Compiling Bayesian Networks by Symbolic Probability Calculation Based on Zero-suppressed BDDs

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Abstract

Compiling Bayesian networks (BNs) is one of the hot topics in the area of probabilistic modeling and processing. In this paper, we propose a new method of compiling BNs into multi-linear functions (MLFs) based on Zero-suppressed BDDs (ZBDDs), which are the graph-based representation of combinatorial item sets. Our method is different from the original approach of Darwiche et. al which encodes BNs into Conjunctive Normal Forms (CNFs) and then translates CNFs into factored MLFs. Our approach directly translates a BN into a set of factored MLFs using ZBDD-based symbolic probability calculation. The MLF may have an exponential size, but our ZBDD-based data structure provides a compact factored form of the MLF, and arithmetic operations can be executed in a time almost linear to the ZBDD size. Our method is not necessary to generate the MLF for the whole network, but we can extract MLFs for only a part of network related to the query, to avoid unnecessary calculation of redundant terms of MLFs. We show experimental results for some typical benchmark examples. Although our algorithm is simply based on the mathematical definition of probability calculation, the performance is competitive to the existing state-of-the-art method.

1 Introduction

Compiling Bayesian Networks (BNs) is one of the hot topics in the area of probabilistic modeling and processing. Recently, the data structures of decision diagrams[9; 4; 5; 6; 2; 10] are effectively used for accelerating probability computation for BNs. Darwiche et. al[6; 2] have shown an efficient method of compiling BNs into the factored forms of Multi-Linear Functions (MLFs), whose evaluation and differentiation solves the exact inference problem. In their method, at first a given BN structure is encoded to a Conjunctive Normal Form (CNF) to be processed in Boolean domain, and then the CNFs are factored under Boolean algebra. The compilation procedure generates a kind of decision diagram representing a compact Arithmetic Circuit (AC) with the symbolic parameters.

In this paper, we propose a new method of compiling BNs into factored MLFs based on Zero-suppressed BDDs (ZBDDs)[7], which are the graph-based representation at first proposed for VLSI logic design applications. Our method is based on a similar MLF modeling with symbolic parameters as well as Darwiche's approach. However, our method does not use CNF representation but directly translates a BN into a set of factored MLFs. Our ZBDD manipulator can generate a new ZBDD as the result of addition/multiplication operations between a pair of ZBDDs. Using such inter-ZBDD operations with a bottom-up manner according to the BN structure, we can produce a set of ZBDDs each of which represents the MLF of each BN nodes. We can see an important property that the total product of the ZBDDs for all BN nodes corresponds to the factored MLF which is basically equivalent to the Darwiche's result. In addition, our method is not necessary to calculate the MLF for the whole network, but we can extract MLFs for only a part of network related to the query, to avoid unnecessary calculation of redundant terms of MLFs.

In this paper, we show experimental results for some typical benchmark examples. Although our algorithm is simply based on the mathematical definition of probability calculation, the performance is competitive to the existing state-of-the-art method.

Our ZBDD-based method can also be compared with the recent work by Sanner and McAllester[10], computing BN probabilities using Affine Algebraic DDs (AADDs). Their method generates AADDs as the results of inter-AADD operations for a given BN and an inference query. This is somehow a similar manner to us, but the semantics of decision diagrams are quite different. We discuss the difference in a later section.

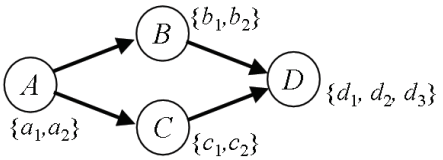
In the following sections, we describe the basic concept of BN compilation and existing method in Section 2. We then show the data structure of ZBDDs for representing MLFs in Section 3. In section 4, we describe the procedure of ZBDD generation and online inference. Experimental result is shown in Section 5, followed by conclusion.

2 Preliminary

Here we briefly review the method of compiling BNs.

2.1 Bayesian networks and MLFs

A *Bayesian network* (BN) is a directed acyclic graph. Each BN node has a network variable X whose domain is a discrete set of values. Each BN node also has a *Conditional Probability Table* (CPT) to describe the conditional probabilities of the variable X to be respective values for respective conditions of the parent BN nodes. Figure 1 shows a small example of BN with CPTs.



