Query the model: precomputations for efficient inference with Bayesian Networks

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ABSTRACT
Probabilistic models learned from a database can be used for the purposes of approximate query processing and predictive querying, two tasks that must be performed at interactive speeds in many real-life settings. In this paper, we propose a novel approach towards speeding up query evaluation over a probabilistic model by materializing a set of probabilistic quantities involved in query evaluation. Specifically, we consider a scenario where a Bayesian network is built over a relational database to represent the joint distribution of data attributes, and we address the problem of choosing a set of intermediate relational tables to materialize so as to maximize the expected efficiency gain in query-response time over a given workload of queries. We provide an optimal polynomial-time algorithm for the problem we consider and further discuss other alternative methods. We validate our technique using Bayesian networks learned from benchmark data. Our experimental results confirm that a small set of materialized factors with modest memory space requirements can lead to significant improvements in the running time of queries, reaching up to an average gain of 70% over a uniform workload of queries.

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1. INTRODUCTION
Research in machine learning has led to powerful methods for building probabilistic models for general predictive tasks [3]. As a result, machine learning is currently employed in a wide range of fields, enabling us to automate tasks that until recently were seen as particularly challenging. Examples include image and speech recognition [25, 26], natural language processing [14], and machine translation [30].

Moreover, as several researchers have pointed out recently, the database management systems (DBMS) [19]. For instance, a database system can employ machine-learning techniques to learn a probabilistic model from the data, such as a Bayesian network, which captures the dependencies among values of different attributes, and subsequently use the model either for approximate query processing, i.e., to produce approximate answers for queries about the data already stored in the database, or to answer predictive queries, i.e., to infer the attributes of future data entries. The case is further illustrated with the application scenarios below.

Approximate query answering: We are interested in analyzing a survey database [29], a small extract of which is shown in Figure 1. The database consists of a single table with variables A (age); indicating the age bracket of a person as young, adult, or old; S (sex): which can be female or male; E (education level): indicating whether a person has finished high-school or university; O (occupation): indicating whether a person is employed or self-employed; R (size of residence city): which can be small or big; and T (means of transportation): which takes values train, car, or other. The database is managed by a DBMS that enables its users to ask queries over the data. For example, consider the following two queries.

Query A: what fraction of the population are young females who commute by car?
Query B: among young females who commute by car, what fraction live in big cities?

To answer each query exactly, the DBMS could simply make a scan over the entire database and evaluate the requested quantity. However, a scan is often too expensive to perform and in many application scenarios exact answers are unnecessary; instead approximate answers are satisfactory. To accomplish this goal, the approximate query-answering component of the DBMS learns a Bayesian-network model over the joint distribution of the data attributes, which approximates the observed data distribution within some error range. When the user submits a query, it is translated into a probabilistic quantity that corresponds to the query, the value of which is calculated from the learned model and serves as an approximate answer to the query. For example, the aforementioned queries correspond to the following marginal and conditional probabilities, respectively.

Query A: Pr(A = young, S = female, T = car)
Query B: Pr(R = big | A = young, S = female, T = car)

Note that answering such queries through the learned model can be vastly more efficient than scanning the entire database.
The use of probabilistic models has been proposed for tasks in the search community assesses existing approaches and searches for new ways forward [3, 10, 13] – with some researchers formalizing the uncertainty associated with approximate answers returned by previous queries. Of course, it should be noted that it is not only recently that the use of probabilistic models is being considered. The network is a directed acyclic graph (each directed edge between two variables represents a dependency of the child on the parent) of a Bayesian network, which can be used to model the joint distribution of database attributes, as they have in 2001 how Bayesian network models could be used for selective estimation that moved beyond simplistic independence assumptions. Our work is in the same spirit of Getoor et al. [12]. In particular, we consider the problem setting that we consider in this paper. We start our development by considering the following.

**Predictive queries**: The same system employs a similar approach for predictive queries such as the following.

**Query A’**: what is the probability that a person added to the database is a young female who commutes by car?

**Query B’**: what is the probability that a person added to the database lives in a big city, given that she is a young female who commutes by car?

Unlike the approximate query-answering scenario, in which queries requested quantities directly measurable from the available data, the two queries above request a prediction over unseen data. Nevertheless, queries A’ and B’ correspond to marginal and conditional probabilities that share the same expression as queries A and B, respectively. The only difference between the two scenarios is that, while for approximate query answering the probabilities are evaluated over a model that is optimized to approximate the existing data, for predictive queries the probabilities are evaluated over a model that is optimized for generalized performance over possibly unseen data.

As the two scenarios above suggest, machine learning finds natural application in the tasks of approximate query processing and predictive querying: learning a probabilistic model for the joint distribution of database attributes allows the system to answer a very general class of queries, the answers to which can be evaluated via probabilistic quantities from the model; with no need for potentially expensive access to the data. Probabilistic models such as Bayesian networks offer several advantages over traditional approximate query-processing approaches that use synopses. In particular, probabilistic models allow us to work with distributions rather than single values. This is useful in cases where we are interested in the variance or modality of numerical quantities. Moreover, these models typically extend gracefully to regions of the data space for which we have observed no data. For example, for predictive queries over relational databases with a large number of attributes, it is important to assign non-zero probability to all possible tuples, even for combinations of attribute values that do not exist in the database, yet. And most importantly, since probabilistic models are learned from data (or, fit to the data), their complexity is adjusted to the complexity of the data at hand. This allows us to have very concise representations of the data distribution even for a large number of attributes. For example, one can typically learn from data a very sparse Bayesian network to represent dependencies among a large number of attributes, while, by comparison, synopses like multi-dimensional histograms would suffer to represent high-dimensional data.

In this work, we opt for Bayesian networks to model the joint distribution of database attributes, as they have intuitive interpretation, adapt easily to settings of varying complexity, and have been studied extensively for many years. In what follows, we do not argue further about why this is a good choice for approximate query processing and predictive queries; the interested reader can find a very good treatment of the topic by Getoor et al. [12]. By contrast, we focus on the issue of efficiency, as inference in Bayesian networks is NP-hard [7], thus one cannot conclude the possibility that the evaluation of some queries proves expensive for practical settings.

How can we mitigate this risk? Our key observations are the following: first, the evaluation of probabilities over the Bayesian-network model involves intermediate results, in the form of relational tables, which are costly to compute every time a query requests them; second, same intermediate tables can be used for the evaluation of many different queries. Based on these observations, we set to precompute and materialize the intermediate relational tables that bring the largest computational benefit, i.e., those that are involved in the evaluation of many expensive queries. The problem formulation is general enough to accommodate arbitrary query workloads and takes as input a budget constraint on the number of intermediate relational tables one can afford to materialize (Section 3).

Our contributions are the following: (i) an exact polynomial-time algorithm to choose an optimal materialization (Section 4.1); (ii) a greedy algorithm with approximation guarantees (Section 4.2); (iii) a pseudo-polynomial algorithm to address the problem under a budget constraint on the space used for materialization (Section 5.1); (iv) a further-optimized computational scheme that avoids query-specific redundant computations (Section 5.2); (v) experi-

**Figure 1**: Learning a probabilistic model for the joint distribution of data attributes allows the system to produce fast, approximate answers to queries about the data, but also answer predictive queries. The survey dataset and corresponding Bayesian network illustrated here are found in the book of Scutari and Denis [29].
ments over real data, showing that by materializing only a few intermediate tables, one can significantly improve the running time of queries, reaching up to an average gain of 70% over a uniform workload of queries (Section 6).

To make the paper self-contained, we review the required background material in Section 3.

2. RELATED WORK

Bayesian networks or “directed graphical models” are probabilistic models that capture global relationships among a set of variables, through local dependencies between small groups of variables [28]. This combination of complexity and modularity makes them suitable for general settings where one wishes to represent the joint distribution of a large number of variables (e.g., the column attributes of a large relational table). Bayesian networks have intuitive interpretation captured by the structure of a directed graph (each directed edge between two variables represents a dependency of the child on the parent variables) and probabilities based on the model can be expressed with compact sums-of-products. For exact inference, i.e., exact computation of marginal and conditional probabilities, the conceptually simplest algorithm is variable elimination [31], which follows directly the formula for joint probability under the model. The main other algorithm for exact inference is the Junction-tree algorithm [16, 20], which is based on “message passing” among variables and is quite more elaborate than variable elimination. For Bayesian networks of tree structure, simpler message-passing algorithms exist, e.g., the sum-product algorithm [4]. As this paper is the first work to address materialization for Bayesian networks, we opt to work with variable elimination [31] due to its conceptual simplicity. However, it is possible to show that a similar approach is applicable for message-passing algorithms.

Machine learning for approximate query processing. Approximate answers to queries are often not only sufficient, but also computable faster than exact answers. Traditionally, approximate query processing is based on data synopses [4] of various types, such as samples, histograms, wavelets, and lately coresets [3]. Synopses are summaries of the data that preserve information about quantities of interest and can be used to answer queries about them. Today, there is renewed interest in approximate query processing, as the research community assesses existing approaches and searches for new ways forward [6, 15, 21] — with some researchers pointing out that probabilistic models are a natural way to formalize the uncertainty associated with approximate answers and existing machine-learning techniques can be used to build and use models for approximate query processing [15, 19, 21]. For example Park et al. [27] use Gaussian Processes to model the similarity of (approximately answered) queries, allowing them to obtain increasingly accurate results to new queries, based on the answers to previous queries. Of course, it should be noted that the use of probabilistic models has also been proposed before for tasks in the context of DBMSs. For example, Getoor et al. [12] explained in 2001 how Bayesian networks can be used for selectivity estimation that moved beyond simplistic independence assumptions. Our work is in the same spirit of Getoor et al. [12] in the sense that it assumes a Bayesian network is used to model dependencies between data attributes, but it addresses a different technical problem, i.e., the problem of optimal materialization for efficient usage of the model.

3. SETTING AND PROBLEM STATEMENT

A Bayesian network $\mathcal{N}$ is a directed acyclic graph (DAG), where nodes represent variables and edges represent dependencies among variables. Each node is associated with a table quantifying the probability that the node takes a particular value conditionally on values of its parents. For instance, if a node associated with a $\nu$-ary variable $a$ has $k$ parents, all of which are $\nu$-ary variables, the associated probability distribution for a is a table with $\nu^{k+1}$ entries.

