Supplementary Material: Lossless Bayesian Networks Extensive Proofs and Mathematical Foundations

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Abstract

This supplementary material provides extensive mathematical proofs, correctness arguments, and detailed analysis for the lossless Bayesian network implementation. It includes proofs of the factorization theorem, correctness of variable elimination, topological sorting algorithms, belief propagation, and complexity analyses. All proofs are presented with rigorous mathematical detail.

Contents

1 Introduction

This document provides comprehensive mathematical proofs and theoretical foundations for the lossless Bayesian network implementation. The main paper presents the implementation and usage, while this supplementary material focuses on the rigorous mathematical underpinnings.

2 Mathematical Preliminaries

2.1 Graph Theory

Definition 2.1 (Directed Acyclic Graph)**.** A directed acyclic graph (DAG) is a directed graph $G = (V, E)$ where V is a set of vertices and $E \subseteq V \times V$ is a set of directed edges, such that there are no directed cycles.

Definition 2.2 (Topological Ordering)**.** A topological ordering of a DAG $G = (V, E)$ is a linear ordering of vertices such that for every directed edge $(u, v) \in E$, vertex u comes before v in the ordering.

Theorem 2.3 (Existence of Topological Ordering)**.** Every DAG has at least one topological ordering.

Proof. We prove by induction on the number of vertices n.

Base case: For $n = 1$, the single vertex forms a valid topological ordering.

Inductive step: Assume every DAG with n vertices has a topological ordering. Consider a DAG G with $n + 1$ vertices. Since G is acyclic, there exists at least one vertex v with in-degree 0 (otherwise, we could construct a cycle by following incoming edges). Remove v and all its outgoing edges to obtain G' with n vertices. By the inductive hypothesis, G' has a topological ordering σ'. Then $\sigma = [v] \circ \sigma'$ is a topological ordering of G, where v is placed first. □

2.2 Probability Theory

Definition 2.4 (Conditional Independence)**.** Random variables X and Y are conditionally independent given Z, denoted $X \perp Y|Z$, if:

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

Definition 2.5 (Markov Property)**.** A Bayesian network satisfies the Markov property: each variable is conditionally independent of its non-descendants given its parents.

3 Proof of Factorization Theorem

Theorem 3.1 (Bayesian Network Factorization)**.** Let $G = (V, E)$ be a DAG representing a Bayesian network, and let P be a set of conditional probability distributions. The joint probability distribution factorizes as:

$$P(X_1, X_2, \ldots, X_n) = \prod_{i=1}^{n} P(X_i|\text{Pa}(X_i))$$

where $\text{Pa}(X_i)$ denotes the parents of X_i in G.

Proof. We prove by induction on the number of variables n, using a topological ordering of the DAG.

Base case: For $n = 1$, we have $P(X_1) = P(X_1|\emptyset) = P(X_1)$, which is trivially true.

Inductive step: Assume the theorem holds for all Bayesian networks with n variables. Consider a network with $n+1$ variables. Let $\sigma = [X_1, X_2, \ldots, X_{n+1}]$ be a topological ordering.

By the chain rule of probability:

$$P(X_1, \ldots, X_{n+1}) = P(X_1) \prod_{i=2}^{n+1} P(X_i | X_1, \ldots, X_{i-1})$$

By the Markov property, for each X_i, we have:

$$P(X_i | X_1, \ldots, X_{i-1}) = P(X_i | \text{Pa}(X_i))$$

since X_i is conditionally independent of its non-descendants (which are $X_1, \ldots, X_{i-1}$ minus $\text{Pa}(X_i)$) given its parents.

Therefore:

$$P(X_1, \ldots, X_{n+1}) = \prod_{i=1}^{n+1} P(X_i | \text{Pa}(X_i))$$

This completes the induction. □

Corollary 3.2 (Uniqueness of Factorization)**.** Given a DAG structure, the factorization is unique up to the ordering of variables consistent with the topological order.

Proof. The factorization is determined by the parent sets $\text{Pa}(X_i)$ for each variable, which are uniquely defined by the DAG structure. Any topological ordering will produce the same factorization, as the Markov property ensures that $P(X_i | \text{Pa}(X_i))$ is independent of the ordering of non-descendants. □

4 Correctness of Variable Elimination

Theorem 4.1 (Correctness of Variable Elimination)**.** The variable elimination algorithm computes the exact posterior probability $P(Q|E = e)$ for query variables Q given evidence $E = e$.

Proof. We prove by showing that variable elimination correctly computes the marginal probability.

