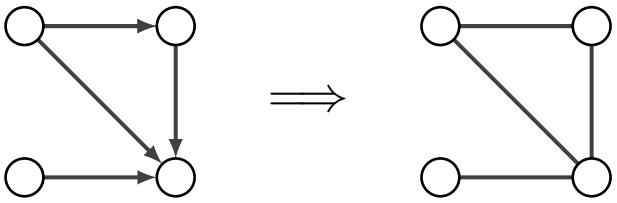


Figure 4.2.1

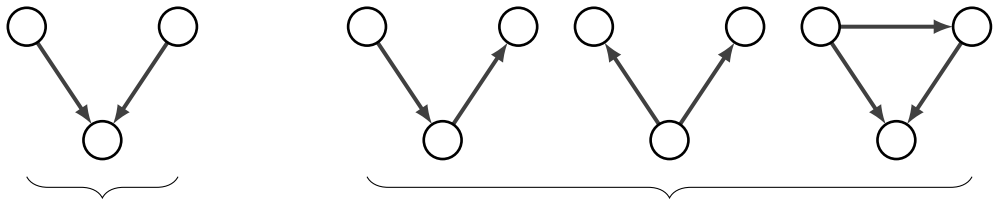
In Figure 4.2.1, for example, the red edge is the only covered edge, since the nodes it connects have a shared set of parents, namely, the single gray node.

Definition 4.2.4 (Skeleton). *Let* $G = (V, E)$ *be a directed graph. The undirected graph* $G' = (V, E')$ *which is constructed by removing the orientation of all edges in* E *is called the* ***skeleton*** *of* G*.*



G $\qquad\qquad$ $G' = \text{skeleton}(G)$

Definition 4.2.5 (v-structure). *A set of three vertices X, Y, Z of a graph $G = (V, E)$ is called a **v-structure** (or immorality) iff $(X, Y) \in E$ and $(Z, Y) \in E$ but X and Z are not adjacent.*



Definition 4.2.6 (Irreversible edge [4]). *Let G be a DAG. A directed edge $(X, Y) \in G$ is called **irreversible** in G if changing (X, Y) to (Y, X) either creates or destroys a v-structure, or creates a directed cycle. An edge which is not irreversible is called **reversible**.*

Lemma 4.2.1 (Criterion for Markov equivalence [8]). *Two graphs are equivalent iff they have the same skeleton and v-structures.*

Proof. The intuition for this Actually this should be cited to the 1989 paper by Pearl et al, (Verma, Geiger)?OR wait, Olmsted? Looks like the real proof is in Smith 1987, Influence Diagrams for Statistical Modelling. □

Lemma 4.2.2 (Covered edges are exactly reversible edges [3]). *Let $G = (V, E)$ be a DAG, let $X, Y \in V$ and let $e = (X, Y) \in E$. Let $G' = (V, E')$ be the DAG constructed from G by reversing the edge (X, Y) to (Y, X). Then G and G' are equivalent iff e is a covered edge in G.*

Proof. Let $G = (V, E)$ be a DAG. A sketch of the proof is as follows (see [3] for the full proof):

(**if**) Suppose $e = (X, Y)$ is a covered edge in G. Let G' be equivalent to G, except that e is reveresed to $e' = (Y, X)$. Then:

- G' is also a DAG. To show this, suppose that G' is not a DAG. Since G and G' only differ by $e' = (Y, X)$, there must be a directed cycle incuding e' in G'. Then there is a path in G from Y to X. By assumption, Y and X have a shared set of parents. However, one can conclude from this that G also contains a cycle, and therefore is not a DAG, a contradiction. By this contradiction, we conclude that G' must be a DAG.

- $G' \sim_M G$. Firstly, G and G' trivially have the same skeleton, since they only differ by the orientation of edge e. Then, if they were *not* Markov equivalent graphs, they would differ by a v-structure. If G' has a v-structure not present in G, it must include the edge (Y, X). However, this would imply that X has a parent which is not a neighbor to Y, contradicting the assumption that e is covered. A similar argument holds for the scenario where G has a v-structre not present in G'.

