Fixed Points of Belief Propagation – An Analysis via Polynomial Homotopy Continuation

Christian Knoll, Student Member, IEEE, Dhagash Mehta, Tianran Chen, and Franz Pernkopf, Senior Member, IEEE

Abstract—Belief propagation (BP) is an iterative method to perform approximate inference on arbitrary graphical models. Whether BP converges and if the solution is a unique fixed point depends on both, the structure and the parametrization of the model. To understand this dependence it is interesting to find all fixed points. In this work, we formulate a set of polynomial equations, the solutions of which correspond to BP fixed points.

To solve such a nonlinear system we present the numerical polynomial-homotopy-continuation (NPHC) method. Experiments on binary Ising models show how our method is capable of obtaining all BP fixed points. We further asses the accuracy of the corresponding marginals and compare them to the exact marginal distribution. Contrary to the conjecture that uniqueness of BP fixed points implies convergence, we find graphs for which BP fails to converge, even though a unique fixed point exists. Moreover, we show that this fixed point gives a good approximation, and the NPHC method is able to obtain this fixed point.

Index Terms—Graphical models, belief propagation, probabilistic inference, sum-product algorithm, Bethe free energy, phase transitions, machine learning, inference algorithms, nonlinear equations.

1 INTRODUCTION

Joint distributions over many random variables (RVs) are often modeled as probabilistic graphical models. Belief propagation (BP) is a prominent tool to determine marginal distributions of such models. On tree-structured models the marginals are exact, while BP provides only an approximation on graphs with loops. Despite the lack of guarantee for convergence, BP has been successfully used for models with many loops, including applications in computer vision, medical diagnosis systems, and speech processing [1], [2], [3]. However, instances of graphs do exist where BP fails to converge. A deeper understanding of the reasons for convergence of BP, and whether and how its non-convergence relates to the number of fixed points may therefore be crucial in understanding BP.

A precise relation among the uniqueness of fixed points, convergence rate, and accuracy is yet to be theoretically understood [4]. Sufficient conditions for uniqueness of fixed points were refined by accounting for both, the potentials as well as the structure of the model [4], [5]. On graphs with a single loop [6] and on small grid graphs [7] accuracy and convergence rate are related; this does, however, not necessarily hold for all graphs. As a consequence using provably convergent variants of BP can still lead to accurate approximations [8], [9]. Changing the BP update schedule can also help to achieve convergence [10], [11], [12]. One can further increase the accuracy of BP by taking not just a single, but multiple fixed points into account [4]. Survey propagation [13] and its efficient approximation scheme [14] represent distributions over BP messages and marginalize over all obtained fixed points.

In this work we are interested in the relation among convergence properties, the number of fixed points, and the accuracy of these fixed points. To get deeper insights into the behavior of BP we aim to find all fixed points – including unstable ones. If BP converges, however, it does only provide a single fixed point. Therefore, in order to find all fixed points, we reformulate the update rules of BP as a system of polynomial equations.

There are indeed several methods to solve such a system of polynomial equations. Numerical solvers (e.g., Newton’s method) are well established, but their ability in obtaining the solutions strongly depends on the initial point. Moreover, such methods only find a single solution at a time, and do not guarantee to find all solutions even with different initial guesses. Symbolic methods, on the other hand, are guaranteed to find all solutions. The Gröbner basis method [15], [16] is widely used, but it is inefficient if the system has irrational coefficients and it suffers from fast growing run time and memory complexity. Moreover the method has a limited scalability in parallel computation. In this paper, we present the numerical polynomial homotopy continuation (NPHC) method [17], [18] that overcomes all the above mentioned problems of both iterative and symbolic methods, yet guarantees to find all solutions of the system. Over the last few decades, this class of methods has been proven to be robust, efficient, and highly parallelizable. We exploit the sparsity of our polynomial system and compute a tight upper bound on the number of complex solutions. This is an essential step to reduce the computational complexity by

• Christian Knoll (christian.knoll@ieee.org) and Franz Pernkopf (pernkopf@tugraz.at) are with the Signal Processing and Speech Communication Laboratory, Graz University of Technology.

• Dhagash Mehta (Dhagash.B.Mehta.13@nd.edu) is with the Department of Applied and Computational Mathematics and Statistics, University of Notre Dame.

• Tianran Chen (ti@nranchen.org) is with the Department of Mathematics and Computer Science, Auburn University at Montgomery.
orders of magnitude so that the systems tackled in this work become tractable.

We apply the NPHC method to different realizations of the Ising model on complete and grid graphs, although it can be used for any other graph structure. These models are appealing because they are well studied in the physics literature, so that we can validate our observations. On these graphs we obtain all BP fixed points and show how the number of fixed points changes at critical regions (i.e., phase transitions) in the parameter space. We further use the obtained fixed points to estimate the approximation of the marginal distribution which we compare to the exact marginal distribution. Our main (empirical) observations are: (i) on loopy graphs BP does not necessarily converge to the best possible fixed point, (ii) on some graphs where BP does not converge we are able to show that there is a unique fixed point, and (iii) if we enforce convergence to this unique fixed point the obtained marginals still give a good approximation.

