Inference with Aggregate Data: An Optimal Transport Approach

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Abstract
We consider inference problems over probabilistic graphical models with aggregate data. In particular, we propose a new efficient belief propagation type algorithm over tree-structured graphs with polynomial computational complexity as well as a global convergence guarantee. This is in contrast to previous methods that either exhibit prohibitive complexity as the population grows or do not guarantee convergence. Our method is based on optimal transport, or more specifically, multi-marginal optimal transport theory. In particular, the inference problem with aggregate observations we consider in this paper can be seen as a structured multi-marginal optimal transport problem, where the cost function decomposes according to the underlying graph. Consequently, the celebrated Sinkhorn algorithm for multi-marginal optimal transport can be leveraged, together with the standard belief propagation algorithm to establish an efficient inference scheme. We demonstrate the performance of our algorithm on applications such as inferring population flow from aggregate observations.

1. Introduction
Probabilistic graphical models (PGMs) (Wainwright & Jordan, 2008) provide a powerful framework for modeling the dependence and relations between probabilistic quantities. Probabilistic inference using PGMs have been widely used in signal processing, computer vision, computational biology, and many other real-world applications (Wainwright & Jordan, 2008; Koller & Friedman, 2009; Box & Tiao, 2011). During the last decades, many inference algorithms have been proposed, among which the belief propagation (BP) algorithms (Pearl, 1988; Yedidia et al., 2001; 2003) have been extremely effective and successful. The standard PGM framework and the associated inference algorithms are suitable for the modeling of distinguishable/labeled individuals as in most standard applications.

Recently, there has been growing interest in applications involving a large population of individuals, e.g., bird migration, where data about individuals are not available. Instead, aggregate population-level observation in the form of counts or contingency tables are provided (Sundberg, 1975; MacRae, 1977; Kalbfleisch et al., 1983; Sheldon & Dietterich, 2011; Luo et al., 2016). A distinct feature of this setting is that the individuals are no longer distinguishable to each other. This restriction in the observations could be due to privacy, security, or economic reasons. For example, in tourist flow analysis, individual trajectories may not be readily accessible, but the number of people in a given area can typically be counted using video surveillance or electronic gates. Similarly, it is much easier to obtain the population sizes of bird migration than tracking the trajectory of each bird. In this setting with aggregate observations, the traditional inference algorithms such as BP in PGMs which heavily depend on individual observation, are thus not directly applicable. The development of reliable and efficient aggregate inference algorithms is of great importance and necessity.

The collective graphical model (CGM) introduced by Sheldon & Dietterich (2011) is a recent framework for inference and learning with aggregate data. A CGM is a graphical model that describes the histograms of individuals directly. Using this model, it was proved (Sheldon et al., 2013) that the complexity of traditional inference algorithms for exact inference scales at least polynomially as the population grows. To circumvent this difficulty, they (Sheldon et al., 2013) proposed an approximate maximum a posteriori (MAP) formulation, which approximates the marginal inference solution well, especially when the size of the population is large. Under some proper assumptions, the approximate MAP formulation is a convex optimization problem and the problem dimension is independent of the population size. To further accelerate the inference, they proposed the non-linear belief propagation (NLBP) (Sun et al., 2015) algorithm. The NLBP algorithm is a message-passing type algorithm relying on interactions between graph nodes. Despite of its similarity to the BP (Pearl, 1988) algorithm, NLBP suffers from instability and lack of convergence. In-
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deed, no convergence guarantee (Sun et al., 2015) has been established so far.