A	Prb(A)
a_1	$\theta_{a_1} = 0.4$
a_2	$\theta_{a_2} = 0.6$

AB	Prb($B\|A$)
a_1b_1	$\theta_{b_1\|a_1} = 0.2$
a_1b_2	$\theta_{b_2\|a_1} = 0.8$
a_2b_1	$\theta_{b_1\|a_2} = 0.8$
a_2b_2	$\theta_{b_2\|a_2} = 0.2$

AC	Prb($C\|A$)
a_1c_1	$\theta_{c_1\|a_1} = 0.5$
a_1c_2	$\theta_{c_2\|a_1} = 0.5$
a_2c_1	$\theta_{c_1\|a_2} = 0.5$
a_2c_2	$\theta_{c_2\|a_2} = 0.5$

BCD	Prb($D\|B,C$)
$b_1c_1d_1$	$\theta_{d_1\|b_1c_1} = 0.0$
$b_1c_1d_2$	$\theta_{d_2\|b_1c_1} = 0.5$
$b_1c_1d_3$	$\theta_{d_3\|b_1c_1} = 0.5$
$b_1c_2d_1$	$\theta_{d_1\|b_1c_2} = 0.2$
$b_1c_2d_2$	$\theta_{d_2\|b_1c_2} = 0.3$
$b_1c_2d_3$	$\theta_{d_3\|b_1c_2} = 0.5$
$b_2c_1d_1$	$\theta_{d_1\|b_2c_1} = 0.0$
$b_2c_1d_2$	$\theta_{d_2\|b_2c_1} = 0.0$
$b_2c_1d_3$	$\theta_{d_3\|b_2c_1} = 1.0$
$b_2c_2d_1$	$\theta_{d_1\|b_2c_2} = 0.2$
$b_2c_2d_2$	$\theta_{d_2\|b_2c_2} = 0.3$
$b_2c_2d_3$	$\theta_{d_3\|b_2c_2} = 0.5$

Figure 1: An example of BN.

The *Multi-Linear Function* (MLF)[5] consists of two types of variables, *indicator variable* λ_x for each value $X = x$, and *parameter variable* $\theta_{x|\mathbf{u}}$ for each parameter Prb($x|\mathbf{u}$). The MLF contains a term for each instantiation of the BN variables, and the term is the product of all indicators and parameters that are consistent with the instantiation. For the example in Fig. 1, the MLF has the following forms.

$$\begin{aligned}
& \lambda_{a_1}\lambda_{b_1}\lambda_{c_1}\lambda_{d_1}\theta_{a_1}\theta_{b_1|a_1}\theta_{c_1|a_1}\theta_{d_1|b_1c_1} \\
+\ & \lambda_{a_1}\lambda_{b_1}\lambda_{c_1}\lambda_{d_2}\theta_{a_1}\theta_{b_1|a_1}\theta_{c_1|a_1}\theta_{d_2|b_1c_1} \\
+\ & \lambda_{a_1}\lambda_{b_1}\lambda_{c_1}\lambda_{d_3}\theta_{a_1}\theta_{b_1|a_1}\theta_{c_1|a_1}\theta_{d_3|b_1c_1} \\
+\ & \lambda_{a_1}\lambda_{b_1}\lambda_{c_2}\lambda_{d_1}\theta_{a_1}\theta_{b_1|a_1}\theta_{c_2|a_1}\theta_{d_3|b_1c_2} \\
+\ & \ldots \\
+\ & \lambda_{a_2}\lambda_{b_2}\lambda_{c_2}\lambda_{d_3}\theta_{a_2}\theta_{b_2|a_2}\theta_{c_2|a_2}\theta_{d_3|b_2c_2}
\end{aligned}$$

Once we have generated the MLF for a given BN, the probability of evidence $\mathbf{e}$ can be calculated by setting indicators that contradict $\mathbf{e}$ to 0 and other indicators to 1. Namely, we can calculate the probability in a linear time to the size of MLF. Obviously the MLF has an exponential size, so the computation requires exponential time and space. The MLF can be factored into an *Arithmetic Circuit* (AC) whose size may not be exponential. If we can generate a compact AC for a given BN, the probability calculation can greatly be accelerated. This means compiling BNs based on MLFs.