The paper is structured as follows: Section 2 provides a brief background on probabilistic graphical models and free energy approximations. In Section 3, we reformulate the message passing equations, and introduce the NPHC method that guarantees to find all BP fixed point solutions. Our experimental results are presented and discussed in Section 4. Finally, we conclude the paper in Section 5.

2 Background

In this section, we briefly introduce probabilistic graphical models and the BP algorithm, and fix our notations. For an in-depth treatment of these topics we refer the reader to [3, 21, 22].

2.1 Probabilistic Graphical Models

We consider a finite set of \( N \) discrete random variables \( X = \{X_1, \ldots, X_N\} \) taking values from the binary alphabet \( x_i \in \mathbb{B} = \{-1, +1\} \). Let us consider the joint distribution \( P(X) = \mathbb{P}(X) \) corresponding to the set of nodes and \( E \) is the set of edges. Between the RVs and the nodes a one-to-one correspondence holds. An interaction between two nodes \( X_i \) and \( X_j \), \( i \neq j \) is represented by an undirected edge \( e_{i,j} \in E \). The set of neighbors of \( X_i \) be defined by \( \partial(X_i) = \{X_j \in X \setminus X_i : e_{i,j} \in E\} \). The joint probability of an undirected graphical model is

\[
P(X = x) = \frac{1}{Z} \prod_{i,j} \Phi_{C_{ij}}(C_{ij}),
\]

where \( \Phi_{C_{ij}} \) are specified over the cliques \( C_{ij} \) of the nodes [11, p.105]. If we restrict all the potentials to consist of at most two variables: then, the joint distribution is factorized according to the normalized product

\[
P(X = x) = \frac{1}{Z} \prod_{i,j} \Phi_{X_i,X_j}(x_i, x_j) \prod_{i=1}^{N} \Phi_{X_i}(x_i).
\]

The first product runs over all edges and the second product runs over all nodes; pairwise potentials and local evidence

1. A complete graph is an undirected graph where each pair of nodes is connected by an edge. A grid graph, or lattice graph, has all edges aligned along the 2D square lattice. Examples are depicted in Fig. 2.

2.2 Belief Propagation

Belief propagation (BP) is an algorithm that approximates marginal probabilities (or beliefs) \( \hat{P}(X_i = x_i) \). The marginals are approximated by recursively updating messages between random variables. This update rule is guaranteed toconverge and return the exact marginals on graphs without loops. Note that such a procedure has been discovered in different fields independently: belief propagation for probabilistic reasoning [11], the sum-product-algorithm in information theory [23, 24], and the Bethe-Peierls approximation in statistical mechanics [20].

The messages from \( X_i \) to \( X_j \) of state \( x_j \) at iteration \( n+1 \) are given by the following update rule:

\[
\mu_{i,j}^{n+1}(x_j) = \alpha_{i,j}^{n} \Phi_{X_i,X_j}(x_i, x_j) \Phi_{X_i}(x_i) \prod_{X_k \in \partial(X_i)} \mu_{k,i}^n(x_i),
\]

where \( \Gamma_{i,j} = \partial(X_i) \setminus \{X_j\} \). Loosely speaking BP collects all messages sent to \( X_i \), except for \( X_j \), and multiplies this product with the local potential \( \Phi_{X_i}(x_i) \) and the pairwise potential \( \Phi_{X_i,X_j}(x_i, x_j) \). The sum over both states of \( X_i \) is sent to \( X_j \). In practice the messages are often normalized by \( \alpha_{i,j}^n \) so as to sum to one.

Lemma 1. Messages being sent from node \( X_i \) to \( X_j, i \neq j \), represent probabilities – provided all messages are initialized to be positive.

Proof. Positive potentials in (2) guarantee that all messages remain positive at every iteration. Consequently, a normalization term \( \alpha_{i,j}^n \) exists so that \( \sum_{x_j \in \mathbb{B}} \mu_{i,j}^{n+1}(x_j) = 1 \). □

The set of all messages at iteration \( n \) is given by \( \mu^n = \{\mu_{i,j}^n(x_j) : e_{i,j} \in E\} \). In a similar manner we collect all normalization terms in \( \alpha^n \). Let the mapping of all messages induced by (2) be denoted as \( \mu^{n+1} = BP[\mu^n] \). If all successive messages show the same value (up to some predefined precision), that is \( \mu^n \approx \mu^{n+1} \), then BP is converged. We refer to converged messages and the associated normalization terms as fixed points \( (\mu^*, \alpha^*) \).