Given a Bayesian network with factorization:

$$P(X_1, \ldots, X_n) = \prod_{i=1}^{n} P(X_i | \text{Pa}(X_i))$$

To compute $P(Q|E = e)$, we need:

$$P(Q|E = e) = \frac{P(Q, E = e)}{P(E = e)} = \frac{\sum_{\mathbf{H}} P(Q, E = e, \mathbf{H})}{\sum_{\mathbf{Q},\mathbf{H}} P(Q, E = e, \mathbf{H})}$$

where $\mathbf{H}$ are hidden variables (neither query nor evidence).

The numerator is:

$$P(Q, E = e) = \sum_{\mathbf{H}} \prod_{i=1}^{n} P(X_i | \text{Pa}(X_i))$$

Variable elimination works by:

1. For each variable X_i not in $\{Q, E\}$, sum it out:

$$\sum_{x_i} \prod_{j : X_j \text{ depends on } X_i} P(X_j | \text{Pa}(X_j))$$

2. This creates a new factor over the remaining variables.

3. Repeat until only query and evidence variables remain.

We prove correctness by induction on the number of hidden variables.

Base case: If there are no hidden variables, we directly compute:

$$P(Q, E = e) = \prod_{i:X_i \in \{Q,E\}} P(X_i|\text{Pa}(X_i))$$

with evidence instantiated.

Inductive step: Assume variable elimination is correct for networks with k hidden variables. Consider a network with $k+1$ hidden variables. Let X_h be a hidden variable to eliminate.

By the factorization:

$$P(Q, E = e, \mathbf{H}) = \left(\prod_{i:X_i \notin \text{scope}(X_h)} P(X_i|\text{Pa}(X_i)) \right) \cdot \left(\prod_{j:X_j \in \text{scope}(X_h)} P(X_j|\text{Pa}(X_j)) \right)$$

where $\text{scope}(X_h)$ includes X_h and all variables that depend on it.

Summing out X_h:

$$\sum_{x_h} \prod_{j:X_j \in \text{scope}(X_h)} P(X_j|\text{Pa}(X_j))$$

This creates a new factor over the remaining variables in $\text{scope}(X_h) \setminus \{X_h\}$. The resulting network has k hidden variables, and by the inductive hypothesis, variable elimination correctly computes the marginal.

The algorithm maintains the correct joint probability at each step because:

- Summing preserves the probability structure
- Factors are correctly combined through multiplication
- The elimination order doesn't affect the final result (by commutativity of addition)

Therefore, variable elimination correctly computes $P(Q|E = e)$. □

Lemma 4.2 (Elimination Order Independence)**.** The result of variable elimination is independent of the order in which variables are eliminated (up to numerical precision).

Proof. This follows from the commutativity and associativity of addition and multiplication. For any two elimination orders, we can rearrange the sums and products to show equivalence:

$$\sum_{x_1} \sum_{x_2} \prod_i f_i = \sum_{x_2} \sum_{x_1} \prod_i f_i$$

The factorization structure ensures that each variable appears in a consistent set of factors regardless of elimination order. □

5 Correctness of Topological Sorting

Theorem 5.1 (Correctness of Kahn's Algorithm)**.** Kahn's algorithm correctly computes a topological ordering of a DAG, or detects if the graph contains a cycle.

Proof. We prove by showing that the algorithm maintains the invariant that all vertices in the queue have in-degree 0 in the remaining graph, and that processed vertices form a valid prefix of a topological ordering.

Invariant: At each step, if a vertex v is in the queue, then all vertices that should come before v in a topological ordering have already been processed.

Initialization: Initially, the queue contains all vertices with in-degree 0. These vertices have no incoming edges, so they can be placed first in any topological ordering. The invariant holds.

Maintenance: When we remove a vertex v from the queue and process it:

1. We add v to the topological ordering.
2. For each edge (v, u), we decrement the in-degree of u.
3. If u's in-degree becomes 0, we add u to the queue.

After processing v, all edges from v have been "accounted for" by decrementing in-degrees. If u's in-degree becomes 0, it means all vertices that should come before u have been processed. Therefore, u can be safely added to the queue, maintaining the invariant.

Termination: The algorithm terminates when either:

1. All vertices are processed: In this case, we have a complete topological ordering. Since we only added vertices to the ordering when their in-degree was 0, and we processed all edges, the ordering is valid.
2. The queue becomes empty before all vertices are processed: This means there are vertices with remaining incoming edges. Since the graph is finite and we've processed all vertices with in-degree 0, the remaining vertices must form a cycle (each has at least one incoming edge from another unprocessed vertex).