2.2 Compiling BNs based on CNFs

Darwiche et. al[6] have shown an efficient method for generating compact ACs without processing an exponential size of MLFs. In their method, at first a given BN structure is encoded to a *Conjunctive Normal Form* (CNF) to be processed in Boolean domain. The CNF is factored by all variables one by one based on Boolean algebra, and a kind of decision diagram is obtained. The result of diagram has a special property called *smooth deterministic Decomposable Negational Normal Form* (smooth d-DNNF)[4], so it can directly be converted to the AC for probability calculation.

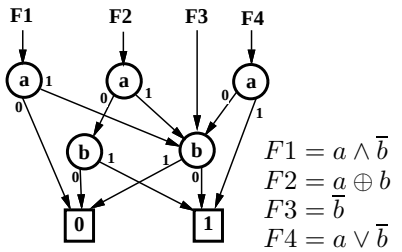


Figure 2: Shared multiple BDDs.

In addition, the following two techniques are used in variable encoding:

- If a parameter is deterministic ($\theta_{x|\mathbf{u}} = 1$ or 0), we do not assign a parameter variable and just reduce the CNF.
- The different parameter variables related to the same BN node do not coexist at the same term of MLF. Therefore, if a CPT contains a number of parameters with a same probability, we do not have to distinguish them and we may assign only one parameter variable to share those. This technique sometimes greatly reduces the CNF.

The experimental results reported that their method succeeded in compiling large-scale benchmark networks, such as "pathfinder" and "Diabetes," with a practical computation time and space. The BN compilation method is one of the hot topics on probabilistic modeling and inference for practical problems.

3 Zero-suppressed BDDs

In this paper, we present a new method of manipulating MLFs using Zero-suppressed BDDs (ZBDDs). Here we describe our data structure.

3.1 ZBDDs and combinatorial item sets

Reduced Ordered BDD (ROBDD)[1] is a compact graph representation of the Boolean function. It is derived by reducing a binary tree graph representing recursive *Shannon's expansion*. ROBDDs provide canonical forms for Boolean functions when the variable order is fixed. (In the following sections, we basically omit "RO" from BDDs.) As shown in Fig. 2, a set of multiple BDDs can be shared each other under the same fixed variable ordering. In this way, we can handle a number of Boolean functions simultaneously in a monolithic memory space.

A conventional BDD package supports a set of basic logic operations (i.e. AND, OR, XOR) for given a pair of operand BDDs. Those operation algorithms are based on hash table techniques, and the computation time is almost linear to the data size unless the data overflows the main memory. By using those inter-BDD operations, we can generate BDDs for given Boolean expressions or logic circuits.

BDDs are originally developed for handling Boolean function data, however, they can also be used for implicit representation of *combinatorial item sets*. A combinatorial item set consists of the elements each of which is a combination of a number of items. There are 2^n combinations chosen from n items, so we have 2^{2^n} variations of combinatorial item sets. For example, for a domain of five items a, b, c, d, and e, we can show examples of combinatorial item sets as:

$$\{ab, e\}, \{abc, cde, bd, acde, e\}, \{1, cd\}, 0.$$

a	b	c	F	
0	0	0	0	As a Boolean function:
1	0	0	0	F(a,b,c) = (a b ~c) V (~b c)
0	1	0	0	As a combinatorial item set:
1	1	0	1	S(a,b,c) = {ab, ac, c}
0	0	1	1	→ ab
1	0	1	1	→ c
0	1	1	0	→ ac
1	1	1	0	

Figure 3: A Boolean function and a combinatorial item set.

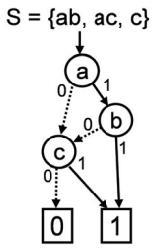


Figure 4: An example of ZBDD.

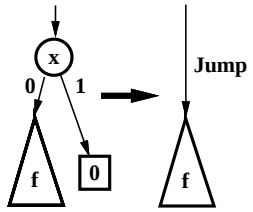


Figure 5: ZBDD reduction rule.

Here "1" denotes a combination of null items, and 0 means an empty set. Combinatorial item sets are one of the basic data structure for various problems in computer science.