The goal of this paper is to establish an efficient and reliable algorithm for marginal inference with aggregate observations. We build on the CGM framework and develop such an aggregate inference algorithm. Our algorithm is based on multi-marginal optimal transport (MOT) (Pass, 2015; Benamou et al., 2015) theory, which involves the transport among multiple marginal distributions. MOT is a generalization of the classical optimal transport (OT) problem (Villani, 2003) of Monge and Kantorovich to find a transport plan from a source distribution to a target one that minimizes the total transport cost. Within the MOT framework, the aggregate observations are viewed as fixed given marginal distributions. We show that the aggregate inference problem in CGM reduces to the special case of entropic regularized formulation of MOT with marginals specified by these aggregate observations. Thanks to this equivalence, the aggregate inference problem can be solved by the popular Sinkhorn a.k.a., iterative scaling algorithm (Sinkhorn, 1964; Franklin & Lorenz, 1989; Cuturi, 2013; Benamou et al., 2015). The Sinkhorn algorithm has the advantages of being extremely easy to implement and parallelize, and has global convergence guarantee (Franklin & Lorenz, 1989; Benamou et al., 2015). We show that the Sinkhorn algorithm for aggregate inference can be further accelerated by leveraging the underlying graphical structure of the inference problems with aggregate observations; a key projection step in the Sinkhorn algorithm, which could be potentially expensive, can be realized efficiently by standard BP for tree-structured graphical models. This accelerated version of our algorithm is named Sinkhorn belief propagation (SBP).

SBP exhibits convergence guarantees when the underlying graph is a tree. We also observed in numerical experiments that SBP has a faster convergence rate compared to NLBP. The contributions of the paper are summarized as follows.

- We discover an equivalent relation between OT theory and marginal inference problems with aggregate observations;

- Based on OT theory and belief propagation, we propose an efficient marginal inference algorithm with aggregate data that has a global convergence guarantee;

- We demonstrate the performance of our algorithm on applications such as inferring population flow from aggregate observations.

Related Work: Early works on aggregate data focused on the learning of the parameters of the underlying models. For example, Sundberg (1975); MacRae (1977); Kalbfleisch et al. (1983) studied the modeling of a single Markov chain by maximizing the aggregate posterior. More recent learning methods from aggregate data include Gangbo & Świech (1998); Pasanisi et al. (2012); Luo et al. (2016). Since the formalism of CGMs by Sheldon & Dietterich (2011) there have been multiple works on inference for aggregate data. The complexity of exact inference in CGMs has been investigated in (Sheldon et al., 2013) and an approximate MAP formulation has been proposed in the same paper. The nonlinear belief propagation algorithm (Sun et al., 2015) is a message passing type algorithm for approximate MAP inference in CGMs, but it does not have a convergence guarantee. The learning of a Markov chain within the CGM framework has been presented in Bernstein & Sheldon (2016). On the other hand, the application of OT theory in filtering and estimation problems have been investigated in (Chen & Karlsson, 2018; Haasler et al., 2019). Another closely related problem is the Schrödinger bridge problem (Léonard, 2014; Chen et al., 2016; 2019), which is essentially equivalent to an entropic OT problem. Our focus in this paper is marginal inference with aggregate data and our method is based on OT and BP. Thus, our work is closest to (Sun et al., 2015).

The rest of the article is organized as follows. In Section 2, we briefly discuss related background including PGMs, standard BP, CGMs, NLBP and MOT. We present our main results and algorithm in Section 3. It is followed by the experimental results in Section 4 and conclusion in Section 5.

2. Background

In this section, we briefly present related concepts including PGMs, standard BP, CGMs, and MOT.

2.1. Probabilistic Graphical Models

Probabilistic graphical models (Wainwright & Jordan, 2008) are graph-based representations of a collection of random vectors that capture the conditional dependencies between them. Consider graphical models with underlying graph $G = (V, E)$ where $V$ and $E$ denotes the set of vertices and edges respectively. Each node $i \in V$ is associated with a random variable $x_i$ which can be either discrete or continuous, though we assume discrete random variables. Assuming that the underlying graph is undirected with $J = |V|$ nodes, the probability of the PGM is given by

$$p(x_1, x_2, \ldots, x_J) = \frac{1}{Z} \prod_{(i,j) \in E} \psi_{ij}(x_i, x_j),$$

(1)

where $\psi_{ij}$ are edge potentials and $Z$ is a normalization constant.