Note that at least one fixed point always exists if all potentials are positive. Existence of fixed points, however, is not sufficient to guarantee convergence; in fact BP may be trapped in limit cycles or show chaotic behavior. Finally, if BP converges to a fixed point, then the marginals are approximated by the normalized product

\[
\hat{P}(X_i = x_i) = \frac{1}{Z_i} \Phi_{X_i}(x_i) \prod_{X_k \in \partial(X_i)} \mu_{k,i}^*(x_i),
\]

where \( Z_i \in \mathbb{R}^+ \) is required so that \( \sum_{x_i} \hat{P}(X_i = x_i) = 1 \).
2.3 Free Energy Approximations

Over the years a fruitful connection between computer science and statistical mechanics was established (cf. [20, 28, 29, 30]). In particular, the relationship between stationary points of the Bethe free energy $\mathcal{F}_B$ and fixed points of BP led to a deeper understanding of BP. We briefly discuss important insights and present differences in notations to circumvent any confusions.

In the Ising model, a popular statistical mechanics model, often used for evaluation of BP, each node $X_i$ has an associated spin taking values in $\mathbb{S} = \{-1, +1\}$. We define the corresponding energy function [20, p.44] by assigning a coupling $J_{i,j} \in \mathbb{R}$ to each edge $e_{i,j} \in E$ and some local field $\theta_i \in \mathbb{R}$ acting on each node $X_i \in \mathbb{X}$. Note that we will drop the subscripts of $J_{i,j}$ and $\theta_i$ whenever they are constant for all edges and nodes. Let the local and pairwise Ising potentials of state $x_i$ be $\Phi_{X_i}(x_i) = \exp(\theta_i x_i)$ and $\Phi_{X_i, X_j}(x_i, x_j) = \exp(J_{i,j} x_i x_j)$. Then by plugging these potentials into (1) the joint distribution is equal to the Boltzmann distribution

$$P(X = x) = \frac{1}{Z} \exp \left( \beta \sum_{(i,j): x_i \neq x_j \in E} J_{i,j} x_i x_j + \sum_{i=1}^N \theta_i x_i \right). \quad (4)$$

We omit the term of the inverse temperature $\beta$ by choosing $\beta = 1$ for the rest of this work.

If the Ising model is not on a path graph, critical regions in the parameter space can exist where phase transitions occur [19, Ch.12]. If all nodes $X_i \in \mathbb{X}$ have equal degree $|\partial(X_i)| = d + 1$, phase transitions can be determined by replacing the graph with a Cayley tree of degree $d$ [31]. Therefore let

$$p(J, d) = \begin{cases} d \arctan \frac{d - 1/w - 1}{d - w} & \text{if } J > \arctanh(d) \\ d \arctan \frac{d - 1/w - 1}{d - w} & \text{if } J < \arctanh(d) \end{cases} \quad (5)$$

where $w = \tanh |J|$. Also, in accordance with [31] and [19, p.247-255], let the phase transitions partition the parameter space $(J, \theta)$ into the following three distinct regions $(I), (II), (III)$:

$$(J, \theta) \in (I) \quad \text{if } J > 0, J > p(J, d) \quad \text{and } |\theta| \leq p(J, d), \quad (6)$$

$$(J, \theta) \in (II) \quad \text{if } J < 0, J < -p(J, d) \quad \text{and } |\theta| < p(J, d), \quad (7)$$

$$(J, \theta) \in (III) \quad \text{if } (J, \theta) \notin (I) \quad \text{and } (J, \theta) \notin (II). \quad (8)$$

In the literature one distinguishes three different interactions on Ising grids. First, if all couplings $J > 0$ the model is ferromagnetic: for ferromagnetic models BP converges to a unique stationary point inside (III). This stationary point becomes unstable and two additional stationary points emerge inside (I) [20, 24]. Second, if all couplings $J < 0$ the model is antiferromagnetic: here, BP only converges inside (III) and not inside (II) [32]. Finally, spin glasses are models containing both positive and negative couplings.

Depending on the graph structure spin glasses and antiferromagnetic models allow for frustrations; i.e., the marginals minimizing the Bethe free energy may correspond to a degenerate joint distribution [27, 20, pp.45].

It turns out that instead of performing BP, one can minimize $\mathcal{F}_B$ to find stationary points directly. $\mathcal{F}_B$ is a convex function for tree-structured graphs and one-loop graphs [5]. For general graphs, however, convexity breaks down and $\mathcal{F}_B$ has multiple local minima. Energy functions with many local minima can be decomposed into a convex and a concave problem (this decomposition is in general not unique) [9]. Alternatively one can construct convex surrogates and minimize these convex functions instead [33].

Sufficient conditions for convexity of $\mathcal{F}_B$ are often used to make statements regarding uniqueness of BP fixed point solutions. This seems to be a rather limiting point of view – it is possible to add loops to a former tree-structured model without changing the distribution [51, pp.2391]. Hence, the number of BP fixed points does not only depend on the structure of the graph but also depends on the potentials.

