Loop Corrected Belief Propagation

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Abstract

We propose a method for improving Belief Propagation (BP) that takes into account the influence of loops in the graphical model. The method is a variation on and generalization of the method recently introduced by Montanari and Rizzo [2005]. It consists of two steps: (i) standard BP is used to calculate *cavity distributions* for each variable (i.e. probability distributions on the Markov blanket of a variable for a modified graphical model, in which the factors involving that variable have been removed); (ii) all cavity distributions are combined by a message-passing algorithm to obtain consistent single node marginals. The method is exact if the graphical model contains a single loop. The complexity of the method is exponential in the size of the Markov blankets. The results are very accurate in general: the error is often several orders of magnitude smaller than that of standard BP, as illustrated by numerical experiments.

1 INTRODUCTION

Belief Propagation (BP), also known as the Sum-Product Algorithm and as Loopy Belief Propagation, is a popular algorithm for approximate inference on graphical models. It often yields surprisingly accurate results, using little computation time. It has strong ties with the Bethe approximation [Yedidia et al., 2001], which was developed in statistical physics [Bethe, 1935]. Belief Propagation is the simplest case in a family of related but more sophisticated algorithms such as Generalized Belief Propagation (GBP) [Yedidia et al., 2005] (which can be used e.g. for the Cluster Variation Method (CVM) [Pelizzola, 2005, Kikuchi, 1951]) and Expectation Propagation (EP) [Minka, 2001].

It is well-known that Belief Propagation yields exact results if the graphical model is a tree. However, if the graphical model contains loops (cycles), the approximate marginals calculated by BP can have large errors. Increasing the cluster size of the approximation (e.g. by using CVM with larger clusters) does not necessarily solve this problem if long, influential loops cannot be completely included in one cluster. Using TreeEP [Minka and Qi, 2004] one can correct for the presence of loops to a certain extent, namely for those loops that consist of part of the base tree and one additional factor. The method we propose here effectively takes into account all the loops in the factor graph, in many cases yielding more accurate approximate marginals as a result.

In the statistical physics community different methods for calculating loop corrections to the Bethe approximation have been proposed recently [Montanari and Rizzo, 2005, Parisi and Slanina, 2005, Chertkov and Chernyak, 2006]. The work we present here is a variation on the theme introduced in [Montanari and Rizzo, 2005]. The alternative that we propose here offers two advantages compared to the original method proposed in [Montanari and Rizzo, 2005]: (i) it has better convergence properties in the case of relatively strong interactions; (ii) it is directly applicable to arbitrary factor graphs, whereas the original method has only been formulated for binary variables with pairwise factors.

This article is organized as follows. First we explain the theory behind the proposed method, discussing differences with the original approach in [Montanari and Rizzo, 2005] along the way. Then we report numerical experiments regarding the quality of the approximation and the computation time, comparing with other approximate inference methods. Finally, we discuss the results and state conclusions. More details and more extensive numerical experiments can be found in [Mooij and Kappen, 2006].

2 THEORY

2.1 GRAPHICAL MODEL CLASS, NOTATIONS

Let $\mathcal{V} := \{1, \ldots, N\}$ be an index set for N random variables $\{x_i\}_{i \in \mathcal{V}}$, where variable x_i takes values in a discrete[1] domain $\mathcal{X}_i$. We will use a multi-index notation, i.e. for any subset $I \subseteq \mathcal{V}$, we write $x_I := (x_{i_1}, x_{i_2}, \ldots, x_{i_m})$ if $I = \{i_1, i_2, \ldots, i_m\}$ and $i_1 < i_2 < \ldots i_m$. We consider probability distributions over $x = (x_1, \ldots, x_N)$ that can be written as a product of factors ψ_I:

$$P(x_1, \ldots, x_N) = \frac{1}{Z} \prod_{I \in \mathcal{F}} \psi_I(x_I). \tag{1}$$

The factors (or "interactions") ψ_I are indexed by subsets of $\mathcal{V}$, i.e. $I \in \mathcal{F} \subseteq \mathcal{P}(\mathcal{V})$. Each factor is a nonnegative function $\psi_I : \prod_{i \in I} \mathcal{X}_i \to [0, \infty)$. This class of probability distributions includes Markov Random Fields as well as Bayesian Networks. In general, the normalizing constant Z is not known and exact computation of Z is infeasible. One can visualize a probability distribution of the form (1) with a *factor graph* (c.f. Figure 1(a)), a bipartite graph having *variable nodes* $i \in \mathcal{V}$ and *factor nodes* $I \in \mathcal{F}$, with an edge between i and I if and only if $i \in I$.