(**only if**) We now show that if $e = (X, Y)$ is not a covered edge in G, we are in one of two cases: either G' contains a directed cycle, or G' is a DAG which is not equivalent to G. If (X, Y) is not a covered edge in G, then at least one of the following hold:

1. There is a node $Z \neq X$ which is a parent of Y but not of X.
2. There s a node W which is a parent of X but not of Y.

Let $Z \neq X$ be a parent of Y in G but not a parent of X in G. IF Z and X are not neighbors, then there is a v-structure consisting of edges (X, Y) and (Y, Z) in G which does not exist in G'. If X is a parent of Z in G, then it must also be a parents of Z in G', which would imply that G' contains a directed cycle and is therefore not a DAG.

The argument for the second case is equivalent, assuming W is a parent of X in G and deriving a v-structure with $(W, X) and (X, Y)$ which exists in G' but not G. We conclude that G would have to contain a directed cycle. In both scenarios, we have derived a contradiction which shows that (X, Y) must be covered in G.

□

Example 4.2.1 (Members of Markov equivalence class [1]). Consider the following four DAGs:
The fact that G_1, G_2, and G_3 are in the same MEC while G_4 is not can be seen by considering the joint probability distribution $p(X, Y, Z)$ of each of the above graphs.

$$
\begin{aligned}
G_1: &\quad p(X,Y,Z) = p(X) \cdot p(Y|X) \cdot p(Z|Y) \\
G_2: &\quad p(X,Y,Z) = p(Y) \cdot p(X|Y) \cdot p(Z|Y) \\
G_3: &\quad p(X,Y,Z) = p(Z) \cdot p(Y|Z) \cdot p(X|Y)
\end{aligned}
$$

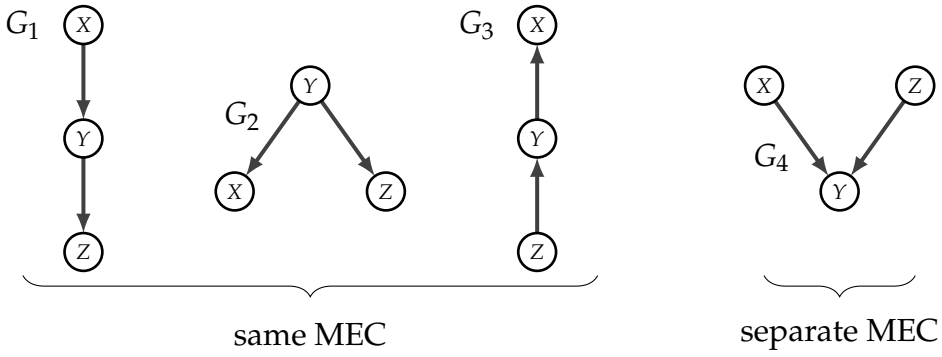


Figure 4.2.2

By Bayes' theorem, all of the values of G_2 can be completely determined from values from G_1:

$$p(X)p(Y|X) = p(X,Y) = p(Y)p(X|Y)$$

and $p(Z|Y)$ is unchanged. A similar application of Bayes' theorem shows that G_3 is completely determined by G_1 and G_2:

$$p(z) \cdot p(Y|Z) = p(Z,Y) = p(Y) \cdot p(Z|Y)$$

where $p(Y)$ can be attained directly from G_2 and $p(Z|Y)$ can be attained from G_1. Therefore, we can conclude that since all three describe the same distribution, they lie in the same equivalence class. In contrast, the joint probability for G_4 is given by

$$p(X,Y,Z) = p(X) \cdot p(Z) \cdot p(Y|X,Z)$$

which can not be determined from the values of G_1, G_2 and G_3. This is because in $[G_1]$ X is conditionally independent from Y and Z, that is, X is only independent in the circumstance that we are given values for Y and Z. Meanwhile, in G_4, X is marginally independent of Z, that is, independent in the circumstance that we ignore Y. Conditional independence does not provide information about marginal independence, and conversely, marginal independence does not imply conditional independence. Therefore, G_4 describes a different distribution, and does not lie in $[G_1]$.