A combinatorial item set can be mapped into Boolean space of n input variables. For example, Fig. 3 shows a truth table of Boolean function: $F = (a\ b\ \overline{c}) \vee (\overline{b}\ c)$, but also represents a combinatorial item set $S = \{ab, ac, c\}$. Using BDDs for the corresponding Boolean functions, we can implicitly represent and manipulate combinatorial item set.

Zero-suppressed BDD (ZBDD)[7] is a variant of BDDs for efficient manipulation of combinatorial item sets. An example of ZBDD is shown in Fig. 4. ZBDDs are based on the following special reduction rules.

- Delete all nodes whose 1-edge directly points to the 0-terminal node, and jump through to the 0-edge's destination, as shown in Fig. 5.
- Share equivalent nodes as well as ordinary BDDs.

The zero-suppressed deletion rule is asymmetric for the two edges, as we do not delete the nodes whose 0-edge points to a terminal node. It is proved that ZBDDs are also gives canonical forms as well as ordinary BDDs under a fixed variable ordering. Here we summarize the properties of ZBDDs.

- The nodes of irrelevant items (never chosen in any combination) are automatically deleted by ZBDD reduction rule.
- Each path from the root node to the 1-terminal node corresponds to each combination in the set. Namely, the number of such paths in the ZBDD equals to the number of combinations in the set.
- When many similar ZBDDs are generated, their ZBDD nodes are effectively shared into a monolithic multi-rooted graph, so the memory requirement is much less than storing each ZBDD separately.

Table 1 shows the most of primitive operations of ZBDDs. In these operations, $\emptyset$, **1**, $P.top$ are executed in a constant time, and the others are almost linear to the size of graph. We can describe various processing on sets of combinations by composing of these primitive operations.

Table 1: Primitive ZBDD operations.

"$\emptyset$"	Returns empty set. (0-termial node)
"**1**"	Returns the set of only null-combination. (1-terminal node)
P.top	Returns the item-ID at the root node of P.
P.factor0(v)	Subset of combinations not including item v.
P.factor1(v)	Gets $P - P$.factor0(v) and then deletes v from each combination.
P.attach(v)	Attaches v to all combinations in P.
$P \cup Q$	Returns union set.
$P \cap Q$	Returns intersection set.
$P - Q$	Returns difference set. (in P but not in Q.)
P.count	Counts number of combinations.

3.2 MLF representation using ZBDDs

An MLF is a polynomial formula of indicator and parameter variables. It can be regarded as a combinatorial item set, since each term is just a combination of variables. For example, the MLF at Node B in Fig. 1 can be written as follows.

$$\begin{aligned} \mathrm{MLF}(B) &= \lambda_{a_1}\lambda_{b_1}\theta_{a_1}\theta_{b_1|a_1} + \lambda_{a_1}\lambda_{b_2}\theta_{a_1}\theta_{b_2|a_1} \\ &+ \lambda_{a_2}\lambda_{b_1}\theta_{a_2}\theta_{b_1|a_2} + \lambda_{a_2}\lambda_{b_2}\theta_{a_2}\theta_{b_2|a_2} \end{aligned}$$

Here, we rename the parameter variables to share the same probabilities.

$$\begin{aligned} \mathrm{MLF}(B) &= \lambda_{a_1}\lambda_{b_1}\theta_{a(0.4)}\theta_{b(0.2)} + \lambda_{a_1}\lambda_{b_2}\theta_{a(0.4)}\theta_{b(0.8)} \\ &+ \lambda_{a_2}\lambda_{b_1}\theta_{a(0.6)}\theta_{b(0.8)} + \lambda_{a_2}\lambda_{b_2}\theta_{a(0.6)}\theta_{b(0.2)} \end{aligned}$$

Then, we show an example of ZBDD for MLF(B) in Fig. 6. In this example, there are four paths from the root node to the 1-terminal node, each of which corresponds to a term in the MLF. Namely, it is an implicit representation of the MLF. At the same time, the structure of ZBDD also represents a compact factored form of MLF. As shown in Fig. 7, each ZBDD decision node can be interpreted as a few AC nodes with the simple mapping rule. This means that a compact AC is quite easily obtained when we have generated a ZBDD for MLF.