In the following, we will use uppercase letters for indices of factors ($I, J, K, \ldots \in \mathcal{F}$) and lowercase letters for indices of variables ($i, j, k, \ldots \in \mathcal{V}$). For simplicity we assume that no pair of variables is contained in more than one factor, i.e. we assume that no loops of length 4 are present in the factor graph.[2] Let $i \in \mathcal{V}$ and $A \subseteq \mathcal{V}$; we slightly abuse notation by writing $A \setminus i$ instead of $A \setminus \{i\}$, $\setminus A$ instead of $\mathcal{V} \setminus A$ and $\setminus i$ instead of $\mathcal{V} \setminus \{i\}$.

2.2 LCBP: A BRIEF OVERVIEW

The main idea of what is known in the statistical physics community as the "cavity method" is to consider modified graphical models in which a single variable is removed, together with all factors in which that variable appears, thus forming a "cavity" (c.f. Figure 1). The removed variable is called the *cavity variable.* The method proposed in [Montanari and Rizzo, 2005] (and our method, which is a variation and generalization thereof) approximates for each variable its corresponding *cavity distribution*, i.e. the marginal probability distribution of the cavity network on the neighborhood (Markov blanket) of the cavity variable. Subsequently, the removed factors are multiplied back in, and we demand consistency of single node marginals. This results in partial cancellation of errors in the approximated cavity distributions, improving the accuracy of the final result. The Bethe approximation is obtained as the special case in which the cavity distributions are assumed to factorize completely. We will now explain the procedure in more detail.

2.3 CAVITIES

Let $i \in \mathcal{V}$. We denote by $\partial i := \{j \in \mathcal{V} : i, j \in I \text{ for some } I \in \mathcal{F}\}$ the set of neighboring variables of i, also called the *Markov blanket* of i. We define $\Delta i := \partial i \cup \{i\}$. We modify the original graphical model (1) by removing variable x_i and all the factors in which it appears (c.f. Figure 1); the probability distribution corresponding to the resulting *cavity network* is thus by definition:

$$\frac{1}{Z_{\setminus i}} \prod_{\substack{I \in \mathcal{F} \\ i \notin I}} \psi_I(x_I). \tag{2}$$

Note that the normalization constant $Z_{\setminus i}$ differs from the normalization constant Z of the original network (1). We will call the marginal distribution of (2) on ∂i (the Markov blanket of i) the *cavity distribution* $P^{\setminus i}$ *of* i:

$$P^{\setminus i}(x_{\partial i}) := \frac{1}{Z_{\setminus i}} \sum_{x_{\setminus \Delta i}} \prod_{\substack{I \in \mathcal{F} \\ i \notin I}} \psi_I(x_I). \tag{3}$$

Writing Ψ_i for the product of the removed factors:

$$\Psi_i(x_{\Delta i}) := \prod_{\substack{I \in \mathcal{F} \\ i \in I}} \psi_I(x_I), \tag{4}$$

the following identity is immediate:

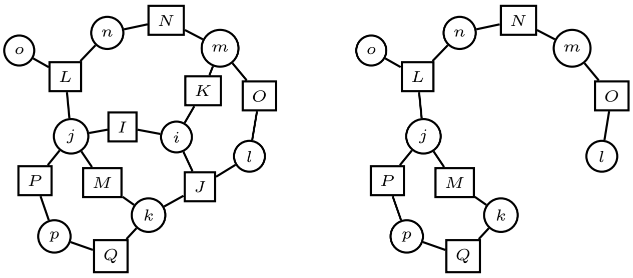
$$P(x_{\Delta i}) \propto P^{\setminus i}(x_{\partial i}) \Psi_i(x_{\Delta i}), \tag{5}$$

i.e. the marginal distribution on Δi of the *original* probability distribution (1) is proportional to the product of the cavity distribution of i and the product of the factors involving x_i.[3] The cavity distribution summarizes the rest of the network; it can be seen as an "effective interaction" on $x_{\partial i}$. In particular, it summarizes information about loops in which variable i is contained. For example, in Figure 1, the cavity distribution $P^{\setminus i}(x_{\partial i})$ contains the interaction ψ_O between x_m and x_l, which is part of the loop $iKmOlJi$ in the original factor graph.