3 Solving BP Fixed Point Equations

We reformulate the message update rules (2) as a system of polynomial equations whose solutions are the fixed points of BP. Whether such systems can be solved in practice depends largely on the chosen method. We list a variety of approaches and describe NPHC that can be applied in practice to obtain all BP fixed points.

3.1 Reformulation of Belief Propagation

For all messages $\mu_{i,j}(x_j) : e_{i,j} \in E$ the residual, i.e., the difference between two successive message values $\mu_{n+1}^i - \mu_n^i$ and the message normalization constraints $\mu_n^i$ are given by the following system of polynomial equations:

$$\mathbf{F}(\mu, \alpha) =$$

$$\begin{align*}
-\mu_{\bar{i,j}}^i(x_j) + \alpha_{x_j}^i \sum_{x_i \in \mathbb{X}} \Phi_{X_i, X_j}(x_i, x_j) \Phi_{X_i}(x_i) & \prod_{X_k \in \Gamma_{i,j}} \mu_{\bar{k,i}}^i(x_i) \\
-\mu_{\bar{i,j}}^j(x_i) + \alpha_{x_i}^j \sum_{x_j \in \mathbb{X}} \Phi_{X_i, X_j}(x_i, x_j) \Phi_{X_j}(x_j) & \prod_{X_k \in \Gamma_{i,j}} \mu_{\bar{k,j}}^j(x_j) \\
\mu_{\alpha}^i(x_j) + \mu_{\alpha}^j(x_i) & - 1.
\end{align*} \quad (9)$$

This system of polynomial equations consist of

$$M = (2|E| \cdot (|S| + 1) \quad (10)$$

equations $(f_1(\mu, \alpha), \ldots, f_M(\mu, \alpha))$. To solve such a polynomial system, it is advantageous to consider it defined over complex variables rather than real variables, in order to apply the NPHC method. Let the set of solutions over complex variables, without accounting for multiplicity, be

$$V(\mathbf{F}) = \{ (\mu, \alpha) \in \mathbb{C} : f_m(\mu, \alpha) = 0 \quad \forall f_m \in \mathbf{F}(\mu, \alpha) \}. \quad (11)$$

We further define the set of solutions $V_{\mathbb{R}^+}(\mathbf{F}) \subset V(\mathbf{F})$ over strictly positive real numbers.

**Theorem 1 (Fixed Points of BP).** Let $(\mu, \alpha)$ be some set of messages and normalization terms. Then, $(\mu, \alpha)$ is a fixed point solution of BP, if and only if $(\mu, \alpha) \in V_{\mathbb{R}^+}(\mathbf{F})$.  

2. A Cayley tree is an infinite tree without loops that captures interactions of a cyclic finite size graph.
Proof. First we show that \( (\mu, \alpha) \in V^*_{\mathbb{R}}(F) \) is sufficient to characterize fixed point solutions. All messages are positive and represent probabilities (Lemma 1). Further, it follows from (9) that \( BP(\mu^\alpha) = \mu^\alpha \), which constitutes a fixed point solution (cf. Section 3).

Conversely, consider some fixed point messages and the corresponding normalization coefficients \( (\mu^\alpha, \mu^*) \), then it follows by definition that \( BP(\mu^*) = \mu^* \) and consequently \( F(\mu, \alpha) = 0 \).

Corollary 1.1. Consider a graph with strictly positive potentials. Then, the solution set \( V^*_{\mathbb{R}}(F) \) is nonempty. Moreover, if \( \Phi_{X_i, X_j} \) and \( \Phi_{X_i} \) are Ising potentials, then \( V^*_{\mathbb{R}}(F) \) is always nonempty.

Proof. For non-negative potentials the average energy is bounded from below and \( \mathbb{F}_B \) has at least one minimum [26, Th. 4]. Minima of the constrained \( \mathbb{F}_B \) correspond to BP fixed point solutions, the existence of which implies non-emptiness of \( V^*_{\mathbb{R}}(F) \) by Theorem 1.

3.2 Solving Systems of Polynomial Equations

Solving systems of (nonlinear) polynomial equations is a classic problem in computational mathematics, and a great variety of approaches have been developed such as iterative solvers, symbolic methods, and homotopy methods.

One basic method for solving systems of nonlinear equations is Newton’s method which is an iterative solver that progressively refines an initial guess to reach a solution. Such iterative solvers find a single solution in the vicinity of an already known initial guess. However, when the initial guess is not sufficiently close to a solution, they may diverge or even exhibit chaotic behavior. Moreover, it is difficult, to obtain the full set of solutions with these methods. Consequently they are not useful in the current setting since we are interested in the entire set of (positive) real solution \( V^*_{\mathbb{R}}(F) \).