We can see an important property that our ZBDD representation for an MLF is basically equivalent to a smooth d-DNNF, obtained by Darwiche's CNF-based method[6; 2]. In the following sections, we show our new method for generating ACs without CNFs but only using ZBDD operations.

3.3 Comparison to AADDs

Sanner and McAllester[10] presented *Affine Algebraic Decision Diagrams* (AADDs), another variant of decision diagram, for computing BN probabilities. AADD is a factored form of ADD, which contains indicator variables for splitting conditions, and the results of respective conditional probabilities are written in the leaves of the graph. This is somehow similar to our approach since they generate AADDs as the result of algebraic operations of AADDs. The most different point is that they numerically calculate the probability values with a floating-point data format, not using symbolic probability parameters as our MLFs. It is an interesting open problem which is more efficient to handle probabilities in symbolic or numerical. It may depend on the instances of probability values written in CPTs.

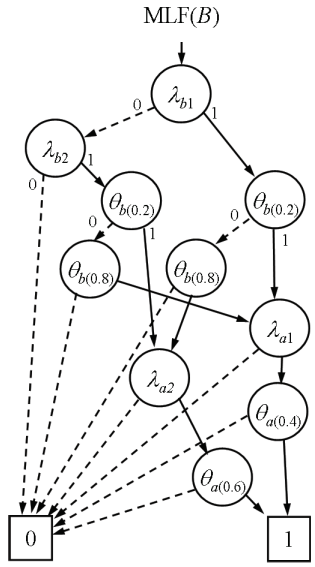


Figure 6: An example of ZBDD for MLF(B).

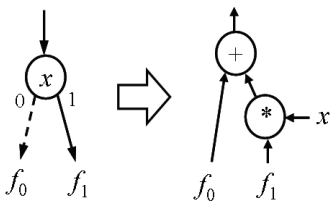


Figure 7: Mapping from a ZBDD node to an AC node.

4 ZBDD-based MLF calculation

4.1 ZBDD construction procedure

BDDs are originally developed for VLSI logic circuit design[1], and the basic technique of BDD construction is shown in Fig. 8. First we make trivial BDDs for the primary inputs F_1 and F_2, and then we apply the inter-BDD logic operations according to the data flow, to generate BDDs for F_3 to F_7. After that, all the BDDs are shared into a monolithic multi-rooted graph. This procedure is called *symbolic simulation* for the logic circuit.

Our ZBDD construction procedure for the MLF is based on a similar manner to the symbolic simulation of logic circuit. The different points are:

- BNs do not only assume binary values. The MLF uses multiple variables at each node for respective values.
- The BN node is not a logic gate. The function of each node is specified by a CPT.

As shown in Fig. 9, we first make MLF(A), and then we generate MLF(B) and MLF(C) using the result of MLF(A). Finally we generate MLF(D) using the results for the node B and C. After the construction procedure, all MLFs for respective nodes are compactly represented by the shared ZBDDs.

On each BN node X, the MLF is calculated by the following operations using the MLFs at the parent nodes of X.

$$\mathrm{MLF}(X_i) = \lambda_{x_i} \cdot \sum_{\mathbf{u} \in \mathrm{CPT(X)}} \left(\theta_{x(P_\mathbf{u})} \cdot \prod_{Y_v \in \mathbf{u}} \mathrm{MLF}(Y_v) \right)$$

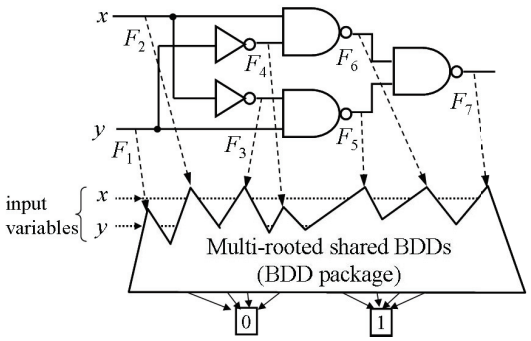


Figure 8: Conventional BDD construction procedure.

