Anytime Exact Belief Propagation

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Abstract
Statistical Relational Models and, more recently, Probabilistic Programming, have been making strides towards an integration of logic and probabilistic reasoning. A natural expectation for this project is that a probabilistic logic reasoning algorithm reduces to a logic reasoning algorithm when provided a model that only involves 0-1 probabilities, exhibiting all the advantages of logic reasoning such as short-circuiting, intelligibility, and the ability to provide proof trees for a query answer. In fact, we can take this further and require that these characteristics be present even for probabilistic models with probabilities near 0 and 1, with graceful degradation as the model becomes more uncertain. We also seek inference that has amortized constant time complexity on a model’s size (even if still exponential in the induced width of a more directly relevant portion of it) so that it can be applied to huge knowledge bases of which only a relatively small portion is relevant to typical queries. We believe that, among the probabilistic reasoning algorithms, Belief Propagation is the most similar to logic reasoning: messages are propagated among neighboring variables, and the paths of message-passing are similar to proof trees. However, Belief Propagation is either only applicable to tree models, or approximate (and without guarantees) for precision and convergence. In this paper we present work in progress on an Anytime Exact Belief Propagation algorithm that is very similar to Belief Propagation but is exact even for graphical models with cycles, while exhibiting soft short-circuiting, amortized constant time complexity in the model size, and which can provide probabilistic proof trees.

1 Introduction
Statistical Relational Models (Getoor and Taskar 2007) and, more recently, Probabilistic Programming, have been making strides towards probabilistic logic inference algorithms that integrate logic and probabilistic reasoning. These algorithms perform inference on probabilistic logical models, which generalize regular logical models by containing formulas that have a probability of being true, rather than always being true.

While Statistical Relational Models and Probabilistic Programming focus on higher-level representations such as relations and data structures, even regular graphical models such as Bayesian networks can be thought of as probabilistic logic models, since conditional probability distributions (or factors, for undirected models) can be described by formulas and therefore thought of as probabilistic formulas. This paper focuses on regular graphical models that will later serve as a basis for higher-level probabilistic logic models (as further discussed in the conclusion).

Naturally, probabilistic inference algorithms must be able to perform inference on purely logic models, since these can be seen as probabilistic logic models whose formulas have probability 1 of being true. In this case, it is desirable that the probabilistic inference algorithms reduce to logic reasoning in a way that exploits the logic structure of the model nearly as efficiently as pure logic reasoning algorithms would. In fact, we should expect even more: if a model (or part of it) is near-certain (with probabilities close to 0 and 1), then the model is very close to a purely logical model and it is reasonable to expect a probabilistic inference algorithm to exploit the logical structure to some degree, with graceful degradation as the model becomes more uncertain.

Short-circuiting is a type of structure that is an important source of efficiency for logic reasoning. A formula is short-circuited if its value can be determined from the value of only some of its sub-formulas. For example, if a model contains the formula \( A \leftrightarrow B \lor C \lor D \) and \( B \) happens to be true, then a logic reasoning algorithm can conclude that \( A \) is true without having to decide whether \( C \) and \( D \) are true. However, if a probabilistic reasoning algorithm knows \( P(A|B \lor C \lor D) = 1 \) and that \( P(B) = 0.9 \), it will typically still need to compute \( P(C) \) and \( P(D) \) in order to compute \( P(A) \), even though it is already possible to affirm that \( P(A) \geq 0.9 \) without any reasoning about \( C \) and \( D \). Providing such a bound can be considered a soft short-circuiting that approximates logical short-circuiting as probabilities get closer to 0 and 1, but such ability is absent from most probabilistic inference methods.

Soft short-circuiting serves as a basis for an anytime, incremental algorithm that trades bound accuracy for time. Given more time, the algorithm may determine that \( P(C) \geq 0.8 \) independently of \( B \), perhaps by recursively processing another rule \( P(C|E \lor F) \), which allows it to increase its lower bound \( P(A) \geq 0.98 \), a tight bound obtained without ever reasoning about some potentially large parts of the model (in this case, rules involving \( D \) or adding information...
There are several probabilistic inference algorithms, discussed in Section 2, that produce bounds on query probabilities. However, we find that most of these algorithms do not exhibit another important property of logic reasoning algorithms: a time complexity for inference that is amortized constant in the size of the entire model (although still exponential on the induced width of the portion of the model that is relevant for computing the current bound). This is achieved by storing formulas in a model in hash tables indexed by the variables they contain, and looking up formulas only as needed during inference as their variables come into play. An important application for probabilistic logic reasoning in the future is reasoning about thousands or even millions of probabilistic rules (for example in knowledge bases learned from the Web such as NELL, (Mitchell et al. 2013)), for which this property will be essential.