Corollary 2. *Lemma 4.2.2 and Lemma 4.2.1 together imply that the graph G' which results from only reversing the orientation of a covered edge $(X,Y) \in G$ is in the MEC of $[G]$.*

Proof. This follows from the fact that edge reversal does not change the skeleton

of the graph G (since no edges are added nor removed) and reversing covered edges does not alter the v-structures of G (Lemma 4.2.2), thus the v-structures and skeleton are unchanged. □

4.3 Effects of Edge Reversal

Lemma 4.3.1. *Given a single directed edge between two parentless nodes in which* $p(X_2) = p(X_1) \cdot p(X_2|X_1)$*, the joint probability after switching edge orientation is given by*

$$p(X_1) \;=\; p(X_2)\frac{p(X_2|X_1)\cdot p(X_1)}{\sum_{X_1} p(X_2|X_1)\cdot p(X_1)}.$$

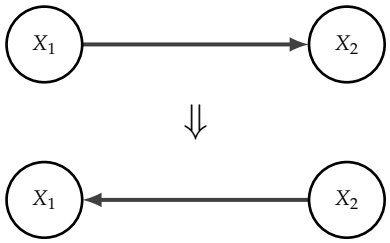


Figure 4.3.1

Proof. This follows directly from Bayes' theorem, which gives us

$$\begin{aligned} p(X_1) &= p(X_2)\cdot p(X_1|X_2) \\ &= p(X_2)\frac{p(X_2|X_1)\cdot p(X_2)}{p(X_2)} \\ &= p(X_2)\frac{p(X_2|X_2)\cdot p(X_2)}{\sum_{X_1} p(X_2|X_1)\cdot p(X_1)}. \end{aligned}$$

□

Lemma 4.3.2. *Given a directed edge between two nodes* X_1 *and* X_2 *with a shared parent node* X_P*, the joint probability after switching edge* (X_1, X_2) *to* (X_2, X_1) *is given by*

$$p(X_1, X_2, X_P) \;=\; p(X_P)\cdot p(X_2|X_P)\cdot p(X_1|X_2, X_P) \;=\; \ldots$$

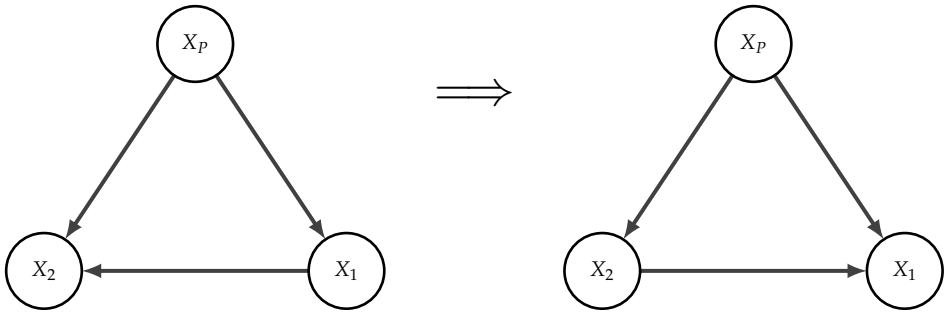


Figure 4.3.2

Remark. Furthermore, because this result does not depend on $p(X_p)$, we can conclude that for a set of shared parents $P = \{X_{P_1}, X_{P_2}, \ldots X_{P_i}\}$ of two nodes X_1 and X_2, the same equality holds. Additionally, note that any reversal of an edge with a set of shared parents is MEC-invariant, since all such edges are covered (corollary 2).