Standard Belief Propagation: Belief propagation (BP) (Pearl, 1988) is an effective message-passing algorithm for Bayesian inference in PGMs. The BP algorithm updates the marginal distribution of each node through communica-
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When the algorithm converges, the node and edge marginals are estimated as

\[ m_{i \rightarrow j}(x_j) \propto \sum_{x_i} \psi_{ij}(x_i, x_j) \prod_{k \in N(i) \setminus j} m_{k \rightarrow i}(x_i), \tag{2} \]

where \( m_{i \rightarrow j}(x_j) \) denotes the message from variable node \( i \) to variable node \( j \), encapsulating the belief of node \( i \) on node \( j \). Here, \( N(i) \) is the set of neighboring nodes of \( i \), and thus \( N(i) \setminus j \) denotes the set of neighbors of \( i \) except for \( j \). The messages in (2) are updated iteratively over the graph. When the algorithm converges, the node and edge marginals are given by

\[ b_i(x_i) \propto \prod_{k \in N(i)} m_{k \rightarrow i}(x_i) \tag{3a} \]

\[ b_{ij}(x_i, x_j) \propto \psi_{ij}(x_i, x_j) \prod_{k \in N(i) \setminus j} m_{k \rightarrow i}(x_i) \prod_{\ell \in N(j) \setminus i} m_{\ell \rightarrow j}(x_j). \tag{3b} \]

When the graph has no cycles it is well-known that the belief propagation algorithm converges globally (Yedidia et al., 2001) and the estimated marginal distributions in (3) recover the true marginals exactly. For general graphs with cycles, convergence is not guaranteed but it works well in practice.

### 2.2. Collective Graphical Models

Collective graphical models (CGMs) were first introduced by Sheldon & Dietterich (2010) as a framework for inference and learning with aggregate data. CGMs describe the distribution of the aggregate counts of a population sampled independently from a discrete graphical model. Assume that the relationships between the random variables \( X_1, X_2, \ldots, X_J \) are captured using an undirected independence graph \( G = (V, E) \). Let \( X = (x_1, \ldots, x_J) \) be a particular assignment to the individual variables, where each variable \( X_i \) takes one of the values from a finite set \( X \) with cardinality \( |X| = d \). The individual pairwise probability model is given by

\[ p(x) = \frac{1}{Z} \prod_{(i,j) \in E} \psi_{ij}(x_i, x_j), \tag{4} \]

where \( \psi_{ij}(x_i, x_j) \) are local pairwise edge potentials and \( Z \) is a normalization constant.

To generate the aggregate data, first assume that \( M \) independent sample vectors \( x^{(1)}, \ldots, x^{(M)} \) are drawn from the individual probability model to represent the individuals in a population. Here, each vector \( x^{(m)} \) takes one of the \( d \) possible states. Let \( X_i^{(m)} \) be the state of the \( m \)th individual at node \( i \), and let \( n_i = \mathbb{R}^d \) be the aggregate node distribution with entries \( n_i(x_i) = \sum_{m=1}^{M} \mathbb{I}[X_i^{(m)} = x_i] \) that count the number of individuals in each state. Here, \( \mathbb{I}[] \) denotes indicator function. Moreover, let \( n_{ij} \) be the aggregate edge distributions with entries \( n_{ij}(x_i, x_j) = \sum_{m=1}^{M} \mathbb{I}[X_i^{(m)} = x_i, X_j^{(m)} = x_j] \). The vectors \( n_1, \ldots, n_J \) constitute the aggregate data and the aggregate edge distributions \( n_{ij} \) represent sufficient statistics of the individual model (Sheldon & Dietterich, 2011). The collection of all the aggregate node distributions \( n_i \) together with the aggregate edge distributions \( n_{ij} \) is denoted as \( n = \{n_i, n_{ij}\} \).

In CGMs, the observation noise is modeled explicitly as a conditional distribution \( p(y | n) \) with \( y \) being the aggregate noisy observations that probabilistically depend on the aggregate data \( n \). The goal of inference in CGMs is to estimate \( n \) from the aggregate noisy observations through the conditional distribution \( p(n | y) \propto p(n)p(y | n) \), where \( p(n) \) is known as the CGM distribution (Sheldon & Dietterich, 2011) which is derived from the individual model (4). For the tree structured graph, the CGM distribution \( p(n) \) equals