Finally, we are also interested in a third important property of logic reasoning algorithms: the ability to produce an intelligible trace of its inference (such as a proof or refutation tree) that serves as a basis for explanations and debugging. In probabilistic reasoning, Belief Propagation is perhaps the closest we get to this, since local message-passing is easily understood and the tree of messages can be used as a proof tree. However, BP only returns correct marginal probabilities for graphical models without cycles, and non-guaranteed approximation and convergence for general graphical models.

In this paper, we present work in progress on Anytime Exact Belief Propagation, an algorithm that exhibits the three properties described above: it incrementally computes bounds on marginal probabilities that can be provided at any time, whose accuracy can be traded off for time, and that eventually converge to the exact marginal; it has time complexity amortized constant in the size of the entire model; and it produces a tree of local messages that can be used to explain its conclusion.

2 Related Work
The most obvious candidates for probabilistic logic reasoning approaches that exhibit logic properties with graceful degradation are the ones based on logic programming: Bayesian Logic Programs (Kersting (2000)), PRISM (Sato and Kameya 1997), Stochastic Logic Programs (Muggleton 1995), and ProbLog (Raedt and Kersting 2004). While these approaches can be used with sampling, they typically derive (by regular logic programming methods) a proof tree for the query and evidence in order to determine which portion of the model is qualitatively relevant to them. Only after that does the probabilistic reasoning starts. This prevents selecting portions of the model based on quantitative relevance.

More recently, the ProbLog group has proposed two methods for anytime inference: (Renkens et al. 2014) successively finds multiple explanations for a query, each of them narrowing bounds on the latter’s probability. However, finding an explanation requires inference on the entire model, or at least on a qualitatively relevant portion that may include quantitatively irrelevant knowledge. (Vlasselaer et al. 2015) proposes a method based on forward reasoning with iterative deepening. Because the reasoning goes forward, there is no clear way to limit the inference to the portion most relevant to a query (which is a form of backward inference), and no selection for more likely proofs.

Our calculation of bounds is equivalent to the one presented in (Leisink and Kappen 2003), but that work does not attempt to focus on relevant portions of a model and does not exploit the graphical model’s factorization as much as our method and Variable Elimination do. Box propagation (Mooij and Kappen 2008) propagates boxes, which are looser bounds than ours and Leisink & Kappen’s bounds. In fact, their method can easily use these tighter bounds, but in any case it does not deal with cycles, stopping the unrolling of the model (the Bethe tree) once a cycle is found. Ihler (Ihler 2007) presents a similar method that does not stop when a cycle is found, but is not guaranteed to converge to the exact marginal.

Liu et al (Lou, Dechter, and Ihler 2017) present a method very similar to ours based on growing an AND-OR search tree from the query and bounding the not-yet-processed remaining of the model. As more of the tree is expanded, the better the bounds become. The main difference from our method is that the AND-OR search tree has a child per value of each random variable, making it arguably less intelligible and harder to use as a proof tree and to generalize to richer representations such as Statistical Relational Models.

3 Background
3.1 Graphical Models
Graphical models are a standard framework for reasoning with uncertainty. The most common types are Bayesian networks and Markov networks. In both cases, a joint probability distribution for each assignment tuple x to N random variables is defined as a normalized product of non-negative real functions \( \{ \phi_i \}_{i=1..K} \), where 1..K is short for \{1, \ldots, K\}, each of them applied to a subtree \( X_i \) of \( X \):

\[
P(X) = \frac{1}{Z} \prod_{i=1}^{K} \phi_i(X_i),
\]

where Z is a normalization constant equal to \( \sum_x \prod_i \phi_i(X_i) \). Functions \( \phi_i \) are called factors and map each assignment on their arguments to a potential, a non-negative real number that represents how likely the assignment \( X_i \) is. This representation is called factorized due to its breaking the joint probability into this product. In Bayesian networks, \( K = N \) and factors are conditional probabilities \( P(X_i | P_{\alpha_i}) \), for each random variable \( X_i \) in \( X \), where \( P_{\alpha_i} \) are its parents in a directed acyclic graph.