One key property of Bayesian networks is that, conditional on the values of its parents, a variable is independent of other variables. This property leads to simple formulas for the evaluation of marginal and conditional probabilities. For example, for the network of Figure 1, the joint probability of all variables is given by

$$\Pr(A, S, E, O, R, T) = \Pr(T \mid O, R) \Pr(O \mid E) \Pr(R \mid E) \Pr(E \mid A, S) \Pr(A) \Pr(S).$$

Each factor on the right-hand side of Equation 1 is part of the specification of the Bayesian network and represents the marginal and conditional probabilities of its variables.

In what follows, we assume that a Bayesian network $\mathcal{N}$ has been learned from a relational database, with each variable corresponding to one relational attribute. While in the example of Figure 1 the Bayesian network has only 6 variables, in many applications we have networks with hundreds or thousands of variables. Here we assume that all variables are categorical; numerical variables can be discretized in categorical intervals. In many cases, access to the probability tables of a Bayesian network can replace access to the original data; indeed, we can answer queries via the Bayesian-network model rather than through direct processing of potentially huge volumes of data. As discussed in the introduction, this approach is not only more efficient, but it can also lead to more accurate estimates as it avoids over-fitting.

Querying the Bayesian network. We consider the task of answering probabilistic queries over the model defined by a Bayesian network $\mathcal{N}$. For instance, for the model shown in Figure 1, example queries are: “what is the probability that a person is a university-graduate female, lives in a small city, and is self employed?” or “for each possible means of transport, what is the probability that a person is young and uses the particular means of transport?” More precisely, we consider queries of the form

$$q = \Pr(X_q, Y_q = y_q),$$

where $X_q \subseteq X$ is a set of free variables and $Y_q \subseteq X$ is a set of bound variables with corresponding values $y_q$. Notice that free variables $X_q$ are the ones for which the query requests a probability for each of their possible values. For the examples above, the first query is answered by the probability $\Pr(S = \text{female}, E = \text{uni}, O = \text{self}, R = \text{small})$, and the second by the distribution $\Pr(T, A = \text{young})$.

We denote by $Z_q = X \setminus (X_q \cup Y_q)$ the set of variables that do not appear in the query $q$. The variables in the set $Z_q$ are those that need to be summed out in order to
compute the query \( q \). Specifically, query \( q \) is computed via the summation
\[
\Pr(X_q, Y_q = y_q) = \sum_{z_q} \Pr(X_q, Y_q = y_q, Z_q). \tag{3}
\]
The answer to the query \( \Pr(X_q, Y_q = y_q) \) is a table indexed by combinations of values of variables \( X_q \). Note that conditional probabilities of the form \( \Pr(X_q | Y_q = y_q) \) can be computed from the corresponding joint probabilities by
\[
\Pr(X_q | Y_q = y_q) = \frac{\Pr(X_q, Y_q = y_q)}{\Pr(Y_q = y_q)} = \frac{\Pr(X_q, Y_q = y_q)}{\sum_{X_q} \Pr(X_q, Y_q = y_q)},
\]
thus without loss of generality, we focus on queries of type (2).

**Answering queries.** The variable-elimination algorithm, proposed by Zhang et al. [31] to answer queries \( q = \Pr(X_q, Y_q = y_q) \), introduces the concept of elimination tree. The algorithm computes \( q \) by summing out the variables \( Z_q \) that do not appear in \( q \), according to Equation (3). When we sum out a variable, we say that we eliminate it. The elimination tree represents the order in which variables are eliminated and the intermediate results that are passed along.

**Variable elimination.** We eliminate variables according to a total order \( \sigma \) on variables that is given as input and considered fixed hereafter. For example, for the Bayesian network of Figure 1, one possible order is \( \sigma = (A, S, T, E, O, R) \).

A query \( q \) can be computed by brute-force elimination in two steps. In the first step, compute into a table \( H \) the joint probability for each combination of values of all variables. In the second step, process variables sequentially in the order of \( \sigma \): for a variable \( a \in Y_q \), select those entries of \( H \) that satisfy the corresponding equality condition in \( Y_q = y_q \); for a variable \( a \in Z_q \) compute a sum over each group of values of variables that have not been processed so far (thus “summing out” the variable); and finally for a free variable \( a \in Y_q \), no computation is needed. The table that results from this process is the answer to query \( q \).

The variable-elimination algorithm by Zhang et al. improves upon brute-force elimination by observing that it is not necessary to compute \( H \). To see why, let us consider again the query \( q = \Pr(T, A = \text{young}) \) and order \( \sigma = (A, S, T, E, O, R) \). In this example, we have \( X_q = \{T\}, Y_q = \{A\} \), and \( Z_q = \{S, E, O, R\} \). The first variable in \( \sigma \) is \( A \in Y_q \). The brute-force algorithm would first compute a natural join over all factors in Equation (1) and then select those rows that match the condition \( (A = \text{young}) \). An equivalent but more efficient computation is to consider first only the tables of those factors that include variable \( A \) and select only the rows that satisfy the equality condition \( (A = \text{young}) \); then perform the natural join over the resulting tables. This computation corresponds to the following two equations.

\[
\psi_A(S, E; A = \text{young}) = \Pr(E | A = \text{young}, S) \Pr(A = \text{young}) \Pr(A = \text{young}, S, E, O, R, T) \psi_S(S, E; A = \text{young}) \Pr(T | O, R) \Pr(O | E) \Pr(R | E) \Pr(S). \tag{4}
\]

The crucial observation is that the equality condition \( (A = \text{young}) \) concerns only two factors of the joint probability formula. After processing variable \( A \) these two factors can be replaced by a factor \( \psi_A(S, E; A = \text{young}) \), a table indexed by \( S \) and \( E \) and containing only entries with \( (A = \text{young}) \).

We can continue repeatedly for the remaining variables. Let us consider how to sum out \( S \in Z_q \), the second variable in \( \sigma \). Instead of a brute-force approach, a more efficient computation is to compute a new factor by summing out \( S \) over only those factors that include \( S \); and use the new factor to perform a natural join with the remaining factors.

\[
\psi_S(E; A = \text{young}) = \sum_S \psi_A(S, E; A = \text{young}) \Pr(S) \Pr(A = \text{young}, S, E, O, R, T) = \psi_S(E; A = \text{young}) \Pr(T | O, R) \Pr(O | E) \Pr(R | E). \tag{5}
\]

Again, the crucial observation is that \( S \) appears in only two factors of Equation (4), which, after the summation over \( S \), can be replaced by a factor \( \psi_S(E; A = \text{young}) \), a table indexed by \( E \) and containing only entries with \( (A = \text{young}) \).

The third variable in \( \sigma \) is the free variable \( T \in X_q \). As with the previous two cases, the processing of a free variable corresponds to the computation of a new factor from the natural join over all factors that involve it. Unlike the previous cases, however, where the natural join was followed by a selection of a subset of entries or a summation, no such operation is applied on the natural join in this case. This computation corresponds to the two equations below.

\[
\Psi_T(O, R; T) = \Pr(T | O, R) \Pr(A = \text{young}, E, O, R, T) = \psi_T(O, R; T) \Pr(O | E) \Pr(R | E). \tag{6}
\]

As in the previous cases, the factors that involve \( T \) (in this example it is only \( \Pr(T | O, R) \)) are replaced with a factor \( \psi_T(O, R; T) \), the table of which is indexed by variables \( O \) and \( R \), but also contains a column for free variable \( T \).

The procedure described above for the first three variables of \( \sigma \) is repeated for the remaining variables, and constitutes the variable-elimination algorithm [31]. To summarize, the variable-elimination algorithm considers variables \( a \) in the order of \( \sigma \). If \( a \in Y_q \) or \( a \in Z_q \), the algorithm computes a natural join over the factors that involve \( a \); it performs a selection or group summation, respectively, and uses the result to replace the factors that involve \( a \).

**Elimination tree.** The variable-elimination algorithm gives rise to a graph, like the one shown in Figure 2, for the example we discussed. Each node is associated with a factor and there is a directed edge between two factors if one is used for the computation of the other. In particular, each leaf node corresponds to one of the factors that define the Bayesian network. In our running example, these are the factors that appear in Equation (1). Each internal node corresponds to a factor that is computed from its children (i.e., the factors that correspond to its incoming edges), and replaces them in the variable-elimination algorithm. Moreover, as we saw, each internal node corresponds to one variable. The last factor computed is the answer to the query.

Notice that the graph constructed in this manner is either a tree or a forest. It is not difficult to see that the elimination graph is a tree if and only if the corresponding Bayesian network is a weakly connected DAG. To simplify our discussion, we will focus on connected Bayesian networks and deal with an elimination tree \( T \) for each query. All our results can be directly extended to the case of forests.
Notice that the exact form of the factor for each internal node of $T$ depends on the query. For the elimination tree in Figure 2 we have factor $\psi_4(S,E,A = \text{young})$ on the node that corresponds to variable $A$. However, if the query contained variable $A$ as a free variable rather than bound to value $A = \text{young}$, then the same node in $T$ would contain a factor $\psi_4(S,E;A)$. And if the query did not contain variable $A$, then the same node in $T$ would contain a factor $\psi_4(S,E)$. On the other hand, the structure of the tree, the factors that correspond to leaf nodes and the variables that index the variables of the factors that correspond to internal nodes are query-independent.

**Note.** The elimination algorithm we use here differs slightly from the one presented by Zhang et al. [31]. Specifically, the variable-elimination algorithm of Zhang et al. computes the factors associated with the bound variables $Y_i$ at a special initialization step, which leads to benefits in practice (even though the running time remains super-polynomial in the worst case). On the other hand, we compute factors in absolute accordance with the elimination order. This allows us to consider the variable-elimination order fixed for all variables independently of the query.

**Materialization of factors.** Materializing factor tables for internal nodes of the elimination tree $T$ can speed up the computation of queries that require those factors. As we saw in the previous example, factors are computed in a sequence of steps, one for each variable, and each step involves the natural join over other factor tables, followed by: (i) either variable summation (to sum-out variables $Z_i$); or (ii) row selection (for variables $Y_i$); or (iii) no operation (for variables $X_i$). In what follows, we focus on materializing factors that involve only variable summation, the first out of these three types of operations. Materializing such factors is often useful for multiple queries $q$ and sufficient to make the case for the materialization of factors that lead to the highest performance gains over a given query workload. Dealing with the materialization of general factors is a rather straightforward albeit non-trivial extension which, due to space constraints, will be the topic of future work.

