Convergence Rates of Smooth Message Passing with Rounding in Entropy-Regularized MAP Inference

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Abstract

Maximum a posteriori (MAP) inference is a fundamental computational paradigm for statistical inference. In the setting of graphical models, MAP inference entails solving a combinatorial optimization problem to find the most likely configuration of the discretevalued model. Linear programming (LP) relaxations in the Sherali-Adams hierarchy are widely used to attempt to solve this problem, and smooth message passing algorithms have been proposed to solve regularized versions of these LPs with great success. This paper leverages recent work in entropy-regularized LPs to analyze convergence rates of a class of edge-based smooth message passing algorithms to ϵ -optimality in the relaxation. With an appropriately chosen regularization constant, we present a theoretical guarantee on the number of iterations sufficient to recover the true integral MAP solution when the LP is tight and the solution is unique.

1 INTRODUCTION

Undirected graphical models are a central modeling formalism in machine learning, providing a compact and powerful way to model dependencies between variables. Here we focus on the important class of discrete-valued pairwise models. Inference in discrete-valued graphical models has applications in many areas including computer vision, statistical physics, information theory, and genome research (Antonucci et al., 2014; Mezard and Montanari, 2009; Wainwright and Jordan, 2008).

We focus on the problem of identifying a configuration of all variables that has highest probability, termed maximum a posteriori (MAP) inference. This problem has an extensive literature across multiple communities, where it is described by various names, including energy minimization (Kappes et al., 2013) and constraint satisfaction (Schiex et al., 1995). In the binary case, the MAP problem is sometimes described as quadraticpseudo Boolean optimization (Hammer et al., 1984) and it is known to be NP-hard to compute exactly (Cooper, 1990; Kolmogorov and Zabin, 2004) or even to approximate (Dagum and Luby, 1993). Consequently, much work has attempted to identify settings where polynomial-time methods are feasible. We call such settings "tractable" and the methods "efficient." A general framework for obtaining tractable methodology involves "relaxation"—the MAP problem is formulated as an integer linear program (ILP) and is then relaxed to a linear program (LP). If the vertex at which the LP achieves optimality is integral, then it provides an exact solution to the original problem. In this case we say that the LP is tight. If the LP is performed over the convex hull of all integral assignments, otherwise known as the marginal polytope \mathcal{M} , then it will always be tight. Inference over the marginal polytope is generally intractable because it requires exponentially many constraints to enforce global consistency.

A popular workaround is to relax the marginal polytope to the local polytope \mathbb{L}_2 (Wainwright and Jordan, 2008). Instead of enforcing global consistency, the local polytope enforces consistency only over pairs of variables, thus yielding pseudo-marginals which are pairwise consistent but may not correspond to any true global distribution. The number of constraints needed to specify the local polytope is linear in the number of edges. More generally, Sherali and Adams (1990) introduced a series of successively tighter relaxations of the marginal polytope, or convex hull, while retaining control on the number of constraints. However, even with these relaxations, it has been observed that standard LP solvers do not scale well (Yanover et al., 2006), motivating the study of solvers that exploit the structure of the problem, such as message passing algorithms.

Of particular interest to this paper are smooth mes-

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sage passing algorithms, i.e. algorithms derived from regularized versions of the relaxed LP (Hazan and Shashua, 2008; Meshi et al., 2012; Ravikumar et al., 2010; Savchynskyy et al., 2011, 2012). These regularized LPs conduce to efficient optimization in practice and have the special property that their fixed points are unique and optimal; however, this comes at the cost of solving an approximation of the true MAP problem and, without rounding, they do not recover integral solutions in general. Non-asymptotic convergence rates to the optimal regularized function value have been studied (Meshi et al., 2012), but guarantees on the number of iterations sufficient to recover the optimal integral assignment of the true MAP problem have not been considered to our knowledge.

In this work we provide a sharp analysis of the entropy-regularized MAP inference problem with Sherali-Adams relaxations. We first characterize the approximation error of the regularized LP in l_1 distance, based on new results on entropy-regularized LPs (Weed, 2018). We then analyze an edge-based smooth message passing algorithm, modified from the algorithms described in Werner (2007) and Ravikumar et al. (2010). We prove a $O(1/\epsilon^2)$ rate of convergence of iterates in l_1 distance. Combining the approximation error and convergence results, we present a guarantee on the number of iterations sufficient to recover of the true integral MAP assignment using a standard vertex rounding scheme when the LP relaxation is tight and the solution is unique.

2 RELATED WORK

The idea of entropy regularization to aid optimization in inference problems is well studied. It is well known that solving a scaled and entropy-regularized linear program over the marginal polytope yields the scaled Gibbs free energy, intimately related to the log partition function, when the temperature parameter equals one (Wainwright and Jordan, 2008). As the temperature parameter is driven to zero, the calculation of the free energy reduces to the value of the MAP problem. However, this problem is intractable due to the difficulty of both computing the exact entropy and characterizing the marginal polytope (Deza and Laurent, 2009). Therefore, there has been much work in trying to turn this observation into tractable inference algorithms. The standard Bethe approximation instead minimizes an approximation of the true entropy (Bethe, 1935). It was show by Yedidia et al. (2003) that fixed points of the loopy belief propagation correspond to its stationary points, but still the optimization problem resulting from this approximation is non-convex and convergence is not always guaranteed.

To alleviate convergence issues, much work has considered convexifying the free energy problem leading to classes of convergent convex belief propagation often derived directly from convex regularizers (Hazan and Shashua, 2008; Heskes, 2006; Johnson and Willsky, 2008; Meshi et al., 2009; Savchynskyy et al., 2012). For instance, Weiss et al. (2007) proposed a general convexified belief propagation and explored some sufficient conditions that enable heuristically recovering the MAP solution of the LP via a convex sum-product variant. However, the approximation error was still unclear and non-asymptotic convergence rates were not considered. A number of algorithms have also been proposed to directly optimize the unregularized LP relaxation often with only asymptotic convergence guarantees such as block-coordinate methods (Globerson and Jaakkola, 2008; Kappes et al., 2013; Kovalevsky and Koval, 1975; Tourani et al., 2018; Werner, 2007) and tree-reweighted message passing (Kolmogorov, 2006; Wainwright et al., 2005). The relationship between the regularized and unregularized problems can equivalently be viewed as applying a soft-max to the dual objective typically considered in the latter to recover that of the former (Nesterov, 2005; Sontag et al., 2011). Many other convergent methods exist such as augmented Lagrangian (Martins et al., 2011; Meshi and Globerson, 2011), bundle (Kappes et al., 2012), and steepest descent (Schwing et al., 2012, 2014) approaches, but again they are difficult to compare without rates.