For succinctness, we often do not explicitly write the arguments to factors:

\[
P(X) = \frac{1}{Z} \prod_i \phi_i(X_i) = \frac{1}{Z} \prod_i \phi_i.
\]

For simplicity, we use the same symbols for both random variables and their values, but the meaning should be clear.
The marginal probability (MAR) problem consists of computing

\[ P(Q) = \sum_{X \notin Q} P(X), \]

where \( Q \) is a subtuple of \( X \) containing queried variables, and \( \sum_{X \notin Q} \) is the summation over all variables in \( X \) but not in \( Q \). It can be shown that \( P(Q) = \frac{1}{Z_Q} \sum_{X} \prod_i \phi_i \) for \( Z_Q \) a normalization constant over \( Q \). Therefore, because \( Z_Q \) is easily computable if \( |Q| \) is small, the problem can be simply reduced to computing a summation over products of factors, which the rest of the paper focuses on.

We denote the variables (or neighbors) of a factor \( \phi \) or set of factors \( M \) as \( Var(\phi) \) and \( Var(M) \). The neighbors \( neighbors_M(V) \) of a variable \( V \) given a set of factors \( M \) is defined as the set of factors \( \{ \phi \in M : V \in Var(\phi) \} \). We call a set of factors a model. The factor graph of a model \( M \) is the graph with variables and factors of \( M \) as nodes and with an edge between each factor and each of its variables.

3.2 Belief Propagation

Belief Propagation (Yedidia, Freeman, and Weiss 2003) is an algorithm that computes the marginal probability of a random variable given a graphical model whose factor graph has no cycles.

Let \( M \) be a set of factors and \( P_M \) be the probability distribution it defines. Then, for a set of variables \( Q \subseteq Var(M) \), we define:

\[ P_M(Q) \propto m^{M}_{\phi \in Q} \]

(\( m^{M}_{\phi \in Q} \) does not depend on \( \phi \)).

\[ m^{M}_{V \leftarrow \phi} = \sum_{S} \phi \prod_{S^j \in S} m^{M^j}_{\phi \in S^j} \]

where \( \{ S^1, \ldots, S^n \} \) \( \equiv \) \( Var(\phi) \setminus V \),

\[ m^{M}_{\phi \leftarrow V} = \prod_{\phi_i \in neighbors_M(V)} m^{M}_{\phi \leftarrow \phi_i} \]

where \( \{ \phi^1, \ldots, \phi^n \} \) \( \equiv \) \( neighbors_M(V) \),

\( M^j \) is the set of factors in \( M \) connected to \( \phi^j \).

Note that each message depends on a number of sub-messages. Since the factor graph is a tree (it has no cycles), each sub-message involves a disjoint set of factors \( M^j \). This is crucial for the correctness of BP because it allows the computation to be separately performed for each branch.

If a graphical model has cycles, an iterative version of BP, loopy BP, can still be applied to it (Yedidia, Freeman, and Weiss 2003). In this case, since a message will eventually depend on itself, we use its value from a previous iteration, with random or uniform messages in the initial iteration. By iterating until a convergence criterion is reached, loopy BP provides distributions, called beliefs, that in practice often approximate the marginal of the query well. However, loopy BP is not guaranteed to provide a good approximation, or even to converge.

3.3 Anytime Belief Propagation

Even though BP is based on local computations between neighboring nodes, it only provides any information on the query’s answer once it has analyzed the entire model, even if some parts of the model have a relatively small influence on the answer. This goes against our initial goal providing information on the query’s answer even after analyzing only a (hopefully more relevant) portion of the model.