[1] The same ideas can be applied for the case of continuous variables. Here we focus on the discrete case.

[2] For a more general approach, see Mooij and Kappen [2006].

[3] Note that equation (5) is *not* one of the DLR equations [Georgii, 1988]. The most similar DLR equation would be $P(x_i) = \sum_{x_{\partial i}} P(x_i \,|\, x_{\partial i}) P(x_{\partial i})$, whereas (5) implies $P(x_i) \propto \sum_{x_{\partial i}} \Psi_i(x_{\Delta i}) P^{\setminus i}(x_{\partial i})$. Although the equations may appear identical at first sight, they are not. Consider



(a) Original factor graph

(b) Cavity graph of i

Figure 1: (a) Original factor graph; (b) cavity graph remaining after variable node i and the factor nodes that contain i (i.e. I,J,K) have been removed. The neighbors of i are $\partial i = \{j, k, l, m\}$ and $\Delta i = \{i, j, k, l, m\}$. The cavity distribution $P^{\setminus i}$ is defined as the marginal on $x_{\partial i}$ of the probability distribution corresponding to (b).

2.4 CONSISTENCY OF SINGLE NODE MARGINALS

Consider two variables $i, j \in \mathcal{V}$ with $i \in \partial j$; let I be the common factor involving both x_i and x_j. The joint marginal on x_i and x_j *in the absence of the factor* I is given by

$$P^{\setminus I}(x_i, x_j) \propto \sum_{x_{\setminus\{i,j\}}} \prod_{\substack{J\in\mathcal{F}\\ J\neq I}} \psi_J(x_J). \qquad (6)$$

We can calculate this joint marginal from the cavity distribution of i:

$$P^{\setminus I}(x_i, x_j) \propto \sum_{x_{\partial i\setminus j}} P^{\setminus i}(x_{\partial i})\Psi_i^{\setminus I}(x_{\Delta i}) \qquad (7)$$

where we defined:

$$\Psi_i^{\setminus I}(x_{\Delta i}) := \prod_{\substack{J\in\mathcal{F}\\ i\in J, J\neq I}} \psi_J(x_J) = \frac{\Psi_i}{\psi_I} \qquad \text{for } i \in I, I \in \mathcal{F}.$$

Alternatively, we can calculate (6) from the cavity distribution of j (interchanging i and j):

$$P^{\setminus I}(x_i, x_j) \propto \sum_{x_{\partial j\setminus i}} P^{\setminus j}(x_{\partial j})\Psi_j^{\setminus I}(x_{\Delta j}). \qquad (8)$$

The results are obviously identical if the cavity distributions $P^{\setminus i}$ and $P^{\setminus j}$ are exact.

In practice, the exact cavity distributions are unavailable and we can only obtain approximations $Q_0^{\setminus k} \approx P^{\setminus k}$. Replacing $\{P^{\setminus k}\}_{k\in\mathcal{V}}$ by their approximations $\{Q_0^{\setminus k}\}_{k\in\mathcal{V}}$ in equations (7) and (8) will yield inconsistent results; the main idea of the method proposed in [Montanari and Rizzo, 2005] is to deform the approximate cavity distributions $\{Q_0^{\setminus k}\}_{k\in\mathcal{V}}$ in such a way that the single node marginals of x_i and x_j in equations (7) and (8) become consistent.[4] In [Montanari and Rizzo, 2005], the single node marginals of the approximate cavity distributions are varied whereas the higher order cumulants are kept fixed.[5] Instead, we propose here to deform the approximate cavity distributions $Q_0^{\setminus i}$ in the following way:

$$Q^{\setminus i}(x_{\partial i}) \propto Q_0^{\setminus i}(x_{\partial i}) \prod_{j\in\partial i} \phi_j^{\setminus i}(x_j). \qquad (9)$$

Thus we change the single variable interactions by multiplying with single node factors but keep higher order interactions fixed. The single node factors $\phi_j^{\setminus i}(x_j)$ are chosen such that the single node marginals of x_i and x_j are consistent in the absence of factor I, i.e. such that

$$\sum_{x_{\Delta i\setminus i}} Q^{\setminus i}(x_{\partial i})\Psi_i^{\setminus I}(x_{\Delta i}) \propto \sum_{x_{\Delta j\setminus i}} Q^{\setminus j}(x_{\partial j})\Psi_j^{\setminus I}(x_{\Delta j}). \qquad (10)$$

This should hold for all pairs of neighboring variables $i, j \in \mathcal{V}$ with $i \in \partial j$. In this way, first order errors in the initial approximate cavity distributions $Q_0^{\setminus k}$ are cancelled out.