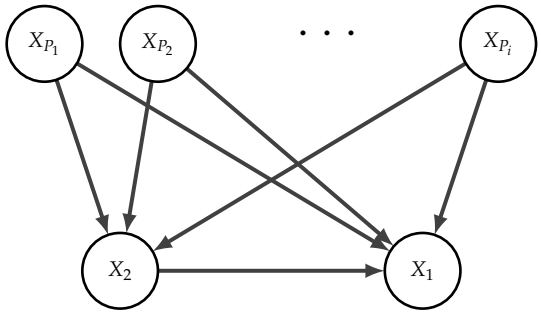


Figure 4.3.3

Proof. From before the edge reversal, we have access to the values $p(X_p), p(X_1|X_p)$, and $p(X_2|X_1, X_p)$. Our goal is to determine the new joint probability distribution $p(X_1, X_2, X_p)$ using this information. Therefore, we must find $p(X_p), p(X_2|X_p)$, and $p(X_1|X_2, X_p)$. First, $p(X_p)$ is already trivially available. Then, to compute $p(X_1|X_1, X_p)$,

$$
\begin{aligned}
p(X_1|X_2, X_p) &= \frac{p(X_1, X_2, X_p)}{p(X_2, X_p)} \\
&= \frac{p(X_2|X_1, X_p) \cdot p(X_1, X_p)}{p(X_2, X_p)} \\
&= \frac{p(X_2|X_1, X_p) \cdot p(X_1, X_p)}{p(X_2, X_p)} \\
&= \frac{p(X_2|X_1, X_p) \cdot p(X_1|X_p) \cdot p(X_p)}{p(X_2|X_1, X_p)} \\
&= \frac{p(X_2|X_1, X_p) \cdot p(X_1 X_p)}{p(X_2|X_p)} \\
&= \frac{p(X_2|X_1, X_p) \cdot p(X_1|X_p)}{p(X_2|X_p)}
\end{aligned}
$$

which depends only on known quantities once we compute

$$
\begin{aligned}
p(X_2|X_p) &= \sum_{X_1} p(X_1|X_p) \cdot p(X_2|X_1, X_p) \\
&= \frac{1}{p(X_p)} \sum_{X_1} p(X_1, X_p) \frac{p(X_2, X_1, X_p)}{p(X_1, X_p)} \\
&= \frac{1}{p(X_p)} \sum_{X_1} p(X_2, X_1, X_p) \\
&= \sum_{X_1} p(X_2, X_p)
\end{aligned}
$$

TO BE CONT.

□

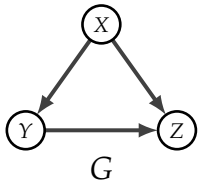
4.4 Find Reversible Edges of a DAG Model

Definition 4.4.1 (Essential edge [4], [2]). *An **essential edge** (also called a compelled edge [3]) of a graph $G = (V, E)$ is an edge $(X, Y) = e \in E$ such that for every graph $G' = (V, E')$ in $[G]$, the orientation of $e \in E$ is unchanged. That is, there is no graph $G' = (V, E')$ in $[G]$ such that $(Y, X) \in E'$.*

Definition 4.4.2 (Essential graph [4]). *The **essential graph** of a Markov equivalence class $[G]$ is a mixed graph G_* such that the only directed edges in G_* are essential edges of $[G]$. That is,*

- *The directed edge $e = (X, Y) \in G_*$ iff $e \in G$ for every graph $G \in [G]$,*
- *The undirected edge $X^-Y \in G_*$ iff there are graphs G_1 and $G_2 \in [G]$ such that (u, v) in G_1 and (Y, X) in G_2.*

Example 4.4.1. In this example, we identify the essential edges of a Markov equivalence class and construct the essential graph. Consider the following DAG $G = (V, E)$:



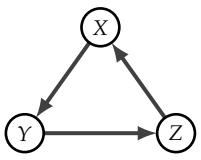
G

Figure 4.4.1

We use the following realizations to show that the graph has no essential edges. If we switch any edge in G, the resulting graph G' becomes one of two cases:

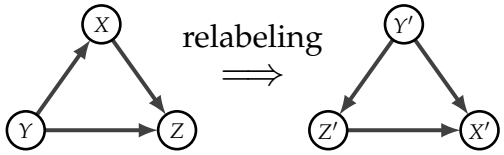
- G' is cyclic, and therefore no longer a DAG, meaning this edge was irreversible.

