Hypertree Decompositions Revisited for PGMs

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Abstract

We revisit the classical problem of exact inference on probabilistic graphical models (PGMs). Our algorithm is based on recent worst-case optimal database join algorithms, which can be asymptotically faster than traditional data processing methods. We present the first empirical evaluation of these new algorithms via JoinInfer, a new exact inference engine. We empirically explore the properties of the data for which our engine can be expected to outperform traditional inference engines refining current theoretical notions. Further, JoinInfer outperforms existing state-of-the-art inference engines (ACE, IJGP and libDAI) on some standard benchmark datasets by up to a factor of 630x. Finally, we propose a promising data-driven heuristic that extends JoinInfer to automatically tailor its parameters and/or switch to the traditional inference algorithms.

1 Introduction

Efficient inference on probabilistic graphical models (PGMs) is a core topic in artificial intelligence (AI) and standard inference techniques are based on tree decomposition [21][13][23][28]. The runtime of such algorithms is exponential in the treewidth (tw) of the underlying graph, which in the worst case, is unavoidable. Over the years, efforts in the logic, database and AI communities to refine tw into a finer-grained measure of complexity have culminated in generalized hypertree decompositions (GHDs) [18][15]. Recently, FAQ/AJAR [4][22] theoretically reconnected such GHD-based algorithms with probabilistic inference and achieved tighter bounds based on a finer-grained notion of width called fractional hypertree width (fhtw).

However, (1) the practical significance of such GHD based PGM inference has met with some skepticism: Dechter et al. [14], via experimental evaluation, conclude that classical treewidth-based algorithms run faster on PGM benchmarks than those optimizing GHD-based measures. Their experiments suggest that the advantages of the latter manifest only in instances with substantial factor sparsity (i.e. large number of factor entries have zero probabilities) and high factor arity. (2) Translating the superior asymptotic bounds of GHDs into practice is a non-trivial challenge. In theory, these algorithms assume that one can exhaustively search over all potential GHDs, which is often untenable due to the combinatorial explosion of possible GHDs with thousands of variables and factors. Indeed, the theoretical runtimes of these algorithms completely ignore the dependence on the number of variables and factors; in practice, their asymptotic advantages may be negated by large constants.
In the current work, we revisit the conclusions in (1) and overcome the challenges of (2) using a proof-of-concept inference engine — JoinInfer — that leverages recently introduced worst case optimal joins \cite{31} in conjunction with improved data structures. In particular, we make the following contributions:

**GHDs revisited.**

- Experimental evaluation in \cite{14} used a ratio of theoretical bounds based on the GHD measure of hypertree width (htw) and the treewidth measure (we call the analogous version of this ratio $R_D$: where we replace htw with fhtw). However, we suggest that the predictions made by $R_D$ are, in practice, contingent upon the total number of entries processed across all bags of the GHD (we call this $\rho$). Engines such as libDAI that use truth-table indices do not scale to higher levels of $\rho$, an insight that is not captured in \cite{14}'s experimental paradigm. For instance, in the top row in Figure 1 (corresponding to high $\rho$), libDAI fails on all datasets while JoinInfer successfully completes on all of them.

- Introduction of $\rho$ shows that GHD based algorithms like JoinInfer may have a wider scope than previously predicted: while \cite{14} predicted that JoinInfer will work well only when $R_D$ is small, we expect it to perform well even when $R_D$ is medium-to-large (provided $\rho$ is high). We expect libDAI to perform well when $R_D$ is medium-to-large and $\rho$ is low (Bands 5 and 6 in Figure 1).

- We use a finer-grained theoretical measure that better predicts JoinInfer’s speed up, thus refining the insights of \cite{14}. For instance, our measure can differentiate between the rows of column ‘$R_D$ small’ in Figure 1 while $R_D$ cannot.

- We show that JoinInfer can be up to 630x faster on networks with small $R_D$ and high $\rho$ (Band 1 in Figure 1). When $R_D$ is large, at the higher threshold of $\rho$ (Band 3 in Figure 1), JoinInfer actually outperforms at non-trivial levels (by upto 2.7x), while the corresponding prediction by \cite{14} expects under-performance by more than $10^{10}$x. IJGP and libDAI fail in this space; ACE is the only other
engine that completes on a subset of the space, since it is designed to accommodate higher levels of \( \rho \).

**Hybrid Architecture.** Given the relative advantages of JoinInfer and libDAI in different spaces, we explore the feasibility of exploiting their strengths in a ‘best-of-all-worlds’ architecture. The hybrid outperforms libDAI, IJGP and ACE for 75% of the networks (ref. Table 1), illustrating its promise.

**Technical Contributions.** Our primary technical contribution in JoinInfer lies in improved data-structures. We introduce two data representations for use in different passes of the algorithm: (i) level-order trie, which collapses a conventional trie into a single array; (ii) (two variants of) an index-based compressed list. We find that the resulting gains more than compensate for the overheads involved in maintaining both data representations.

## 2 Related Work

Several streams of inquiry have emerged in the exact inference setting. One such stream involves *conditioning algorithms* [32, 11] that adopt a case-based reasoning approach. *Cutset conditioning* [32] attempts to reduce a network into a tree structure so as to make inference tractable, while another approach *recursive conditioning* [11] recursively decomposes a network into smaller subnetworks that are solved independently.

Another class of algorithms seeks to exploit local structure [26, 33], where [10, 20] exploit factor sparsity by going beyond the listing representation (i.e., they only store tuples with non-zero probability). In particular, the goal in these aforementioned works is to represent the factors compactly via *algebraic* structures. Among related representations, *arithmetic circuits* or ACs [9] are still a very active research area [34]. At a very high level, these circuits work best when the PGM variables themselves are Boolean. However, the ‘compilation’ process (to AC representation) becomes more expensive for larger domain sizes. Although our algorithm also seeks to exploit factor sparsity, it works directly with the much simpler listing representation, making it much more efficient.

An emerging area *lifted probabilistic inference* [12, 29, 24], exploits symmetric structures within graphs to speed up inference. Thus far, this has been undertaken primarily in the relational learning paradigm, whereas our current work is propositional.

Yet another stream runs along the lines of variable elimination [13, 35], which undertakes a sequential marginalization of variables to compute posterior probabilities. Another stream involves tree decomposition-based routines [21, 23, 28] where the original network is decomposed into a hypertree and inference is performed using a two-phase message passing routine on this decomposed tree. The runtime complexity of most of these algorithms is dictated by the treewidth of the underlying graph. JoinInfer improves on this class of algorithms, with its complexity bounded by a finer notion of fractional hypertree width.

Finally, past work in PGMs has also focused on approximate inference [25]; we believe that the advancements introduced in JoinInfer could enhance existing approximate engines by, for instance, applying it to models in the emerging tractable learning paradigms [7] such as thin junction trees [6].
3 JoinInfer: An Overview

Below we (a) give a brief overview of the background concepts, (b) outline the theoretical algorithm and (c) identify the implementation challenges and present our solutions.

3.1 Background

**Definition 1** A (discrete) probabilistic graphical model can be defined by the triplet $(\mathcal{H}, D, \mathcal{K})$ where hypergraph $\mathcal{H} = (V, E)$ represents the underlying graphical structure (note $E \subseteq 2^V$). There are $n = |V|$ discrete random variables on finite domains $D = \{D(U) : U \in V\}$ and $m = |E|$ factors $\mathcal{K} = \{\phi_e | e \in E\}$, where each factor $\phi_e$ is a mapping: $\phi_e : \prod_{U \in e} D(U) \rightarrow \mathbb{R}_+$. For instance Figure 2 is a hypergraph representing a PGM with variables $V = \{A, B, C, D\}$, edges $E = \{e = (A, B), f = (A, C), g = (B, C, D)\}$ and factors $\mathcal{K} = \{\phi_e(A, B), \phi_f(A, C), \phi_g(B, C, D)\}$.

**Definition 2** For any factor $\phi$, the size of $\phi$ is its support size, i.e., the number of entries with non-zero probabilities. Storing only the non-zero entries (as well as their $\phi$ values) is called the listing representation of $\phi$. Factor sparsity is defined as $N/\prod_{U \in \phi} |D(U)|$, where $N$ is the size of factor $\phi$.

![Figure 2: The PGM query hypergraph (left), factor graph (middle) and a GHD for it (right). We use hypergraphs instead of factor graphs for notational ease.](image)

A typical inference task in PGMs is to compute the marginal estimates given by: $\forall F \subseteq V, \ y \in \prod_{U \in F} D(U)$,

$$\phi_F(y) = \frac{1}{Z} \sum_{z \in \prod_{U \in F \setminus F} D(U)} \prod_{S \in E} \phi_S(x_S), \quad (1)$$

where $x = (y, z)$, $x_S$ denotes the projection of $x$ onto the variables in $S$ and $Z$ is a normalization constant. Variable/factor marginals are a special case of $[1]$; $F = \{U\}$ for $U \in V$ for variable marginals and $F \in E$ for factor marginals.

Exact inference in PGMs is usually performed by propagating on a **generalized hypertree decomposition (GHD)** of the underlying hypergraph $\mathcal{H}$.