From a completely different point of view, the symbolic methods [15] (e.g. Gröbner basis method, Wu’s method, and methods of sparse resultant) rely on symbolic manipulation of the equations and successive elimination of variables to obtain a simpler but equivalent form of the equations. In a sense, these methods can be considered as various generalizations of the Gaussian elimination method for linear systems into nonlinear settings. In the past several decades, symbolic methods, especially the Gröbner basis method, has seen substantial development. Still it has a worst case complexity that is double exponential in the variables [34], [35]. This and the limited scalability in parallel computation limits the application of symbolic methods to smaller systems.

3.3 Numerical Polynomial Homotopy Continuation

Another important approach for solving a system of nonlinear equations is the numerical polynomial homotopy continuation (NPHC) method [17], [18]. The “target” system \( F(\mu, \alpha) \) in (9), which we intend to solve, is continuously deformed into a closely related “starting system” \( Q(\mu, \alpha) = (q_1(\mu, \alpha), \ldots, q_M(\mu, \alpha)) \) that is trivial to solve. With an appropriate construction, the corresponding solutions also vary continuously under this deformation forming “solution paths” that connect the solutions of the trivial system to the desired solutions of the target system.

For instance, a basic form of linear homotopy for the target system can be given by

\[
H(\mu, \alpha, t) = (1-t)Q(\mu, \alpha) + tF(\mu, \alpha) = 0.
\]

Clearly, at \( t = 0 \) the homotopy reduces to the starting system \( Q(\mu, \alpha) \) and at \( t = 1 \) it reduces to \( F(\mu, \alpha) \). As \( t \) varies continuously from \( t = 0 \) to \( t = 1 \), the homotopy represents a deformation from the starting system to the target system. For a generic complex \( \gamma \), the above procedure is guaranteed to find all isolated complex solutions of \( F(\mu, \alpha) \) [18, pp.91].

Even though only positive real solutions \( V^*_{\mathbb{R}}(F) \) are of interest in the current study, the homotopy method benefits from extending the domain to the field of complex numbers. Only then smooth solution paths emerge towards the desired solutions. Each of these solution paths can be tracked independently making this approach being pleasantly parallelizable; this is essential in dealing with large polynomial systems.

3.4 Polyhedral Homotopy

More advanced “nonlinear” homotopies can be constructed where the parameter \( t \) appears in nonlinear form. Among a great variety of polynomial homotopy constructions, the polyhedral homotopy method, developed by B. Huber and B. Sturmfels [35], is particularly suited for the present study as it is capable of finding all isolated nonzero complex solutions, which must include all BP fixed points \( V^*_{\mathbb{R}}(F) \). This advantage and the level of parallel scalability are the main motivation for applying the polyhedral homotopy method.

In applying the NPHC method to solve (9), the choice of \( Q(\mu, \alpha) \) (the trivial system of equations that the target system is deformed into) plays an important role in the overall efficiency of the approach since different choices may induce a vastly different number of solution paths one has to track. The crucial part is to come up with a good upper bound on the number of solutions and to create an appropriate start system. Once this is solved, every solution can be tracked completely independently in parallel in order to reach all desired solutions.

In our experiments, we observed that despite the rather high total degree \( d_t \) [18, pp.118], the number of solution paths to be tracked to solve (9) is relatively small. The number of solution paths one has to track when using the polyhedral homotopy method for solving a system of polynomial equations is given by the so-called BKK bound: fixing the list of monomials that appear in the polynomial system, it is an important yet surprising fact in algebraic

3. Here, “nonzero complex solutions” refer to complex solutions of a system of polynomial equations where each variable is nonzero. A solution is considered to be isolated if it has no degree of freedom, i.e., there is an open set containing it but no other solutions.

4. The total degree of a system of polynomial equations is the product of the degrees of each equation. It is a basic fact in algebraic geometry that the total number of isolated complex solutions a polynomial system has is bounded by its total degree (i.e., Bezout bound). Therefore the total degree serves as a crude measure of the complexity of the polynomial system.
Fig. 1: (a) Number of fixed points (yellow: unique fixed point, red: three fixed points). (b) Number of real solutions, including negative ones. The increase in number of both, real solutions and positive real solutions, indicates a phase transition.

Fig. 2: Structure of Ising graphs considered: (a) grid graph with 9 RVs; (b) fully connected graph.

We apply (3) to the positive real solutions to obtain the marginals and compare them with marginals obtained by an implementation of BP without damping [44], we further compare these results with the exact marginals obtained by the junction tree algorithm [45]. Combining properly weighted marginals can lead to accuracy improvements [13, 14]. We do not follow this path, because we apply the NPHC method in order to rigorously analyze the individual fixed points of BP.