To calculate the values for the corrections $\phi_j^{\setminus i}(x_j)$, we use Algorithm 1, which is a simple fixed-point algorithm based on equations (10). After convergence, we calculate single node marginals $q_i(x_i) \approx P(x_i)$ from the final deformed approximate cavity distributions $Q_\infty^{\setminus i}$ using:

$$q_i(x_i) \propto \sum_{x_{\partial i}} Q_\infty^{\setminus i}(x_{\partial i})\Psi_i(x_{\Delta i}).$$

In our experiments, Algorithm 1 always converged to a reproducible fixed point, even without damping. Note

e.g. a star-shaped model with a central variable i coupled to its neighbors by pairwise factors. In that case, $P^{\setminus i}(x_{\partial i})$ is completely factorized, whereas $P(x_{\partial i})$ is not.

[4] Instead of demanding consistency of single node marginals x_i and x_j in the *absence* of the factor I connecting x_i with x_j, one could alternatively demand consistency of the single node marginals in the presence of all factors, i.e. demanding that $\sum_{x_{\partial i\setminus j}} P^{\setminus i}(x_{\partial i})\Psi_i(x_{\Delta i}) \propto \sum_{x_{\partial j\setminus i}} P^{\setminus j}(x_{\partial j})\Psi_j(x_{\Delta j})$ for all $i \in \mathcal{V}, j \in \partial i$. This might appear more natural, but it turns out that the resulting method is inferior to the one presented here if factors involving more than two variables are present (see also section 4).

[5] Cumulants are called "connected correlations" in [Montanari and Rizzo, 2005] and are defined as certain polynomial combinations of moments $\sum_{x_{\partial i}} P^{\setminus i}(x_{\partial i}) \prod_{j\in\mathcal{A}} x_j$ with $\mathcal{A} \subseteq \partial i$, where all variables are assumed to be ±1-valued.

that if we would start with the exact cavity distributions, i.e. $Q_0^{\setminus i} = P^{\setminus i}$ for all i, the algorithm would terminate immediately because the single node marginals would already be consistent. Obviously, one can use other update schemes than the parallel one given in Algorithm 1; in our experiments, we have used a sequential update scheme.

2.5 COMPUTING $Q_0^{\setminus i}$

We have discussed in the previous subsection how to deform the initial approximate cavity distributions $Q_0^{\setminus i}$ to make them consistent; we now discuss how to obtain the $Q_0^{\setminus i}$ in the first place.

In [Montanari and Rizzo, 2005] it is suggested to initialize the second-order cumulants of the approximate cavity distribution using BP in combination with linear response and to assume higher order cumulants to be zero (although in principle one could use higher order linear response estimates for the higher order cumulants).

Here, instead, we propose to initialize the approximate cavity distributions by using standard BP on a "clamped" network. This means that for each cavity variable i, we fix some setting $x_{\partial i}$ of its Markov blanket, use BP to calculate the corresponding Bethe free energy $F_{Bethe}(x_{\partial i})$ for that particular setting, iterate over all possible settings, and finally calculate the approximate cavity distribution

$$Q_0^{\setminus i}(x_{\partial i}) \propto e^{-F_{Bethe}(x_{\partial i})}. \tag{11}$$

In this way we capture all effective interactions, also higher order ones, in the initial cavity distributions.

One can think of many other ways to approximate the initial cavity distributions. The procedure described above is exponential in the size of the cavity. An alternative way of initializing the cavity distributions is to estimate the pair marginals $P^{\setminus i}(x_j, x_k)$ for each pair $(j,k) \in \partial i^2$. This can be done by clamping x_j to some value, using BP to approximate $P^{\setminus i}(x_k \,|\, x_j)$ and $F_{Bethe}(x_j)$. An approximation of $P^{\setminus i}(x_j, x_k)$ is then given by

$$q_0^{\setminus i}(x_j, x_k) \propto P^{\setminus i}(x_k \,|\, x_j) e^{-F_{Bethe}(x_j)}.$$

The approximate cavity distribution $Q_0^{\setminus i}$ is then simply the product of all approximated pair marginals:

$$Q^{\setminus i}(x_{\partial i}) \propto \prod_{\substack{\{j,k\} \\ j,k \in \partial i}} q_0^{\setminus i}(x_j, x_k) \tag{12}$$

This procedure is quadratic in cavity size. However, the update equations are still exponential in the cavity size.