Most closely related to our work is recent work in convergence analysis of certain smoothed message passing algorithms that aim to solve the regularized LP objective. Savchynskyy et al. (2011) proposed an accelerated gradient method that achieves $O(1/\epsilon)$ convergence to the optimal regularized dual objective value. Convergence of the primal iterates was only shown asymptotically. Meshi et al. (2012) considered a general dual coordinate minimization algorithm based on the entropy-regularized MAP objective. They proved upper bounds on the rate of convergence to the optimal regularized dual objective value; however, closeness to the true MAP assignment was not formally characterized. Furthermore, convergence in the dual objective value again does not make it easy to determine when the true MAP assignment can be recovered. Meshi et al. (2015) later studied the benefits of adding a quadratic term to the LP objective instead and proved similar guarantees. Ravikumar et al. (2010) also considered entropic and quadratic regularization, using a proximal minimization scheme with inner and outer loops. They additionally provided rounding guarantees to recover true primal solutions. However, as noted by the authors, the inexact calculation of the inner loop prevents a convergence rate analysis once combined with the outer loop. Additionally, rates on the inner

loop convergence were not addressed.

The approach of this paper can be understood as the bridging the gap between Meshi et al. (2012) and Ravikumar et al. (2010). Our first contribution is a characterization of the approximation error of the entropy-regularized MAP inference problem. We then study an edge-based message passing algorithm that solves the regularized LP, which is essentially a smoothed max-sum diffusion (Werner, 2007) or the inner loop of the proximal steps of Ravikumar et al. (2010). For our main contribution, we provide non-asymptotic guarantees to the integral MAP assignment for this message passing algorithm when the LP is tight and the solution is unique. To our knowledge, this is the first analysis with rates guaranteeing recovery of the true MAP assignment for smooth methods.

3 BACKGROUND

We denote the d-dimensional probability simplex as $\begin{array}{l} \Sigma_d \stackrel{\mathrm{def.}}{=} \left\{ p \in \mathbb{R}_+^d : \sum_i p_i = 1 \right\}. \quad \text{The set of joint distributions which give rise to } p,q \in \Sigma_d \text{ is defined as } \mathcal{U}_d(p,q) \stackrel{\mathrm{def.}}{=} \left\{ P \in \mathbb{R}_+^{d \times d} : P\mathbb{1} = p, \ P^\top \mathbb{1} = q \right\}. \ \text{For} \end{array}$ any two vectors or matrices p and q having the same number of elements, we use $\langle p, q \rangle$ to denote the dot product, i.e. elementwise multiplication then sum over all elements. We use $||p||_1$ to denote the sum of absolute values of the elements of p. The Bregman divergence between $p, q \in \mathbb{R}^d_+$ with respect to a strictly convex function $\Phi: \mathbb{R}^d_+ \mapsto \mathbb{R}$ is $\mathcal{D}_{\Phi}(p,q) \stackrel{\text{def.}}{=} \Phi(p) - \Phi(q) - \langle \nabla \Phi(q), p - q \rangle$. We will consider the Bregman divergence with respect to the negative entropy $\Phi(p) = -H(p) \stackrel{\text{def.}}{=} \sum_{i} p_i (\log p_i - 1)$, where p need not be a distribution. When p is a distribution, this corresponds to the Kullback-Leibler (KL) divergence. The Bregman projection with respect to Φ of $q \in \mathbb{R}^d_{\perp}$ onto the set \mathcal{X} is defined as $\mathcal{P}_{\mathcal{X}}(q) \stackrel{\text{def.}}{=} \arg\min_{p \in \mathcal{X}} \mathcal{D}_{\Phi}(p,q)$. The Hellinger distance between $p,q \in \Sigma_n$ is defined as $h(p,q) \stackrel{\text{def.}}{=} \frac{1}{\sqrt{2}} \|\sqrt{p} - \sqrt{q}\|_2$, where $\|\cdot\|_2$ is the l_2 -norm. We denote the square of the Hellinger distance by $h^2(p,q)$. We will often deal with marginal vectors which are ordered collections of joint and marginal distributions in the form of matrices and vectors, respectively.

3.1 Pairwise Models

For a set of vertices, $\mathcal{V} = \{1, \dots, n\}$, and edges \mathcal{E} , a pairwise graphical model, $\mathcal{G} \stackrel{\text{def.}}{=} \{\mathcal{V}, \mathcal{E}\}$, is a Markov random field that represents the joint distribution of variables $X_{\mathcal{V}} \stackrel{\text{def.}}{=} (X_i)_{i \in \mathcal{V}}$, taking on values from the set of states $\chi = \{0, \dots, d-1\}$. We assume that each vertex has at least one edge.

For pairwise models, the joint distribution can be written as a function of doubletons and singletons: $p_{\theta}(x_{\mathcal{V}}) \propto \exp\left(\sum_{i \in \mathcal{V}} \theta_i(x_i) + \sum_{ij \in \mathcal{E}} \theta_{ij}(x_i, x_j)\right)$. We wish to find maximum a posteriori (MAP) estimates of this model. That is, we consider the integer program:

$$\max_{x_{\mathcal{V}} \in \chi^n} \sum_{i \in \mathcal{V}} \theta_i(x_i) + \sum_{i j \in \mathcal{E}} \theta_{ij}(x_i, x_j).$$
 (Int)