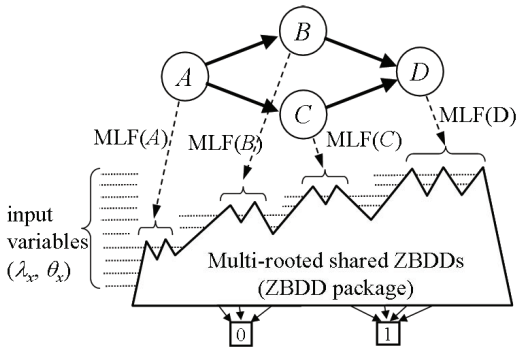


Figure 9: ZBDD construction procedure for BN.

Here MLF(X_i) denotes the MLF for the node X to be a value x_i. Namely, MLF(X) = $\sum$ MLF(X_i).

When calculating this expression using the ZBDD operations, we have to consider the differences between the arithmetic algebra and combinatorial set algebra. For considering arithmetic sum, we may use *union* operation to perform arithmetic sum, because the MLF does not contain the same term more than once. We should be more careful for arithmetic product operation. Product of two MLFs produces all possible combinations of two terms from the respective MLFs. Here, probabilistic algebra does not produces x^2 for duplicate variables, but just returns x. In addition, λ_{x_i} and λ_{x_j} (same node but different values) cannot coexist in one term since at least either becomes zero.

4.2 Multi-valued multiplication algorithm

The multiplication algorithm is a key technique in our compiling method. The conventional algorithm for product of two ZBDDs has been presented in the article[8]. The sketch of the algorithm is shown in Fig. 10. This algorithm is based on a divide-and-conquer manner, with the two recursive calls for the sub-graphs obtained by assigning 0 and 1 into the top variable. It also uses a hash-based cache technique to avoid duplicated recursive calls. The computation time is almost linear to the ZBDD size.

Unfortunately, the conventional algorithm does not consider multi-valued variable encoding, so the result of ZBDD may contain redundant terms, such as one both λ_{x_i} and λ_{x_j} coexist. Such redundant MLFs are still correct expressions for probability calculation, however, the redundant terms cause a significant overhead of computation time. For exam-

```
procedure(F · G)
{  if (F.top < G.top) return (G · F) ;
     if (G = 0) return 0 ;
     if (G = 1) return F ;
     H ← cache("F · G") ;
     if (H exists) return H ;
     v ← F.top ; /* the highest item in F */
     (F_0, F_1) ← factors of F by v ;
     (G_0, G_1) ← factors of G by v ;
     H ← ((F_1 · G_1) ∪ (F_1 · G_0) ∪ (F_0 · G_1)).attach(v)
        ∪(F_0 · G_0) ;
     cache("F · G") ← H ;
     return H ;
}
```

Figure 10: Conventional multiplication algorithm.

```
procedure(F · G)
{  if (F.top < G.top) return (G · F) ;
     if (G = 0) return 0 ;
     if (G = 1) return F ;
     H ← cache("F · G") ;
     if (H exists) return H ;
     v ← F.top ; /* the highest item in F */
     (F_0, F_1) ← factors of F by v ;
     (G_0, G_1) ← factors of G by v ;
     F_Z ← F_0 ; G_Z ← G_0 ;
     while(F_Z.top and v conflict) F_Z ← F_Z.factor0(F_Z.top) ;
     while(G_Z.top and v conflict) G_Z ← G_Z.factor0(G_Z.top) ;
     H ← ((F_1 · G_1) ∪ (F_1 · G_Z) ∪ (F_Z · G_1)).attach(v)
        ∪(F_0 · G_0) ;
     cache("F · G") ← H ;
     return H ;
}
```

Figure 11: Improved multiplication algorithm.

ple, we analyzed our MLF construction for a BN in the benchmark set. It is a typical case that we have the two ZBDDs F and G each of which has about 1,000 decision nodes, and the product $(F \cdot G)$ grows as much as 200,000 nodes of ZBDD, but it can be reduced to only 400 nodes after eliminating redundant terms. This observation indicates that, the redundant terms consume 500 times of overhead time and space in this case.