4.1 Grid Graph with Random Factors (Spin Glass)
Consider a grid graph of size $N = 3 \times 3$ (Fig. 2a) with randomly distributed potentials. All pairwise and local potentials are sampled uniformly; i.e., $(J_{i,j}, \theta_i) \sim \mathcal{U}(-K, K)$. The larger the support of the uniform distribution is, the more difficult the task of inference becomes. For $K = 3$ inference is sufficiently difficult (cf. [12]).

According to (10) the system of equations consists of $M = 72$ equations and 72 unknowns. More specifically, (9) consists of 24 linear (i.e., normalization constraints), 40 quadratic, and 8 cubic equations; the total degree bounds the number of solutions by $d = 12^4 \cdot 2^{10} \cdot 3^8 \approx 7.2 \cdot 10^{15}$. Tracking such an amount of solution paths is not feasible in practice, even with a parallel implementation of the NPHC method. The system of equations in (9), however, is very sparse. We can exploit this sparsity that is induced by the graph structure if we consider the BKK bound and reduce the computational complexity. The number of complex solutions for this graph is bounded by $BKK = 608$. After creating a suitable start system the problem is straightforward to solve with the NPHC method. It actually turns out that the BKK bound is tight for all graphs considered.

In particular we evaluated 100 grid graphs with random factors: on 99 graphs BP converged after at most $10^4$ iterations. Although the grid graph has multiple loops and the constrained $F_B$ is not convex [5 Corr.2], we observe that all 100 graphs have a unique positive real solution corresponding to a unique BP fixed point.

4.2 Grid Graph with Uniform Factors
We further analyze the convergence properties of BP on grid graphs of size $N = 3 \times 3$ (Fig. 2a) with constant potentials...
among all nodes and edges; i.e., for all edges \( J_{i,j} = J \) and for all nodes \( \theta_i = \theta \). We apply BP and NPHC for 1681 graphs in the parameter region \( (J, \theta) \in \{-2, -1.9, \ldots, 1.9, 2\} \).

The number of solutions in \( V_{\mathcal{G}_d}(\mathbf{F}) \) is presented in Fig. 3a. In the well-behaved region of the parameter space (III) a unique fixed point exists, whereas 3 fixed points exist in (I) and (II) — this is in accordance with statistical mechanics [20, p.43]. Interestingly, we observe a close relation between the onset of phase transitions and the increase in the number of real solutions in Fig. 4. Most of these solutions, however, correspond to negative message values which violate the first axiom of probability (moreover, by Lemma 1 negative message values are not feasible).

BP converges to some fixed point on all 1681 graphs within at most \( 10^4 \) iterations. This raises the question: what is the approximation error of BP if it converges to the best possible fixed point? Or, speaking in terms of free energies, how large is the gap between the global minimum of the constrained \( \mathcal{F}_B \) and the Gibbs free energy? To answer this question we evaluate the correctness of the approximated marginals, averaging the mean squared error (MSE) of all fixed points (yellow: unique fixed point, red: three fixed points).

Looking at all parameter regions separately we can see that BP does converge to the global optimum in (III), as well as in (I). In the antiferromagnetic region (II) BP converges to a fixed point that does not necessarily give the best possible approximation.

### 4.3 Fully Connected Graph with Uniform Factors

We consider a fully connected Ising model with \( |X| = 4 \) binary RVs (Fig. 2b). Among all four nodes we apply uniform factors \( J_{i,j} = J \) and \( \theta_i = \theta \). This type of graph is particularly interesting because one can derive exact conditions where phase transitions occur (cf. Section 2.3). For \((J, \theta) \in (III)\) BP has a unique fixed point, which is a stable attractor in the whole message space [32]. In (I) three fixed points satisfy (9), two of which are symmetric, i.e., \( \tilde{P}_1(\mathbf{X} = \mathbf{x}) = \tilde{P}_2(\mathbf{X} = \tilde{\mathbf{x}}) \). BP converges to one of these fixed points. In the antiferromagnetic case BP does only converge inside (III) and not inside (II) (Fig. 3b). We can see two interesting effects: first in Fig. 4 the number of real solutions increases at the onset of phase transitions; secondly, even though BP does not converge, a unique fixed point exists inside (II) (Fig. 3b).

We further assess the accuracy of the marginals obtained by NPHC and BP; averaged over all graphs, and for each distinct region (Table 2). Indeed, inside region (II) the marginals obtained by NPHC give much better approximations than BP does.