The maximization in (Int) can be written as a linear program by defining a marginal vector $\boldsymbol{\mu}$ over variable vertices $\{\boldsymbol{\mu}_i\}_{i\in\mathcal{V}}$ and variable edges $\{\boldsymbol{\mu}_{ij}\}_{ij\in\mathcal{E}}$. The vector $\boldsymbol{\mu}_i \in \mathbb{R}_+^d$ represents the marginal distribution probabilities on vertex i while the matrix $\boldsymbol{\mu}_{ij} \in \mathbb{R}_+^{d\times d}$ represents the joint distribution probabilities shared between vertices i and j. We follow the notation of Globerson and Jaakkola (2008) and denote indexing into the vector and matrix variables with parentheses, e.g. $\boldsymbol{\mu}_{ij}(x_i, x_j)$ for $x_i, x_j \in \chi$. The set of marginal vectors that are valid probability distributions is known as the marginal polytope and is defined as

$$\mathcal{M} \stackrel{\text{def.}}{=} \left\{ \boldsymbol{\mu} : \exists \mathbb{P}, \begin{array}{l} \mathbb{P}_{X_i}(x_i) = \boldsymbol{\mu}_i(x_i), \ \forall i, x_i \\ \mathbb{P}_{X_i, X_j}(x_i, x_j) = \boldsymbol{\mu}_{ij}(x_i, x_j), \\ \forall ij, x_i, x_j \end{array} \right\} (1)$$

We can think of \mathcal{M} as the set of mean parameters of the model for which there exists a globally consistent distribution \mathbb{P} . We abuse notation slightly and dually view θ as a potential "vector." The edge matrix $\theta_{ij} \in \mathbb{R}^{d \times d}$ is indexed as $\theta_{ij}(x_i, x_j)$, indicating the element at the x_i th row and x_j th column. The vertex vector θ_i is indexed as $\theta_i(x_i)$, indicating the x_i th element. The MAP problem in (Int) can be shown to be equivalent to the following LP (Wainwright and Jordan, 2008):

$$\max \langle \theta, \boldsymbol{\mu} \rangle \quad \text{s.t.} \quad \boldsymbol{\mu} \in \mathcal{M}$$
where $\langle \theta, \boldsymbol{\mu} \rangle = \sum_{i \in \mathcal{V}} \sum_{x_i} \theta_i(x_i) \boldsymbol{\mu}_i(x_i) + \sum_{ij \in \mathcal{E}} \sum_{x_i, x_j} \theta_{ij}(x_i, x_j) \boldsymbol{\mu}_{ij}(x_i, x_j).$

3.2 Sherali-Adams Relaxations

The number of constraints in \mathcal{M} is unfortunately superpolynomial (Sontag, 2010). This motivates considering relaxations of the marginal polytope to outer polytopes that involve fewer constraints. For example, the *local outer polytope* is obtained by enforcing consistency only on edges and vertices:

$$\mathbb{L}_{2} \stackrel{\text{def.}}{=} \left\{ \boldsymbol{\mu} \geq 0 : \begin{array}{cc} \boldsymbol{\mu}_{i} \in \Sigma_{d} & \forall i \in \mathcal{V} \\ \boldsymbol{\mu}_{ij} \in \mathcal{U}_{d}(\boldsymbol{\mu}_{i}, \boldsymbol{\mu}_{j}) & \forall ij \in \mathcal{E} \end{array} \right\} (2)$$

Relaxations of higher orders have also been studied, in particular by Sherali and Adams (1990) who introduced a hierarchy of polytopes by enforcing consistency on joint distributions of increasing order up to n: $\mathbb{L}_2 \supseteq \mathbb{L}_3 \supseteq \ldots \supseteq \mathbb{L}_n \equiv \mathcal{M}$. The corresponding Sherali-Adams LP relaxation of order m is then

$$\max \langle \theta, \boldsymbol{\mu} \rangle \quad \text{s.t.} \quad \boldsymbol{\mu} \in \mathbb{L}_m, \quad \text{(LP)}$$

where $1 \leq m \leq n$. Because \mathbb{L}_m is an outer polytope of \mathcal{M} , we no longer have that the solution to (LP) recovers the true MAP solution of (Int) in general. However if the solution to (LP) is integral, then $x_i = \arg\max_x \boldsymbol{\mu}_i(x)$ recovers the optimal solution of the true MAP problem. In this case, we say \mathbb{L}_m is tight.

4 ENTROPY-REGULARIZED MAP

In this section, we present our first main technical contribution, characterizing the approximation error in the entropy-regularized MAP problem for Sherali-Adams relaxations. In contrast to solving the exact (LP), we aim to solve the entropy-regularized LP:

min
$$\langle C, \boldsymbol{\mu} \rangle - \frac{1}{\eta} H(\boldsymbol{\mu})$$
 s.t. $\boldsymbol{\mu} \in \mathbb{L}_m$, (Reg)

where $C \stackrel{\text{def.}}{=} -\theta$ and $H(\mu) = \langle \mu, -\log \mu + 1 \rangle$. The hyperparameter η adjusts the level of regularization. Denote by μ_{η}^* the solution of (Reg) where we omit the reference to m to alleviate notation. In addition to their extensive history in inference problems, entropy-regularized LPs have arisen in a number of other fields to aid optimization when standard LP solvers are insufficient. For example, recent work in optimal transport has relied on entropy regularization to derive alternating projection algorithms (Benamou et al., 2015; Cuturi, 2013) which admit almost linear time convergence guarantees in the size of the cost matrix (Altschuler et al., 2017). Some of our theoretical results draw inspiration from these works.

4.1 Approximation Error

When \mathbb{L}_m is *tight* and the solution is unique, we show that approximate solutions from solving (Reg) are not necessarily detrimental because we can apply standard vertex rounding schemes to yield consistent integral solutions. It was shown by Cominetti and San Martín (1994), and later refined by Weed (2018), that the approximation error of general entropy-regularized linear programs converges to zero at an exponential rate in η . Furthermore, it is possible to determine how large η should be chosen in order for rounding to exactly recover the optimal solution to (Int). The result is summarized in the following extension of Theorem 1 of Weed (2018)¹.