Algorithm 1 LCBP update algorithm (parallel updates)

```
$t \leftarrow 0$
repeat
    for all $i, j \in \mathcal{V}$ s.t. $i, j \in I$ for some $I \in \mathcal{F}$ do
        $Q_{t+1}^{\setminus j} \propto Q_t^{\setminus j} \frac{\sum_{x_{\partial i}} Q_t^{\setminus i} \; \Psi_i^{\setminus I}}{\sum_{x_{\Delta j \setminus i}} Q_t^{\setminus j} \; \Psi_j^{\setminus I}}$
    end for
    $t \leftarrow t + 1$
until convergence
```

As a side note, one can show that by simply taking completely factorized initial cavity distributions (i.e. $Q_0^{\setminus i}(x_{\partial i}) \propto \prod_{j \in \partial i} q_j^{\setminus i}(x_j)$ for arbitrary $q_j^{\setminus i}$), fixed points of BP are fixed points of Algorithm 1 (see [Mooij and Kappen, 2006] for a detailed proof). Thus LCBP can indeed be regarded as a loop correction scheme for the Bethe approximation.

2.6 EXACTNESS IN CASE OF ONE LOOP

It was shown in [Montanari and Rizzo, 2005] that the method proposed there is exact if the graphical model contains only one loop, possibly attached to treelike structures. Using a similar argument, we can show that a similar result holds for our alternative method. Suppose the graphical model contains exactly one loop. Consider first the case that i is part of the loop; removing i will break the loop and the remaining cavity graph will be singly connected, hence the cavity distribution calculated by BP will be exact. On the other hand, if i is not part of the loop, removing i will divide the network into several connected components, one for each neighbor of i; this implies that the cavity distribution calculated by BP contains no higher order interactions, i.e. $Q_0^{\setminus i}$ is exact modulo single node interactions. Hence, after running the LCBP update algorithm, all cavity distributions will be exact, which obviously implies that the final single node marginals will be exact.

3 EXPERIMENTS

We have performed numerical experiments to compare the quality of the results and the computation time of the following approximate inference methods:

BP Standard BP, using the recently proposed update scheme [Elidan et al., 2006], which converges also for difficult problems without damping.

CVM-Δ A double-loop implementation [Heskes et al., 2003] of CVM using the sets $\{\Delta i\}_{i \in \mathcal{V}}$ as outer clusters.[6]

CVM-4 A double-loop implementation of CVM using as outer clusters all factors together with all loops in the factor graph that consist of up to 4 different variables.

TreeEP TreeEP [Minka and Qi, 2004], without damping.

LCBP-CUM The original cumulant-based loop correction scheme described in [Montanari and Rizzo, 2005]. Response propagation (i.e. linear response) is used to approximate the initial second-order cavity cumulants; the update equations are the exact equations with the assumption that cumulants of order higher than two are zero.

LCBP LCBP with cavities initialized as in (11).

LCBP-PAIR LCBP with cavities initialized as in (12).

To be able to assess the errors of the various approximate methods, we limited ourselves to problems for which exact inference (using a standard junction tree method) was still feasible.

For each approximate inference method, we have calculated the maximum error in the approximate single node marginals q_i as follows:

$$\max_{i \in \mathcal{V}} \max_{x_i \in \mathcal{X}_i} |q_i(x_i) - p_i(x_i)| \tag{13}$$

where $p_i(x_i) = P(x_i)$ is the exact marginal.[7]

The computation time was measured as CPU time in seconds on a 2.4 GHz AMD Opteron 64bits processor with 4 GB memory. The timings should be seen as indicative, as we have only optimized BP. The implementations of the other approximate inference can still be optimized for speed, which may alter the timings reported here by some constant depending on the method.[8]

We have studied three different model classes: (i) random graphs with fixed degree $d = 5$ and binary variables; (ii) periodic square grids with binary variables; (iii) the ALARM network. For more extensive numerical experiments, see also Mooij and Kappen [2006].