To formalize our discussion, let us introduce some notation. Given a node $u \in V$ in an elimination tree $T$, we write $T_u$ to denote the subtree of $T$ that is rooted in node $u$. We also write $X_u$ to denote the subset of variables of $X$ that are associated with the nodes of $T_u$. Finally, we write $A_u$ to denote the set of ancestors of $u$ in $T$, that is, all nodes between $u$ and the root of the tree $T$, excluding $u$.

Computing a factor for a query $q$ incurs a computational cost. We distinguish two notions of cost: first, if the children factors of a node $u$ in the elimination tree $T$ are given as input, computing $u$ incurs a partial cost of computing the factor of $u$ from its children; second, starting from the factors that define the Bayesian network, the total cost of computing a node includes the partial costs of computing all intermediate factors, from the leaf nodes to $u$. Formally, we have the following definitions.

**Definition 1 (Partial-Cost).** The partial cost $c(u)$ of a node $u \in V$ in the elimination tree $T = (V,E)$ is the computational effort required to compute the corresponding factor given the factors of its children nodes.

**Definition 2 (Total-Cost).** The total cost of a node $u \in V$ in the elimination tree $T = (V,E)$ is the total cost of computing the factor at node $u$, i.e.,

$$b(u) = \sum_{x \in T_u} c(x),$$

where $c(x)$ is the partial cost of node $x$.

When we say that we materialize a node $u \in V$, we mean that we materialize the factor that is the result of summing out all variables below it on $T$. When is a materialized factor useful for a query $q$? Intuitively, it is useful if it is one of the factors computed during the evaluation of $q$, in which case we save the total cost of computing it from scratch, provided that there is no other materialized factor that could be used in its place, with greater savings in cost. The following definition of usefulness formalizes this intuition.

**Definition 3 (Usefulness).** Let $q = \Pr(X_q; Y_q = y_q)$ be a query, and $R \subseteq V$ a set of nodes of the elimination tree $T$ that are materialized. We say that a node $u \in V$ is useful for the query $q$ with respect to the set of nodes $R$, if (i) $u \in R$; (ii) $X_u \subseteq Z_q$; and (iii) there is no other node $v \in A_u$ for which conditions (i) and (ii) hold.

To indicate that a node $u$ is useful for the query $q$ with respect to a set of nodes $R$ with materialized factors, we use the indicator function $\delta_q(u; R)$. That is, $\delta_q(u; R) = 1$ if node $u \in V$ is useful for the query $q$ with respect to the set of nodes $R$, and $\delta_q(u; R) = 0$ otherwise.

When a materialized node is useful for a query $q$, it saves us the total cost of computing it from scratch. Considering a query workload, where different queries appear with different probabilities, we define the benefit of a set of materialized nodes $R$ as the total cost we save in expectation.

![Figure 2: The elimination tree $T$ for query $q = \Pr(T, A = \text{young})$ and order of variables $\sigma = (A, S, T, E, O, R)$.](image)
**Definition 4 (Benefit).** Consider an elimination tree \( T = (V, E) \), a set of nodes \( R \subseteq V \), and query probabilities \( \Pr(q) \) for the set of all possible queries \( q \). The benefit \( B(R) \) of the node set \( R \) is defined as:

\[
B(R) = \sum_q \Pr(q) \sum_{u \in R} \delta_q(u; R) b(u)
\]

\[
= \sum_{u \in R} \Pr(\delta_q(u; R) = 1) b(u)
\]

\[
= \sum_{u \in R} E[\delta_q(u; R)] b(u).
\]

**Problem definition.** We can now define formally the problem we consider: for a space budget \( K \), our goal is to select a set of factors to materialize to achieve optimal benefit.

**Problem 1.** Given a Bayesian network \( \mathcal{N} \), an elimination tree \( T = (V, E) \) for answering probability queries over \( \mathcal{N} \), and budget \( K \), select a set of nodes \( R \subseteq V \) to materialize, whose total size is at most \( K \), so as to optimize \( B(R) \).

For simplicity of exposition we also consider a version of the problem where we are given a total budget \( k \) on the number of nodes that we can materialize. We first present algorithms for Problem 2 in Section 4.2 and discuss how to address the more general Problem 1 in Section 5.

**Problem 2.** Given a Bayesian network \( \mathcal{N} \), an elimination tree \( T = (V, E) \) for answering probability queries over \( \mathcal{N} \), and an integer \( k \), select at most \( k \) nodes \( R \subseteq V \) to materialize so as to optimize \( B(R) \).

### 4. ALGORITHMS

This section focuses on algorithms for Problem 2. Section 4.1 presents an exact polynomial-time dynamic-programming algorithm; and Section 4.2 discusses a greedy algorithm, which yields improved time complexity but provides only an approximate solution, yet with quality guarantee.

#### 4.1 Dynamic programming

We discuss our dynamic-programming algorithm in three steps. First, we introduce the notion of partial benefit that allows us to explore partial solutions for the problem. Second, we demonstrate the optimal-substructure property of the problem, and third, we present the algorithm.

**Partial benefit.** In Definition 1, we defined the (total) benefit of a subset of nodes \( R \subseteq V \) (i.e., a potential solution) for the whole elimination tree \( T \). Here we define the partial benefit of a subset of nodes \( R \) for a subtree \( T_u \) of a given node \( u \) of the elimination tree \( T \).

**Definition 5 (Partial benefit).** Consider an elimination tree \( T = (V, E) \), a subset of nodes \( R \subseteq V \), and probabilities \( \Pr(q) \) for the set of all possible queries \( q \). The partial benefit \( B_u(R) \) of the node set \( R \) at a given node \( u \in V \) is

\[
B_u(R) = \sum_{v \in R \cap T_u} E[\delta_q(v; R)] b(v).
\]

The following lemma states that, given a set of nodes \( R \), and a node \( u \in R \), the probability that \( u \) is useful for a random query with respect to \( R \) depends only on the lowest ancestor of \( u \) in \( R \).

**Lemma 1.** Consider an elimination tree \( T = (V, E) \) and a set \( R \subseteq V \) of nodes. Let \( u, v \in R \) such that \( v \in A_u \) and path(\( u, v \)) \( \cap R = \emptyset \). Then we have:

\[
E[\delta_q(u; R)] = E[\delta_q(u; v)],
\]

where the expectation is taken over a distribution of queries \( q \).

**Proof.** To prove the lemma, we will show that for any query \( q \), it is \( \delta_q(u; R) = 1 \) if and only if \( \delta_q(u; v) = 1 \).

We first show that \( \delta_q(u; R) = 1 \) implies \( \delta_q(u; v) = 1 \). From Definition 3, we have that \( \delta_q(u; R) = 1 \) if \( X_u \subseteq Z_q \) and there is no \( w \in A_u \cap R \) such that \( X_w \subseteq Z_q \). Given that \( \delta_q(u; R) = 1 \) and \( v \in A_u \cap R \), it follows that \( X_v \subseteq Z_q \), hence, \( \delta_q(u; v) = 1 \). Conversely, we show that \( \delta_q(u; v) = 1 \) implies \( \delta_q(u; R) = 1 \). Notice that \( \delta_q(u; v) = 1 \) if \( X_u \subseteq Z_q \) and \( X_v \subseteq Z_q \) since \( X_v \subseteq X_w \). Given also that path(\( u, v \)) \( \cap R = \emptyset \), we have that for all \( w \in R \cap A_u \), it is \( X_w \subseteq Z_q \), hence, \( \delta_q(u; R) = 1 \).

Given the one-to-one correspondence between the set of queries in which \( \delta_q(u; R) = 1 \) and the set of queries in which \( \delta_q(u; v) = 1 \), we have \( \sum_q \Pr(q) \delta_q(u; R) = \sum_q \Pr(q) \delta_q(u; v) \), hence, the result follows.

Building upon Lemma 1 we arrive to Lemma 2 below, which states that the partial benefit \( B_u(R) \) of a node-set \( R \) at a node \( u \) depends only on (i) the nodes of \( T_u \) that are included in \( R \), and (ii) the lowest ancestor \( v \) of \( u \) in \( R \), and therefore it does not depend on what other nodes “above” \( v \) are included in \( R \).

For the proof of Lemma 2 we introduce some additional notation. Let \( T = (V, E) \) be an elimination tree, \( u \) a node of \( T \), and \( T_u \) the subtree of \( T \) rooted at \( u \). Let \( R \subseteq V \) be a set of nodes. For each node \( w \in T_u \cap R \), we define \( a_w^R \) to be the lowest ancestor of \( w \) that is included in \( R \).

**Lemma 2.** Consider an elimination tree \( T = (V, E) \) and a node \( u \in V \). Let \( v \in A_u \) be an ancestor of \( u \). Consider two sets of nodes \( R \) and \( R' \) for which

(i) \( v \in R \) and \( v \in R' \);

(ii) \( T_u \cap R = T_u \cap R' \); and

(iii) path(\( u, v \)) \( \cap R = \text{path}(u, v) \cap R' = \emptyset \).

Then, we have: \( B_u(R) = B_u(R') \).

**Proof.** From direct application of Lemma 1, we have \( E[\delta_q(w; R)] = E[\delta_q(w; a_w^R)] \), for all \( w \in T_u \cap R \), and similarly, we have \( E[\delta_q(w; R')] = E[\delta_q(w; a_w^{R'})] \) for all \( w \in T_u \cap R' \). Now, given that \( T_u \cap R = T_u \cap R' \) and path(\( u, v \)) \( \cap R = \text{path}(u, v) \cap R' = \emptyset \), we have \( a_w^R = a_w^{R'} \), for all \( w \in T_u \cap R \); and similarly \( a_w^R = a_w^{R'} \), for all \( w \in T_u \cap R' \). It then follows that for all \( w \in T_u \cap R \), we have \( E[\delta_q(w; R)] = E[\delta_q(w; R')] \).

Putting everything together, we get

\[
B_u(R) = \sum_{w \in R \cap T_u} E[\delta_q(w; R)] b(w)
\]

\[
= \sum_{w \in R \cap T_u} E[\delta_q(w; R')] b(w) = B_u(R').
\]
adds $\epsilon$ into $A_u$. Notice that $\text{path}(u, \epsilon)$ corresponds to the set of ancestors of $u$ including the root $r$, i.e., $\text{path}(u, \epsilon) = A_u$.