Theorem 1. Let $\mathcal{R}_1 = \max_{\boldsymbol{\mu} \in \mathbb{L}_m} \|\boldsymbol{\mu}\|_1$, $\mathcal{R}_H = \max_{\boldsymbol{\mu}, \boldsymbol{\mu}' \in \mathbb{L}_m} H(\boldsymbol{\mu}) - H(\boldsymbol{\mu}')$, \mathcal{V}_m be the set of vertices of \mathbb{L}_m , and $\mathcal{V}_m^* \subseteq \mathcal{V}_m$ the set of optimal vertices with respect to C. Let $\Delta = \min_{V_1 \in \mathcal{V}_m \setminus \mathcal{V}_m^*, V_2 \in \mathcal{V}_m^*} \langle C, V_1 \rangle$ –

 $\langle C, V_2 \rangle$ be the smallest gap in objective value between an optimal vertex and any suboptimal vertex of \mathbb{L}_m . Suppose \mathbb{L}_m is tight and $|\mathcal{V}_m^*| = 1$. If $\eta \geq \frac{2\mathcal{R}_1 \log 64\mathcal{R}_1 + 2\mathcal{R}_1 + 2\mathcal{R}_H}{\Delta}$, the following rounded solution is a MAP assignment:

$$\left(\operatorname{round}(\boldsymbol{\mu}_{\eta}^*)\right)_i := \underset{x \in \chi}{\operatorname{arg\,max}}(\boldsymbol{\mu}_{\eta}^*)_i(x)$$

Proof. Define $\widetilde{C}=C+\mathbf{1}\frac{1}{\eta}$, where $\mathbf{1}$ denotes an all-ones vector with the same dimensions as C. If $\eta\geq\frac{4\mathcal{R}_1}{\Delta}$ then $\widetilde{\mathcal{V}}_m^*$, the set of optimal vertices of \mathbb{L}_m with respect to \widetilde{C} , satisfies $\widetilde{\mathcal{V}}_m^*=\mathcal{V}_m^*$ and $\min_{V_1\in\mathcal{V}_m\backslash\widetilde{\mathcal{V}}_m^*,V_2\in\widetilde{\mathcal{V}}_m^*}\langle C,V_1\rangle-\langle C,V_2\rangle\geq\frac{\Delta}{2}$. If $V\in\widetilde{\mathcal{V}}_m^*$; and $V'\in\mathcal{V}_m\backslash\widetilde{\mathcal{V}}_m^*$, then $\langle\widetilde{C},V'\rangle-\langle\widetilde{C},V\rangle\geq\Delta-\frac{1}{\eta}\|V'-V\|_1\geq\frac{\Delta}{2}$. Let $\widetilde{\Delta}=\frac{\Delta}{2}$. If $\eta\geq\frac{\mathcal{R}_1\log 64\mathcal{R}_1+\mathcal{R}_1+\mathcal{R}_H}{\widetilde{\Delta}}$, and $|\widetilde{\mathcal{V}}_m^*|=1$ then $2\mathcal{R}_1\exp\left(-\eta\frac{\widetilde{\Delta}}{\mathcal{R}_1}+\frac{\mathcal{R}_1+\mathcal{R}_H}{\mathcal{R}_1}\right)\leq\frac{1}{32}$. And therefore, by Corollary 9 of Weed (2018) $\min_{\boldsymbol{\mu}\in\mathcal{V}_m^*}\|\boldsymbol{\mu}-\boldsymbol{\mu}_\eta^*\|_1\leq\frac{1}{32}$. Since \mathbb{L}_m is assumed to be tight and $\widetilde{\mathcal{V}}_m^*=\mathcal{V}_m^*$ contains a single integral vertex $\boldsymbol{\mu}^*$, the last equation implies $\operatorname{round}(\boldsymbol{\mu}_\eta^*)=\boldsymbol{\mu}^*$.

Consequently, since $\mathcal{R}_1 \leq \sum_{j=1}^m \binom{n}{j} d^j$ and $\mathcal{R}_H \leq \sum_{j=1}^m \binom{n}{j} \log(d^j)^2$, we have:

Corollary 1. If \mathbb{L}_m is tight, $|\mathcal{V}_m^*| = 1$, and $\eta \geq \frac{\log(8mn^md^m) + 2mn^md^m}{\Delta}$, the rounded solution round($\boldsymbol{\mu}_{\eta}^*$) is a MAP assignment.

In general the dependence of Δ on η suggested by Theorem 1 is not improvable (Weed, 2018). Nevertheless, when m=2 and d=2, since all vertices in \mathcal{V}_2 have entries equal to either $0, \frac{1}{2}$ or 1—see Padberg (1989) or Theorem 3 of Weller et al. (2016)—if the entries of C are all integral, we have $\Delta \geq \frac{1}{2}$, thus yielding a more concrete guarantee. The disadvantage of choosing exorbitantly large η is that efficient computation of solutions often becomes more difficult in practice (Altschuler et al., 2017; Benamou et al., 2015; Weed, 2018). Thus, in practice, there exists a trade-off between computation time and approximation error that is controlled by η . We will provide a precise theoretical characterization of the trade-off in Section 6. In our guarantees, multiplying C by a constant a (and therefore multiplying Δ by a) is equivalent to multiplying η by the same value.

4.2 Equivalent Bregman Projection

The objective (Reg) can be interpreted as a Bregman projection. This interpretation has been explored by

 $^{^{1}}$ The entropy is defined without the linear offset in Weed (2018).

²For m = 2 we can get tighter bounds corresponding to the number of edges in the graph \mathcal{G} .

Ravikumar et al. (2010) as a basis for proximal updates and also Benamou et al. (2015) for the optimal transport problem. The objective is equivalent to

min
$$\mathcal{D}_{\Phi}(\boldsymbol{\mu}, \exp(-\eta C))$$
 s.t. $\boldsymbol{\mu} \in \mathbb{L}_m$, (Proj)

where $\Phi := -H$. The derivation, based on a mirror descent step can be found in the appendix. The projection, however, cannot be computed in closed form in general due to the complex geometry of \mathbb{L}_m .

Ravikumar et al. (2010) proposed using the Bregman method (Bregman, 1966), which has been applied in many fields to solve difficult constrained problems (Benamou et al., 2015; Goldstein and Osher, 2009; Osher et al., 2005, 2010), to compute $\mathcal{P}_{\mathbb{L}_m}(\exp(-\eta C))$ for the inner loop calculation of their proximal algorithm. While the outer loop proximal algorithm can be shown to converge at least linearly, the inner loop rate was not analyzed and the constants (possibly dependent on dimension) were not made clear. Furthermore, the Bregman method is in general inexact, which makes the approximation and the effect on the outer loop unclear (Liu and Ihler, 2013).