**Definition 3** A GHD of $\mathcal{H} = (V, E)$ is defined by a triple $\langle T, \chi, \lambda \rangle$, where $T = (V(T), E(T))$ is a tree, $\chi : V(T) \rightarrow 2^V$ is a function associating a set of vertices $\chi(v) \subseteq V$ to each node $v$ of $T$, and $\lambda : V(T) \rightarrow 2^E$ is a function associating a set of hyperedges to each node $v$ of $T$ such that the following properties hold (i) for each $e \in E$, there is a node $v \in V(T)$ such that $e \subseteq \chi(v)$ and $e \in \lambda(v)$; and (ii) for each $t \in V$, the set $\{v \in V(T) | t \in \chi(v)\}$ is connected in $T$.
3.1.1 Existing GHD-based message passing algorithms

As illustrated in Figure 2, a GHD can be thought of as a labeled (hyper)tree $T$, where sets assigned to each node in $T$ are called bags of the hypertree. Inference propagation on $T$ involves a two-pass ‘message-passing’ algorithm [21]. In the first pass (message-up), messages are propagated ‘up’ from leaf (child) to root (parent). Subsequently in the second pass (message-down), they are propagated ‘down’ from root (parent) to leaf (child).

A message $\phi_{m_{v,u}}$ from node $v$ to node $u$ can be viewed as a marginal estimate where variables $U \not\in \chi(v) \cap \chi(u)$ are summed out of the factor product of node $v$, which is given by:

$$\phi'_v = \prod_{e \in \lambda(v)} \phi_e \cdot \prod_{u \in \Gamma(v)} \phi'_{m_{u,v}},$$

where $\Gamma(v)$ represents Children$(v)$ or Parent$(v)$ depending on the propagation direction. Upon completion of both propagation passes variable marginals for all $U \in \chi(v)$ can be retrieved using label $\chi(v)$, and factor marginals for all $e \in \lambda(v)$ can be retrieved from each node $v$ using the label $\lambda(v)$.

3.2 Joins based theoretical inference algorithm

The above GHD based messaging passing framework (also known as junction tree algorithms) forms the structure of JoinInfer as outlined in Algorithm 1 (in standard algorithms $R$ is always 0, and in FAQ/AJAR $R$ is always 1). To compute the GHD in Line 3 we build a junction tree using the MinFill heuristic, rooting it arbitrarily and determine the parent-child relationship for every node. We assume that each input factor in $\mathcal{K}$ is assigned to a unique bag in the GHD. In particular, for every node $v$, $\alpha(v)$ denotes the factors in $\mathcal{K}$ assigned to it.

**Algorithm 1 JoinInfer**

1: **Input:** A PGM $\mathcal{P} = (\mathcal{H}, D, \mathcal{K})$.
2: **Output:** Variable and Factor Marginals.
3: Create a GHD $G = ((V, E), \chi, \lambda)$ for $\mathcal{P}$. $\triangleright$ Using MinFill variable ordering.
4: $R \leftarrow$ HYJAR$(G)$ $\triangleright R : V \rightarrow \{0, 1, 2\}$.
5: $\{\phi'_v, v \in V, \{\phi'_{m_{v,Paren(v)}} \mid v \in V\} \} \leftarrow$ JoinInferUp$(G, R)$
6: $\{\phi'_v, v \in V \} \leftarrow$ JoinInferDown$(G, \{\phi'_v, v \in V, \{\phi'_{m_{v,Paren(v)}} \mid v \in V\} \})$
7: Compute variable and factor marginals from $\{\phi'_v, v \in V\}$

3.2.1 Message-Up Phase

**Computation Within a Single Bag.** The upward pass propagates messages or marginalized factor products from leaf-nodes (child bags) to root-nodes (parent bags) along the hypertree. This involves computing factor products at every node (bag) of the hypertree. The runtime complexity of junction tree algorithms is dominated by these bag-wise factor product computations, and, it is here that JoinInfer lends its core contribution: it uses a novel algorithm different from previously proposed exact inference algorithms to compute the factor products inside each bag. By exploiting the correspondence between computing database joins and computing factor marginals[1] it uses worst-case optimal join algorithms.

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[1]If the probability values in the factor entries are Boolean, i.e., just 0 or 1, the factor product would reduce to a join.
WCOJA) to compute the factor products within each bag. The key idea behind these algorithms is that, unlike the traditional approach of computing factor products via a sequence of pairwise products, WCOJA undertake a multi-way product, i.e., the product of all relevant factors are computed simultaneously. Moreover, they work on a listing representation of the factors thereby exploiting the inherent factor sparsity of a PGM. The multi-way product algorithm used by JoinInfer is outlined in Algorithm[2] which is essentially from [31].

The inputs to Algorithm [2] are: a product flag that decides between the Multiway Product algorithm of [31] and Algorithm[3], the set of variables $V$ whose product $\phi'$ needs to be computed, the corresponding factors $\mathcal{E}$, factor tables $\mathcal{K}$ and finally, the set of free variables $\mathcal{F}$. When the product flag is 2, we run the traditional Pairwise Product algorithm. Otherwise, we run our algorithm whose description we provide here. We assume that $V$, $\mathcal{E}$, $\mathcal{K}$ and $\mathcal{F}$ are all sorted in input order. We now start with $V_1$ and find a value $y \in D(V_1)$ that is present in all the factor tables of factors which contain $V_1$. We then fix this value as a potential candidate for $V_1$ in the factor product and continue the process for $V_2$ and so on. If we get a potential candidate from every variable in $V$, we have a vector that we add to the final factor product. On the other hand, if we don't get a potential candidate in a given variable say $V_y$, we backtrack and find a new potential candidate for $V_{k-1}$ (i.e. a value that is present in all factor tables of factors containing $V_{k-1}$) and so on (until $V_1$). We obtain two outputs from this algorithm: the factor product $\phi'$ and its marginal on $\mathcal{F}$ denoted by $\phi'_\mathcal{F}$.

**Example 1** Let us look at the triangle query $\psi(A, B, C) = \phi(A, B) \cdot \phi(B, C) \cdot \phi(C, A)$ for a bag. For simplicity, let $|D(U)| = D$ for all $U \in \{A, B, C\}$ and $|\phi_e| = N \leq D^2$ for all $e \in \{(A, B), (B, C), (C, A)\}$. Standard algorithms compute this query in time $O(D^3)$. On the other hand, we obtain a runtime bound of $O(N^{3/2})$, a bound that becomes especially useful in the presence of factor sparsity i.e., $N < D^2$ (in the worst case $N = D^2$, we recover the bound $O((D^2)^{3/2} = O(D^3)$).

**Computation Across Multiple Bags.** Another significant difference stems from the ‘factors’ that are included in the bag-wise product computation [14]. Standard algorithms process (a) the input factors mapped to the bag and (b) the messages received by the bag from its children. In addition to the above two, JoinInfer also includes factors called ‘01-projections’ that are not originally mapped to the bag, but have non-trivial intersections with the variables in the bag. In other words, such factors are computed across multiple bags in the hypertree. In the presence of sparsity, this ‘look-ahead’ maneuver helps prune unproductive entries from factor products early on. Further, using 01-projections is central to realizing the asymptotically better bounds in FAQ/AJAR (see Section[3.2.3]).

**Example 2** Consider the bag $\{A, B, C\}$ of the GHD in Figure[2] (where assume $F = \{B, C\}$) representing a product over two factors, $\phi'(a, b, c) = \phi_e(a, b) \cdot \phi_f(a, c)$. The 'up' pass would propagate $\phi'(b, c) = \sum_a \phi'(a, b, c)$, a marginal on $\{B, C\}$ to the root bag $(B, C, D)$. The worst-case output size of this factor product is given by $|\phi_e(a, b) \cdot \phi_f(a, c)| \leq |\phi_e(a, b)| \cdot |\phi_f(a, c)| = N^2$ and consequently the runtime bound is $O(N^2)$. However, we are able to obtain a much better bound by also utilizing factor $\phi_g(B, C, D)$ in the product computation (as both B and C participate in this factor), $\psi(A, B, C) = \phi_e(A, B) \cdot \phi_f(A, C) \cdot \phi_{01}(B, C)$, where $\phi_{01}(b, c) = 1$, $\exists d$ s.t. $\phi_g(b, c, d) \neq 0$ and 0 otherwise. By employing this 01-projection in our factor product computation, we can get a bound of $N^{3/2}$ on the output size (recall Example[1]) and consequently a runtime bound of $O(N^{3/2})$ for the above query (detailed illustration and formal definition of 01-projections are provided later in Appendix[4.7]).
Algorithm 2 MultFacProd

1: **Input:** Product Flag $P$, Variables $V$, Factors $\mathcal{E}$, Factor Tables $\mathcal{K}$ (as tries) and Free variables $\mathcal{F}$. $\triangleright$ All these are sorted in the input order.

2: **Output:** Factor Product $\phi'$ and its marginal on $\mathcal{F}$, denoted by $\phi'_\mathcal{F}$.

3: if $P = 2$ then
4: $(\phi', \phi'_\mathcal{F}) \leftarrow$ PairwiseProd$(V, \mathcal{E}, \mathcal{K}, \mathcal{F})$ $\triangleright$ Algorithm 3.
5: return $(\phi', \phi'_\mathcal{F})$

6: Initialize a vector $x$ of size $|V|$ to all 0s. $\triangleright$ The entries of $\phi'$ will be added one-by-one as a vector $(x)$, probability pair.