To address this problem, we implemented an improved multiplication algorithm devoted to the multi-valued variable encoding. Figure 11 shows a sketch of new algorithm. Here we assume that the indicator variables for a same BN node have the consecutive positions in the ZBDD variable ordering. This algorithm does not produce any redundant terms in the recursive procedure, and we can calculate MLFs without any overhead related to the multi-valued encoding.

4.3 Online inference based on ZBDDs

After the compilation procedure, each BN node has its own ZBDD for the MLF. The MLF(X) on a node X contains only the variables at the ancestor nodes of X, since the other variables are irrelevant to the probabilities on X.

Here we describe the online inference method based on ZBDDs. To obtain the joint probability for evidence $\mathbf{e}$, we first compute the product of MLF(X_v) for all $X_v \in \mathbf{e}$ by the ZBDD multiplication operation. The contradicting terms are automatically eliminated by our multiplication algorithm, so the result of ZBDD contains only the variables related to the joint probability computation. We then set all indicators to 1 and calculate the AC directly converted from the ZBDD.

For example, to compute Prb(b_1, c_2) for the BN of Fig. 1, the two MLFs are the follows:

$$\text{MLF}(B_1) = \lambda_{a_1}\lambda_{b_1}\theta_{a(0.4)}\theta_{b(0.2)} + \lambda_{a_2}\lambda_{b_1}\theta_{a(0.6)}\theta_{b(0.8)},$$
$$\text{MLF}(C_2) = \lambda_{a_1}\lambda_{c_2}\theta_{a(0.4)}\theta_{c(0.5)} + \lambda_{a_2}\lambda_{c_2}\theta_{a(0.6)}\theta_{c(0.5)},$$

and then

$$\text{MLF}(B_1)\cdot\text{MLF}(C_2) = \lambda_{a_1}\lambda_{b_1}\lambda_{c_2}\theta_{a(0.4)}\theta_{b(0.2)}\theta_{c(0.5)} + \lambda_{a_2}\lambda_{b_1}\lambda_{c_2}\theta_{a(0.6)}\theta_{b(0.8)}\theta_{c(0.5)}.$$

Finally we can obtain the probability as: $0.4 \times 0.2 \times 0.5 + 0.6 \times 0.8 \times 0.5$.

In our method, each multiplication requires a time almost linear to the ZBDD size, however, the ZBDD size may not glow larger in repeating multiplications for the inference, because many of terms contradict the evidence and they are eliminated. Therefore, the computation cost for the inference will be much smaller than the cost for compilation.

An interesting point is that the above MLF for Prb(b_1, c_2) does not contain the variables at the node D since they are irrelevant to the joint probability. In other word, our inference method provides dependency checking for a given query.

As another strategy, we can generate the MLF for the whole networks by performing product of all MLF(X). Such a global MLF is basically equivalent to the result of Darwiche's compilation[2]. After generating the global MLF, we do not have to perform product of MLFs any more. However, the MLF contains the parameters of all the BN nodes, and we should sum up the parameters even if they are irrelevant to the query. Having a set of local MLFs will be more efficient than the global one since we can avoid unnecessary calculation of parameters not related to the query.

Finally we note that our method can save the result of partial product of MLFs in the shared ZBDD environment, so we do not have to re-compute ZBDDs for the same evidence set.

5 Experimental Results

For evaluating our method, we implemented a BN compiler based on our own ZBDD package. We used a Pentium-4 PC, 800MHz, 1.5GB of main memory, with SuSE Linux 9 and gnu C++ compiler. In this platform, we can manipulate up to 40,000,000 nodes of ZBDDs with up to 65,000 different variables. We applied our method to the practical size of BN examples provided at http://www.cs.huji.ac.il/labs/compbio/Repository.

The experimental results are shown in Table 2. In this table, the first four columns shows the network specifications, such as BN name, the number of BN nodes, the indicator variables, and the parameter variables to be used in the MLF. The next three columns present the results of our compiling method. "|ZBDDs|(total)" shows the number of decision nodes in the multi-rooted shared ZBDDs representing the set of MLFs. "|ZBDD|(a node)" is the average size of ZBDD on each BN node. Notice that the total ZBDD size is usually much less than numerical product of each ZBDD size because their sub-graphs are shared each other.