**Optimal substructure.** In Lemma 3, we present the optimal-substructure property for Problem 2. Lemma 3 builds upon Lemma 2 and states that among nodes of the optimal solution, the subset of nodes that fall within a given subtree depends only on the nodes of the subtree and the lowest ancestor of the subtree that is included in the optimal solution.

**Lemma 3 (Optimal Substructure).** Given an elimination tree $T = (V, E)$ and an integer $k$, let $R^*$ denote the optimal solution to Problem 2. Consider a node $u \in V$ and let $v \in A_u$ be the lowest ancestor of $u$ that is included in $R^*$. Let $R_u^* = T_u \cap R^*$ denote the set of nodes in the optimal solution that reside in $T_u$ and let $r_u^* = |T_u \cap R^*|$. Then,

$$R_u^* = \arg \max_{R_u \subseteq T_u} \{B_u(R_u \cup \{v\})\}.$$  

**Proof.** First, notice that the sets $R^*$ and $R_u^* \cup \{v\}$ satisfy the pre-conditions of Lemma 2 and thus,

$$B_u(R^*) = B_u(R_u^* \cup \{v\}). \quad (7)$$

Now, to achieve a contradiction, assume that there exists a set $R_u \neq R_u^*$ such that $|R_u^*| = r_u^*$ and

$$B_u(R_u^* \cup \{v\}) < B_u(R_u \cup \{v\}). \quad (8)$$

Let $R' = (R^* \setminus R_u^*) \cup R_u$ denote the solution obtained by replacing the node set $R_u^*$ in $R^*$ by $R_u$. Again $R'$ and $R_u^* \cup \{v\}$ satisfy the preconditions of Lemma 2 and thus,

$$B_u(R') = B_u(R_u^* \cup \{v\}). \quad (9)$$

As before, for $w \in R^* \setminus R_u^*$ we define $a_w^{R^*}$ and $a_w^{R_u^*}$ to be the lowest ancestor of $w$ in $R^*$ and in $R_u^*$, respectively. Given that $w \notin T_u$, we have $a_w^{R_u^*} = a_w^{R'}$, hence, for all $w \in R^* \setminus R_u^*$:

$$E[\delta_q(w; R^*)] = E[\delta_q(w; R')] \quad (10)$$

Putting together Equations (7-10) we get

$$B(R') = \sum_{w \in R'} E[\delta_q(w; R')] b(w)$$

$$= \sum_{w \in R_u} E[\delta_q(w; R_u)] b(w) + \sum_{w \in R^* \setminus R_u^*} E[\delta_q(w; R')] b(w)$$

$$= B_u(R_u^* \cup \{v\}) + \sum_{w \in R^* \setminus R_u^*} E[\delta_q(w; R')] b(w)$$

$$> B_u(R_u^* \cup \{v\}) + \sum_{w \in R^* \setminus R_u^*} E[\delta_q(w; R^*)] b(w)$$

$$= \sum_{w \in R_u^*} E[\delta_q(w; R^*)] b(w) + \sum_{w \in R^* \setminus R_u^*} E[\delta_q(w; R^*)] b(w)$$

$$= B(R^*)$$

which is a contradiction since $R^*$ is the optimal solution of Problem 2 and thus, $B(R') \geq B(R^*)$.

The following lemma provides a bottom-up approach to combine partial solutions computed on subtrees. We note that in the rest of the section, we present our results on binary trees. This assumption is made without any loss of generality as any $d$-ary tree can be converted into a binary tree by introducing dummy nodes; furthermore, by assigning appropriate cost to dummy nodes, we can ensure that they will not be selected by the algorithm.

**Lemma 4 (Additivity).** Consider an elimination tree $T = (V, E)$, a node $u \in V$, and a set $R_u$ of nodes in $T_u$. Let $r(u)$ and $\ell(u)$ be the right and left children of $u$, and let $R_{r(u)} = T_{r(u)} \cap R_u$ and $R_{\ell(u)} = T_{\ell(u)} \cap R_u$. Then, for any node $v \in A_u$ it is

$$B_u(R_u \cup \{v\}) = \begin{cases} B_u(\{u, v\}) + B_{r(u)}(R_{r(u)} \cup \{u\}) + B_{\ell(u)}(R_{\ell(u)} \cup \{v\}), & \text{if } u \in R_u \setminus R_{r(u)} \\ B_u(\{u, v\}) + B_{r(u)}(R_{r(u)} \cup \{u\}) + B_{\ell(u)}(R_{\ell(u)} \cup \{\ell(u)\}), & \text{otherwise.} \end{cases}$$

**Proof.** We show the result in the case of $u \in R_u$: notice that since $u \in R_u$ the node $v$ cannot be the lowest solution ancestor of any node in $R_{r(u)} \cup R_{\ell(u)}$. Given also that no node in $R_{r(u)}$ can have an ancestor in $R_{\ell(u)}$ and vice versa, following Lemma 1 we have:

$$B_u(R_u \cup \{v\}) = \sum_{w \in R_u} E[\delta_q(w; R_u \cup \{v\})] b(w)$$

$$= E[\delta_q(u; v)] b(u) + \sum_{w \in R_{r(u)}} E[\delta_q(w; R_{r(u)} \cup \{u\})] b(w)$$

$$+ \sum_{w \in R_{\ell(u)}} E[\delta_q(w; R_{\ell(u)} \cup \{u\})] b(w)$$

$$= B_u(\{u, v\}) + B_{r(u)}(R_{r(u)} \cup \{u\}) + B_{\ell(u)}(R_{\ell(u)} \cup \{u\}).$$

The case $u \notin R_u$ is similar and we omit the details for brevity. □

**Dynamic programming.** Finally, we discuss how to use the structural properties shown above in order to devise the dynamic-programming algorithm. We first define the data structures that we use. Consider a node $u$ in the elimination tree, a node $v \in A_u$, and an integer $\kappa$ between 1 and $\min\{k, |T_u|\}$. We define $F(u, \kappa, v)$ to be the optimal value of partial benefit $B_u(R)$ over all sets of nodes $R$ that satisfy the following three conditions:

(i) $|T_u \cap R| \leq \kappa$;

(ii) $v \in R$; and

(iii) $\text{path}(u, v) \cap R = \emptyset$.

Condition (i) states that the node set $R$ has at most $\kappa$ nodes in the subtree $T_u$; condition (ii) states that node $v$ is contained in $R$; and condition (iii) states that no other node between $u$ and $v$ is contained in $R$, i.e., node $v$ is the lowest ancestor of $u$ in $R$.

For all $u$, $v$, $\kappa$, and sets $R$ that satisfy conditions (i)-(iii) we also define $F^+(u, \kappa, v)$ and $F^-(u, \kappa, v)$ to denote the optimal partial benefit $B_u(R)$ for the cases when $u \in R$ and $u \notin R$, respectively. Hence, we have

$$F(u, \kappa, v) = \max\{F^+(u, \kappa, v), F^-(u, \kappa, v)\}.$$
Algorithm 1 ConstructSolution($u, \kappa, v$)

1: if $F(u, \kappa, v) = F^+(u, \kappa, v)$ then  
2: print $u$  
3: if $\kappa = 1$ then  
4: return  
5: $(\kappa^*_u, \kappa^*_v) \leftarrow \arg \max_{\kappa + \kappa_v = 1} F(\ell(u), \kappa, u) + F(r(u), \kappa_v, u)$  
6: ConstructSolution$(\ell(u), \kappa^*_u, v)$  
7: ConstructSolution$(r(u), \kappa^*_v, u)$  
8: else  
9: $(\kappa^*_u, \kappa^*_v) \leftarrow \arg \max_{\kappa + \kappa_v = 1} F(\ell(u), \kappa, v) + F(r(u), \kappa_v, v)$  
10: ConstructSolution$(\ell(u), \kappa^*_u, v)$  
11: ConstructSolution$(r(u), \kappa^*_v, v)$

Moreover, each entry $F(u, \kappa, v)$ indicates whether $u$ would be included in any solution $R$ in which (i) $\kappa$ nodes are selected from $T_u$ into $R$ and (ii) $v \in R$ and path $(u,v) \cap R = \emptyset$. Once we fill all the entries of the table, the optimal solution is constructed by Algorithm 1 that performs a BFS traversal of the tree: the decision to select each visited node into $R^*$ is given based on its inclusion state indicated by the entry $F(u, \kappa^*_u, a^*_u)$, where $a^*_u$ is the lowest ancestor of $u$ in solution $R^*$ that is added to the solution before visiting $u$ and $\kappa^*_u$ is the optimal partial budget allowance for $T_u$, which are both determined by the decisions taken in previous layers before visiting node $u$.  

Notice that for each node $u$ the computation of the entries $F(u, \kappa, v)$ requires the computation of partial benefit values $B_u((u, v))$ for pairs of nodes $(u, v)$, which in turn, require access to or computation of values $E[\delta(u; v)]$. As Lemma 5 below shows, the latter quantity can be computed from $E[\delta(u; \emptyset)]$ and $E[\delta(u; v)]$, for all $u \in V$ and $v \in A_u$. In practice, it is reasonable to consider a setting where one has used historical query logs to learn empirical values for $E[\delta(u; \emptyset)]$ and thus for $E[\delta(u; v)]$.

LEMMA 5. Let $u \in V$ be a given node in an elimination tree $T$ and let $v \in A_u$ denote an ancestor of $u$. Then,  

$$E[\delta(u; v)] = E[\delta(u; \emptyset)] - E[\delta(u; v)] .$$

PROOF. Notice that for any possible query $q$, whenever $X_v \subseteq Z_q$, we also have $X_u \subseteq Z_q$, since $T_u \subseteq T_v$. This suggests that given any query $q$ for which $\delta_u(q; \emptyset) = 1$, we also have $\delta_u(q; \emptyset) = 1$. On the other hand, when $\delta_u(q; \emptyset) = 1$, there can be two cases: (i) $X_u \subseteq Z_q$, which implies $\delta_u(q; v) = 0$, and (ii) there exists a node $w \in T_u \setminus T_u$ such that $X_u \subseteq Z_q$, which implies $\delta_u(q; v) = 1$. The latter suggests that the event $\{\delta_u(q; \emptyset) = 1\}$ occurs for a subset of queries $q$ for which the event $\{\delta_u(q; \emptyset) = 1\}$ occurs. The lemma follows.