3.1 RANDOM REGULAR GRAPHS WITH BINARY VARIABLES

We have compared various approximate inference methods on random graphs with fixed degree $|\partial i| = 5$ with ± 1-valued variables. Random graphs are special in the sense that the number of short loops is relatively small. As single node factors we took $\psi_i(x_i) = \exp(\theta_i x_i)$ for i.i.d. weights θ_i drawn from a $\mathcal{N}(0, \beta)$ distribution. For the pairwise factors we took $\psi_{ij}(x_i, x_j) = \exp(J_{ij} x_i x_j)$ for i.i.d. weights J_{ij}, also drawn from a $\mathcal{N}(0, \beta)$ distribution. The parameter β controls the strength of the interactions and the difficulty of the inference problem.

Figure 2 shows the results for $\beta = 0.5$. BP is the fastest method (taking less than 0.01 s for almost all N) but is not very accurate. CVM-Δ performs remarkably bad, being the slowest and the least accurate method of all. This is remarkable, since one would expect that it should at least improve on BP because it uses larger clusters. It shows that although both LCBP and CVM-Δ use identical clusters, the nature of both approximations is very different.[9] TreeEP is more accurate than BP but still very efficient in terms of computation time. LCBP is the most accurate method and its improvement upon BP is often more than one order of magnitude. The quality of the LCBP-PAIR, LCBP-CUM, CVM-4 and TreeEP results does not differ substantially in this case. For $N \geq 70$, the tree size became so large that exact inference was infeasible, whereas the approximate methods can still be used for larger N.

Figure 3 shows the results for higher interaction strengths $\beta = 0.8$. The picture largely remains the same, with the notable difference that in this case, LCBP-CUM does not converge for the majority of instances. LCBP-PAIR and LCBP have no convergence problems; LCBP is still the most accurate method.

For weaker interaction strengths (not shown), the relative improvement of LCBP over TreeEP and BP increases.

[6] We have used a double-loop implementation of CVM instead of GBP because the former is guaranteed to convergence to a local minimum of the Kikuchi free energy [Heskes et al., 2003], whereas the latter often only would converge with strong damping, where the required damping constant is not known *a priori*.

[7] We have considered other error measures as well (average maximum single node error, maximum and average Kullback-Leibler divergence). We do not report these results here because of space constraints and because the choice of error measure does not affect our conclusions. Furthermore, by use of Scheffe's theorem, the ℓ_1 norm can be used to obtain bounds on the probabilities of events.

[8] Our C++ implementations of the various algorithms are released as free/open source software, licensed under the GNU Public License, at `http://www.mbfys.ru.nl/~jorism/libDAI/`

[9] Indeed, the similarity between LCBP and CVM-Δ is only superficial: CVM tries to estimate the dependencies in a cluster as the algorithm runs, instead of in a preprocessing phase, and CVM passes multi-variable messages, while LCBP passes single-variable messages.

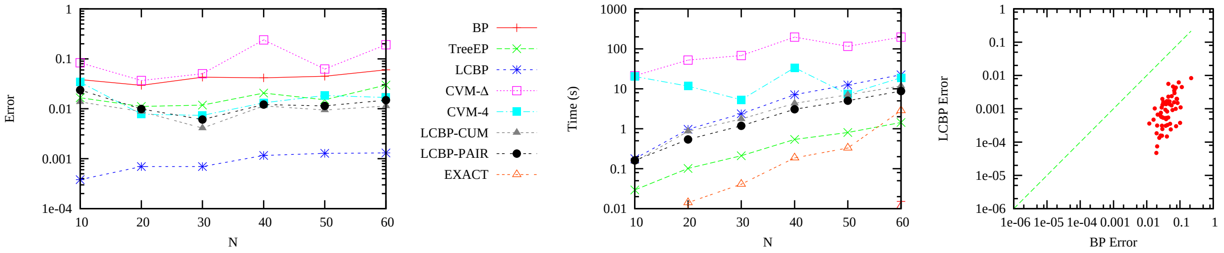


Figure 2: Errors and computation times for random graphs with degree 5 and interaction strength $\beta = 0.5$. Left: errors of single node marginals vs. graph size. Middle: computation time vs. graph size. Right: LCBP error vs. BP error. Each point in the left and middle plots is an average (in the log-domain) over 10 randomly generated instances.