Anytime BP (de Salvo Braz et al. 2009) is an algorithm based on (loopy) BP that computes iteratively improved bounds on a message. A bound (following definitions in (Mooij and Kappen 2008)) on a message \( m \) is any set of messages to which \( m \) is known to belong. Anytime BP (and, later, Anytime Exact BP) only use bounds that are convex sets of messages, and that can therefore be represented by a finite number of messages (the bounds extremas), the convex hull of which is the entire bound. Initially, the bound on a message on a variable \( V \) is the simplex \( \mathcal{P}(V) \), the set of all possible probability distributions on \( V \), and whose extremas are the distributions that place the entire probability on a single value. For example, if \( V \) is a boolean random variable, its simplex is the set \( \{ \text{if } V = \text{true} \text{ then } 1 \text{ else } 0, \text{if } V = \text{false} \text{ then } 1 \text{ else } 0 \} \).

It turns out that the computation of a message \( m \) given its sub-messages is a convex function. Therefore, given the bounds on sub-messages represented by their extremes, we can compute a bound \( b(m) \) on \( m \) by computing the extremes of this bound, each extreme being equal to the message computed from a combination of extremes to the sub-messages. This provides a finite set of extremum messages that define \( b(m) \) and can be used to compute further bounds.

Figure 1 shows an example of Anytime Belief propagation on a factor network. The algorithm provides increasingly improving bounds on the belief \( m(A) \) on query \( A \), by first returning the simplex \( \mathcal{P}(A) \) as a bound, then returning the bound computed from simplex sub-messages, and then successively refining this bound by selecting one or more of the sub-messages, obtaining tighter bounds on these sub-messages, and recomputing a tighter bound for \( m(A) \). At every step from (b) to (d), factors are included in the set so as to complete some random variable’s blanket (we do not show the expansions from (d) to (e), however, only their consequences). We include the table for factor \( \phi_1 \) but omit the others. For simplicity, the figure uses binary variables only and shows bounds as the interval of possible probabilities for value 1, but it applies to multi-valued variables as well.

This incrementally processes the model from the query, eventually processing it all and producing an exact bound.
3.4 Cycle Cutset Conditioning

If a graphical model has cycles, an iterative version of BP, loopy BP, can still be applied to it (Yedidia, Freeman, and Weiss 2003). However, loopy BP is not guaranteed to provide a good approximation, or even to converge.

Cycle cutset conditioning (Pearl 1988) is a way of using BP to solve a graphical model $M$ with cycles. The method uses the concept of absorption: if a factor $\phi_i(X_i)$ has some of its variables $V \subseteq X_i$ set to an assignment $v$, it can be replaced by a new factor $\phi'_{i}$, defined on $X \setminus V$ and $\phi'(X_i \setminus V) = \phi_i(X_i \setminus V, v)$. Then, cutset conditioning consists of selecting $C$, a cycle cutset random variables in $M$ such that, when fixed to a value $c$, gives rise through absorption in all factors involving variables in $C$ to a new graphical model $M_c$ without cycles and defined on the other variables $X \setminus C$ such that $P_{M_c}(X \setminus C) = P_{M}(X \setminus C, c)$. The marginal $P_{M_c}(Q)$ can then be computed by going over all assignments to $C$ and solving the corresponding $M_c$ with BP:

$$P_{M_c}(Q) = \sum_{X \setminus Q} P_M(X)$$
$$= \sum_{c} \sum_{X \setminus (Q \cup C)} P_M(X \setminus C, c)$$
$$= \sum_{c} \sum_{X \setminus (Q \cup C)} P_{M_c}(X \setminus C)$$
$$= \sum_{c} P_{M_c}(Q)$$

Figure 2(a) shows a model with a cycle. Panel (b) shows how cutset conditioning for cutset {A} can be used to compute $P(Q)$: we successively fix $A$ to each value $a$ in its domain, and use absorption to create two new factors $\phi_1(C, a) = \phi_1(C, a) = \phi_2(E, a)$. This new model does not contain any cycles and BP computes $P(Q, a)$. The overall $P(Q)$ is then computed as $\sum_{a} P(Q, a)$. Now, consider that the messages computed across the reduced model that depend on $a$ can be thought of as functions of $a$. From that angle, the multiple applications of BP for each $a$ can be thought of as a single application of BP in which $A$ is a fixed, free variable that is not eliminated and becomes a parameter in the propagated messages (panel (c)). This has the advantage of computing all messages that do not depend on $a$ only once.