5 SMOOTH MESSAGE PASSING

We are interested in analyzing a class of algorithms closely inspired by max-sum diffusion (MSD) as presented by Werner (2007) and the proximal updates of Ravikumar et al. (2010) to solve (Proj) over the \mathbb{L}_2 polytope. We describe it in detail here, with a few minor modifications and variations to facilitate theoretical analysis. In \mathbb{L}_2 , the constraints occur only over edges between vertices³. Given an edge $ij \in \mathcal{E}$, we must enforce the constraints prescribed by (2), which is the intersection of the following sets:

(a)
$$\mathcal{X}_{ij\to i} = \{\boldsymbol{\mu} : \boldsymbol{\mu}_{ij}\mathbb{1} = \boldsymbol{\mu}_i\}$$

(b)
$$\mathcal{X}_{ii,i} = \{ \boldsymbol{\mu} : \boldsymbol{\mu}_i^\top \mathbb{1} = 1, \ \mathbb{1}^\top \boldsymbol{\mu}_{ii} \mathbb{1} = 1 \}$$

(c)
$$\mathcal{X}_{ij \to j} = \{ \boldsymbol{\mu} : \boldsymbol{\mu}_{ij}^{\top} \mathbb{1} = \boldsymbol{\mu}_{i} \}$$

(d)
$$\mathcal{X}_{ij,j} = \{ \boldsymbol{\mu} : \boldsymbol{\mu}_i^\top \mathbb{1} = 1, \ \mathbb{1}^\top \boldsymbol{\mu}_{ij} \mathbb{1} = 1 \}.$$

The normalization of the joint distribution μ_{ij} in (b) and (d) is actually a redundant constraint, but it facilitates analysis as we demonstrate in Section 6. For each of these affine constraints, we can compute the Bregman projections in closed form with simple multiplicative updates.

Proposition 1. For a given edge $ij \in \mathcal{E}$, the closed-form solutions of the Bregman projections for each of the above individual constraints are given below.

Algorithm 1 EMP-cyclic (C, η, ϵ)

```
1: \boldsymbol{\mu} \leftarrow \text{NORMALIZE}(\exp(-\eta C))
2: k \leftarrow 1
3: while \max_{ij} \left\{ \begin{array}{l} \max\{\|\boldsymbol{\mu}_{ij}^{(k)}\mathbb{1} - \boldsymbol{\mu}_{i}^{(k)}\|_{1}, \\ \|(\boldsymbol{\mu}_{ij}^{(k)})^{\top}\mathbb{1} - \boldsymbol{\mu}_{j}^{(k)}\|_{1} \end{array} \right\} \geq \epsilon \text{ do}
4: \boldsymbol{\mu} \leftarrow \boldsymbol{\mu}^{(k)}
5: for ij \in \mathcal{E} do
6: \boldsymbol{\mu} \leftarrow (\mathcal{P}_{\mathcal{X}_{ij,j}} \circ \mathcal{P}_{\mathcal{X}_{ij\to j}} \circ \mathcal{P}_{\mathcal{X}_{ij,i}} \circ \mathcal{P}_{\mathcal{X}_{ij\to i}})(\boldsymbol{\mu})
7: end for
8: \boldsymbol{\mu}^{(k+1)} \leftarrow \boldsymbol{\mu}
9: k \leftarrow k+1
10: end while
11: return ROUND(\boldsymbol{\mu}^{(k)})
```

Figure 1: The EMP-cyclic algorithm (Ravikumar et al., 2010) projects on all edges in order until the constraints are satisfied up to ϵ in l_1 distance. The operator \circ denotes the composition of the projection operations.

(a) Left consistency: If
$$\mu' = \mathcal{P}_{\mathcal{X}_{ij\to i}}(\mu)$$
, then for all $x_i, x_j \in \chi$, $\mu'_{ij}(x_i, x_j) \leftarrow \mu_{ij}(x_i, x_j) \sqrt{\frac{\mu_i(x_i)}{\sum_x \mu_{ij}(x_i, x)}}$ and $\mu'_i(x_i) \leftarrow \mu_i(x_i) \sqrt{\frac{\sum_x \mu_{ij}(x_i, x)}{\mu_i(x_i)}}$.

(b) Left normalization: If
$$\mu' = \mathcal{P}_{\mathcal{X}_{ij,i}}(\mu)$$
, then for all $x_i \in \chi$, $\mu'_i \leftarrow \frac{\mu_i}{\sum_x \mu_i(x)}$ and $\mu'_{ij} \leftarrow \frac{\mu_{ij}}{\sum_{x_i,x_j} \mu_{ij}(x_i,x_j)}$.

(c) Right consistency: If
$$\boldsymbol{\mu}' = \mathcal{P}_{\mathcal{X}_{ij\to j}}(\boldsymbol{\mu})$$
, then for all $x_i, x_j \in \chi$, $\boldsymbol{\mu}'_{ij}(x_i, x_j) \leftarrow \boldsymbol{\mu}_{ij}(x_i, x_j) \sqrt{\frac{\boldsymbol{\mu}_j(x_j)}{\sum_x \boldsymbol{\mu}_{ij}(x, x_j)}}$ and $\boldsymbol{\mu}'_j(x_j) \leftarrow \boldsymbol{\mu}_j(x_j) \sqrt{\frac{\sum_x \boldsymbol{\mu}_{ij}(x, x_j)}{\boldsymbol{\mu}_j(x_j)}}$.

(d) Right normalization: If
$$\mu' = \mathcal{P}_{\mathcal{X}_{ij,j}}(\mu)$$
, then for all $x_j \in \chi$, $\mu'_j \leftarrow \frac{\mu_j}{\sum_x \mu_j(x)}$ and $\mu'_{ij} \leftarrow \frac{\mu_{ij}}{\sum_{x_i,x_j} \mu_{ij}(x_i,x_j)}$.

These update rules are similar to a number of algorithms throughout the literature on LP relaxations. Notably, they can be viewed as a smoothed version of MSD (Kovalevsky and Koval, 1975; Werner, 2007) in that the updates enforce agreement between variables on the edges and vertices. Nearly identical smoothed updates were also initially proposed by Ravikumar et al. (2010). As in MSD, it is common for message passing schemes derived from LP relaxations to operate on dual objective instead. We presented the primal view here as the Bregman projections lend semantic meaning to the updates and ultimately the stopping conditions in the algorithms. An equivalent dual view is presented in Appendix C.1.

Based on these update rules, we formally outline the algorithms we wish to analyze, which we call *edge-based message passing* (EMP) for convenience. We

³Written explicitly, the constraints actually occur between any pair of vertices, but these variables play no role in the objective or constraints.