7: $x_1 \leftarrow -\infty$, $k \leftarrow 0$
8: while $x_1 < \infty$ do
9: $y \leftarrow x_k + 1$
10: while (true) do
11: for all $S \in \mathcal{E}_k : S \cap V_{k+1} \neq \emptyset$ do $\triangleright$ All factors that contain the variable $V_{k+1}$.
12: $y^S_{k+1} \leftarrow \min\{x_{k+1}(x_{k+1} > y) \land (x_{k+1} \in \mathcal{K}_{S_{k+1}})\}$ $\triangleright$ Here, $\mathcal{K}_S$ is the factor table corresponding to $S$. Among all $x_{k+1} \in D(V_{k+1}) : x_{k+1} > y$ having at least one entry in $\mathcal{K}_S$, we pick the smallest one (using galloping).
13: $y \leftarrow \max_S\{y^S_{k+1}\}$
14: if ($y = \min_S\{y^S_{k+1}\}$) then $\triangleright$ Check if the value $y$ is present in all factor tables of factors that contain $V_{k+1}$.
15: $x_{k+1} \leftarrow y$
16: break
17: else
18: $y \leftarrow y - 1$
19: if ($x_{k+1} \neq \infty$) then
20: if $k + 1 < |V|$ then
21: $k \leftarrow k + 1$ $\triangleright$ The value for variable $V_k$ is fixed as $x_k$ and we move on to the next variable.
22: $x_{k+1} \leftarrow -\infty$
23: else
24: $\phi' \leftarrow \phi' \cup \{(x, \prod_{S \in \mathcal{E}_k} \mathcal{K}_S(x_S))\}$
25: else
26: if $k > 0$ then
27: $k \leftarrow k - 1$ $\triangleright$ We don't have any potential candidates for $V_{k+1}$ and we backtrack.
28: if $\mathcal{F} \neq \emptyset$ then
29: $\phi'_{\mathcal{F}} \leftarrow \sum_{q \in \mathcal{V} \setminus \mathcal{F}} \phi'$ $\triangleright$ We marginalize out $\phi'$ on all the variables in $\mathcal{F}$, resulting in a set of vector, probability pairs.
30: return $(\phi', \phi'_\mathcal{F})$
than WCOJA.

traditional algorithms in lines 13 and 14 use a pairwise product algorithm, which is asymptotically slower
in Line 7 is always satisfied while in traditional algorithms, the condition is never satisfied. Further,
the bag’ s factor product. A detailed description on how to compute an in-place HashProduct follows.
up and down messages sent/received by the bag, and then, between the result of the previous step with
the bag’s factor product. This is step is computed using LibDAI’s API for marginalizing out variables from a
Factor/Cluster Product.

The upward message propagation in JoinInfer is outlined in Algorithm 4. In FAQ/AJAR, the condition
in Line 7 is always satisfied while in traditional algorithms, the condition is never satisfied. Further,
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traditional algorithms in lines 13 and 14 use a pairwise product algorithm, which is asymptotically slower than WCOJA.

Algorithm 3 PairwiseProd

1: **Input:** Variables $V$, Factors $\mathcal{E}$, Factor Tables $\mathcal{K}$, Free variables $\mathcal{F}$. $\triangleright$ All these are sorted in the input
order.
2: **Output:** Factor Product $\phi'$ and its marginal on $\mathcal{F}$, denoted by $\phi'_{\mathcal{F}}$
3: $\phi' \leftarrow \emptyset$
4: **for all** $e \in \mathcal{E}$ **do**
5:  **if** $\phi' == \emptyset$ **then**
6:   $\phi' \leftarrow \mathcal{K}_e$
7:  **else**
8:   $\phi' \leftarrow \phi' \cdot \mathcal{K}_e$ $\triangleright$ This step is computed using LibDAI’s API for pairwise product.
9: $\phi'_{\mathcal{F}} = \sum_{q \in V \setminus \mathcal{F}} \phi'$ $\triangleright$ This is step is computed using LibDAI’s API for marginalizing out variables from a
Factor/Cluster Product.
10: **return** ($\phi'$, $\phi'_{\mathcal{F}}$)

Algorithm 4 JoinInferUp

1: **Input:** GHD $\mathcal{G} = ((V, E), \chi, \lambda)$ and the map $R$.
2: **Output:** Factor Products $\{\phi'_v\}_{v \in V}$ and Up Messages $\{\phi'_{m_{u \rightarrow \text{parent}(v)}}\}_{v \in V}$ both as tries.
3: **for all** nodes $v \in V$ **do:** $\triangleright$ This is done in a level-order traversal from leaves-to-root.
4: $\mathcal{E}_v \leftarrow \lambda(v), \mathcal{K}_v, \{\phi_e : e \in \lambda(v)\}$ $\triangleright$ Initialize the PGM Query corresponding to $v$’s Factor Product.
5: **for all** $w \in \text{Children}(v)$ **do** $\triangleright$ We add all the messages sent to $v$ from its children.
6: $\mathcal{E}_v \leftarrow \mathcal{E}_v \cup \{\chi(v) \cap \chi(w)\}, \mathcal{K}_v \leftarrow \mathcal{K}_v \cup \{\phi'_{m_{w \rightarrow v}}\}$
7: **if** $R(v) = 1$ **then** $\triangleright$ We include the 0/1 projections while computing the Factor Product for $v$.
8:  **for all** $e \in \mathcal{E} \setminus \lambda(v)$ **do**
9:   **if** $e \cap \chi(v) \neq \emptyset$ **then**
10:    $\mathcal{E}_v \leftarrow \mathcal{E}_v \cup \{e \cap \chi(v)\}, \mathcal{K}_v \leftarrow \mathcal{K}_v \cup \{\phi'_{e \cap \chi(v)}\}$
11: **if** $v$ is not a root **then**
12:  Let $u = \text{Parent}(v), \phi'_{m_{u \rightarrow v}}$ be $\sum_{q \in \chi(v) \setminus \chi(u)} \phi'_u$ and $\mathcal{F}_v = \chi(v) \cap \chi(u)$.
13:  $(\phi'_u, \phi'_{m_{u \rightarrow v}}) \leftarrow \text{MultFacProd}(R_u, \chi(v), \mathcal{E}_v, \mathcal{K}_v, \mathcal{F}_v)$
14:  **else** $\phi'_{\mathcal{F}} \leftarrow \text{MultFacProd}(R, \chi(v), \mathcal{E}_v, \mathcal{K}_v, \chi(v))$
15: **return** $\{(\phi'_v)_{v \in V}, (\phi'_{m_{u \rightarrow \text{parent}(v)}})_{v \in V}\}$

3.2.2 Message-Down phase

Since the Message-Down phase (Algorithm 5) involves updating factor products for each bag (except the root) using down messages, we perform two in-place HashProducts for each such bag: first, between the up and down messages sent/received by the bag, and then, between the result of the previous step with the bag’s factor product. A detailed description on how to compute an in-place HashProduct follows.
Consider any two factors \( e_1 \) and \( e_2 \), whose corresponding factor tables are denoted by \( \phi_{e_1} \) and \( \phi_{e_2} \) respectively. (Note that cluster products/messages can be treated as factor tables as well.) Recall that the factor tables are stored as a list of \( \langle \text{index}, \text{probability} \rangle \) pairs. We start by assuming that one of \( \phi_{e_1} \) or \( \phi_{e_2} \) is stored as a hash-table with index as key and probability as value respectively. \(^2\) Without loss of generality, let’s assume that \( \phi_{e_1} \) is stored as a hash table. Our goal is to compute \( \phi_{e_1} \cdot \phi_{e_2} \) in-place. To this end, we iterate through each entry in \( \phi_{e_2} \) and probe the corresponding index in \( \phi_{e_1} \)’s hash table. If it is present, then we multiply the probabilities and store the result in the corresponding entry in \( \phi_{e_2} \). Otherwise, we discard the entry from \( \phi_{e_1} \). It follows that by the end of this procedure, we would have computed \( \phi_{e_1} \cdot \phi_{e_2} \) and the result is stored in \( \phi_{e_2} \). Note that probing in the Hash Table is an amortized constant time operation and entry removal in \( \phi_{e_2} \) can be done in constant time as well, concluding that the time complexity of our algorithm is \( O(|\phi_{e_2}|) \).

**Algorithm 5 JoinInferDown**

1: **Input:** GHD \( \mathcal{G} = ((V,E), \chi, \lambda) \). Factor Products \( \{\phi'_v\}_{v \in V} \) and Up Messages \( \{\phi'_{m \nonumber \text{Parent}(v)}\}_{v \in V} \) converted to listing representation from tries.
2: **Output:** Final Factor Products \( \{\phi'_v\}_{v \in V} \).
3: Set \( f[v] ← 0 \) for every \( v \in V \).
4: **for all** nodes \( v \in V \) do:
   - **This is done as a level-order traversal from root-to-leaf.**
5:   **for all** \( w \in \text{Children}(v) : f[w] = 0 \) do
6:     \( \phi''_{m_{w,v}} ← \sum_{q \in \chi(v) \setminus \chi(w)} \phi'_v \) \hspace{1em} \( \triangleright \) Compute the Down Message from \( v \) to \( w \) by summing out variables not in \( \chi(w) \).
7:   \( \phi'_m_{v,w} ← \text{HashProduct}(\phi''_{m_{w,v}}, \phi'_{m_{v,w}}) \) \hspace{1em} \( \triangleright \) We divide the Down Message by its corresponding Up Message.
8:   **for all** \( w \in \text{Children}(v) : f[w] = 0 \) do
9:     \( \phi'_w ← \text{HashProduct}(\phi'_w, \phi'_{m_{w,v}}) \) \hspace{1em} \( \triangleright \) We multiply \( w \)’s cluster product with \( \phi'_{m_{w,v}} \).
10: \( f[w] ← 1. \)
11: **return** \( \{\phi'_v\}_{v \in V} \).