While cutset conditioning solves graphical models with cycles exactly, it has some disadvantages. Like standard BP, cutset conditioning requires the entire model to be processed before providing useful information. In fact, simply finding a cutset already requires going over the entire model, before inference proper starts. Besides, its cost grows exponentially in the size of the cutset, which may be larger than the induced tree width. Our main proposal in this paper, Anytime Exact Belief Propagation, counters those disadvantages by processing the model in an incremental way, providing a hard bound around the exact solution, determining the cutset during inference, and summing out cutset variables as soon as possible as opposed to summing them out only at the end.

4 Anytime Exact Belief Propagation

We are now ready to present the main contribution of this paper, Anytime Exact Belief Propagation (AEBP). Like cutset conditioning, the algorithm applies to any graphical models, including those with cycles. Unlike cutset conditioning, it does not require a cutset to be determined in advance, and instead determines it on the fly, through local message-passing. It also performs a gradual discovery of the model, providing bounds on the final result as it goes. This is similar to Anytime BP, but Anytime Exact BP, as the name implies, provides bounds on the exact query marginal probability and eventually converges to it.

We first provide the intuition for Anytime Exact BP through an example. Consider the graphical model in Figure 4 (the full model is shown in (e)). If we simply apply Anytime BP to compute $P(Q)$, messages will be computed in an
infinite loop. This occurs because Anytime BP has no way of identifying loops. AEBP, on the other hand, takes an extra measure in this regard: when it requests a new bound from one of the branches leading to a node, it also provides the set of factors known so far to belong to the other branches. Any variable that is in the branch and is connected to these external factors must necessarily be a cutset variable. Upon finding a cutset variable $C$, AEBP considers it fixed and does not sum it out, and resulting messages are functions of $C$ (as well we the regular variable for which we have a message). Branches sharing a cutset variable $C$ will therefore return bounds that are functions of $C$. Cutset variables are summed out only after messages from all branches containing $C$ are collected.

While the above procedure is correct, delaying the sum over cutset variables until the very end is exponentially expensive in the number of them. Figure 4 shows an example in which a cutset variable ($G$) that occurs only in an inner cycle is summed out when that cycle is processed (at node $E$), while the more global cutset variables ($C$ and $F$) are summed out at the end, when the more global cycle is processed (at node $A$).

Algorithm 1 presents the general formulation. It works by keeping track of each component, that is, a branch of the factor graph rooted in either a variable or factor, its Node, and computing a message from Node to some other requesting node immediately outside the component. Each component is initially set with the external factors that have already been selected by other components. The message is on a variable $V$ (this is Node itself if Node is a variable, and some argument of Node if it is a factor). In the first update, the component sets the bound to the simplex on $V$ and creates its children components: if Node is a variable, the children components are based on the factors on it that are not already external; if it is a factor, they are based on its argument variables.

From the second update on, the component selects a child, updates the child’s external factors by including that child’s siblings external factors, updates the child’s bound, updates its own set of factors by including the child’s newly discovered factors, and computes a new bound. If Node is a factor, this is just the product of the bounds of its children. If Node is a variable, this is obtaining by multiplying $\phi$ and children bounds, and summing out the set of variables $S$. $S$ is the set of variables that occur only inside $C$, (which excludes $V$ and cutset variables connected to external factors, but does include cutset variables that occur only inside this component). This allows cutset variables to be eliminated as soon as possible in the process. To compute the marginal probability for a query $Q$, all that is needed is to create a component for $Q$ without external factors and update it successively until it converges to an exact probability distribution. During the entire process, even before convergence, this component tree can be used as a trace of the inference process, indicating how each message has been computed from sub-messages so far, similarly to a probabilistic proof or refutation tree in logic reasoning.

**UPDATE($C$)**

$C$ is a component, defined as a tuple $(V, \text{Node}, \text{Bound}, M, \text{ExteriorFactors}, \text{Children})$ where:

- $V$: the variable for which a message is being computed
- $\text{Node}$: a variable or factor from which the message on variable $V$ is being computed
- $\text{Bound}$: a bound on the computed message
- $\text{Factors}$: the set of factors selected for this message already
- $\text{ExteriorFactors}$: set of factors already observed outside the component, and used to identify new cutset variables.
- $\text{Children}$: components for the sub-messages of this message.