Algorithm 2 EMP-greedy (C, η, ϵ)

```
1: \boldsymbol{\mu} \leftarrow \text{NORMALIZE}(\exp(-\eta C))
2: k \leftarrow 1
3: while \max_{ij} \left\{ \begin{array}{l} \max\{\|\boldsymbol{\mu}_{ij}^{(k)}\mathbb{1} - \boldsymbol{\mu}_{i}^{(k)}\|_{1}, \\ \|(\boldsymbol{\mu}_{ij}^{(k)})^{\top}\mathbb{1} - \boldsymbol{\mu}_{j}^{(k)}\|_{1} \end{array} \right\} \geq \epsilon \text{ do}
4: ij \leftarrow \text{GREEDYEDGE}(\boldsymbol{\mu}^{(k)})
5: if \|\boldsymbol{\mu}_{ij}^{(k)}\mathbb{1} - \boldsymbol{\mu}_{i}^{(k)}\|_{1} > \|(\boldsymbol{\mu}_{ij}^{(k)})^{\top}\mathbb{1} - \boldsymbol{\mu}_{j}^{(k)}\|_{1} \text{ then}
6: \boldsymbol{\mu}^{(k+1)} \leftarrow (\mathcal{P}_{\mathcal{X}_{ij,i}} \circ \mathcal{P}_{\mathcal{X}_{ij\to i}})(\boldsymbol{\mu}^{(k)})
7: else
8: \boldsymbol{\mu}^{(k+1)} \leftarrow (\mathcal{P}_{\mathcal{X}_{ij,j}} \circ \mathcal{P}_{\mathcal{X}_{ij\to j}})(\boldsymbol{\mu}^{(k)})
9: end if
10: k \leftarrow k+1
11: end while
12: return \text{ROUND}(\boldsymbol{\mu}^{(k)})
```

Figure 2: The EMP-greedy algorithm selects the edge and direction with the greatest constraint violation and projects until all constraints are satisfied up to ϵ in l_1 distance.

consider two variants: EMP-cyclic (Algorithmic 1), which cyclically applies the updates to each edge in each iteration and EMP-greedy (Algorithmic 2), which applies a single projection update to only the edge with the greatest constraint violation in each iteration. We emphasize that these algorithms are not fundamentally new, but our analysis in the next section is our main contribution. EMP-cyclic is the Bregman method, almost exactly the inner loop proposed by Ravikumar et al. (2010). In both variants, $\mu^{(1)}$ is defined as the normalized value of $\exp(-\eta C)$. The GREEDYEDGE operation in EMP-greedy is defined as

$$\text{GreedyEdge}(\boldsymbol{\mu}) = \operatorname*{arg\,max}_{ij \in \mathcal{E}} \left\{ \begin{array}{l} \max\{\|\boldsymbol{\mu}_{ij}^{(k)}\mathbbm{1} - \boldsymbol{\mu}_{i}^{(k)}\|_1, \\ \|(\boldsymbol{\mu}_{ij}^{(k)})^\top \mathbbm{1} - \boldsymbol{\mu}_{i}^{(k)}\|_1 \} \end{array} \right\}$$

These procedures are then repeated again until the stopping criterion is met, which is that $\mu^{(k)}$ is ϵ -close to satisfying the constraint that the joint distributions sum to the marginals for all edges. Both algorithms also conclude with a rounding operation. Any fixed point of EMP must correspond to an optimal μ_{η}^* (see details in appendix). Computationally, EMP-greedy requires a search over the edges to identify the greatest constraint violation, which can be efficiently implemented using a max-heap (Nutini et al., 2015).

6 THEORETICAL ANALYSIS

We now present our main contribution, a theoretical analysis of EMP-cyclic and EMP-greedy. This result combines two aspects. First, we present a convergence guarantee on the number of iterations sufficient to solve (Proj), satisfying the \mathbb{L}_2 constraints with $\epsilon > 0$ error in l_1 distance. We note that, in finite iterations, the pseudo-marginals of EMP are not primal feasible

in general due to this ϵ -error. We then combine this result with our guarantee on the approximation error in Theorem 1 to show a bound on the number of iterations sufficient to recover the true integral MAP assignment by rounding, assuming the LP is tight and the solution is unique. This holds with sufficient iterations and a sufficiently large regularization constant even though the pseudo-marginals may not be primal feasible. We emphasize that these theorems are a departure from usual convergence rates in the literature (Meshi et al., 2012, 2015). Prior work has guaranteed convergence in objective value to the optimum of the regularized objective (Proj), making it unclear whether the optimal MAP assignment can be recovered, e.g. by rounding. We address this ambiguity in our results.

We begin with the upper bound iterations to obtain ϵ -close solutions, which is the result of two facts which we show. The first is that the updates in Proposition 1 monotonically improve a Lyapunov (potential) function by an amount proportional to the constraint violation as measured via the Hellinger distance. The second is that the difference between the initial and optimal values of the Lyapunov function is bounded.

Let $\deg(\mathcal{G})$ denote the maximum degree of graph \mathcal{G} and define:

$$S \stackrel{\text{def.}}{=} \sum_{ij\in\mathcal{E}} \left[\log \sum_{x_i, x_j \in \chi} e^{-\eta C_{ij}(x_i, x_j)} + \sum_{x_i, x_j \in \chi} \frac{\eta}{d^2} C_{ij}(x_i, x_j) \right]$$
$$+ \sum_{i\in\mathcal{V}} \left[\log \sum_{x\in\chi} e^{-\eta C_{i}(x)} + \sum_{x\in\chi} \frac{\eta}{d} C_{i}(x) \right].$$

Theorem 2. For any $\epsilon > 0$, EMP is guaranteed to satisfy $\|\boldsymbol{\mu}_{ij}\mathbb{1} - \boldsymbol{\mu}_i\|_1 < \epsilon$ and $\|\boldsymbol{\mu}_{ij}^{\top}\mathbb{1} - \boldsymbol{\mu}_j\|_1 < \epsilon$ for all $ij \in \mathcal{E}$ in $\lceil \frac{4S_0(\deg(\mathcal{G}_k)+1)}{\epsilon^2} \rceil$ iterations for EMP-cyclic and $\lceil \frac{4S_0}{\epsilon^2} \rceil$ iterations for EMP-greedy.