  Example: reversing edge (X, Z) as in **(A)** creates a cycle.



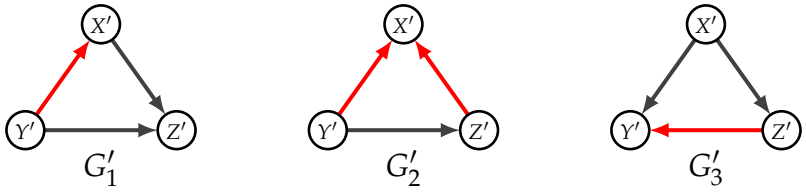
(A)

- G' is equivalent to G up to relabeling, and therefore in the same MEC.
  Example: reversing (X, Y) and changing labels according to $X \to Y'$, $Y \to Z'$, and $Z \to X'$, as in **(B)**.

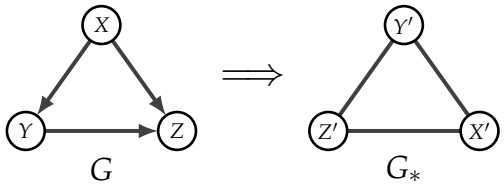


(B)

Thus the following graphs are included in $[G]$, though they are not the entire MEC. The red edges in each are those with orientation which differs from edges in G. Notice, however, that some relabeling was required, meaning these edges do not necessarily correspond (under this new labeling) to covered edges.



Therefore, under some circumstance, for every edge $(U, V) = e \in G$, there is a DAG $G' \in [G]$ such that $(V, U) \in G'$. This means that G has no essential edges. We construct the essential graph G_* of G by removing the orientation of all non-essential edges in G:



Remark. Andersson et. al. [4] demonstrate that essential graphs are consistent across a MEC and unique to it, meaning an essential graph can be used as a representative for a given MEC. Furthermore, essential graphs are not necessarily DAGs, and therefore do not generally belong to the MEC that they represent.

This can be seen by the fact that the distinction between two MECs lies entirely in either differences in their skeletons or in the orientations of their compelled edges.

"It is only in the heart that one can see rightly; what is essential is invisible to the eye."
-Antoine de Saint-Exupéry, The Little Prince.

Remark. One should take care to note the distinction between implications about non-essential edges versus covered edges:

- For $G = (V, E)$, an edge $e \in E$ is non-essential iff there exists a graph G' in $[G]$ such that e is reversed,
- An edge e in G is covered iff the graph G' derived from *only* reversing e, is in the MEC of G. (Follows from corollary 2.)

That is, reversing e *exclusively* while remaining in the MEC of G requires e to be covered. Meanwhile, a non-essential edge $e \in G$ may require other edges in G to be reversed as well to remain in the same MEC. This means that not all non-essential edges can be reversed at a given time. The following example demonstrates that some configurations of non-essential edge reversals are not possible if we wish to remain in the MEC of G.

Example 4.4.2. Again consider members of the Markov equivalence class seen in example 4.2.1. The positions of the nodes are visually rearranged for clarity, but no properties are changed.