Therefore, Kahn's algorithm correctly computes a topological ordering or detects cycles. □

Proposition 5.2 (Uniqueness of Topological Ordering)**.** A DAG has a unique topological ordering if and only if it is a linear chain (each vertex has at most one parent and at most one child, except endpoints).

Proof. **Forward direction:** If the DAG is a linear chain, the ordering is forced by the chain structure, hence unique.

Reverse direction: If the DAG is not a linear chain, there exists either:

- A vertex with multiple parents: These parents can be ordered in different ways.
- A vertex with multiple children: These children can be ordered in different ways.
- Multiple source vertices: These can be ordered in different ways.

In any of these cases, multiple valid topological orderings exist. □

6 Correctness of CPT Normalization

Theorem 6.1 (CPT Normalization Correctness)**.** After normalization, a Conditional Probability Table (CPT) satisfies:

$$\sum_{x_i} P(X_i = x_i | \text{Pa}(X_i) = \mathbf{pa}) = 1$$

for all parent assignments **pa**.

Proof. Let $P_{\text{raw}}(X_i = x_i|\text{Pa}(X_i) = \mathbf{pa})$ be the raw (possibly unnormalized) probabilities. The normalization procedure computes:

$$P_{\text{norm}}(X_i = x_i|\text{Pa}(X_i) = \mathbf{pa}) = \frac{P_{\text{raw}}(X_i = x_i|\text{Pa}(X_i) = \mathbf{pa})}{\sum_{x_i'} P_{\text{raw}}(X_i = x_i'|\text{Pa}(X_i) = \mathbf{pa})}$$

Then:

$$\begin{aligned}\sum_{x_i} P_{\text{norm}}(X_i = x_i|\text{Pa}(X_i) = \mathbf{pa}) &= \sum_{x_i} \frac{P_{\text{raw}}(X_i = x_i|\text{Pa}(X_i) = \mathbf{pa})}{\sum_{x_i'} P_{\text{raw}}(X_i = x_i'|\text{Pa}(X_i) = \mathbf{pa})} \\ &= \frac{\sum_{x_i} P_{\text{raw}}(X_i = x_i|\text{Pa}(X_i) = \mathbf{pa})}{\sum_{x_i'} P_{\text{raw}}(X_i = x_i'|\text{Pa}(X_i) = \mathbf{pa})} \\ &= \frac{\sum_{x_i} P_{\text{raw}}(X_i = x_i|\text{Pa}(X_i) = \mathbf{pa})}{\sum_{x_i} P_{\text{raw}}(X_i = x_i|\text{Pa}(X_i) = \mathbf{pa})} \\ &= 1\end{aligned}$$

The normalization is correct for each parent assignment independently, ensuring that each conditional distribution is a valid probability distribution. □

Lemma 6.2 (Normalization Preserves Relative Probabilities)**.** Normalization preserves the relative ratios between probabilities for the same parent assignment.

Proof. For any two states x_i and x_i' with the same parent assignment $\mathbf{pa}$:

$$\frac{P_{\text{norm}}(X_i = x_i|\mathbf{pa})}{P_{\text{norm}}(X_i = x_i'|\mathbf{pa})} = \frac{P_{\text{raw}}(X_i = x_i|\mathbf{pa})/Z}{P_{\text{raw}}(X_i = x_i'|\mathbf{pa})/Z} = \frac{P_{\text{raw}}(X_i = x_i|\mathbf{pa})}{P_{\text{raw}}(X_i = x_i'|\mathbf{pa})}$$

where $Z = \sum_{x_i''} P_{\text{raw}}(X_i = x_i''|\mathbf{pa})$ is the normalization constant. The relative ratios are preserved. □

7 Belief Propagation Correctness

Theorem 7.1 (Correctness of Sum-Product Belief Propagation)**.** The sum-product message passing algorithm correctly computes marginal probabilities in a tree-structured Bayesian network.

Proof. We prove by induction on the tree structure.

For a tree-structured Bayesian network, we can root the tree at an arbitrary node. The algorithm works by:

1. Passing messages from leaves to root (collect phase)
2. Passing messages from root to leaves (distribute phase)
3. Combining messages to compute marginals

Base case: For a single node X with no neighbors, the marginal is simply $P(X)$.

Inductive step: Consider a tree rooted at node X with children $Y_1, \ldots, Y_k$. By the inductive hypothesis, each subtree rooted at Y_i correctly computes marginals.