Finally, the running time of the algorithm can be easily derived by the time needed to compute all entries of the dynamic-programming table.

THEOREM 2. The running time of the dynamic-programming algorithm is $O(nhk^2)$, where $n$ is the number of nodes in the elimination tree, $h$ is its height, and $k$ is the number of nodes that we ask to materialize.

PROOF. Notice that we have $O(nhk)$ subproblems, where each subproblem corresponds to an entry $F(u, v)$ of the three-dimensional table. To fill each entry of the table, we need to compute the two distinct values of $\kappa_u$ and $\kappa_v$ that maximize $F^+(u, \kappa, v)$ (subject to $\kappa_u + \kappa_v = k$) and $F^-(u, \kappa, v)$ (subject to $\kappa_u + \kappa_v = k$), respectively. Thus, it takes $O(k)$ time to fill each entry of the table in a bottom-up fashion, hence, the overall running time is $O(nhk^2)$.

### 4.2 Greedy algorithm

In this section, we first point out that the benefit function $B : 2^V \rightarrow \mathbb{R}_{\geq 0}$ is monotone and submodular. We then exploit these properties to provide a greedy algorithm that achieves an approximation guarantee of $(1 - \frac{1}{e})$. In the discussion that follows, we’ll be using the notion of marginal benefit to refer to the benefit we gain by adding one extra node to the solution set.
Definition 6 (Marginal Benefit). Consider an elimination tree \( T = (V, E) \), a set of nodes \( R \subseteq V \), a node \( u \in V \setminus R \), and a probability distribution \( \Pr(q) \) over the set of all possible queries. The marginal benefit \( B(u \mid R) \) of the node \( u \) with respect to the solution set \( R \) is defined as:

\[
B(u \mid R) = B(R \cup \{u\}) - B(R).
\]

Marginal benefits can be computed via the closed-form expression provided by the following Lemma.

Lemma 6. Consider an elimination tree \( T = (V, E) \), a set of nodes \( R \subseteq V \), a node \( u \in V \setminus R \), and a probability distribution \( \Pr(q) \) over the set of all possible queries. Let \( D_u^R = \{v \mid v \in T_u \cap R \land \text{path}(v, u) \cap R = \emptyset\} \) denote the set of descendants of \( u \) in \( R \cup \{u\} \) whose lowest ancestor in \( R \cup \{u\} \) is \( u \), and let \( a_u^R \in A_u \) denote the lowest ancestor of \( u \) in \( R \). Then, the marginal benefit \( B(u \mid R) \) of node \( u \) with respect to the set \( R \) is given by:

\[
B(u \mid R) = \mathbb{E}\left[\delta_q^u(u; a_u^R)\right] \left(b(u) - \sum_{v \in D_u^R} b(v)\right).
\]

Proof. Notice that for all nodes \( v \in R \setminus D_u^R \), the lowest ancestor \( a_u^R \) of \( v \) in \( R \) remains unchanged in \( R \cup \{u\} \). On the other hand, for each node \( v \in D_u^R \), we have \( a_u^R = a_u^R \). Thus, using Lemmas 1 and 3, we have:

\[
B(u \mid R) = B(R \cup \{u\}) - B(R) \\
= \sum_{v \in R \cup \{u\}} \mathbb{E}\left[\delta_q^u(v; R \cup \{u\})\right] b(v) \\
- \sum_{v \in R} \mathbb{E}\left[\delta_q^u(v; R)\right] b(v) \\
= \mathbb{E}\left[\delta_q^u(u; a_u^R)\right] b(u) \\
+ \sum_{v \in D_u^R} \left(\mathbb{E}\left[\delta_q^u(v; u)\right] - \mathbb{E}\left[\delta_q^u(v; a_u^R)\right]\right) b(v) \\
= \mathbb{E}\left[\delta_q^u(u; a_u^R)\right] \left(b(u) - \sum_{v \in D_u^R} b(v)\right).
\]

The main result of this section is the following.

Lemma 7. The benefit function \( B : 2^V \to \mathbb{R}_{\geq 0} \) is monotone and submodular.

Proof. We will first show that the benefit function \( B \) is monotone, i.e., \( B(u \mid R) \geq 0 \) for any given \( R \subseteq V \) and \( u \in V \setminus R \). In light of Lemma 6, it suffices to show that \( b(u) \geq \sum_{v \in D_u^R} b(v) \) for any \( u \) and for any possible set \( D_u^R \) of its descendants whose lowest ancestor in \( R \cup \{u\} \) is \( u \). Notice that for any node \( v \in D_u^R \), by definition we have \( \text{path}(v, u) \cap R = \emptyset \), which means that no ascendant or descendant of \( v \) can be in \( D_u^R \). Now, remember that by definition we have:

\[
b(u) = \sum_{x \in T_u} c(x).
\]

Using this definition, we equivalently have

\[
b(u) = b(u) + b(\ell(u)) + b(r(u)),
\]

which implies that the utility of a parent node is always greater than the sum of the utilities of its children. Given also that for any \( v \in D_u^R \), no ascendant or descendant of \( v \) can be in \( D_u^R \), we have

\[
\sum_{v \in D_u^R} b(v) \leq b(\ell(u)) \quad \text{and} \quad \sum_{v \in D_u^R} b(v) \leq b(r(u)).
\]

and therefore

\[
b(u) \geq \sum_{v \in D_u^R} b(v) + \sum_{v \in D_u^R} b(v) = \sum_{v \in D_u^R} b(v),
\]

concluding the proof of monotonicity.

We proceed to show that \( B \) is submodular, i.e., that for any \( R \subseteq S \subseteq V \) and \( u \in V \setminus S \), we have \( B(u \mid R) \geq B(u \mid S) \). For any given \( R \) and node \( w \notin R \), let \( S = R \cup \{w\} \). We consider two cases: (i) \( w \in A_u \), or (ii) \( w \in T_u \). Notice that the case of \( w \) being neither an ascendant or descendant of \( u \) is trivial, since we would then have \( B(u \mid R) = B(u \mid S) \).

First consider the case \( w \in A_u \). In this case, it could be that either (i) \( w \in \text{path}(u, a_u^R) \), which implies \( w = a_u^R \), or (ii) \( w \in \text{path}(a_u^R, \epsilon) \) which means that the lowest ancestor of node \( u \) in \( S \) is the same as in \( R \). It is easy to see that in the latter case we have \( B(u \mid R) = B(u \mid S) \), hence, we only consider the case in former. Notice that \( w = a_u^R \) implies that \( a_u^R \in A_w \), which, by Lemma 5, further implies that \( \mathbb{E}\left[\delta_q(a_u^R; \emptyset)\right] \leq \mathbb{E}\left[\delta_q(w; \emptyset)\right] \). Then we have:

\[
\mathbb{E}\left[\delta_q^u(u; a_u^R)\right] = \mathbb{E}\left[\delta_q(u; \emptyset)\right] - \mathbb{E}\left[\delta_q^u(a_u^R; \emptyset)\right] \\
\geq \mathbb{E}\left[\delta_q(u; \emptyset)\right] - \mathbb{E}\left[\delta_q(w; \emptyset)\right] \\
= \mathbb{E}\left[\delta_q(u; w)\right].
\]

Hence, by Lemma 5 we have:

\[
B(u \mid R) = \mathbb{E}\left[\delta_q^u(u; a_u^R)\right] \left(b(u) - \sum_{v \in D_u^R} b(v)\right) \\
\geq \mathbb{E}\left[\delta_q(u; w)\right] \left(b(u) - \sum_{v \in D_u^R} b(v)\right) \\
= B(u \mid S).
\]

Now we consider the case \( w \in T_u \). In this case, if \( w \notin D_u^R \) then it trivially follows that \( B(u \mid R) = B(u \mid S) \), hence, we only consider the case in which \( w \in D_u^R \). Notice that if \( w \in D_u^R \) then either (i) \( T_w \cap D_u^R = \emptyset \), or (ii) \( T_w \cap D_u^R \neq \emptyset \).
Algorithm 2 Greedy Algorithm

1: $R \leftarrow \emptyset$
2: while $|R| < k$ do
3: \[ u \leftarrow \arg \max_{v \in V \setminus R} B(R \cup \{v\}) - B(R) \]
4: \[ R \leftarrow R \cup \{u\} \]
5: return $R$

First, consider the case $T_u \cap D_u^R = \emptyset$ which implies that $D_u^R = D_u^R \cup \{w\}$. Then we have:

\[
B(u \mid R) = E\left[\delta_q(u; a_u^R)\right] \left( b(u) - \sum_{v \in D_u^R} b(v) \right) \\
\geq E\left[\delta_q(u; a_u^R)\right] \left( b(u) - \sum_{v \in D_u^R \cup \{w\}} b(v) \right) \\
= B(u \mid S).
\]

Next, consider the case $T_u \cap D_u^R \neq \emptyset$. In this case, it holds that $D_u^R = \{v \in D_u^R : \text{path}(v, u) \cap S = w\}$ and $D_u^S = (D_u^R \setminus D_u^R) \cup \{w\}$. Remember that, as given by Eq. 12, the utility of a parent node is always greater than the sum of utilities of its children. Given also that, for any $v \in D_u^R$, no ascendant or descendant of $v$ can be in $D_u^R$, we have

\[
b(w) \geq \sum_{v \in D_u^S} b(v),
\]

which implies that $\sum_{v \in D_u^R} b(v) \leq \sum_{v \in D_u^S} b(v)$, since we have $D_u^S = (D_u^R \setminus D_u^R) \cup \{w\}$. Thus, we have:

\[
B(u \mid R) = E\left[\delta_q(u; a_u^R)\right] \left( b(u) - \sum_{v \in D_u^R} b(v) \right) \\
\geq E\left[\delta_q(u; a_u^R)\right] \left( b(u) - \sum_{v \in D_u^S} b(v) \right) \\
= B(u \mid S).
\]

This concludes the proof. \(\square\)

Consider now the greedy algorithm that creates a solution set incrementally, each time adding the node with the highest marginal benefit into the solution set until the cardinality budget is consumed, as shown in Algorithm 2. It is easy to show that the algorithm comes with a constant factor approximation guarantee.