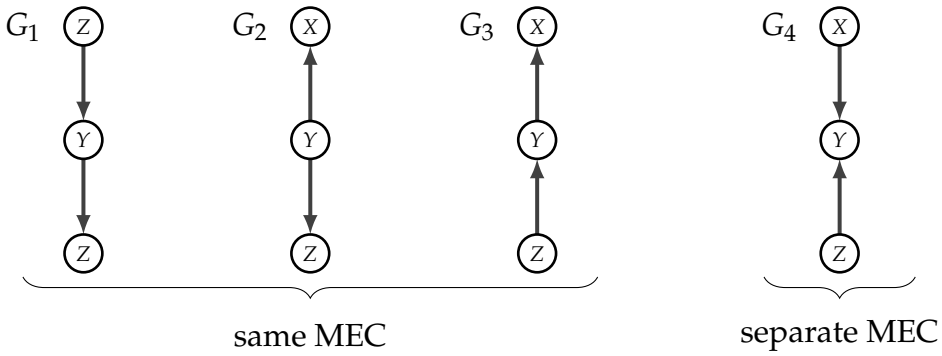


Figure 4.4.2

Notice that edge $(Y, Z) \in G_1$ is non-essential, since there exists another graph (namely G_3) in $[G_1]$ such that $(Z, Y) \in G_3$. Therefore, we know that there exists some combination of edge reversals such that (Y, Z) can be reversed without leaving $[G_1]$. However, if we choose to switch only (Y, Z) to (Z, Y), we have exactly graph G_4, which is no longer in the same MEC. Therefore, the fact that an edge is non-essential does not provide information about the circumstances in which the edge can be reversed without altering the MEC; only that in some context, it can be. This realization leads us to corollary 3.

Corollary 3. *Let E_c be the set of covered edges in G, and let E_e be the set of essential edges in G. Then $E_c \subseteq \bar{E}_e$, the set of non-essential edges in G.*

Proof. This follows directly from the realization that non-essential edges can be switched while remaining in the same MEC under the correct conditions, while covered edges can be switched immediately, without regard to other edge conditions (the conditions for their reversal are always met). □

Example 4.4.3. We use the graph G from example 4.4.1 to demonstrate corollary 3. Of course, this is not sufficient for a proof, but rather helps to contextualize the lemma.

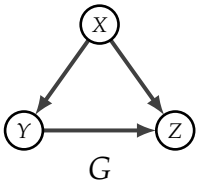


Figure 4.4.3

In example 4.4.1 we determined that all edges $e_i \in E$ of $G = (V, E)$ are non-essential, so the set of non-essential edges $E_G^N = \{(X,Y),(Y,Z),(X,Z)\}$. We can quickly see that the only covered edge of G is (Y,Z) since Y and Z share a single parent X, not including Z itself. Then, indeed, $\{(Y,Z)\} \subset E_G^N$.

Remark. There are two scenarios we consider for finding reversible edges, that is, edges which can be reversed without altering the MEC of the graph:

- Firstly, we may wish to find the set of edges which can be immediately reversed in one step, without regard to other edges in the graph. This coincides with the set of covered edges.
- Secondly, we may wish to find the set of edges which can ever be reversed within a graph, under the correct conditions of other edges being reversed beforehand/simultaneously. This coincides with the set of non-essential edges.

Theorem 4.4.1 (Edge reversal sequence. [3]). *Given two Markov equivalent DAGs G and G', there exists a sequence of distinct edge reversals in G with the following properties:*

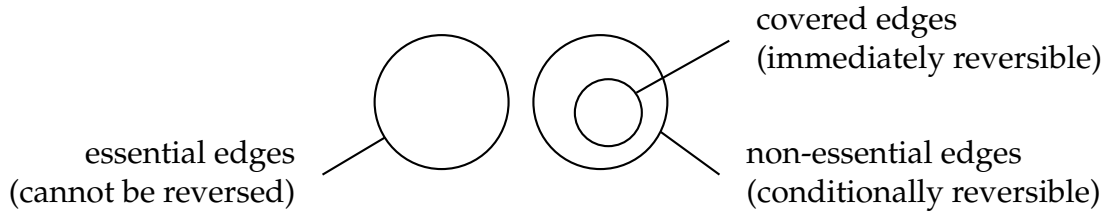


Figure 4.4.4

- *Each edge reversed in G is a covered edge,*
- *After each reversal, G is a DAG and* $G \sim_M G'$
- *After all reversals,* $G = G'$.

That is, we can transform G into G' *via a finite sequence of covered edge reversals, such that all of the intermittently resulting graphs* $G_1, G_2, ...G_n \sim_M G, G'$.