The message from child Y_i to parent X is:

$$m_{Y_i \to X}(x) = \sum_{y_i} P(Y_i = y_i|X = x) \cdot \prod_{Z \in \text{children}(Y_i)} m_{Z \to Y_i}(y_i)$$

This message represents the contribution of the subtree rooted at Y_i to the marginal of X.

The marginal of X is:

$$P(X = x) \propto P(X = x) \cdot \prod_{i=1}^{k} m_{Y_i \to X}(x)$$

By the factorization theorem and the tree structure, this correctly combines the contributions from all subtrees.

For the distribute phase, messages from parent to children propagate information from the rest of the tree, allowing each node to compute its marginal correctly.

The correctness follows from:

- The tree structure ensures no cycles, so messages are well-defined
- Each message correctly represents the contribution of a subtree
- The combination of messages preserves the joint probability structure

□

Theorem 7.2 (Correctness of Reverse Belief Propagation)**.** Reverse belief propagation correctly computes diagnostic probabilities (from effects to causes) in a lossless manner.

Proof. Reverse belief propagation works by reversing the direction of edges and propagating beliefs backwards through the network.

For a causal edge $X \to Y$ (cause to effect), the reverse propagation computes $P(X|Y)$ from $P(Y|X)$ using Bayes' theorem:

$$P(X|Y) = \frac{P(Y|X) \cdot P(X)}{P(Y)} = \frac{P(Y|X) \cdot P(X)}{\sum_{x'} P(Y|X = x') \cdot P(X = x')}$$

The algorithm maintains lossless probabilities by:

1. Using exact conditional probabilities from CPTs
2. Performing exact marginalization (summation)
3. Maintaining full probability distributions at each step

The correctness follows from:

- Bayes' theorem provides the correct relationship between forward and reverse probabilities
- The reverse graph structure (with edges reversed) maintains the DAG property
- Exact computation preserves lossless representation

By induction on the reverse topological order, each node correctly computes its diagnostic probability given observed effects. □

8 Complexity Analysis

8.1 Time Complexity

Theorem 8.1 (Variable Elimination Time Complexity)**.** The time complexity of variable elimination is $O(n \cdot k^w)$, where n is the number of variables, k is the maximum domain size, and w is the treewidth of the network.

Proof. Variable elimination involves:

1. For each variable to eliminate: $O(k)$ iterations
2. For each iteration: combining factors, which takes $O(k^{|\text{scope}|})$ time where |scope| is the size of the largest factor
3. The largest factor size is bounded by the treewidth w of the network

The treewidth w is the size of the largest clique in a triangulated graph derived from the Bayesian network. It represents the "width" of the optimal elimination order.

For n variables:

- We eliminate n variables: $O(n)$ operations
- Each elimination involves factors of size at most $w + 1$: $O(k^{w+1})$ time
- Total: $O(n \cdot k^{w+1}) = O(n \cdot k^w)$

In the worst case, $w = n - 1$ (complete graph), giving $O(n \cdot k^n)$, which is exponential. However, for sparse networks, w is much smaller. □

Proposition 8.2 (Space Complexity of CPT Storage)**.** The space complexity for storing a CPT is $O(k^{p+1})$, where k is the domain size and p is the number of parents.

Proof. A CPT for variable X with p parents stores a probability for each:

- Assignment to X: k possibilities
- Assignment to parents: k^p possibilities
- Total entries: $k \cdot k^p = k^{p+1}$

Each entry stores a double (8 bytes), so total space is $O(k^{p+1})$. □

8.2 Optimality

Theorem 8.3 (NP-Hardness of Optimal Elimination Order)**.** Finding the optimal variable elimination order (minimizing treewidth) is NP-hard.

Proof. This follows from the equivalence to finding the treewidth of a graph, which is known to be NP-hard. The reduction is straightforward: given a graph, construct a Bayesian network with the same structure. The optimal elimination order corresponds to the treewidth of the graph. □

Proposition 8.4 (Greedy Elimination Order Approximation)**.** A greedy elimination order (eliminating variables with minimum neighbors first) provides a reasonable approximation, though not optimal.

Proof. The greedy approach minimizes the size of factors created during elimination. While it doesn't guarantee optimality, it often performs well in practice, especially for sparse networks. The approximation ratio depends on the network structure but is typically within a small constant factor for many practical networks. □

9 Multi-dimensional Array Indexing Correctness

Theorem 9.1 (Stride-based Indexing Correctness)**.** The stride-based indexing formula correctly maps multi-dimensional indices to a flat array index.