\[ \frac{M!}{\prod_{i \in V} \prod_{(i,j) \in E} \binom{n_i(x_i)!}{d_i-1} \prod_{(i,j) \in E} \psi_{ij}(x_i, x_j)^{n_{ij}(x_i, x_j)}}, \]

where \( d_i \) is the number of neighbors of node \( i \) in \( G \) and

\[ \frac{1}{Z_M} \prod_{(i,j) \in E} \prod_{x_i, x_j} \psi_{ij}(x_i, x_j)^{n_{ij}(x_i, x_j)} \]

is the joint probability of the entire population. Moreover, the support of the CGM distribution \( p(n) \) is such that each entry of \( n \) is an integer and satisfies the following constraints

\[ \sum_{x_i} n_i(x_i) = M, \quad \forall i \in V \]

\[ n_i(x_i) = \sum_{x_j} n_{ij}(x_i, x_j), \quad \forall i \in V, \; j \in N(i). \tag{5} \]

Exact inference of \( n \) based on \( p(n | y) \) is unrealistic for large populations as the computational complexity scales at least polynomially as population size \( M \) grows (Sheldon et al., 2013). It was first discovered in Sheldon et al. (2013) that \( -\ln p(n | y) \) can be approximated by (up to a constant addition and multiplication) the CGM free energy

\[ F_{\text{CGM}}(n) = U_{\text{CGM}}(n) - H_{\text{CGM}}(n), \tag{6} \]

where \( U_{\text{CGM}}(n) \) equals

\[ - \sum_{(i,j) \in E} n_{ij}(x_i, x_j) \ln \psi_{ij}(x_i, x_j) - \ln p(y | n), \]

and

\[ H_{\text{CGM}}(n) = - \sum_{(i,j) \in E} n_{ij}(x_i, x_j) \ln n_{ij}(x_i, x_j) + \sum_{i \in V} (d_i - 1) \sum_{x_i} n_i(x_i) \ln n_i(x_i). \]
After relaxing the constraints that $n_i(x_i), n_{ij}(x_i, x_j)$ are integers and under the assumption that the observation model $p(y | n)$ is log-concave, the resulting problem of minimizing $F_{\text{CGM}}$ is a convex optimization problem. This is the approximate MAP (Sheldon et al., 2013) framework for CGMs. Note that the problem size of minimizing $F_{\text{CGM}}$ is independent of the population size $M$.

**Non-linear Belief Propagation:** Even though the approximate MAP framework is insensitive to population size, its complexity grows rapidly as the number of variables $J$ increases. One algorithm that is designed to solve the approximate MAP problems more efficiently is non-linear belief propagation (NLBP) (Sun et al., 2015). The NLBP (Sun et al., 2015) algorithm addresses the aggregate inference problem by establishing a connection between the Bethe free energy (Yedidia et al., 2005) and the objective function (6) for approximate MAP inference in CGMs. NLBP (Sun et al., 2015) is a message passing type algorithm for aggregate MAP inference. The steps of the NLBP algorithm are listed in Algorithm 1.

**Algorithm 1 Non-Linear Belief Propagation (NLBP)**

1. Initialize messages $m_{i\rightarrow j}(x_j)$ potentials $\hat{\psi}_{ij}(x_i, x_j)$, $\forall (i, j) \in E, \forall x_i, x_j$
2. Repeat
   - Update the following in any order
     
     $\hat{\psi}_{ij}(x_i, x_j) = \exp \left( - \frac{\partial U_{\text{CGM}}(n)}{\partial n_{ij}(x_i, x_j)} \right)$
     
     $m_{i\rightarrow j}(x_j) \propto \sum_{x_i} \hat{\psi}_{ij}(x_i, x_j) \prod_{k \in N(i)\setminus j} m_{k\rightarrow i}(x_i)$
     
     $n_{ij}(x_i, x_j) \propto \hat{\psi}_{ij}(x_i, x_j) \prod_{k \in N(i)\setminus j} m_{k\rightarrow i}(x_i) \prod_{\ell \in N(j)\setminus i} m_{\ell\rightarrow j}(x_j)$

   until convergence

After convergence of the messages in Algorithm 1, the aggregate marginals can be estimated as

$$n_i(x_i) \propto \prod_{k \in N(i)} m_{k\rightarrow i}(x_i).$$

(7)