Summing up, our inference algorithm is a standard tree propagation algorithm with two modifications: (1) We adapt WCOJA to compute factor-products in the bags, and (2) We modify the factor products in bags using 01-projections.

### 3.2.3 Runtime complexity

With the above steps we obtain a two-pass inference routine whose runtime bound follows from a recent improved bound (AGM) on size of factor product \( [31] \). For a hypergraph \( \mathcal{H} = (\mathcal{V}, \mathcal{E}) \), let \( B \subseteq \mathcal{V} \) be any subset of vertices and let \( x \in \mathbb{R}^{|\mathcal{E}|} \) be a vector indexed by edges, such that \( x^*(B) = (x^*_S(B))_{S \in \mathcal{E}} \) be the optimal solution to the linear program

\[
\begin{align*}
\min & \quad \sum_{S \in \mathcal{E}} x_S \log_2 |\phi_S| \\
\text{s.t.} & \quad \sum_{S : v \in S} x_S \geq 1, \forall v \in B; x_S \geq 0, \forall S \in \mathcal{E}.
\end{align*}
\]

Then, the quantity

\[
\text{AGM}_{\mathcal{H}}(B) := \prod_{S \in \mathcal{E}} |\phi_S|^{x^*_S(B)}
\]

\( \triangleright \) The up/down messages are stored as hash tables.
is called the AGM-bound of $B$ using edges in $\mathcal{H}$. The WCOJA used in JoinInfer meets the AGM-bound thus giving our GHD (Definition 3) based algorithm a runtime complexity of

$$\sum_{v' \in V(T)} \text{AGM}_{\mathcal{H}}(\chi(v')).$$  

(5)

Upper-bounding each $|\phi_S|$ by $N = \max_{S \in \mathcal{E}} |\phi_S|$ in the above equation and maximizing (instead of summing) over all bags in the GHD gives us an asymptotic bound of $N^{\text{fhtw}(T)}$. $\text{fhtw}(T)$ is guaranteed to be smaller than $\text{htw}(T)$ or $\text{tw}(T)$ (hypertree width or tree width) for the same GHD, giving us the best known theoretical bounds for exact inference in PGMs. (Formal definitions for $\text{fhtw}(T), \text{htw}(T), \text{tw}(T)$ can be found in Appendix A.2.)

**Example 3** In Example 2, the original hypergraph structure, $\psi'(A, B, C)$, consisted of only two edges $(A, B)$ and $(A, C)$. The AGM-bound from the optimal solution $x^* = \{1, 1\}$ translates to a bound of $N^2$. However, by employing 01-projections the induced hypergraph, $\psi(A, B, C)$, has three edges $(A, B), (A, C)$ and $(B, C)$ and the optimal solution $x^* = \{1/2, 1/2, 1/2\}$ gives us an asymptotically better bound of $N^{3/2}$. For the GHD $T$, $\text{fhtw}(T) = 3/2, \text{htw}(T) = \text{tw}(T) = 2$.

Note that (5) gives a finer grained measure for our runtime: $\sum_{v' \in V(T)} \prod_{S \in \mathcal{E}} |\phi_S|^{x^*_S(\chi(v'))}$. Recall that the asymptotic bounds for tw based algorithms is given by $D^{\text{tw}}$, where $D = \max_{U \in V} |D(U)|$. However, a more realistic measure here would be $\rho = \sum_{v' \in V(T)} \prod_{U \in \chi(v')} |D(U)|$. This gives us a finer grained ratio (as compared to [14]) to evaluate JoinInfer against classical engines:

$$R_J = \frac{\sum_{v' \in V(T)} \prod_{S \in \mathcal{E}} |\phi_S|^{x^*_S(\chi(v'))}}{\rho}.$$  

(6)

Replacing the numerator with the upper bound $N^{\text{fhtw}}$ and the denominator with the upper bound $D^{\text{tw}}$ in (6) gives us

$$R_D = \frac{N^{\text{fhtw}}}{D^{\text{tw}}}.$$  

(7)

This ratio is analogous to the one in [14], which was based on hypertree width:

$$R = \log_{10} \left( \frac{N^{\text{htw}^*}}{D^{\text{tw}}} \right).$$

Since computing $\text{htw}$ is NP-Hard, [14] used an approximation for it (denoted by $\text{htw}^*$). In our measure $R_D$, we overcome this issue by using $\text{fhtw}$ over $\text{htw}$. Using $\text{fhtw}$ offers two significant advantages – one, it is a more fine-grained measure (see (8)) and two, $\text{fhtw}$ is polynomially computable (basically, solve the LP from (3)). We compute the numerator in $R_D$ as described in Appendix A.2. We show in the Experiments Section that $R_J$ is a better predictor than $R_D$ on most bands since it exploits the fact that factors/factor tables and variables in a bag can have different sizes and domain sizes respectively.
3.3 Challenges and Our Solutions

3.3.1 Factor Representations

Consistent with WCOJA, we use a listing representation \[19, 26\] to store data, i.e., we only store factor entries with non-zero probabilities. It has been shown that tries are sufficient for theoretical bounds. While computing the factor product of a bag, Algorithm 4 adopts a back-tracking based search routine over multiple tries (MultiFacProd). However, ‘multi-level’ tries impose considerable random access costs during the back-tracking search; they are also unsuitable for message propagation. We resolve these two problems via two novel factor-representations.

**Within Bag Computation.** First, we introduce ‘level-order’ tries for the back-tracking search in Algorithm 4. Essentially, we flatten the trie into a single-level contiguous block and redesign the search to mimic the original multi-level traversal. This re-design enabled us to simultaneously (i) exploit the compact storage of tries for sparse factors and (ii) the caching advantages of contiguous memory blocks. Initial experimental runs showed a gain of \(\sim 10x\) in runtime using level-order tries.

**Message Propagation Between Bags.** Second, in addition to storing each factor as a trie, we also store it as a list of \(\langle\text{index value, probability}\rangle\) pairs where each factor tuple is converted into a single number: their index value. We use two variants (i) which stores only ‘reverse’ indices, i.e., indices computed in reverse variable order and (ii) which stores forward and reverse indexes (for representing intermediary messages). These multiple representations enable us to optimize Algorithms 4 and 5: the reverse index enables efficient construction of tries in the up-phase and in decoding message entries over all children in a single pass in the down-phase. Moreover, the reverse indices of the up-messages act as placeholders for down-messages, enabling the re-use of data-structures. Finally, the forward indexes are used while merging down-messages with cluster products, thus reducing redundant decoding/encoding steps.

**01-projections.** To obtain the asymptotically better theoretical bounds, FAQ/AJAR uses 01-projections for all bag-wise computations. However, in practice they impose significant computational costs since interconnected factors generate a large number of projections per bag; building and maintaining these are costly. Firstly, since the utility of a 01-projection lies in its sparseness we filter out dense projections at each bag-wise computation. Secondly, instead of pre-computing all projections, we compute projections on the fly and amortize it (cache-and-reuse) over subsequent computations.

3.3.2 Hybrid Architecture

In Bands 5 and 6 (Figure 1), libDAI’s pairwise product implementation demonstrates distinct advantages over JoinInfer’s multi-way product. We explore the feasibility of leveraging the respective advantages of both these strategies in a new (HY)brid (J)oin (AR)chitecture (HYJAR). To build such a system, we use the native structure of JoinInfer and import only the pairwise-product functionality from libDAI (we do not integrate the entire engine). Given the high costs of switching between the data-structures required for JoinInfer and libDAI, the main challenge here was to devise a system that not only optimally chooses between the strategies per bag, but at the same time minimizes the switches between bags. We overcome this challenge by introducing a deterministic heuristic (Algorithm 6) that decides the optimal strategy.