After compilation, we evaluated the performance of online inference. In our experiment, we randomly select a pair of BN nodes with random values (x_i, y_j), then generate a ZBDD as the product of the two ZBDDs $(\text{MLF}(X_i) \cdot \text{MLF}(Y_j))$. After that we counted the number of decision nodes "|ZBDD|(product)" and the number of the MLF terms. We repeated this process for 100 times and show the average time and space. The inference time shown here is

Table 2: Experimental results.

BN name	BN nodes	indicator vars.	parameter vars.	offline compile			inference (ave. for 100 cases)			CNF-based[2](*)	
				|ZBDDs| (total)	|ZBDD| (a node)	time (sec)	|ZBDD| (product)	MLF terms	time (sec)	comp. time	inf. time
alarm	37	105	187	34,299	1,863	0.2	4,139	3.70×10^8	0.04	0.52	0.01
hailfinder	56	223	835	294,605	4,427	3.0	9,799	1.00×10^{17}	0.19	0.86	0.06
mildew	35	616	6,709	15,310,511	2,684,245	8019.4	593,469	6.60×10^{16}	43.43	7,483.80	3.35
pathfinder(pf1)	109	448	1,839	16,808	155	20.1	337	667	0.01	20.36	0.07
pathfinder(pf23)	135	520	2,304	17,557	135	19.6	188	212	0.01	(no data)	(no data)
pigs	441	1,323	1,474	73,543	237	2.9	993	3.27×10^7	0.01	17.84	1.60
water	32	116	3,578	25,629	611	6.1	974	6,295	0.02	4.83	0.21
diabetes	413	4,682	17,622	–	–	(>36k)	–	–	–	2,269.05	16.27
munin1	189	995	4,249	–	–	(>36k)	–	–	–	1,534.97	44.91
munin2	1,003	5,376	22,866	9,936,191	86,267	1,247.8	–	–	(>360)	225.46	6.59
munin3	1,044	5,604	24,116	11,191,778	100,640	777.7	–	–	(>360)	151.72	3.65
munin4	1,041	5,648	24,242	5,724,468	46,989	4,951.1	–	–	(>360)	677.92	7.70

(*) uses a PC twice faster than ours.

the total time of ZBDD multiplication and traversing every decision node once in the ZBDD for calculating probability. From the experimental results, we can observe that the size of "|ZBDD|(product)" is dramatically smaller than "|ZBDDs|(total)." This indicates that we can avoid calculating so many redundant terms of MLFs, by using a product of local MLFs instead of the global MLF.

In the last two columns, we referred the results of CNF-based method[2]. For some of examples, our results are competitive or better than theirs. Notice that we cannot directly compare to their results because (1) the experimental setting of online inference would be different, (2) we may use a different variable ordering since it is not shown in [2], and (3) for larger examples, they applied another technique called *decomposition tree*(dtree)[3], to reduce the original network of CPTs

Currently, our simple variable ordering strategy is that a variable appears at earlier stage of calculation will get a lower position (near to the leaf) in ZBDDs. The ZBDD size is sometimes very sensitive to the variable ordering. For example, we have observed that the ZBDDs for "munin2" can easily be reduced to a half by ad-hoc exchange of variable ordering. We expect that a good variable ordering will bring a significant improvement to the current results.

Our method is too time-consuming for larger examples, such as "diabetes" and "munin"s. This would be because we have not applied the dtree-based CPT network reduction. This technique is independent of our ZBDD-based data structure, so we hope it will be effective as well as for the CNF-based method.

6 Conclusion

We have presented a new method of compiling BNs, not using CNF encoding but directly calculate MLFs by using ZBDDs. Our method is not necessary to generate MLFs for the whole networks, but we can extract MLFs for only selective BN nodes related to the query, to avoid unnecessary calculation of redundant terms of MLFs. Our computation algorithm is quite simple and just based on the mathematical definition of probability calculation, and still efficiently calculates an exponential size of MLFs in a compact ZBDD representation. Our method will be improved more in combining with state-of-the-art techniques developed in the history of BN processing.

In this paper, we have shown that the BN compilation process has a similarity to the symbolic simulation of VLSI logic circuits. There have been so many heuristic techniques on BDDs in VLSI logic design area, and some of them would be useful for probabilistic inference on BNs or Markov Decision Processes.

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