One of the major drawbacks of the NLBP algorithm is that it does not exhibit any convergence guarantee. The major factor affecting the convergence of NLBP is the update of the potentials $\hat{\psi}_{ij}$ which requires gradient computations of $p(y | n)$. These gradients depend on the observation model at hand and might cause the explosion or saturation of potential updates based on the smoothness of the model $p(y | n)$. To stabilize the NLBP to some degree, it was proposed (Sun et al., 2015) to dampen the estimates $n$ as

$$n = (1 - \alpha)n + \alpha n^{\text{new}}$$

in each iteration, where $0 < \alpha \leq 1$ and $n^{\text{new}}$ is the estimate in the current iteration. However, the selection of the parameter $\alpha$ has to be done carefully to ensure appropriate potential updates (Sun et al., 2015).

### 2.3. Multimarginal Optimal Transport

The multimarginal optimal transport (MOT) (Nenna, 2016; Pass, 2012) problem aims to find a transport plan among a set of marginal distributions, depending on an underlying given cost function. We consider discrete settings where the marginal distributions are described by vectors $\mu_j \in \mathbb{R}^d$, $j \in \{1, 2, \ldots, J\}$ and we denote the cost function and the transport plan by the $J$-mode tensors $C, B \in \mathbb{R}^{d \times \cdots \times d}$. The Kantorovich formulation of MOT with constraints on a subset of marginals $\Gamma \subset \{1, 2, \ldots, J\}$ reads (Elvander et al., 2020)

$$\min_{B \in \mathbb{R}^{d \times \cdots \times d}} \langle C, B \rangle \quad \text{s. t. } P_j(B) = \mu_j, \text{ for } j \in \Gamma,$$

(8)

where $\langle C, B \rangle = \sum_{i_1, \ldots, i_J} C_{i_1, \ldots, i_J} B_{i_1, \ldots, i_J}$, and the projection on the $j$-th marginal of $B$ is defined by

$$P_j(B) = \sum_{i_1, \ldots, i_{j-1}, i_{j+1}, \ldots, i_J} B_{i_1, \ldots, i_{j-1}, i_{j+1}, \ldots, i_J}.$$

(9)

Note that the standard OT problem with two marginals is a special case of (8) with $J = 2$ and $\Gamma = \{1, 2\}$.

For faster computations, it was proposed by Cuturi (2013); Benamou et al. (2015) to add a regularizing entropy term

$$H(B) = -\sum_{i_1, \ldots, i_J} \log(B_{i_1, \ldots, i_J})$$

(10)

to the objective. This results in the strongly convex problem

$$\min_{B \in \mathbb{R}^{d \times \cdots \times d}} \langle C, B \rangle - \epsilon H(B) \quad \text{s. t. } P_j(B) = \mu_j, \text{ for } j \in \Gamma,$$

(11)

where $\epsilon > 0$ is a regularization parameter.

It can be shown that the optimal solution to (17) is of the form

$$B = K \odot U,$$

(12)

where $K = \exp(-C/\epsilon)$ and $U = u_1 \odot u_2 \odot \cdots \odot u_J$. The Sinkhorn scheme for finding the vectors $u_j$, given that they are initialized to be $\exp(-1/J)1$ ($1$ denotes the vector of all entries being $1$), is to iteratively update them according to

$$u_j \leftarrow u_j \odot \mu_j / P_j(K \odot U),$$

(13)

for all $j \in \Gamma$. This scheme may for instance be derived as Bregman iterations (Benamou et al., 2015) or dual block
Algorithm 2 Sinkhorn Algorithm for MOT

Compute $K$

Initialize $u_1, u_2, \ldots, u_J$ to $\exp(-1/J)1$

repeat

for $j \in \Gamma$ do

$U \leftarrow u_1 \otimes u_2 \otimes \cdots \otimes u_J$

$u_j \leftarrow u_j \otimes \mu_j / P_j(K \otimes U)$

end for

until convergence

coordinate ascend (Elvander et al., 2020). All the steps of Sinkhorn iterations are listed in Algorithm 2. It is worth noting that the update step (13) in Algorithm 2 is a scaling step that ensures that the $j$-th marginal of the updated tensor $K \odot U$ satisfies the constraint in (11), i.e., $P_j(K \odot U) = \mu_j$.