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\[A\] trie is a multi-level data structure where each factor tuple corresponds to a unique path from root to leaf and the probability value associated with each tuple are stored in the leaf.
JoinInfer (with or without 01-projections) or Pairwise Product (Algorithm 3) without any 0/1 projections respectively. We first consider the case when $\rho \leq 10^9$ – we iterate through all nodes $v \in V$ with $|\alpha(v)| \geq 1$ (i.e. at least one input factor table assigned) in the decreasing order of their corresponding product of domain sizes. In particular, we run JoinInfer and Pairwise Product without 0/1 projections (i.e. the first and third algorithms) with only pre-assigned factor tables determined by $\alpha(v)$. For the second algorithm, since we include 0/1 projections, we include all factor tables whose variables have a non-empty intersection with the union of variables in the pre-assigned factors in the current bag. Once these three runs are done, we assign the fastest strategy to node $v$. We then propagate this decision to all nodes in its subtree for which no decision has been made so far. However, even after this procedure, there could be some nodes, which don’t have an $R$ value assigned. In order to address this issue, we repeat the same procedure for the root i.e., we make an arbitrary choice of strategy for it and then propagate this choice along the remaining GHD. Finally, for the case when $\rho > 10^9$, running JoinInfer without 0/1 projections could turn out to be very expensive (since we don’t consider the

---

**Algorithm 6 HYJAR**

1: **Input:** GHD $\mathcal{G} = ((V, E), \chi, \lambda)$, Sum of product of domains $\rho$.
2: **Output:** A map $R$ that maps every node $v \in V$ to 0 (MultFacProd w/o 0/1), 1 (MultFacProd 0/1) or 2 (PairwiseProd).
3: Initialize $R_v$ to $-1$ for every $v \in V$.
4: if $\rho \leq 10^9$ then
5: for all nodes $v \in V$ with $|\alpha(v)| \geq 1$ do: \>
6: \> $\mathcal{E}_v \leftarrow \alpha(v), \mathcal{K}_v \leftarrow \{\phi_e : e \in \alpha(v)\}$
7: \> $T_0 \leftarrow$ Time taken to run MultFacProd $\{0, \chi(v), \mathcal{E}_v, \mathcal{K}_v, \chi(v)\}$
8: \> $\mathcal{E}'_v \leftarrow \{S \cap \chi(v) | S \in E\}, \mathcal{K}'_v \leftarrow \{\phi_e : e \in \mathcal{E}'_v\}$
9: \> $T_1 \leftarrow$ Time taken to run MultFacProd $\{0, \chi(v), \mathcal{E}'_v, \mathcal{K}'_v, \chi(v)\}$
10: \> $T_2 \leftarrow$ Time taken to run MultFacProd $\{2, \chi(v), \mathcal{E}_v, \mathcal{K}_v, \chi(v)\}$
11: \> $R_v \leftarrow i$, where $\min(T_0, T_1, T_2) = T_j$.
12: for all $w \in$ subtree($v$): $R_w = -1$ do \>
13: \> Propagate the decision obtained for $v$ to all unassigned nodes in its subtree.
14: \> $R_w \leftarrow R_v$
15: else
16: for all nodes $v \in V$ do
17: \> $R_v \leftarrow$ Random(0, 1)
18: return $R$

(JoinInfer (with or without 01-projections) or PairwiseProd) for each bag $v$ in the GHD that has at least one input factor assigned to it (i.e. $\alpha(v) \geq 1$)\(^4\). We then propagate this decision along the subtree of $v$, until it reaches a bag that was already assigned a decision. To decide the order of preference, we consider bags $v$ in decreasing order of $\prod_{U \in \chi(v)} |D(U)|$, with the intuition being that the larger bags dominate the runtime of libDAI. A detailed description of Algorithm 6 follows.
messages). Thus, for each cluster, we randomly choose between JoinInfer without 0/1 projections and with 0/1 projections. Note that we don’t run Pairwise Product for this case since LibDAI crashes when $\rho > 10^9$.

4 Experimental Evaluation

In this section, we empirically validate JoinInfer and outline features that influence JoinInfer’s performance. Specifically, we describe our empirical setup and on standard benchmarks, we (i) demonstrate the scope of JoinInfer vis-a-vis state-of-the-art systems, (ii) document performance gains of the hybrid setting and (iii) evaluate our technical contributions.

4.1 Experimental Setup

Datasets. To create a testbed that spans the full range of cases illustrated in Figure 1, we sample from three publicly available benchmark datasets: UAI’06 [8], PIC 2011 [16] and the BN Learns dataset [1] (which subsumes the IJCAI’05 networks [9]). Our testbed contains 52 networks. For Band 1, we selected the CELAR subset from PIC 2011. From the UAI’06 benchmarks, we selected grids (BN_30-41) for Band 2, iscas89 (BN_47-68) for Band 3, the Speech Recognition DBNs (BN_20-25) for Band 4 and, iscas85 (BN_42-46) for Band 6. We left out networks CELAR-SUB4, BNs 65, 66 and 68 in Bands 1 to 3 because JoinInfer does not (yet) support the precision to compute very large indices ($> 2^{63} - 1$). Finally, we selected networks from BN Learns which had more than 30 variables (i.e., we filtered out the smaller ones); these populated Bands 4, 5 and 6.

In order to improve the tractability of some of the larger networks for exact inference (high $\rho$ cases), we randomly induce factor table sparsity. Further, to ensure that all final cluster tables are non-empty, for every factor $e \in \mathcal{E}$, we force the entry $(i)_{U \in e}$ in the corresponding factor table $\mathcal{K}_e$ for every $i \in \{\min_{U \in e} |D(U)|\}$. These sparsity levels are consistent with the ranges found in other networks in the benchmark. In particular, for the CELAR subsets, the induced median factor sparsity is at 20% and 40% (original median sparsity was 100%). However, for the networks in Bands 2 and 3, we ensure that the induced median factor table sparsity remains close to the original value of 50%. (Note that inducing sparsity to improve model tractability is a well-accepted procedure in many practical settings [27, 26]).

Comparison Engines. We compare JoinInfer against three state-of-the-art systems: ACE [9], an engine that explicitly exploits determinism, and, libDAI [30] and IJGP [28], two award winning systems in the UAI 2010 inference challenge. Since JoinInfer is for exact inference, we compare against the exact inference ‘settings’ in these models: the ‘Junction Tree’ algorithm in libDAI and the ‘Join-Tree’ propagation in IJGP (since it computes exact marginals only when the join-graph is a tree). In particular, IJGP requires the ‘degree’ parameter to be set high, which we set to the number of variables in the network (see Table 1’s description for more details). For ACE, we follow the recommended settings outlined for the IJCAI networks and the standard settings for the others – commands ‘compile’ and ‘evaluate’ to compile the AC and run inference respectively. The compile/run commands for these engines can be found in Appendix B.1.

Inference Queries. The inference query we evaluate is the computation of (all) variable marginals. We observed that while JoinInfer, IJGP and ACE process evidence (requiring it to be input separately), lib-
DAI does not. Further, JoinInfer, IJGP and ACE perform SAT-based singleton consistency and treat the resulting variables as evidence, which again libDAI doesn't. Hence, in order to ensure a fair comparison, we incorporate the evidence and singleton-consistency directly into the input given to the engines. In particular, we remove both these types of variables from the input network (note that this could remove some factors from the query as well). We then provide the updated network resulting from this procedure to all four engines in their respective formats: libDAI (.fg), IJGP (.uai), ACE (.uai) and JoinInfer. We compare our marginal outputs with these engines, with an error limit of 0.00001.

**Evaluation Metrics and Settings.** We evaluate the systems on the time taken to compute variable marginals. We repeat each experimental run 5 times and report the average of the runs. Additionally, we set a timeout of 60 minutes for our experimental runs. We would like to note here that ACE requires separate compilation of the arithmetic circuit representing the input network (a non-standard design). For a fair comparison with other engines with end-to-end computations, we report both (i) the total of compilation and inference times and (ii) only the inference time for ACE. We ran all our experiments on a Linux server (Ubuntu 14.04 LTS) with Intel Xeon E5-2640 v3 CPU @ 2.60GHz and 64 GB RAM.

**Error Codes in Table 1.** We describe the error codes in Table 1 here. ‘T’ denotes engine-time out (60 mins). LibDAI and IJGP crash on all benchmarks where \( \rho > 10^9 \), due to huge pre-memory allocation and this is denoted by ‘F’. For ACE, we observed that for benchmarks BN_30-39 in Band 2, it compiles successfully but throws a runtime exception due to precision issues. We believe that this is due to large treewidth (\( \geq 39 \)) on these datasets. We denote this by ‘E’. For IJGP, we observed that it does approximate inference in benchmarks Munin1 and BN_43-46 respectively. In particular, we recorded its final treewidth using the MinFill ordering on all benchmarks and compared it with JoinInfer’s and libDAI’s treewidth (both using the MinFill ordering) respectively. We noticed that the final treewidth reported by IJGP was much smaller than the treewidth reported by JoinInfer and libDAI. Recall that we preprocess evidence and SAT-based singleton consistency on these benchmarks and thus, we concluded that IJGP does Approximate Inference on these datasets (which we denote by ‘A’).

**4.2 Experimental Results**

**4.2.1 Benchmark experiments**

**Benchmark Comparisons.** The results in Table 1 are laid out along the lines of Figure 1. These networks span over a wide range of sparsity (20% - 100%), domain sizes (2 -100) and factor arity levels (1-10).