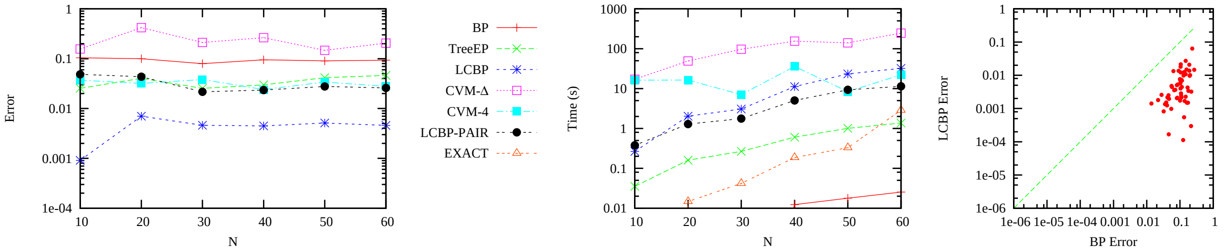


Figure 3: Similar setup as in Figure 2, now with higher interaction strength $\beta = 0.8$. LCBP-CUM did not converge within 10000 iterations in the majority of the cases and is therefore not plotted, whereas all other methods converged in all cases.

3.2 PERIODIC SQUARE GRIDS

The next class of models are periodic square grids (i.e. square grids on a torus) with binary variables. These models have many short loops, making them difficult problems for approximate inference. The special topology of these graphical models allows for a natural choice of the outer clusters for CVM, namely 2×2 plaquettes. Thus in addition to CVM-Δ (which in this case uses +-shaped clusters consisting of 5 variables), we compare with CVM-4, a double-loop implementation of CVM using the 2×2 plaquettes. We took the same kind of interactions as for the random graphs.

The results can be found in Figure 4. CVM-Δ was so slow that we did not consider it. As for random graphs, the fastest method is BP, and TreeEP improves significantly on BP using little computation time. Again LCBP uses more computation time but improves the accuracy even more. The CVM-4 method shows a surprising behavior: its accuracy improves as the grids get larger, and for large grids it is the most accurate of all methods that were considered. Note that the tree width quickly increases with N and for $N = 121$ computation time for exact inference already exceeds that of the slowest approximate inference methods. Note that LCBP uses less computation time than CVM-4, although for larger N the difference becomes smaller.

3.3 ALARM NETWORK

The ALARM network[10] is a well-known Bayesian network consisting of 37 variables and higher order factors. In addition to the usual approximate inference methods, we have compared with GBP, using maximal factors as outer clusters. The results are reported in Table 1. Apart from the error measure (13) ("Max MAD"), we also report the average maximum absolute deviation of the single node marginals ("Avg MAD").

The accuracy of GBP is almost identical to that of BP on this model. Again we see that simply enlarging the cluster size (CVM-Δ) does not improve the results, it even makes them worse. CVM-4, which uses clusters that contain small loops, does lead to an improvement, but needs much time to converge. TreeEP is very fast and obtains a comparable improvement. LCBP-PAIR also obtains a similar improvement, using more time than TreeEP but less than CVM-4. LCBP takes even longer but obtains an impressive improvement: the error is reduced by a factor of about 400. LCBP-CUM is not applicable because the network contains variables with more than two possible values and factors consisting of more than two variables.

[10] `http://compbio.cs.huji.ac.il/Repository/Datasets/alarm/alarm.dsc`

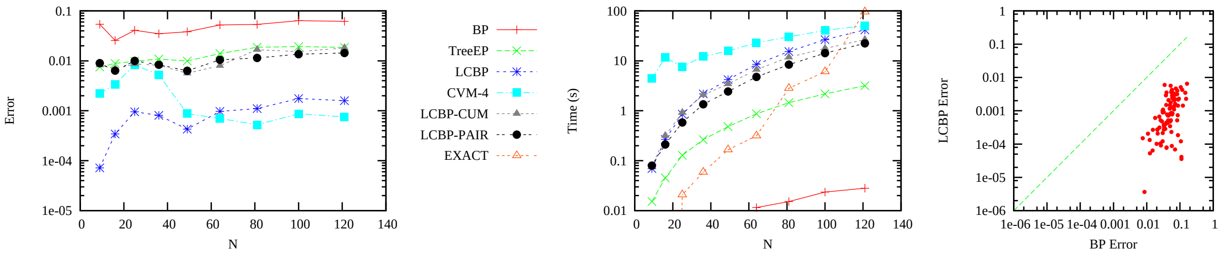


Figure 4: Periodic square grids, $\beta = 0.6$. Left: errors of single node marginals vs. graph size. Middle: computation time vs. graph size. Right: LCBP error vs. BP error. Each point in the left and middle plots is an average (in the log-domain) over 10 randomly generated instances.