**Theorem 3.** Algorithm 2 achieves an approximation guarantee of $(1 - 1/e)$.

**Proof.** As shown in Lemma 7, the non-negative benefit function $B$ is monotone and submodular. Hence, the $(1 - 1/e)$ approximation guarantee for the greedy method follows from the classic result of Nemhauser et al. \(\square\)

5. EXTENSIONS

5.1 Space budget constraints

The algorithms we presented in the previous section address Problem 2 where a budget $k$ is given on the number of nodes to be materialized. A more realistic and practical scenario is Problem 1 where a budget $K$ is given on the total space required to materialize the selected nodes. In this case, for each node $u$ of the elimination tree $T$ the space $s_u$ required to materialize the probability table at node $u$ is specified as input.

Both of the algorithms we presented in the previous section, dynamic-programming and greedy, can be extended to address this more general version of the problem. In both cases the extension is fairly standard, and for lack of space we only describe it here in brief.

For the dynamic-programming algorithm the idea is to create an entry $F(u, \kappa, v)$ for nodes $u$ and $v$, and index $\kappa$ taking values from 1 to $\min\{K, s_u\}$, where $s_u$ is the total space required to materialize the probability tables of all nodes in $T_u$. We then evaluate the entry $F(u, \kappa, v)$ by considering the maximum benefit over all possible values $\kappa, \kappa$, such that $\kappa + \kappa = \kappa - s_u$, where $s_u$ is the space required to materialize node $u$.

The modified algorithm provides the exact solution, and the running time is $O(n \log K^2)$. Note, however, that unlike the previous case (Problem 2) where $k$ is bounded by $n$, the value of $K$ is not bounded by $n$. As the running time is polynomial in the value of $K$, which can be specified by $O(\log K)$ bits, it follows that the algorithm is in fact pseudo-polynomial. However, the technique can be used to obtain a fully-polynomial approximation scheme (FPTAS) by rounding all space values into a set of smaller granularity and executing the dynamic programming algorithm using these rounded values.

For the greedy algorithm, in each iterative step we select to materialize the node $u$ that maximizes the normalized marginal gain $(B(R \cup \{u\}) - B(R)) / s_u$. The modified greedy algorithm has the same running time and yields the same approximation guarantee $(1 - 1/e)$.

5.2 Accounting for redundant variables

In our algorithms so far we have considered a fixed elimination tree $T$ and elimination order $\sigma$. The elimination tree $T$ specifies the order in which sums-of-products evaluations are performed, with one summation for every variable in $N$. One can observe, however, that it is not necessary to involve every variable in the evaluation of a query. For example, for the Bayesian network $N$ shown in Figure 3 the query $q_1 = \Pr(b = b_0, c)$ can be computed from the sub-network $N_1 \subseteq N$, while the query $q_2 = \Pr(c \mid b = b_0)$ can be computed from the sub-network $N_2 \subseteq N$.

Previous work \cite{11,20,31} provides methods to determine the variables that are redundant for the evaluation of a query.
q allowing us to perform computations based on a “shrunk” Bayesian network. The characterization of variables into redundant and non-redundant is given in Theorem 4 based on the following two definitions.

**Definition 7 (Moral graph)**. The moral graph $M$ of a Bayesian network $N$ is the undirected graph that results from $N$ after dropping edge directions and adding one edge for all pairs of nodes that share a common child.

**Definition 8 ($m$-separated variables)**. Two variables $a$ and $b$ in a Bayesian network $N$ are said to be $m$-separated by variables $U$ if removing $U$ from the moral graph $M$ of $N$ leaves no (undirected) path between $a$ and $b$ in $M$. This property is denoted as $\text{sep}(a, b, U)$.

**Theorem 4 (Redundant Variables)**. Let $N$ be a Bayesian network and $q = \Pr(X_q, Y_q = y_q | Y'_q = y'_q)$ a query. Let $A$ be the union of ancestors in $N$ of all variables in $q$:

$$A = \cup_{i \in X_q \cup Y_q} A_i.$$  

Also, let $R_m$ be all variables outside $A$, i.e., $R_m = X \setminus A$, and $R_c$ all ancestor nodes $A$ that are $m$-separated from $X_q \cup Y_q$ by $Y'_q$, i.e.,

$$R_c = \{ a \in A | \text{sep}(a, b, Y'_q) \text{ for all } b \in X_q \cup Y_q \}.$$  

The variables in $R = R_m \cup R_c$ are redundant, and no other variables are redundant.

Given a Bayesian network $N$ and a query $q$ we write $\text{shrink}(q, N)$ (or $\text{shrink}(q)$ when $N$ is understood from the context) to denote the Bayesian network that results from the removal of all redundant variables as per Theorem 4. We can evaluate the query $q$ on a shrunk Bayesian network $N_s$, such that $\text{shrink}(q) \subseteq N_s \subseteq N$, by building an elimination tree $T'$ on $N_s$ and obtain immediate efficiency gains. However, the elimination tree $T'$ that is built on $N_s$ codifies different computations than the tree $T$ built on $N$, even if $T' \subseteq T$. Therefore, the tables of factors we materialize for $T$ using the algorithms of Section 4 do not generally correspond to factor tables for $T'$. In the next section we discuss how to address the issue of evaluating different queries while accounting for redundant variables.

### 5.2.1 Redundancy-aware scheme

The main idea of our redundancy-aware scheme is to materialize different probability tables for a set of “shrunk” Bayesian networks obtained through removal of redundant variables. The scheme consists of the following components:

**Lattice of Bayesian networks.** Consider a set of Bayesian networks $\mathcal{L} = \{N_0, N_1, N_2, \ldots, N_\ell\}$ that includes the input Bayesian network $N = N_0$ and $\ell$ of its subnetworks, each of which is induced by a subset of variables:

$$N_i \subseteq N, \text{ for all } i = 1, \ldots, \ell.$$  

The set $L$ can be represented as a lattice where edges are added between each network and its maximal subnetworks in $L$ (see an example in Figure 4).

**Query-network mapping.** Consider a function $M: \mathcal{Q} \to \mathcal{L}$ (where $\mathcal{Q}$ is the set of all possible queries) that maps a query $q \in \mathcal{Q}$ to a Bayesian network $N_q \in \mathcal{L}$ from which the answer to $q$ can be computed exactly. Notice that there is always such a Bayesian network in the lattice, namely the input Bayesian network $N_0 = N$.

#### Algorithm 4 Map($\mathcal{L}, q$)

1: Let $S := \text{shrink}(q)$
2: Let $Q := [N]$  
3: Let $N_s := N$
4: while $Q \neq \emptyset$ do
5: $N' = \text{dequeue}(Q)$
6: if $|N'| < N_s$ then
7: $N_s := N'$
8: for $N'' \in \text{children}(N')$ do
9: $\text{enqueue}(N'', Q)$
10: end
11: return $N_s$

**Query workloads.** Each Bayesian network $N_i \in \mathcal{L}$ is associated with a query workload, characterized by: (i) the probability $\pi_i$ that a random query is mapped to $N_i$; (ii) a probability distribution $\Pr_i(q) = \Pr(q | N_i)$ over the queries that are mapped to $N_i$.

We now discuss how the scheme operates and how its components are built. When a query arrives it is mapped to one network in the lattice from which its value is computed exactly. As we discuss below, this mapping operation can be performed efficiently. In this scheme, offline optimization considerations include the choice of networks to include in the lattice, as well as the materialization of factors for each network. We discuss them below.

**An algorithm for query-network mapping.** Algorithm 4 finds the smallest Bayesian network $N_s$ in the lattice such that $\text{shrink}(q) \subseteq N_s \subseteq N$ that can be used to answer a query $q$. The algorithm proceeds as follows: first, at line 3 it computes the smallest shrunk network $S = \text{shrink}(q)$ that can be used to answer query $q$ exactly; then, it performs a breadth-first-search on the lattice $L$ starting from the top element but does not extend search paths on which it encounters networks $N'$ that do not include $S$ as subnetwork.

To test whether $S \subseteq N'$, it is sufficient to test whether the intersection of the (labeled) edge-sets of the two networks is not empty, which can be done in time $O(|E| \log(|E|))$. The algorithm finds the correct network in the lattice since, by construction, if it has visited a Bayesian network $N'$ that contains the target $N_s$ as subnetwork, there is a path from $N'$ to $N_s$, and this condition holds for the best (smallest Bayesian network that contains $S$) discovered up to any point during the execution of the algorithm. The total running time in terms of subnetwork tests is $O(\ell |E| \log(|E|))$.

**Building the lattice.** We build the lattice $L$ off-line, in three phases. During the first phase, we consider the full lattice $L^+$ that includes all sub-networks of $N$ and estimate the
probability $\rho_i$ that a random query $q$ has $N_i = \text{shrink}(q) \in \mathcal{L}^+$ as its corresponding “shrunk” network. Notice that, for the full lattice, $\rho_i$ is also the probability that a random query is mapped by Algorithm 4 to Bayesian network $N_i \in \mathcal{L}^+$. In practice, we consider a sample of queries $q$ (either from a query-log or a probabilistic model) and estimate $\rho_i$ as the relative frequency with which network $N_i$ is the “shrunk” network that can be used to evaluate $q$.

During the second phase, we choose a small number $\ell$ of networks from $\mathcal{L}^+$ to form lattice $\mathcal{L}$. We want to build a lattice of networks that captures well the distribution $\rho$. In practice, we use a greedy approach, successively choosing to add to $\mathcal{L}$ the network that optimizes the utility of the lattice. During the third phase, we follow an approach similar to the first phase to estimate anew the probability $\pi_i$, that a random query $q$ has $N_i = \text{shrink}(q) \in \mathcal{L}$ as its corresponding “shrunk” Bayesian network, as well as the probability distribution $Pr_i(q) = Pr(q \mid N_i)$ over the queries $q$ that are mapped to $N_i$.

### Optimal materialization

Given the set $\mathcal{L}$ of networks contained in the lattice, a query workload $(\pi_i, Pr_i(q))$ over the networks, and a budget $k$, we wish to materialize $k_i$ factors for Bayesian network $N_i$, with $\sum_i k_i \leq k$, so that $G(k_i) = \sum_i \pi_i B_i(k_i)$ is maximized, where $B_i(k_i)$ is the optimal benefit obtained by solving problem 2 for Bayesian network $N_i$ with budget $k_i$. Let $OPT_{m,k}$ be the optimal value of $G(\cdot)$ for the first $m$ networks of $\mathcal{L}$, with budget $k$. Then the following equation holds

$$OPT_{m+1,k} = \max_{n} \{ \pi_{m+1} B_n(k) + OPT_{m,k-n} \},$$

and defines a dynamic-programming algorithm to compute the optimal materialization over a set of networks $\mathcal{L}$.