\( \rho \) **high.** The measure \( R_D \) from [14] predicts superior performance for JoinInfer only in Band 1 (CElar). However, in this region of high \( \rho \), JoinInfer performs consistently better than the predictions in [14]. In Band 1 it is be up to 630x faster on subsets where ACE completes. In Band 2, it is up to 2x faster and in Band 3 where the corresponding predictions of [14] is under-performance by \( 10^{10}x \) - \( 10^{20}x \), it can be up to 2.7x faster than ACE (libDAI and IJGP fail in this space). libDAI fails in these bands since it relies primarily on truth-table indices for its speed which do not scale to these levels of \( \rho \). On the other hand, ACE that takes advantage of factor sparsity using arithmetic circuits is the only other engine that completes; that said, compiling these structures is costly. We surmise that JoinInfer’s performance advantages are rooted in the use of multi-way products. Further, applying multi-way products directly on a listing-representation accentuates the gains.
Table 1: Benchmark Comparisons: The first column denotes the range of $\rho$, followed the band of the datasets (see Figure[1] and the dataset name. The fourth column denotes the number of variables/factors, followed by $R_J$ for $R_D$. We report three runtimes for JoinInfer: without 0/1 projections, with all 0/1 projections and HYJAR, followed by our comparison engines – LibDAI, IJGP and ACE (Total Time and Inference Time). (All runtimes are in seconds.) Further, we report the median and mean sparsity for every dataset, followed by fractional hypertree width (fhtw) and tree-width (tw) (computed for the same GHD). The fractional hypertreewidth (fhtw) numbers were generated by solving the linear program [9] using Google OR-Tools [17]. Finally, we report the maximum domain value (D) and maximum factor table (non-zero) entry size (N). 'T' denotes engine-time out (60 mins). Engine crash due to huge pre-memory allocation is denoted by 'F'. Runtime exceptions due to precision issues is denoted by 'E'. When an engine does Approximate Inference due to large treewidth, we denote it by ‘A’). See Section 4.1 for a detailed description of these error-codes.

| $\rho$ | Band | Dataset | Var/Factors | $R_J$ | $R_D$ | JoinInfer | HYJAR | LibDAI | IJGP | ACE | Sparsity (in %) | fhtw | tw | D/N |
|------|------|---------|-------------|-------|-------|-----------|-------|--------|------|-----|--------------|------|-----|-----|
|      |      |         |             |       |       |            |       |        |      |     |              |      |     |     |
| $> 10^5$ |      |         |             |       |       |            |       |        |      |     |              |      |     |     |
| CELAR6-SUB0_20 | 16/57 | 2.00E-03 | 1.00E-03 | 0.17 | 0.16 | 0.19 | F | F | 97.24 | 0.36 | 20/20 | 4 | 8 | 44/387 |
| CELAR6-SUB1_20 | 14/75 | 3.00E-04 | 3.00E-04 | 2.57 | 2.58 | 2.59 | F | F | 444.38 | 0.99 | 20/20 | 5 | 10 | 44/387 |
| CELAR6-SUB2_15 | 16/89 | 1.00E-04 | 1.00E-04 | 1.05 | 1.04 | 1.07 | F | F | 653.33 | 0.74 | 20/20 | 5 | 11 | 44/387 |
| CELAR6-SUB0_40 | 18/106 | 3.00E-02 | 2.50E-02 | 3.72 | 3.69 | 3.67 | F | F | 1219.09 | 0.78 | 20/20 | 5 | 11 | 44/387 |
| CELAR6-SUB0_60 | 16/57 | 3.00E-02 | 2.50E-02 | 4.55 | 4.59 | 4.17 | F | F | 855.12 | 1.2 | 40/40 | 4 | 8 | 44/377 |
| CELAR6-SUB1_60 | 14/75 | 3.00E-02 | 2.50E-02 | 3.92 | 3.88 | 3.84 | F | F | 444.38 | 1.2 | 40/40 | 5 | 10 | 44/377 |
| CELAR6-SUB2_60 | 16/89 | 3.00E-02 | 2.50E-02 | 4.49 | 4.48 | 4.44 | F | F | 444.38 | 1.2 | 40/40 | 5 | 11 | 44/377 |

| $\rho$ | Band | Dataset | Var/Factors | $R_J$ | $R_D$ | JoinInfer | HYJAR | LibDAI | IJGP | ACE | Sparsity (in %) | fhtw | tw | D/N |
|------|------|---------|-------------|-------|-------|-----------|-------|--------|------|-----|--------------|------|-----|-----|
|      |      |         |             |       |       |            |       |        |      |     |              |      |     |     |
| $> 10^5$ |      |         |             |       |       |            |       |        |      |     |              |      |     |     |
| CELAR6-SUB0_20 | 16/57 | 2.00E-03 | 1.00E-03 | 0.17 | 0.16 | 0.19 | F | F | 97.24 | 0.36 | 20/20 | 4 | 8 | 44/387 |
| CELAR6-SUB1_20 | 14/75 | 3.00E-04 | 3.00E-04 | 2.57 | 2.58 | 2.59 | F | F | 444.38 | 0.99 | 20/20 | 5 | 10 | 44/387 |
| CELAR6-SUB2_15 | 16/89 | 1.00E-04 | 1.00E-04 | 1.05 | 1.04 | 1.07 | F | F | 653.33 | 0.74 | 20/20 | 5 | 11 | 44/387 |
| CELAR6-SUB0_40 | 18/106 | 3.00E-02 | 2.50E-02 | 3.72 | 3.69 | 3.67 | F | F | 1219.09 | 0.78 | 20/20 | 5 | 11 | 44/387 |
| CELAR6-SUB0_60 | 16/57 | 3.00E-02 | 2.50E-02 | 4.55 | 4.59 | 4.17 | F | F | 855.12 | 1.2 | 40/40 | 4 | 8 | 44/377 |
| CELAR6-SUB1_60 | 14/75 | 3.00E-02 | 2.50E-02 | 3.92 | 3.88 | 3.84 | F | F | 444.38 | 1.2 | 40/40 | 5 | 10 | 44/377 |
| CELAR6-SUB2_60 | 16/89 | 3.00E-02 | 2.50E-02 | 4.49 | 4.48 | 4.44 | F | F | 444.38 | 1.2 | 40/40 | 5 | 11 | 44/377 |

| $\rho$ | Band | Dataset | Var/Factors | $R_J$ | $R_D$ | JoinInfer | HYJAR | LibDAI | IJGP | ACE | Sparsity (in %) | fhtw | tw | D/N |
|------|------|---------|-------------|-------|-------|-----------|-------|--------|------|-----|--------------|------|-----|-----|
|      |      |         |             |       |       |            |       |        |      |     |              |      |     |     |
| $> 10^5$ |      |         |             |       |       |            |       |        |      |     |              |      |     |     |
| CELAR6-SUB0_20 | 16/57 | 2.00E-03 | 1.00E-03 | 0.17 | 0.16 | 0.19 | F | F | 97.24 | 0.36 | 20/20 | 4 | 8 | 44/387 |
| CELAR6-SUB1_20 | 14/75 | 3.00E-04 | 3.00E-04 | 2.57 | 2.58 | 2.59 | F | F | 444.38 | 0.99 | 20/20 | 5 | 10 | 44/387 |
| CELAR6-SUB2_15 | 16/89 | 1.00E-04 | 1.00E-04 | 1.05 | 1.04 | 1.07 | F | F | 653.33 | 0.74 | 20/20 | 5 | 11 | 44/387 |
| CELAR6-SUB0_40 | 18/106 | 3.00E-02 | 2.50E-02 | 3.72 | 3.69 | 3.67 | F | F | 1219.09 | 0.78 | 20/20 | 5 | 11 | 44/387 |
| CELAR6-SUB0_60 | 16/57 | 3.00E-02 | 2.50E-02 | 4.55 | 4.59 | 4.17 | F | F | 855.12 | 1.2 | 40/40 | 4 | 8 | 44/377 |
| CELAR6-SUB1_60 | 14/75 | 3.00E-02 | 2.50E-02 | 3.92 | 3.88 | 3.84 | F | F | 444.38 | 1.2 | 40/40 | 5 | 10 | 44/377 |
| CELAR6-SUB2_60 | 16/89 | 3.00E-02 | 2.50E-02 | 4.49 | 4.48 | 4.44 | F | F | 444.38 | 1.2 | 40/40 | 5 | 11 | 44/377 |
Table 2: Real-World Experiments: Memory Consumed (in MB)

| Band   | Datasets | JoinInfer | IJGP   | libDAI | ACE   |
|--------|----------|-----------|--------|--------|-------|
|        | BN_23    | 305       | T      | 2.35x  | 7.41x |
| Band 3 | BN_24    | 293       | T      | 1.67x  | 6.83x |
|        | BN_25    | 294       | T      | 1.71x  | 6.95x |
| Band 5 | Munin2   | 395       | 0.56x  | 0.33x  | 3.01x |
|        | Munin3   | 394       | 0.61x  | 0.31x  | 3.05x |
|        | Munin4   | 1038      | 1.03x  | 0.45x  | 1.37x |

The networks in these bands (1, 2 and 3) cover a sparsity range of 20%-50% and have factor arity between 1 to 4. Further, in Band 1, given that ACE requires the 20% sparsity levels to complete, we present results at two levels of sparsity for CELAR (20% and 40%).

ρ low. $R_D$ predicts superior performance for JoinInfer in Band 4, which it achieves. It is up to 5.29x faster than libDAI (it's closest competitor) and up to 5.4x faster than ACE (on the subsets that ACE completes on). IJGP times-out on almost all of the networks. Finally, in Bands 5/6, the two unfavorable settings, JoinInfer is on an average faster than ACE by 5.8x/9.5x and IJGP by 3.06x/2.28x respectively. It is on average slower than libDAI by 4.8x/10x respectively: libDAI’s truth-table indexing advantages clearly manifest in these two bands. We would like to note however, that the corresponding predictions of [14] for JoinInfer is under performance by 10x - $10^8$x for Band 5, and $10^{20}$x - $10^{28}$x for Band 6, i.e., several orders of magnitude worse.

Secondly, our fine-grained measure $R_J$ (Column 4) is a better predictor for JoinInfer’s performance than $R_D$ (Column 5) on most networks. Consider the Bands 3, 4 and 5 in Table[1]. While $R_D$ overestimates our performance in Band 4, $R_J$ provides a more realistic measure that correlates with our performance. On the other hand, in Bands 3 and 5, while $R_D$ severely underestimates our performance (sometimes by orders of magnitude), $R_J$’s predictions are generally tighter. On Bands 1 and 2, its predictions are comparable to $R_D$. The only place where it fails to make good estimates is Band 6.