Here, $S_0 = \min(\|\eta C/d + \exp(-\eta C)\|_1, S)$. In this theorem, we give our guarantee in terms of l_1 distance rather than function value convergence. As we will see, this is significant, allowing us to relate this result to Theorem 1 in order to derive the main result. The proof is similar in style to Altschuler et al. (2017). We leave the full proof for EMP-cyclic for the appendix due to a need to handle tedious edge cases, but we state several intermediate results and sketch the proof for EMP-greedy for intuition as it reveals possibly how similar message passing algorithms can be analyzed. We first introduce a Lyapunov function written in terms of dual variables (λ, ξ) , indexed by the edges and vertices to which they belong in \mathbb{L}_2 . We denote the iterationindexed dual variables as $(\lambda^{(k)}, \xi^{(k)})$. For a given edge $ij \in \mathcal{E}$, constraints enforcing row and column consistency correspond to $\lambda_{ij}, \lambda_{ji} \in \mathbb{R}^m$, respectively. Normalizing constraints correspond to $\xi_i, \xi_i, \xi_{ij} \in \mathbb{R}$. The Lyapunov function, $L(\lambda, \xi)$, is shown in Figure 3.

$$L(\lambda, \xi) = -\sum_{ij \in \mathcal{E}} \sum_{x_i, x_j \in \chi} \exp\left(-\eta C_{ij}(x_i, x_j) - \lambda_{ij}(x_i) - \lambda_{ji}(x_j) - \xi_{ij}\right)$$

$$-\sum_{i \in \mathcal{V}} \sum_{x \in \chi} \exp\left(-\eta C_i(x) - \xi_i + \sum_{j \in N_r(i)} \lambda_{ij}(x) + \sum_{j \in N_c(i)} \lambda_{ji}(x)\right)$$

$$-\sum_{ij \in \mathcal{E}} \xi_{ij} - \sum_{i \in \mathcal{V}} \xi_i + \sum_{ij \in \mathcal{E}} \sum_{x_i, x_j \in \chi} \exp\left(-\eta C_{ij}(x_i, x_j)\right) + \sum_i \sum_{x \in \chi} \exp\left(-\eta C_i(x)\right)$$
(3)

Figure 3: The proposed Lyapunov function. $N_r(i)$ denotes the set of neighboring vertices of i where row consistency is enforced. $N_c(i)$ is the same for column consistency. The Lyapunov function L can be derived from the dual objective of (Proj). A full derivation is provided in the appendix.

We note that maximizing L over (λ, ξ) satisfies all constraints and yields the solution to (Proj) by first-order optimality conditions. We now present a result that establishes the monotone improvement in L due to the updates in Proposition 1.

Lemma 1. For a given edge $ij \in \mathcal{E}$, let μ' and (λ', ξ') denote the updated primal and dual variables after a projection from one of (a)–(d) in Proposition 1. We have the following improvements on L. If μ' is equal to:

(a)
$$\mathcal{P}_{\mathcal{X}_{ij\to i}}(\boldsymbol{\mu})$$
, then $L(\lambda', \xi') - L(\lambda, \xi) = 2h^2(\boldsymbol{\mu}_{ij}\mathbb{1}, \boldsymbol{\mu}_i)$

- (b) $\mathcal{P}_{\mathcal{X}_{ij,i}}(\boldsymbol{\mu})$, then $L(\lambda', \xi') L(\lambda, \xi) \geq 0$
- (c) $\mathcal{P}_{\mathcal{X}_{ij\to j}}(\boldsymbol{\mu})$, then $L(\lambda', \xi') L(\lambda, \xi) = 2h^2(\boldsymbol{\mu}_{ij}^{\top}\mathbb{1}, \boldsymbol{\mu}_j)$
- (d) $\mathcal{P}_{\mathcal{X}_{ij,j}}(\boldsymbol{\mu})$, then $L(\lambda',\xi') L(\lambda,\xi) \geq 0$.

This result shows that L improves monotonically after each of the four updates in Proposition 1. Furthermore, at every update, L improves by twice the squared Hellinger distance of the constraint violation between the joint and the marginals.

Lemma 2. Let λ^* , ξ^* denote the maximizers of L. The difference in function value between the optimal value of L and the first iteration value is upper bounded

$$L(\lambda^*, \xi^*) - L(\lambda^{(1)}, \xi^{(1)}) \le S_0.$$

Turning to Theorem 2, the result is obtained by observing that as long as the constraints are violated by an amount $\epsilon > 0$ (i.e., the algorithm has not terminated), then the Lyapunov function must improve by a known positive amount at each iteration. We provide a proof sketch for EMP-greedy.

Proof Sketch of Theorem 2 for EMP-greedy. We now show how to combine the results of Lemma 1 and Lemma 2 to obtain Theorem 2. Let k^* be the first iteration such that the termination condition in Algorithm 2 holds with respect to some $\epsilon > 0$. Then, for any k satisfying $1 \le k < k^*$, we have that GREEDYEDGE(μ) selects ij such that either $\|\mu_{ij}\mathbb{1} - \mu_i\|_1 \ge \epsilon$ or $\|\mu_{ij}^{\mathsf{T}}\mathbb{1} - \mu_j\|_1 \ge \epsilon$.

Without loss of generality, suppose $\|\boldsymbol{\mu}_{ij}\mathbb{1} - \boldsymbol{\mu}_i\|_1 \ge \|\boldsymbol{\mu}_{ij}^{\top}\mathbb{1} - \boldsymbol{\mu}_j\|_1$. Therefore, we have

$$\frac{\epsilon^2}{4} \le \frac{1}{4} \|\boldsymbol{\mu}_{ij} \mathbb{1} - \boldsymbol{\mu}_i\|_1^2 \le 2h^2(\boldsymbol{\mu}_{ij} \mathbb{1}, \boldsymbol{\mu}_i),$$

where again $h^2(\mu_{ij}1, \mu_i)$ denotes the squared Hellinger distance and the last inequality is the Hellinger inequality. Since μ_{ij} and μ_i are normalized for each iteration, this inequality is valid. Thus, L improves by $2h^2(\mu_{ij}1, \mu_i)$ when $\mathcal{P}_{\mathcal{X}_{ij\to i}}$ occurs and by a nonnegative amount when $\mathcal{P}_{\mathcal{X}_{ij,i}}$ occurs by Lemma 1. Therefore, we can guarantee improvement of at least $\frac{\epsilon^2}{4}$ each iteration. Since the optimality gap is at most \mathcal{S}_0 by Lemma 2, this means the algorithm must terminate in $\lceil \frac{4\mathcal{S}_0}{\epsilon^2} \rceil$ iterations.