### 6. EXPERIMENTS

We demonstrate the benefit of factor materialization by experiments on real-world Bayesian networks. We remind that due to space constraints, we consider materializing only the factors that involve natural joins and variable summations, while a more general choice could involve materializing factors resulting from natural joins combined with a choice of operation per variable (variable summation, row selection, or no operation), as explained in Section 3. Naturally, this self-imposed constraint limits the benefit of materialization, since we do not materialize any type of factor. This point is important to keep in mind when discussing our experimental results.

#### 6.1 Setup

**Datasets.** We use eight real-world Bayesian networks, whose statistics are listed in Table 1. The column “parameters” refers to the total number of table entries of the factors that define the corresponding Bayesian network.

**PATHFINDER** [13] is a Bayesian network used in an expert system that assists surgical pathologists with the diagnosis of lymph-node diseases. **DIABETERS** [1] is used to model insulin dose adjustment. **MILDREW** is a Bayesian network used to predict the necessary amount of fungicides to be used against mildew in wheat. **LINK** [15] models the linkage between a gene associated with a rare heart disease (the human LQT syndrome) and a genetic marker gene. **MUNIN** [2], **ANDES** [3], and **PATHFINDER** [29] are two subnetworks of **MUNIN**. **ANDES** [5] is a Bayesian network used in an expert electromyography assistant and **MUNIN**#1 and **MUNIN**#2 are two subnetworks of **MUNIN**. **DIABETERS** [4] is a Bayesian network used in an intelligent tutoring system that teaches Newtonian physics to students. All datasets are publicly available online.

### Elimination order

As explained in Section 3, elimination trees are built according to a given variable-elimination order. However, finding the optimal variable-elimination order is NP-hard [17], and several heuristics have been proposed to construct an order that does not lead to exponential space blowup. Among these heuristics, greedy algorithms have been shown to perform well in practice [10]. Given a Bayesian network $\mathcal{N}$, such a greedy algorithm begins by initializing a graph $H$ from the “moralization” of $\mathcal{N}$, i.e., by connecting the parents of each node and dropping the direction of the edges. Then at the $i$-th iteration, a node that minimizes a heuristic cost function is selected as the $i$-th variable in the ordering. The selected variable is then removed from $H$ and undirected edges are introduced between all its neighbors in $H$. In this paper, we consider heuristics where the cost of a node is: min-neighbors (MN): the

#### Table 1: Statistics of Bayesian networks.

| Network | nodes | edges | parameters | avg. degree |
|---------|-------|-------|------------|-------------|
| MILDREW | 35    | 46    | 547K       | 2.63        |
| PATHFINDER | 109   | 195   | 98K        | 2.96        |
| MUNIN#1 | 186   | 273   | 19K        | 2.94        |
| ANDES   | 220   | 338   | 2.3K       | 3.03        |
| DIABETERS | 413   | 602   | 461K       | 2.92        |
| LINK    | 714   | 1125  | 20K        | 3.11        |
| MUNIN#2 | 1003  | 1244  | 84K        | 2.94        |
| MUNIN   | 1041  | 1397  | 98K        | 2.68        |

#### Table 2: Parameter size of factors created with different elimination orders (K: thousand, M: million).

| Network | MN avg | MN max | MF avg | MF max | WMF avg | WMF max |
|---------|--------|--------|--------|--------|---------|---------|
| MILDREW | 15K    | 170K   | 10K    | 170K   | 57K     | 1M      |
| PATHFINDER | 570   | 16K    | 568K   | 16K    | 643K    | 16K     |
| MUNIN#1 | 749K   | 59M    | 375K   | 39M    | 367K    | 39M     |
| ANDES   | 2K     | 131K   | 1.4K   | 66K    | 1.4K    | 66K     |
| DIABETERS | 9K    | 194K   | 4K     | 194K   | 325K    | 33M     |
| LINK    | 109K   | 17M    | 31K    | 4M     | 633K    | 268M    |
| MUNIN#2 | 40K    | 31M    | 1.7K   | 168K   | 1.8K    | 168K    |
| MUNIN   | 9.5K   | 588K   | 5K     | 392K   | 3K      | 112K    |

#### Table 3: Statistics of elimination trees.

| Tree | nodes | height | max. # children |
|------|-------|--------|-----------------|
| MILDREW (MF) | 70 | 17 | 3 |
| PATHFINDER (MF) | 218 | 12 | 54 |
| MUNIN#1 (WMF) | 372 | 23 | 7 |
| ANDES (MF) | 440 | 38 | 5 |
| DIABETERS (MF) | 826 | 77 | 4 |
| LINK (MF) | 1428 | 56 | 15 |
| MUNIN#2 (MF) | 2006 | 23 | 8 |
| MUNIN (WMF) | 2082 | 24 | 8 |

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2 The model was developed by Finn V. Jensen, Jørgen Olesen, and Uffe Kjærulff.

3 Available at http://www.bnlearn.com/bnrepository/ [29]
number of neighbors it has in $H$; **min-weight (MW):** the product of domain cardinalities of its neighbors in $H$; **min-fill (MF):** the sum of the number of edges that need to be added to $H$ due to its removal; and **weighted-min-fill (WMF):** the sum of the weights of the edges that need to be added to $H$ due to its removal, where the weight of an edge is the product of the domain cardinalities of its endpoints [17].

Table 2 shows statistics for the factors in the elimination trees created under elimination orders generated by the best three of the aforementioned heuristics. For each Bayesian network, we select the elimination order that induces the smallest average parameter size and use the maximum parameter size as a tie-breaker. Table 3 reports statistics of the elimination trees obtained from the chosen elimination order for each dataset. In all the trees, the average number of children is found to be consistently close to 1, therefore we do not report it in the table.

**Cost values.** To solve Problem 2, we must assign partial cost values $c(u)$ to the nodes $u$ of elimination trees, and these values must represent the computational cost of computing the corresponding factor from its children in the elimination tree (see Section 3, Definition 1). Following the time-complexity analysis of Koller et al. [17], we estimate $c(u)$ to be proportional to the cost of the corresponding natural join operation. For our implementation of joins, we adopt the technique of one-dimensional representation of factor tables described by Murphy [22], which makes use of a constant-time arithmetic mapping between the indices of the one-dimensional factor table and the combinations of values of variables in its multi-dimensional counterpart. For this implementation, the cost of the natural join operation is twice the resulting size of join, which can be calculated from the sizes of the joined tables without actually performing the join. We confirm experimentally that the theoretical cost estimates align almost perfectly with the empirical execution times (Pearson $r \geq 0.99$).

**Query workload.** The optimization problem we consider assumes a query workload, i.e., a probability distribution $Pr(q)$ of queries $q$. In practice, it is reasonable to consider a setting where one has access to a historical query log to learn a distribution $Pr(q)$. In the absence of such a log for the networks of Table 1, we consider a general setting for $Pr(q)$. In particular, for simplicity of presentation, we consider queries $q = Pr(X_q, Y_q = y_q)$ where $Y_q = \emptyset$, i.e., no variables are bound, but all variables are either free ($X_q$) or summed-out ($Z_q$). We note that the setting $Y_q = \emptyset$ is a worse-case scenario as it leads to computationally more intensive queries, since, by not selecting any subsets of rows associated with $Y_q = y_q$, we need to generate larger factors. Moreover, we consider uniform workloads, where each variable of a Bayesian network has equal probability to be a member of $X_q$. For each dataset, we generate a total of 250 random queries, with 50 queries for each query size $q_r$, i.e., $r_q = |X_q| \in [1, 5]$, under this scheme. In addition, we experimented with a skewed-workload scheme, in which the variables appearing earlier in the elimination ordering, i.e., the variables associated with the nodes that are closer to the leaves of the elimination tree $T$, are more likely to appear among the summed-out variables $Z_q$ rather than the free variables $X_q$. Specifically, in this scheme, a variable that appears $\ell$ levels above another in $T$ is $\ell$ times more likely to be placed among the free variables $X_q$. We do not show results for workload distributions with opposite skew: since we focus on materialized tables that involve only summed-out variables, it is easy to see that having free variables close to the leaves of the elimination tree $T$ would usually render them not useful.

**Execution system.** All experiments were executed on a 64-bit SUSE Linux Enterprise Server with Intel Xeon 2.90 GHz CPU and 264 GB memory. Our implementation is available online.

### 6.2 Results

We now report the performance gains due to materialization. The main results for the uniform scheme are shown in Figure 5. Each plot corresponds to one dataset, with the $x$-axis showing the number of factors that are materialized (budget $k$) and the $y$-axis showing the cost savings in query running time, expressed as a percentage of the query running time when no materialization is used. The reported savings are averages over the query workload and each bar within each plot corresponds to a different query size $q_r$. Moreover, the numbers on the bars indicate the percentage of cost savings relative to the materialization of all the factors in the tree in the uniform-workload scheme.

We observe in Figure 6 that, consistently in all the datasets, a small number of materialized factors can achieve cost savings almost as well as in the case of materializing all the factors of the elimination tree. This result is expected as the submodularity property of the benefit function implies a diminishing-returns behavior. This result is also desirable as it shows that we can achieve significant benefit by materializing only a small number of factors. Another observation, common to all the datasets, is that, as the number $r_q$ of variables in a query increases, the savings from materialization decreases. Given our choice of limiting the materialization operation to factors that involve only joins and variable summation, this trend is expected: with higher $r_q$, the probability that a materialized factor does not contain any free variable in its subtree decreases, limiting the materialization benefit.