01-Projections. In theory, 01-projections are central to realizing the asymptotic bounds of FAQ/AJAR. However, we find that in practice they offer mixed results: we found they help in 20/52 networks (average gains of 20%), they make no difference in 3 networks and marginally hurt in 29 networks (average loss of 7%).

Memory Usage. To examine memory usage, we selected three large networks (> 1000 variables) from Bands 4 and 5 (results in Table[2]. We found that in the former set JoinInfer consumed the least memory: on average libDAI consumed 2.35x and ACE consumed 7x more. In the latter set, libDAI consumed the least memory: on average JoinInfer consumed 2.82x, IJGP 1.98x and ACE 7.29x more. In summary, this underscores that JoinInfer is comparable to classical inference frameworks on the memory consumption metric.

Hybrid Architecture. Since JoinInfer is the only engine that completes on all networks when $\rho$ is high, we now focus on low $\rho$ conditions. As evident from Table[1] HYJAR helps exploit the relative strengths of
each strategy—multiway or pairwise products—into a single architecture, yielding consistent performance across a majority of networks (26/28). Of these, in 9 cases (e.g., munin1, munin, barley, mildew) HYJAR’s completion times are faster than its nearest standalone competitors (JoinInfer or libDAI), in 10 cases it is less than 2.5x slower and in 7 cases it is between 2.5x - 4.5x slower. BN_42 and BN_44 are the only two networks where HYJAR’s strategy does not lead to a notable improvement. Further, follow up analyses indicate that HYJAR consistently switches between strategies at the bag level. We present a detailed analysis of our results in Appendix B.2.

Table 3: We report JoinInfer w/o 0/1, with all 0/1, HYJAR, Pairwise and LibDAI runtimes (in seconds) along with the total number of clusters, followed by the average % of clusters running Multiway w/o 0/1, with all 0/1 and Pairwise (i.e., we set $R_v = 2$ for all $v \in V$ in Algorithm 1). All runtimes are in seconds.

| Band  | Dataset          | JoinInfer | HYJAR | Pairwise | LibDAI | Clusters | JoinInfer Clusters (%) | Pairwise Clusters (%) |
|-------|------------------|-----------|-------|----------|--------|----------|------------------------|-----------------------|
|       |                  | w/o 0/1   | 0/1   |          |        |          |                        |                       |
|       |                  | 14.94     | 14.47 | 22.73    | 1825   | 0        | 27                     | 73                    |
| Band 4| BN_20            | 4.52      | 4.53  | 15.47    | 14.86  | 23.37    | 1825                   | 0                     |
|       | BN_22            | 2.15      | 2.22  | 2.98     | 2.59   | 3.77     | 1513                   | 9                     |
|       | BN_23            | 2.16      | 2.24  | 3        | 2.56   | 3.74     | 1513                   | 8                     |
|       | BN_24            | 1.31      | 1.43  | 1.74     | 1.43   | 2.11     | 908                    | 0                     |
|       | BN_25            | 1.34      | 1.47  | 1.76     | 1.36   | 2.12     | 908                    | 0                     |
|       | Pathfinder       | 0.16      | 0.27  | 0.29     | 0.1    | 0.11     | 91                     | 0                     |
| Band 5| Alarm            | 0.03      | 0.04  | 0.05     | 0.05   | 0.02     | 27                     | 4                     |
|       | Hepar2           | 0.05      | 0.04  | 0.06     | 0.04   | 0.02     | 58                     | 4                     |
|       | Mildew           | 0.81      | 0.76  | 0.24     | 0.21   | 0.27     | 29                     | 6                     |
|       | Munin            | 13.34     | 13.61 | 1.98     | 1.74   | 3.14     | 872                    | 0                     |
|       | Munin1           | 600.86    | 630.22| 20.6     | 19.44  | 39.01    | 158                    | 0                     |
|       | Munin4           | 16.91     | 17.18 | 2.06     | 1.89   | 2.93     | 869                    | 0                     |
|       | Diabetes         | 3.31      | 3.36  | 0.72     | 0.6    | 0.89     | 337                    | 0                     |
|       | Munin2           | 2.74      | 2.31  | 0.68     | 0.6    | 0.79     | 866                    | 1                     |
|       | Munin3           | 2.72      | 2.27  | 0.7      | 0.64   | 0.95     | 901                    | 1                     |
|       | Pigs             | 1.01      | 0.93  | 0.36     | 0.22   | 0.23     | 368                    | 1                     |
|       | Link             | 18.02     | 19.91 | 14.27    | 3.28   | 3.44     | 591                    | 22                    |
|       | Barley           | 26.8      | 27.12 | 1.13     | 0.8    | 1.45     | 36                     | 0                     |
|       | Hailfinder       | 0.03      | 0.05  | 0.06     | 0.04   | 0.02     | 43                     | 1                     |
|       | Water            | 0.18      | 0.15  | 0.27     | 0.28   | 0.31     | 19                     | 0                     |
|       | Win95pts         | 0.04      | 0.03  | 0.05     | 0.06   | 0.03     | 50                     | 19                    |
| Band 6| Andes            | 0.59      | 0.59  | 0.19     | 0.12   | 0.14     | 178                    | 1                     |
|       | BN_42            | 32.63     | 33.01 | 35.15    | 2.48   | 2.66     | 789                    | 13                    |
|       | BN_43            | 65.47     | 64.03 | 4.37     | 4.36   | 4.43     | 789                    | 12                    |
|       | BN_44            | 227.87    | 216.98| 133.5    | 16.29  | 12.82    | 789                    | 18                    |
|       | BN_45            | 67.05     | 68.21 | 8.07     | 8      | 6.95     | 788                    | 14                    |
|       | BN_46            | 45.98     | 46.01 | 20.16    | 5.64   | 5.85     | 446                    | 18                    |

Takeaways. (i) In our investigation, we identified a threshold for $\rho$ at $10^9$ reflecting the current memory limits for truth tables (on our machine). While the absolute value of the threshold may change depending on machine configurations, such a threshold will always exist. (ii) In this work, we show that $R_f$ is a better predictor of JoinInfer’s performance than $R_D$. (iii) Of the 52 networks in the test-bed, HYJAR outperforms libDAI, IJGP and ACE on 39 (i.e., on 75% of networks). libDAI is the next largest winner with wins on 11 datasets. HYJAR thus offers promise as a practically relevant architecture for building a robust, broadly applicable inference engine.
Table 4: Descriptive Experiment: Input Processing. We implement and compare two methods for constructing tries: first using a forward index (Old Tries) and then, using a reverse index (based on reverse input order, New Tries). All runtimes are in seconds.

| Dataset | Num Var/D | Old Tries | New Tries |
|---------|-----------|-----------|-----------|
| BN_20   | 2843/91   | 0.1       | 0.27x     |
| BN_21   | 2843/91   | 0.1       | 0.33x     |
| BN_22   | 2425/91   | 0.09      | 0.37x     |
| BN_23   | 2425/91   | 0.09      | 0.38x     |
| BN_24   | 2425/91   | 0.09      | 0.36x     |
| BN_25   | 2425/91   | 0.09      | 0.36x     |

4.2.2 Factor Representations

As described in Section 3.3.1, a secondary representation for our factors is a list of \( \langle \text{index}, \text{probability} \rangle \) pairs. Specifically, we use two variants of the list that store indices computed in two variable orders: forward and reverse. We perform three descriptive experiments on the UAI speech recognition datasets (BN_20-25) with these new data structures/algorithms, comparing with their corresponding alternatives. Note that the data is stored as compressed indices the memory blowup is only 1.3x (and not 2x) with respect to tries.

**Forward vs Reverse Index.** We compare our new method of constructing tries using a reverse index (based on reverse input order) as opposed to the way of constructing tries with a forward index. In particular, this new method removes significant computational/storage overhead and is on an average 3x faster than the older method (see Table 4).

**Upward Pass.** During the upward pass (Algorithm 4), we store the up message as a hash-table of \( \langle \text{forward index}, \text{reverse index, probability} \rangle \) tuples. Further, we store the cluster tables as lists of \( \langle \text{reverse index, probability} \rangle \) pairs. Overall, this design gives us an average 3x speed gains in Algorithm 4 (see Table 5) compared to a version that stores both the up messages and cluster tables as lists of \( \langle \text{forward index, probability} \rangle \) pairs.

**Downward Pass.** Finally, for the downward pass (Algorithm 5), we perform an in-place HashProduct and compare it with a version implementing Sort-MergeProduct. In particular, we observe that using HashProducts instead of Sort-MergeProduct gives us an average speedup of 1.6x (see Table 6).