Proof. Chickering's [3] proof defines the procedure **Procedure Find-Edge** which takes a DAG G as input. At each step, the procedure identifies a next edge to reverse. To be reversible, such an edge must be covered, by Lemma 4.2.2. The proof demonstrates that such an edge is identifiable when G and G' remain unequal, and each reversal reduces the number of edges in total which must be reversed, eventually transforming G into G'. □

Chapter 5

Exploiting Markov Equivalence using Greedy Strategy

5.1 Motivation

One complication of considering Markov equivalence is that Markov equivalence classes can be quite large. None of the graphs in the MEC is necessarily a more natural representation of the probabilistic dependencies than the others.

We therefore begin by exploring a *greedy* strategy. The idea behind this strategy takes advantage of Theorem 4.4.1:

> *Given two arbitrary graphs G and G' in a family of Markov equivalent graphs, G can be transformed into G' through a finite sequence of transformations such that 1) each step in the sequence involves reversing a single directed edge, and 2) after each edge reversal, the resulting graph is contained within the same Markov equivalence class.*

This result allows us to develop the greedy strategy, an algorithm in which each step entails searching for a single edge that can be reversed without leaving the original Markov equivalence class, and simultaneously reduces the number of variables which must be sampled to answer our original query.

There are two aspects we wish to consider while searching for a reversible edge which reduces the cost of answering a query:

- Does reversing the edge alter existing v-structures in the graph, either by creating a new v-structure or destroying an existing one?

- Does switching the edge indeed benefit our query, ie, reduce the number of variables that must be considered while computing the probabilities?

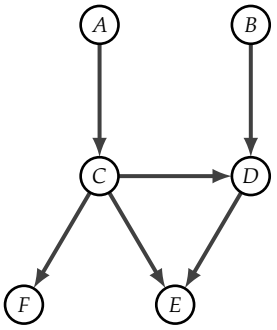
In this section, we present some relevant background, utilize a procedure from Chickering [3] to identify reversible edges, develop a framework for when edge switching is beneficial, and analyze the efficacy of the procedure for minimization.

5.2 Greedy strategy background

Chickering's [3] proof of Theorem 4.4.1 uses the algorithm Procedure Find Edge which returns and edge that can be reversed at each step. We will exploit this same algorithm to find reversible edges for our minimization, and proceed to evaluate whether the reversal is beneficial. In order to undertand the procedure, we must first make use of the following definition.

Definition 5.2.1. *Let $G = (V, E)$ be a DAG. A topological sort on G is a linear ordering of V such that for every edge $(X, Y) \in E$, vertex X comes before vertex Y in the ordering. The node with the smallest value with respect to the sort is called **minimal**. Likewise, the highest valued node is called **maximal**.*

Example 5.2.1. Topological sorts are not necessarily unique. To see this, consider the graph $G = (V, E)$ from Figure 5.2.1.



G

Figure 5.2.1

One can quickly verify that all of the following assignments of values to vertices are valid topological sorts. This is not an exhaustive list, but demonstrates that multiple orderings are possible.

A	B	C	D	E	F
1	2	3	4	6	5
2	1	4	3	5	6
2	1	5	3	5	6

Lemma 5.2.1. *All DAGS have at least one valid topological ordering.*

Algorithm 1: COVERED EDGES returns a covered edge in a DAG

Input: Two equivalent DAGs $G = (V, E)$ and $G'(V', E')$ that differ by at least one edge

Output: An edge which differs between G and G'

1 Perform a topological sort on the nodes in G.

2 Let Y be the minimal node with respect to the topological sort for which $\prod_Y^G \neq \emptyset$.

3 Let X be the maximal node with respect to the sort for which $X \in \prod_Y^P$.

return (X, Y)

Lemma 5.2.2. *The edge (X, Y) output from Algorithm 1 is a covered edge.*

5.3 Implementation

5.4 Cost

Chapter 6

Comparison of methods

A comparison of the speed of normal querying VS the speed of the new query + time required to exploit ME.
Ultimately trying to answer the questions:

- Can we do faster inference?
- Under what circumstances is it possible/effective?
- How much faster is it?
- Maybe include a section on future work in this chapter.

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