The datasets where we observe considerably small savings are MUNIN#1, ANDES, LINK, and DIABETES. In all these datasets except DIABETES, we find that a small number of factors contribute to the largest part of the computational cost when $k = 0$, due to their large number of entries: we observe that 5 out of 372 factors in MUNIN#1 and 6 out of 1428 factors in LINK contribute to almost 90% of the computational cost, while for ANDES, 5 out of 440 factors

| Network | $r_q=1$ | $r_q=2$ | $r_q=3$ | $r_q=4$ | $r_q=5$ | all |
|---------|---------|---------|---------|---------|---------|-----|
| MILDW   | 11.2    | 33.5    | 97.5    | 122.7   | 177.3   | 77.0|
| PATHFINDER | 0.2    | 0.2     | 0.2     | 0.3     | 0.4     | 0.2 |
| MUNIN#1 | 319.4   | 408.4   | 474.7   | 656.6   | 767.2   | 438.2|
| ANDES   | 1.1     | 1.6     | 2.6     | 4.8     | 7.6     | 3.5 |
| DIABETES| 18.0    | 95.7    | 332.3   | 621.0   | 801.9   | 162.3|
| LINK    | 119.4   | 215.8   | 313.8   | 391.1   | 532.0   | 287.1|
| MUNIN#2 | 7.1     | 11.6    | 14.5    | 12.9    | 25.8    | 14.4|
| MUNIN   | 15.1    | 16.7    | 25.8    | 30.3    | 38.5    | 25.3|

\footnote{https://github.com/aslayci/qtm}
contribute to 75%. This suggests that the same computational burden of creating these large factor tables carries to the case of \( k > 0 \) whenever none of the materialized factors are useful during query processing. We indeed observe that the average cost savings, among the queries in which the variables associated to these large factors are summed out, is greater than 90% in these datasets. On the other hand, for Diabetes, we find that the number of entries in the factor tables are almost uniformly distributed, however, we observe that the structure of the elimination tree has large chain components, as reflected by its larger height relative to other similar-sized trees, which makes it rare for any chosen factor to be useful for queries.

We also report in Table 4 the average query-processing times when no materialization is used (i.e., \( k = 0 \)) under the uniform scheme. We observe that the running time increases with the number \( r_q \) of free variables in a query. This is expected because free variables lead to larger factor tables during variable elimination.

Figure 6 reports the average cost savings per query size \( r_q \) for varying number of materialized factors in the skewed-workload scheme. As in the case of uniform-workload scheme, we observe that a small number of materialized factors can achieve cost savings almost as well as in the case of materializing all the factors of the elimination tree under the skewed-workload scheme. We also observe that, while the relative performance of materialization, indicated by the numbers on the bars, do not differ significantly between the uniform and skewed-workload schemes, the savings over the case of no materialization significantly improves in the skewed-workload scheme. Figure 7 reports the overall comparison between the uniform and skewed-workload schemes.
We observe that the performance gains due to materialization under the skewed-workload scheme are significantly higher than the uniform-workload scheme for all the datasets. This trend is especially visible for the datasets MUNIN#1, Andes, and Link, all of which contain only a small number of factors contributing to the majority of the computational cost as explained before: we observed that these large factors reside in middle layers of their elimination trees, hence, are less likely to be associated to free variables under the skewed-workload scheme than its uniform counterpart. This implies that, since a random set of free variables under the skewed-workload scheme are more likely to be associated to the ancestors of the materialized factors, the skewed-workload scheme can obtain higher benefit from materialization. This suggests that constructing an elimination order that is tuned to a given query workload can provide significant boost to the query-processing performance when only factors that are the result of variable summation are materialized.

For Mildew, we found average savings to be slightly higher than 10% under the uniform-workload scheme: when we drill down to savings specific to query size, as provided in Figure 3, we see that for queries of size 1, 2, and 3, the savings are around 70%, 35%, and 25% respectively, and have a sharp decrease to under 10% for queries of size 4 and 5, resulting an average around 10% over all the queries. We remind that Mildew only has 35 variables which translate to a small elimination tree, making it especially hard to find useful factors for large value of $r_k$ under the uniform workload. We see that the savings significantly improve to an average of 50% under the skewed-workload scheme for Mildew. On the other hand, for Diabetes, we see that the average savings under both workload schemes remain around 10%, due to its elimination tree that is composed of large chain components, limiting the extent we can exploit materialization. For the rest of the datasets, Pathfinder, MUNIN#2, and Munin, we observed relatively high savings under the uniform-workload scheme, where the average savings for $k = 20$ was found to be 70% for Pathfinder, and 50% for the latter two that are the largest Bayesian networks used in the experiments.

Lastly, we report statistics regarding the offline materialization phase. For each dataset, we report the results for maximum possible $k$ where all the factors are materialized. In all the datasets except MUNIN#1 and Link, selection and computation of the factors to materialize took less than 10 seconds while for MUNIN#1 and Link it took 270 and 100 seconds respectively. The maximum materialized table size on disk was found to be 240 MB for MUNIN#1, 54 MB Link, and less than 2MB for the rest of the datasets. We conclude that by materializing a small number of tables with modest memory requirements, we can obtain significant performance gains in the query-processing time, reaching up to an average gain of 70% under the uniform-workload scheme and 80% under the skewed-workload scheme.

7. CONCLUSIONS

State-of-the-art machine learning techniques allow us to build probabilistic models, such as Bayesian networks, and use them to perform approximate query processing and predictive querying over very large databases. Well-trained model instances are more concise than the data they were built from, and so queries performed over the model can offer large efficiency gains—and robustness—compared to queries evaluated directly over the data. To make such an approach even more scalable, it is crucial to consider what expensive model computations can be performed in a preprocessing step, so as to make query answering more efficient.

In this paper, we addressed the problem of materializing factor tables for Bayesian networks and provided efficient algorithms to choose the optimal factor tables under a budget constraint. Our experimental results show that appropriate materialization can offer significant speed-up.

Several directions for future work open up ahead. One direction is to extend the results of this paper, e.g., by optimizing the redundancy-aware scheme of Section 5.2.1 accommodating numerical variables, and developing algorithms for special cases of conditional distributions. We believe though that the larger theme of work to follow this paper is that of addressing the problem of materialization for other probabilistic models.
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APPENDIX

A. GENERALITY OF PROBLEM SETTING

We formulated Problems 1 and 2 in terms of an elimination tree, without specifying any constraints on its structure. However, in the context where we’re addressing Problem 2, elimination trees are defined by a Bayesian network and an elimination order. At this point, we should consider the question of whether the elimination trees that are input to Problem 1 and 2 are of general structure — if they were not, then this would leave room for faster algorithms that take advantage of the special structure.

Lemma 8 states that the internal nodes of an elimination tree form a tree of general structure. Note that we use the term “internal subtree” to refer to the subgraph of a tree that is induced by internal (non-leaf) nodes. For an elimination tree $T$, its internal subtree corresponds to the nodes that correspond to the variables of the Bayesian network.

**Lemma 8.** Consider any tree $T$ and its internal subtree $T_{in}$. There is a Bayesian network and an elimination order that define an elimination tree $T'$ with $T'_{in} \simeq T_{in}$.

**Proof.** Assume that $T_{in}$ is rooted at node $\omega$ with subtrees rooted at nodes $u_a, u_b, \ldots , u_z$. Consider a Bayesian Network $N$ that has one corresponding variable $\omega, a, b, \ldots, z$ for each node of $T_{in}$, and conditional probabilities in the opposite direction compared to the respective edges of $T_{in}$ — i.e., if $T_{in}$ contains a directed edge $(u_a, u_b)$, the Bayesian network $N$ contains the edge $(\omega, a)$ with associated conditional probability $Pr(a | \omega)$. Let $\sigma$ be the elimination ordering of variables corresponding to the post-order traversal of $N'$. Consider the directed edges $(\omega, a), (\omega, b), (\omega, c)$ etc., coming out of $\omega$ (see Figure 8). The elimination ordering we chose ensures that variables $a, b, c, \text{etc}.$, are eliminated before $\omega$. It also ensures that the factor that results from the elimination of variable $a$ is a function of $\omega$ but of none of the other variables $b, c, \text{etc}$, that depend on $\omega$, by construction. The elimination of $\omega$ happens after that of each variable $a, b, c, \text{etc}$, it connects to, leading to an elimination tree $T'$ with an edge from each of those variables to $\omega$ — and therefore to an internal subtree $T'_{in}$ that is isomorphic of $T_{in}$. □

We can also show, however, that if we limit ourselves to elimination orderings that follow a pre-order traversal (pot) of the Bayesian network, we end up with elimination trees of linear structure. Note that the Bayesian network $N$ we consider is generally a directed acyclic graph (DAG) and not necessarily a tree. It is therefore possible to have multiple roots in $N$ — i.e., multiple variables that do not depend on other variables. For any variable $\omega$, consider the set of variables $a, b, \ldots, z$ that depend on $\omega$. A pot of $N$ is any ordering of its variables such that $\omega$ precedes $a, b, \ldots, z$. The breadth-first-search of $N$ that starts from the roots of $N$ is a pot.

**Lemma 9.** For a Bayesian Network $N$, let $T$ be the elimination tree obtained for the elimination order defined by any pre-order traversal of $N$. The internal subgraph $T_{in}$ of $T$ is linear.

**Proof.** For any variable $\omega$, let us consider the set of variables $\{a, b, \ldots, z\}$ that depend on $\omega$ — as well as “co-dependents” of $\omega$, i.e., variables $\{\omega'\}$ that depend on variables that overlap with the variables that $\omega$ depends on (see Figure 9). Notice that, in a pre-order traversal of $N$, these are the only variables that can follow $\omega$ in the traversal. During elimination, node $\omega$ passes along a potential that involves all its dependents $\{a, b, \ldots, z\}$ and co-dependents $\{\omega'\}$ that have not been eliminated yet. As a result, at every transition in the pre-order traversal, the factor that results from the latest elimination is a function of the next variable in the traversal, until the traversal of the last variable. This leads to a directed edge in $T$ from the current node in the elimination tree to the node that corresponds to the next variable in the traversal. These directed edges form the subgraph of internal nodes of $T$ — which is thus a linear graph that follows the pre-order traversal of $N$ exactly. □

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**Figure 8:** The tree on the left represents $T_{in}$, the subtree of elimination tree $T$ induced by its internal nodes. The Bayesian Network in the figure, constructed by reversing the direction of edges in $T_{in}$, along with its post-order traversal $(a, b, \ldots, z)$ define $T$ as the elimination tree.

**Figure 9:** Consider the Bayesian Network in the figure, along with its pre-order traversal $\sigma = (\xi, \omega, \omega', a, b, \ldots, z)$. The two define the elimination tree shown in the figure, which includes a linear graph over the internal nodes.