5 Conclusion and Future Directions

This paper demonstrates that in a wide range of PGM benchmarks, GHD based inference algorithms offer much promise in terms of performance and prior conclusions on their practical (ir)relevance [14] might have to be re-visited. Further, the HYJAR architecture shows great promise in integrating the benefits of the traditional inference engines along with JoinInfer. Improving the data structures of JoinInfer to facilitate this integration is one of our future work. The following are other future research directions that seem promising: (1) Incorporate Single Instruction Multiple Data (SIMD) instructions to speed up the
Table 5: Descriptive Experiment: Upward Pass. We implement and compare two data structures for storing the up messages/cluster tables: one by storing the up messages as hash-tables of \( \langle \text{forward index, reverse index, probability} \rangle \) tuples and cluster tables as lists of \( \langle \text{reverse index, probability} \rangle \) pairs and the other, by storing both up messages/cluster tables as lists of \( \langle \text{forward index, probability} \rangle \) pairs. All runtimes are in seconds.

| Dataset | Num Var/D | New Data Structures | Slowdown of Older Data Structures |
|---------|-----------|---------------------|-----------------------------------|
| BN_20   | 2843/91   | 1.17                | 7.26x                             |
| BN_21   | 2843/91   | 1.11                | 6.22x                             |
| BN_22   | 2425/91   | 0.27                | 1.33x                             |
| BN_23   | 2425/91   | 0.29                | 1.21x                             |
| BN_24   | 2425/91   | 0.27                | 1.44x                             |
| BN_25   | 2425/91   | 0.28                | 1.46x                             |

Table 6: Descriptive Experiment: Downward Pass. We implement and compare two algorithms for computing products in the downward pass: HashProduct and SortMergeProduct. All runtimes are in seconds.

| Dataset | Num Var/D | HashProduct | Slowdown of Sort-MergeProduct |
|---------|-----------|-------------|-------------------------------|
| BN_20   | 2843/91   | 0.53        | 3.02x                         |
| BN_21   | 2843/91   | 0.52        | 2.58x                         |
| BN_22   | 2843/91   | 0.11        | 1.18x                         |
| BN_23   | 2843/91   | 0.12        | 1.17x                         |
| BN_24   | 2843/91   | 0.17        | 1.06x                         |
| BN_25   | 2843/91   | 0.18        | 1.06x                         |
computation in a bag (this has been successful in database joins [3]); and (2) utilize JoinInfer to speed up approximate inference engines (there are currently no known approximate extensions for the multi-way product algorithm).

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A Missing Details in Section 3

A.1 01-Projections

As stated earlier, using 01-Projections is central to realizing the asymptotically better bounds in FAQ/AJAR. Moreover, this gain is accentuated when we deal with sparsity: the key idea is to exploit the sparsity of all the input factors and not just those encompassed by the query corresponding to the current bag. We highlight this aspect in an example where the gain is more dramatic than Example 2.

Example 4 For instance, say we are processing the bag of a GHD T at node v that contains k factors $\mathcal{X}_v = \{\phi_1(X_1, X_2), \phi_2(X_1, X_3), ..., \phi_k(X_1, X_{k+1})\}$ and $k + 1$ variables $\chi(v) = \{X_1, X_2, ..., X_{k+1}\}$, and, that the query for the bag involves marginalizing out variable $X_1$ to create an intermediary factor/message $\phi'(X_2, X_3, ..., X_{k+1})$. The optimal fractional cover (recall the LP in (3)) for the query hypergraph would be 1 for all k edges making the runtime complexity of processing this query $O(N^k)$, a bound that could be significant depending on the value of k.

Now suppose the original PGM hypergraph $\mathcal{H}$ contains a factor $\psi(X_2, X_3, ..., X_{k+1}) \not\in \lambda(v)$ that would be encountered somewhere along the tree T in subsequent computations. We could employ this factor upfront while computing query at v to avoid redundant computations at a later stage. With the addition of this factor support the optimal fractional cover of the induced query hypergraph would be $1 - \frac{1}{k}$ for the new hyperedge $\{X_2, X_3, ..., X_{k+1}\}$ and $\frac{1}{k}$ for the other k edges incident on $X_1$. This makes the AGM bound go to $O(N^{2 - \frac{1}{k}})$, a dramatic improvement in the runtime bound especially if N and k are large.

However, employing this factor as-is could lead to double counting of probabilities while processing the additional factor. Hence, we need to find a way of incorporating such support factors without changing the computation.

We accomplish this goal using 01-projections defined by:

Definition 4 For each $S \in \mathcal{E}$ and any set $U \subseteq V$ such that $S \cap U \neq \emptyset$, define the 01-projection of $\phi_S$ onto U as the function

$$\phi_{S/\mathcal{U}} : \prod_{U' \in S \cap U} D(U') \rightarrow \{0, 1\},$$

where

$$\phi_{S/\mathcal{U}}(x_{S \cap U}) = \begin{cases} 1 & \text{if there exists } y_S \text{ s.t. } \phi_S(y_S) \neq 0 \text{ and } y_S \cap U = x_{S \cap U} \\ 0 & \text{otherwise} \end{cases}$$

Two key improvements afforded by 01-projections can be summarized as follows:

- In terms of computation: there could be potential wastage in computing entries that would eventually be annihilated. We avoid this redundancy by computing only those entries that we know will not be eliminated. When dealing with very large factors exploiting factor sparsity via projections could lend substantial reductions in computation.

- The above also implies better theoretical bounds: by incorporating support factors using 01-projections while processing the query corresponding to each bag, we are now bounded by the fractional cover of the induced hypergraph formed by using the projection of edges incident on $\chi(v)$ in addition to edges in $\lambda(v)$. This gain as illustrated in Example 4 can be substantial.
A.2 GHD: Notions of Width

We describe three notions of width here – treewidth (tw), hypetree-width (htw) and fractional hyper-tree-width (fhtw) for a GHD $G = (T, \chi, \lambda)$ (recall Definition 3). The treewidth of a GHD is given by 

$$\text{max}_{v \in V(T)}(|\chi(v)|).$$

The notions htw and fhtw used in this paper can be derived from the concept of edge covers of a hypergraph $[4, 5]$. To this end, for a hypergraph $H = (V, E)$, let $B \subseteq V$ be any subset of vertices. We define $\gamma_H(B)$ and $\gamma^*_H(B)$ to be the minimum integral edge cover and the minimum fractional edge cover respectively of $B$ using edges in $E$. In particular, $\gamma^*_H(B)$ is the optimal objective value of LP (3) obtained by replacing $|\phi_S|$ with max$_{S \in E} |\phi_S|$ for every $S \in E$. Finally, $\gamma_H(B)$ is the optimal objective value of the following integer program:

$$\min \sum_{S \in E} x_S$$

s.t. $\sum_{S \in E} x_S \geq 1, \forall v \in B$

$$x_S \in \{0,1\}, \forall S \in E.$$

Then, we have $\text{htw} = \text{max}_{v \in V} \gamma_H(\chi(v))$ and $\text{fhtw} = \text{max}_{v \in V} \gamma^*_H(\chi(v))$. Note that the following inequality is always true for a fixed $G$:

$$\text{fhtw} \leq \text{htw} \leq \text{tw}. \quad (8)$$

B Missing Details in Section 4

B.1 Comparison Engines: Compile and Run Commands

We outline the commands that we use to run the various inference engines.

To run IJGP, we run 

```
./ijgp -i-bound <No_of_Variables> -order min-fill <InputFilename.uai> <EmptyEvidenceFile>
```

To run LibDAI, we run 

```
./example <InferenceFlag=0> <InputFilename.fg> <OutputFilewith Marginals>
```

For ACE with IJCAI-2005 Datasets in the BN Learn repository (Munin1-4 and diabete)s, we run compile 

```
-compile -cd05 -dtClauseMinfill <InputFilename.uai>
```

followed by evaluate 

```
<InputFilename.uai>
```

setting a memory limit of 54GB (which is 85% of our total RAM capacity as recommended in [2]).

For ACE with other IJCAI-2005 Datasets in the BN Learn repository than the above, we run compile 

```
-compile -cd05 -dtBnMinfill <InputFilename.uai>
```

followed by evaluate 

```
<InputFilename.uai>
```

setting a memory limit of 54GB (which is 85% of our total RAM capacity as recommended in [2]).

For ACE with all other datasets, we run compile 

```
<InputFilename.uai>
```

followed by evaluate 

```
<InputFilename.uai>
```

Whenever we run into a memory error, we set it to 54GB ([2]) and rerun our code (if it runs into the same error in this run, we stop).

B.2 Detailed Analysis of Table 3

From Table 3 we first observe that HYJAR picks mixtures of the three choices (JoinInfer (with/without 01) and PairwiseProd) on most benchmarks i.e., it frequently switches between the strategies on most

5The standard definition of treewidth is $\text{max}_{v \in V(T)}(|\chi(v)|) - 1$ but we use our modified definition throughout the paper.
networks. When our Algorithm 6 leans more consistently towards the better strategy, HYJAR demonstrates good gains – for example, consider the Munin subsets 1-4, Barley and Diabetes. In these networks, our heuristic actually picks PairwiseProd for 95% of the bags on average. On the other hand, when the algorithm leans less strongly towards the better strategy, for instance, in datasets like BN_20/21 and BN_42,45, HYJAR does not make significant gains. In some cases, the cost of switching between data structures needed for MultFacProd and PairwiseProd is not compensated for by the benefits of the hybrid system. Further, our numbers reveal very interesting insights – for example, consider the networks BN_43 and BN_45. In both of them multiway products are much slower compared to pairwise, but the overall HYJAR numbers are extremely competitive (in spite of running multiway products on more than a third of the clusters). Overall, we believe that HYJAR is promising in the direction of building adaptive inference engines that are optimal for a given input PGM, automatically tuning themselves to its characteristics.