We now turn to our main theoretical result. We combine our approximation and iteration convergence guarantees to fully characterize the convergence of EMP for \mathbb{L}_2 to the optimal MAP assignment when the relaxation is tight and the solution is unique.

Theorem 3. Let $\eta \geq \frac{2\log(16n^2d^2)+16|\mathcal{E}|d^2}{\min(\Delta,\frac{1}{128})}$, and $\epsilon^{-1} > (25d \deg(\mathcal{G})|\mathcal{E}|)^2 \max(\eta \|C\|_{\infty}, 68)$. If \mathbb{L}_2 is tight and $|\mathcal{V}_2^*| = 1$, the EMP algorithm returns a MAP assignment after $\lceil \frac{4S_0(\deg(\mathcal{G}_k)+1)}{\epsilon^2} \rceil$ iterations for EMP-cyclic and after $\lceil \frac{4S_0}{\epsilon^2} \rceil$ iterations for EMP-greedy.

When C is integral, $\Delta \geq \frac{1}{2}$, yielding a bound of all known parameters. The main technical challenge in producing this result is to relate the termination condition of EMP to the l_1 distance between $\mu^{(k)}$ and μ^* (the MAP assignment), as this may lie outside the polytope \mathbb{L}_2 . It does not suffice to provide convergence guarantees in function value as the goal of MAP inference is to produce integral assignments. The proof proceeds in two steps. First we show that $\mu^{(k)}$ is the entropy-regularized solution to objective C over a "slack" polytope $\mathbb{L}_2^{\nu^{(k)}}$. Where the slack vector $\nu^{(k)}$ corresponds to the constraint violations of $\mu^{(k)}$. We use this characterization to "project" $\mu^{(k)}$ onto a nearby \mathbb{L}_2 feasible point $\mu^{(k)}(2)$. Second, we can use the properties of the primal objective to bound $\mu^{(k)}(2)$ and μ_n^* . The proof is in the appendix.

7 NUMERICAL EXPERIMENTS

We illustrate our theoretical results in a practical application of the EMP algorithms. Ravikumar et al. (2010) already gave empirical evidence that the basic EMP-

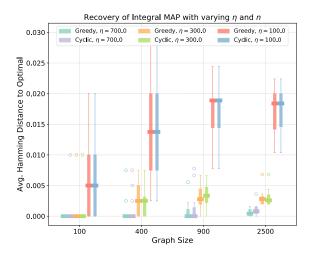


Figure 4: A box-plot showing the effect of graph size (x-axis) and regularization on the quality of rounded solutions for both algorithm variants after 80 iterations. Thick horizontal bars indicate the median over 20 trials each. For large η (cyan and purple), the true MAP is almost always recovered.

cyclic is competitive with standard solvers. Therefore, the objective of these experiments is to understand how graph and algorithm properties affect approximation (Theorem 1) and convergence (Theorem 2). We consider the family of multi-label Potts models (Wainwright et al., 2005) with d=3 labels on \mathbb{L}_2 . For each trial, the cost vector is $C_i(x_i) = \alpha_i(x_i)$, $\forall i, x_i$ and

$$C_{ij}(x_i, x_j) = \begin{cases} \beta_{ij} & x_i = x_j \\ 0 & \text{otherwise} \end{cases} \quad \forall ij, x_i, x_j$$

where the parameters are random $\alpha_i(x_i) \sim \text{Unif}(-0.5, 0.5)$ and $\beta_{ij} \sim \text{Unif}\{-0.1, 0.1\}$. The graphs considered are structured as $\sqrt{n} \times \sqrt{n}$ grids (Erdogdu et al., 2017; Globerson and Jaakkola, 2008; Ravikumar et al., 2010) and as Erdős-Rényi random graphs with edge probability $p = \frac{1.1 \log n}{n}$. To evaluate recovery of the optimal MAP assignment, we first solved each graph with the ECOS LP solver (Domahidi et al., 2013) and selected graphs that were tight. Solving the LP to find the ground-truth was the main computational bottleneck. Further details can be found in Appendix E.

Approximation In Figure 4, we evaluate the effect of regularization and graph size on the quality of the nearly converged solution from EMP for over 80 iterations on grids. The box-plots indicate that large choices of η often yield the exact MAP solution (cyan and purple). Moderate choices still yield competitive solutions but not optimal for larger graphs (orange and green). Low choices generally give poor solutions with high spread for all graph sizes (red and blue).

Convergence We then investigate the effects of regularization on convergence for both variants. Figure 5

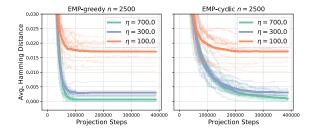


Figure 5: On grids of size n=2500, convergence rates to the optimal MAP assignment of greedy and cyclic variants are shown. The lines on each plot indicate choices of η .

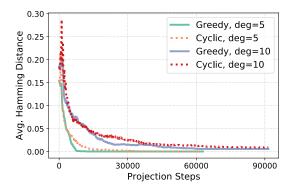


Figure 6: The algorithm variants on Erdős-Rényi random graphs with $n=400, \eta=700.0$, and maximum degrees $\deg(G)=5,10$. The higher degree graphs (red and blue) take longer to converge to the optimal MAP assignment.

illustrates the distance of the rounded solution to the optimal MAP solution over projection steps on grids of size n=2500. EMP-greedy converges sharply and varying regularization has less of an effect on its convergence rate. Finally, in Figure 6, we look at Erdős-Rényi random graphs to observe the effect of the graph structure for both variants. We considered degree-limited random graphs with $\deg(\mathcal{G})=5$ and $\deg(\mathcal{G})=10$. The figure shows convergence over projection steps for graphs of size n=400. For both variants, the convergence rate deteriorates for higher degrees.

8 CONCLUSION

In this paper, we investigated the approximation effects of entropy regularization on MAP inference objectives. We combined these approximation guarantees with a convergence analysis of an edge-based message passing algorithm that solves the regularized objective to derive guarantees on the number of iterations sufficient to recover the true MAP assignment. We also showed empirically the effect of regularization and graph propertise on both the approximation and convergence. In future work, we wish to extend the analyses and proof techniques to higher order polytopes and general block-coordinate minimization algorithms.

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