### TABLE 1: MSE OF THE MARGINALS OBTAINED BY BP AND NPHC FOR THE GRID GRAPH WITH UNIFORM FACTORS

| Couplings | Local Field | BP   | NPHC |
|-----------|------------|------|------|
| \( J \in [-2, 2] \) | \( \theta \in [-2, 2] \) | 0.197 | 0.016 |
| \( J \in (I) \) | \( \theta \in (I) \) | 0.010 | 0.010 |
| \( J \in (II) \) | \( \theta \in (II) \) | 0.836 | 0.050 |
| \( J \in (III) \) | \( \theta \in (III) \) | 0.006 | 0.006 |

Note that the graph under consideration is of finite size and thus \( |\theta(\mathbf{X}_i)| \) varies among the nodes. As a consequence the partitioning according to [6] - [8] are only approximations.
One key feature of our framework is to come up with a favorable upper bound on the number of solutions. In particular the BKK bound utilizes the sparsity of the polynomial system induced by the graph structure and is tight in all our experiments. Finally, to obtain all fixed points, we create an appropriate start system and track all solution paths in parallel. On fully connected graphs and grid graphs with binary Ising factors we empirically show an accuracy-gap between fixed points of BP and the best fixed points obtained by NPHC. In practice this justifies the exploration of multiple fixed points and selecting one that leads to the best approximation of the marginals. We further show how the number of fixed points evolves over a large parameter region. When applied to graphs where BP does not converge, the NPHC method reveals that for some cases a unique fixed point does exist – consequently, uniqueness of BP fixed points is by no means sufficient to guarantee convergence of BP. While, in practice, fixed points have to be positive, we empirically showed that there is a close relation between the occurrence of phase transitions and an increase in the number of real solutions. One requirement of NPHC to be efficient is a tight upper bound on the number of solutions. The determination of this bound limits our current investigations to relatively small graphs. In future we aim to exploit the graph structure in order to reduce the complexity of identifying an upper bound on the number of solutions.

ACKNOWLEDGMENTS

Research supported in part by NSF under Grant DMS 11-15587. This work was supported by the Austrian Science Fund (FWF) under the project number P28070-N33.

REFERENCES

[1] J. Pearl, Probabilistic Reasoning in Intelligent Systems: Networks of Plausible Inference.
[2] D. Batra, P. Yadollahpour, A. Guzman-Rivera, and G. Shakhnarovich, “Diverse m-best solutions in markov random fields,” in Computer Vision—ECCV 2012. Springer, 2012, pp. 1–16.
[3] F. Pernkopf, R. Peharz, and S. Tschiatschek, Introduction to Probabilistic Graphical Models. Academic Press Library in Signal Processing, 2014.
[4] J. Mooij and H. Kappen, “Sufficient conditions for convergence of the sum–product algorithm,” IEEE Trans. on Information Theory, vol. 53, no. 12, pp. 4422–4437, 2007.
[5] T. Heskes, “On the uniqueness of loopy belief propagation fixed points,” Neural Comp., vol. 16, no. 11, 2004.
[6] Y. Weiss, “Correctness of local probability propagation in graphical models with loops,” Neural Comp., vol. 12, no. 1, 2000.
[7] A. Ihler, “Accuracy bounds for belief propagation,” in Proceedings of UAI, Jul. 2007, pp. 183–190.
[8] K. Murphy, Y. Weiss, and M. Jordan, “Loopy belief propagation for approximate inference: An empirical study,” in Proceedings of UAI, 1999, pp. 467–475.
[9] A. Yuille and A. Rangarajan, “The concave-convex procedure,” Neural Comp., vol. 15, no. 4, pp. 915–936, 2003.
[10] G. Elidan, I. McGraw, and D. Koller, “Residual belief propagation: Informed scheduling for asynchronous message passing,” in Proceedings of UAI, 2006.
[11] C. Knoll, M. Rath, S. Tschiatschek, and F. Pernkopf, “Message scheduling methods for belief propagation,” in Machine Learning and Knowledge Discovery in Databases. Springer, 2015, pp. 295–310.
[12] C. Sutton and A. McCallum, “Improved dynamic schedules for belief propagation,” in Proceedings of UAI, 2007.
[13] A. Braunstein, M. Mezard, and R. Zecchina, “Survey propagation: An algorithm for satisfiability,” Random Structures & Algorithms, vol. 27, no. 2, pp. 201–226, 2005.
[14] C. Srinivasa, S. Ravanbakhsh, and B. Frey, “Survey propagation beyond constraint satisfaction problems,” in Proceedings of the 19th International Conference on Artificial Intelligence and Statistics (AISTATS), 2016, pp. 286–295.
[15] D. Cox, J. Little, and D. O’Shea, Ideals, Varieties, and Algorithms. Springer, 1992, vol. 3.
[16] ——. Using Algebraic Geometry. Springer Science & Business Media, 2005, vol. 185.
[17] T. Li, “Solving polynomial systems by the homotopy continuation method,” Handbook of numerical analysis, vol. 11, pp. 209–304, 2003.
[18] A. Sommese and C. Wampler, The Numerical Solution of Systems of Polynomials Arising in Engineering and Science. World Scientific, 2005, vol. 99.
[19] H. Georgii, Gibbs Measures and Phase Transitions, 2011, vol. 9.
[20] M. Mezard and A. Montanari, Information, Physics, and Computation. Oxford Univ. Press, 2009.
[21] D. Koller and N. Friedman, Probabilistic Graphical Models: Principles and Techniques. MIT press, 2009.
[22] M. Jordan, “Graphical models,” Statistical Science, pp. 140–155, 2004.
[23] R. Gallager, Information Theory and Reliable Communication. Springer, 1968, vol. 2.
[24] F. Kschischang, B. Frey, and H. Loeliger, “Factor graphs and the sum-product algorithm,” IEEE Trans. on Information Theory, vol. 47, no. 2, pp. 498–519, 2001.
[25] A. Ihler, J. Fisher, and A. Willsky, “Loopy belief propagation: Convergence and effects of message errors,” in Journal of Machine Learning Research, 2005, pp. 905–936.
[26] J. Yedidia, W. Freeman, and Y. Weiss, “Constructing free-energy approximations and generalized belief propagation algorithms,” IEEE Trans. on Information Theory, vol. 51, no. 7, 2005, pp. 2282–2312.
[27] D. MacKay, “A conversation about the Bethe free energy and sum-product,” Tech. Rep. of MRL, 2001.
[28] M. Welling and Y. Teh, “Approximate inference in boltzmann machines,” Artificial Intelligence, vol. 143, no. 1, pp. 19–50, 2003.
[29] S. C. Tatikonda and M. I. Jordan, “Loopy belief propagation and gibbs measures,” in Proceedings of UAI, 2002, pp. 493–500.
[30] A. Weller and T. Jebara, “Approximating the bethe partition function,” in Proceedings of UAI, 2014.
[31] N. Taga and S. Mase, “On the convergence of belief propagation algorithm for stochastic networks with loops,” Citeseer, 2004.
[32] J. Mooij and H. Kappen, “On the properties of the Bethe approximation and loopy belief propagation on binary networks,” Journal of Statistical Mechanics: Theory and Experiment, vol. 2005, no. 11, p. P11012, 2005.
[33] O. Meshi, A. Jaimovich, A. Globerson, and N. Friedman, “Converifying the Bethe free energy,” in Proceedings of UAI, 2009, pp. 402–410.
[34] E. Mayr and A. Meyer, “The complexity of the word problems for commutative semigroups and polynomial ideals,” Advances in mathematics, vol. 46, no. 3, pp. 305–329, 1982.
[35] H. Möller and F. Mora, “Upper and lower bounds for the degree of Gröbner bases,” EUROSAM 84, pp. 172–183, 1984.