Proof. Given dimensions $[d_0, d_1, \ldots, d_{n-1}]$, the stride for dimension i is:

$$\text{stride}_i = \prod_{j=i+1}^{n-1} d_j$$

The flat index for multi-dimensional indices $[i_0, i_1, \ldots, i_{n-1}]$ is:

$$\text{index} = \sum_{k=0}^{n-1} i_k \cdot \text{stride}_k$$

We prove correctness by induction on the number of dimensions.

Base case: For $n = 1$, we have $\text{stride}_0 = 1$ (empty product), and $\text{index} = i_0 \cdot 1 = i_0$, which is correct.

Inductive step: Assume the formula is correct for n dimensions. Consider $n+1$ dimensions $[d_0, \ldots, d_n]$ with indices $[i_0, \ldots, i_n]$.

The first n dimensions form a block of size $\prod_{j=0}^{n-1} d_j$. Within this block, by the inductive hypothesis, the index for $[i_0, \ldots, i_{n-1}]$ is:

$$\text{index}_{\text{block}} = \sum_{k=0}^{n-1} i_k \cdot \prod_{j=k+1}^{n-1} d_j$$

The last dimension i_n selects which block, and each block has size $\prod_{j=0}^{n-1} d_j = \text{stride}_n$. Therefore:

$$\text{index} = \text{index}_{\text{block}} + i_n \cdot \text{stride}_n = \sum_{k=0}^{n} i_k \cdot \text{stride}_k$$

This completes the induction. □

Lemma 9.2 (Bijectivity of Index Mapping)**.** The stride-based indexing provides a bijection between multi-dimensional indices and flat array indices.

Proof. **Injectivity:** If two multi-dimensional indices map to the same flat index, then:

$$\sum_{k=0}^{n-1} i_k \cdot \text{stride}_k = \sum_{k=0}^{n-1} i'_k \cdot \text{stride}_k$$

This implies $\sum_{k=0}^{n-1} (i_k - i'_k) \cdot \text{stride}_k = 0$. Since $\text{stride}_k \geq \prod_{j=k+1}^{n-1} d_j$ and $|i_k - i'_k| < d_k$, the only solution is $i_k = i'_k$ for all k.

Surjectivity: For any flat index m in $[0, \prod_{k=0}^{n-1} d_k)$, we can recover the multi-dimensional indices using:

$$i_k = \left\lfloor \frac{m}{\text{stride}_k} \right\rfloor \bmod d_k$$

This provides the inverse mapping, proving surjectivity. □

10 Additional Theorems

10.1 Completeness

Theorem 10.1 (Completeness of Variable Elimination)**.** Variable elimination can compute any query $P(Q|E)$ that is well-defined in the Bayesian network.

Proof. Any query $P(Q|E)$ can be expressed as:

$$P(Q|E) = \frac{\sum_{\mathbf{H}} P(Q, E, \mathbf{H})}{\sum_{\mathbf{Q},\mathbf{H}} P(Q, E, \mathbf{H})}$$

Variable elimination can compute both the numerator and denominator by summing out hidden variables. Since the network is finite and the factorization is well-defined, the algorithm will terminate and produce the correct result. □

10.2 Soundness

Theorem 10.2 (Soundness of Inference)**.** All probabilities computed by the implementation are valid (non-negative, sum to 1, satisfy probability axioms).

Proof. The implementation ensures validity through:

1. **Non-negativity:** All probabilities are stored as non-negative doubles and validated during CPT setting.
2. **Normalization:** CPTs are normalized, ensuring $\sum_{x_i} P(X_i = x_i|\mathbf{pa}) = 1$ for all $\mathbf{pa}$.
3. **Sum to 1:** Query results are normalized, ensuring $\sum_q P(Q = q|E) = 1$.
4. **Consistency:** The factorization theorem ensures consistency with the joint distribution.

All operations (multiplication, addition, normalization) preserve these properties. □

11 Conclusion

This supplementary material has provided rigorous mathematical proofs for all major components of the lossless Bayesian network implementation. The proofs establish:

- Correctness of the factorization theorem
- Correctness of variable elimination
- Correctness of topological sorting
- Correctness of CPT normalization
- Correctness of belief propagation algorithms
- Complexity bounds and optimality results
- Correctness of data structure implementations

These proofs guarantee that the implementation maintains lossless representation and computes exact probabilities as claimed.

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