4 DISCUSSION AND CONCLUSIONS

We have proposed a method for improving BP that corrects for the influence of all the loops in the factor graph, which is a variation of the one proposed in [Montanari and Rizzo, 2005]. We have shown that it can significantly outperform other approximate inference methods in terms of accuracy. On the downside, the computation time is rather high and application is limited to graphical models with small cavities. Further we have shown that simply increasing the cluster size in CVM (GBP) does not guarantee better results. In fact, often the results were even worse than for the simplest cluster choice (i.e. the outer clusters being the maximal factors, which coincides with BP in case of pairwise factors). Because LCBP and CVM-Δ use identical clusters, one might think naïvely that both approximation method will behave similarly; however, as we have shown, this is not the case, and the nature of both approximations appears to be completely different.

For all instances that we considered, LCBP gave significantly smaller marginal errors than both BP and TreeEP. Only for grids we encountered an approximate inference method that appears to be structurally better than LCBP (at least for large N). Here, CVM with 2×2 plaquettes outperforms LCBP. A possible explanation may be that in this case the shortest and most important loops are included in an outer cluster each (although this does not explain why the error is larger for smaller grids).

Table 1: ALARM Network Results

Method	Max MAD	Avg MAD	Time (s)
BP	0.203	0.0081	0.00
GBP	0.203	0.0076	0.18
CVM-Δ	0.223	0.074	296.0
CVM-4	0.035	0.0064	161.0
TreeEP	0.039	0.0109	0.22
LCBP	0.00054	0.000015	23.4
LCBP-PAIR	0.033	0.0009	13.2
LCBP-CUM	n/a	n/a	n/a

The most important difference between the method proposed here and the original one in [Montanari and Rizzo, 2005] is that we assume that the cavity distributions contain no higher order *interactions* (i.e. interactions involving more than two cavity variables), whereas the original proposal is to assume that higher order *cumulants* vanish. Both approaches are identical to first order in the corrections $\phi_j^{\setminus i}(x_j)$. However, the cumulant-based formulation has several disadvantages. First, it is difficult to work with in practice, because it leads to rather complicated expressions. Further, it is not obvious how to generalize it beyond the binary, pairwise case, although this should be possible in principle. Finally, the approximation of vanishing higher order cumulants turns out to break down in the regime of strong interactions, whereas our interaction-based approximation still works in that regime.

There still appears to be room for improvement of the LCBP method as formulated here. In particular, various alternatives to the LCBP update equations (line 4 of Algorithm 1) are possible and can give even better results. As an example, consider altered update equations in which the connecting factor ψ_I is *not* divided out (equivalent to demanding consistency of single node marginals for the original, unmodified, probability distribution (1)). This does not significantly alter the results for weak, pairwise factors, but appears to be more robust if the factors are stronger. On the other hand, in the presence of factors involving more than two variables, this alternative approach leads to significantly worse results. This observation suggests the possible existence of update equations in the same spirit as line 4 in Algorithm 1, but which give better results in general.[11]

[11] Another update equation that gives better results in the case of interactions involving more than two variables is considered in [Mooij and Kappen, 2006].

Another important direction for future research would be to extend and generalize the loop correction framework (e.g. by considering other clusters than cavities) in order to find different tradeoffs between computation time and accuracy. In particular, the fact that computation time is exponential in the cavity size limits applicability of the current method.

Finally, many approximate inference methods (Mean Field, BP, GBP, EP) can be derived by minimizing an appropriate "free energy" (e.g. BP can be derived from the Bethe free energy). It is thus natural to expect that the method presented here can also be derived from an appropriate free energy. However, despite some efforts, we have not yet been able to find such a free energy. Furthermore, we have not yet found an expression for the loop corrected approximation of the normalization constant Z in (1) within this framework.

Concluding, the LCBP method proposed in this work appears to be ideally suited to compute with high accuracy single node marginals for graphical models having small cavities, especially when the graph has "long" loops which cannot easily be taken into account exactly using CVM or other region-based methods. On these graphical models, the quality of the results turned out to be superior to the other approximate inference methods we compared with. For large graphs, where exact inference can become intractable, LCBP may provide a viable alternative (provided the cavities are small) that in our experience often gives highly accurate results.

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