TABLE 2: MSE OF THE MARGINALS OBTAINED BY BP AND NPHC FOR THE FULLY CONNECTED GRAPH

| Couplings | Local Field | BP | NPHC |
|-----------|-------------|----|------|
| $J \in [-2, 2]$ | $\theta \in [-2, 2]$ | 0.069 | 0.007 |
| $J \in (I)$ | $\theta \in (I)$ | 0.034 | 0.033 |
| $J \in (II)$ | $\theta \in (II)$ | 0.304 | 0.004 |
| $J \in (III)$ | $\theta \in (III)$ | 0.003 | 0.003 |
[36] B. Huber and B. Sturmfels, “A polyhedral method for solving sparse polynomial systems,” *Mathematics of computation*, vol. 64, no. 212, pp. 1541–1555, 1995.

[37] D. Bernstein, “The number of roots of a system of equations,” *Funkts. Anal. Pril.*, vol. 9, pp. 1–4, 1975.

[38] A. Khovanski, “Newton polyhedra and the genus of complete intersections,” *Funkts. Anal. Pril.*, vol. 12, no. 1, pp. 51–61, 1978.

[39] A. Kushnirenko, “Newton polytopes and the bezout theorem,” *Funkts. Anal. Pril.*, vol. 10, no. 3, 1976.

[40] T.-Y. Li, “Numerical solution of multivariate polynomial systems by homotopy continuation methods,” *Acta numerica*, vol. 6, pp. 399–436, 1997.

[41] T. Chen, T. Lee, and T. Li, “Hom4ps-3: a parallel numerical solver for systems of polynomial equations based on polyhedral homotopy continuation methods,” in *Mathematical Software–ICMS 2014*. Springer, 2014, pp. 183–190.

[42] T. Chen and D. Mehta, “On the network topology dependent solution count of the algebraic load flow equations,” *arXiv preprint arXiv:1512.04987*, 2015.

[43] T. Chen, D. Mehta, and M. Niemerg, “A network topology dependent upper bound on the number of equilibria of the kuramoto model,” *arXiv preprint arXiv:1603.05905*, 2016.

[44] J. Mooij, “libdai: A free and open source c++ library for discrete approximate inference in graphical models,” *The Journal of Machine Learning Research*, vol. 11, 2010.

[45] S. Lauritzen and D. Spiegelhalter, “Local computations with probabilities on graphical structures and their application to expert systems,” *Journal of the Royal Statistical Society. Series B*, pp. 157–224, 1988.