1. if first update
   2. $\text{Bound} \leftarrow P(V)$
   3. if Node is variable
      4. $\text{Factors} \leftarrow \text{factors with } \text{Node} \text{ as argument and not in } \text{ExteriorFactors}$
     5. $\text{Children} \leftarrow \text{components based on each factor in } \text{Factors}$
        and $\text{ExteriorFactors}$ set to $C.\text{ExteriorFactors}$
   6. else // Node is factor $\phi$
      7. $\text{Bound} \leftarrow \sum_{\text{Children}} \phi \prod_{\text{Ch.Factors}}$
     8. $\text{Children} \leftarrow \text{components based on each variable argument (that is, neighbor) of } \phi$
        and $\text{ExteriorFactors}$ set to $C.\text{ExteriorFactors} \setminus \{\phi\}$
   9. else
     10. $\text{Child} \leftarrow \text{chooseNonConvergedChild(Children)}$
     11. $\text{Child.\text{ExteriorFactors}} \leftarrow \text{ExteriorFactors} \cup \bigcup_{\text{Ch.Factors}}\text{Children.\text{Factors}}$
     12. **UPDATE($\text{Child}$)**
     13. $\text{Factors} \leftarrow \text{Factors} \cup \text{Child.\text{Factors}}$
     14. $\text{ChildrenBoundProduct} \leftarrow \prod_{\text{Ch.\text{Factors}}} \text{Ch.\text{Bound}}$
     15. if Node is variable
         16. $\text{Bound} \leftarrow \text{ChildrenBoundProduct}$
     17. else // Node is factor $\phi$
         18. $S \leftarrow \text{variables in } \text{ChildrenBoundProduct}$
            not in any factor in $\text{ExteriorFactors}$
         19. $\text{Bound} \leftarrow \sum_{S} \phi \prod_{\text{Ch.\text{Factors}}} \text{Ch.\text{Bound}}$

Algorithm 1: Anytime Exact Belief Propagation.

### 5 Conclusion

We presented our preliminary work on Anytime Exact Belief Propagation, an anytime, exact inference method for graphical models that provides hard bounds based on a neighborhood of a query. The algorithm aims at generalizing the advantages of logic reasoning to probabilistic models, even for dependencies that are not certain, but near certain.

Future work includes finishing the implementation, evaluating it on benchmarks, and generalizing it higher-level logic representations such as relational models and probabilistic programs. To achieve that, we will employ techniques from the lifted inference literature (Poole 2003; de Salvo Braz 2007) [Milch et al. 2008] [Van den Broeck et al. 2011].
Figure 3: Discovering a cutset in AEBP. $Q$ requests a bound on $Q$ from $\phi_1$ while telling it that no factors have been observed (in red) in other components (empty set $\{\}$) (a). The bound is computing by only assuming that the message from $A$ is the simplex $P(A)$. It then requests a bound from $\phi_2$, this time telling it about $\phi_1$ having already been observed in a different component (b). In (c), it requests a better bound from $\phi_1$, this time telling it about having $\phi_2$, which triggers a request from $\phi_3$ to $A$ with information of having previously observed $\{\phi_1, \phi_2\}$. In (d), a request goes all the way to $B$ with information having observed, among others, $\phi_3$. When $B$ requests a bound from $\phi_4$ (e), it is detected that $\phi_4$’s argument $C$ is also an argument of previously observed factor $\phi_3$, which leads to making $C$ a cutset variable. Bounds are then computed as a function of $C$, as opposed of summing it out, all the way back to $Q$, where $C$ will eventually be summed out.

Figure 4: An example of AEBP that eliminates portions of the cutset separately. The dashed lines show how branches are followed from both $A$ and $E$. $G$ is detected as a cutset variable with respect to $E$ because it connects two branches of $E$, so it is summed out along with $E$ when producing the bound towards $A$. $F$ is also detecting while exploring the branches of $E$, but it connects to a branch of $A$ so it is not summed out when $E$ is finished, being instead summed out when $A$ is finished. $C$ connects two branches of $A$ so it is also summed out along with $A$.

Kersting 2012 as well as probabilistic inference modulo theories [de Salvo Braz et al. 2016].

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