3. Main Results

We consider marginal inference problems with aggregate data as in CGMs. Assume that the graph $G = (V, E)$ encodes the relationships among the node variables $X_1, X_2, \ldots, X_J$ of each individual, which consists of unobserved as well as observed variables, and let $\Gamma \subset V$ be the set of observation nodes. Let the unobserved individual variables take values in a finite set $X_u$ and the observations come from another finite set $X_o$, where in general, $X_u \neq X_o$. The joint distribution of individual variables is assumed to be factored as

$$p(x) = \frac{1}{Z} \prod_{i,j} \psi_{ij}(x_i, x_j), \tag{14}$$

where $\psi_{ij}$ are pairwise potentials and $Z$ is a normalization constant. Then similar to the generative model of aggregate data in CGMs, by drawing $M$ independent samples from the individual model, the aggregate counts corresponding to each node is generated. Therefore, the aggregate data constitute $n_1, n_2, \ldots, n_J$ (here $J = |V|$). We assume that the system is closed (Kalbfleisch et al., 1983), i.e., the population size $M$ remains fixed. In such closed settings, the aggregate data can be thought of as probability distributions when normalized with the population size. This normalization is carried out for the ease of explanation only and can be neglected. With this setup, when the underlying graph structure is a tree, the aggregate variables have the same graph structure as of the individual probability model; this is due to the hyper-Markov property (Sheldon et al., 2013). Now, we have the aggregate distributions constituting $n_1, n_2, \ldots, n_J$ with the underlying structure $G$. Suppose aggregate observations are made from a subset of nodes $\Gamma \subset V$ and let these aggregate observation be $y_i, \forall i \in \Gamma$, then our goal is to infer the aggregate marginals $n_i, \forall i \notin \Gamma$. Without loss of generality, we assume that the observation nodes can only be leaves, otherwise, we can always split the graph over the observation node and then each subgraph will have this observation node as a leaf.

Note that in our setting, the observation model is a subset of the underlying graph as opposed to the original CGM setting, where the observation model is treated separately. Figure 1 depicts this difference between the noise models. In (Sheldon et al., 2013), the observation model we use here was regarded as exact observation since the aggregate measurements are exact marginal distributions of the associated node variable. We argue that this type of observation can also handle measurement noise. Taking Figure 1 as an example, $X_4$ is treated as a measurement node of $X_1$, therefore, the measurement noise is already encoded in the edge potential between them. Indeed, this is the measurement noise model used in standard hidden Markov models (HMMs) (Fine et al., 1998). As a side note, the algorithms developed in Sheldon et al. (2013); Sun et al. (2015) do not apply to the cases with “exact observation”. Taking the limit of those algorithms designed for “noisy observation” with vanishing noise will cause ill-conditioning issues in the updates.

We denote the joint aggregate distribution as $n$ in this section. Now, the aggregate inference problem, with fixed aggregate observations $y_i, \forall i \in \Gamma$ can be posed as an optimization problem via the variational principle. The variational principle seeks an approximate aggregate distribution $n(x)$ which is close to the original distribution $p(x)$ given by (14) in terms of KL divergence. This leads to the following aggregate inference problem subject to the aggregate observation constraints

$$\min_n \quad KL(n || \prod_{(i,j) \in E} \psi_{ij}(x_i, x_j))$$

s. t. $$P_j(n) = y_j, \quad \forall j \in \Gamma.$$
3.1. Multimarginal Optimal Transport Approach

When treating the pairwise potentials of the graphical model as the local components of the cost function in MOT, i.e.,
\[ C(x) = -\sum_{i,j} \ln \psi_{ij}(x_i, x_j), \]  
(16)

the aggregate inference problem (15) can be viewed as a regularized MOT problem. Indeed, the regularized MOT problem (11) can be rewritten as
\[ \min_{B \in \mathbb{R}^{|\mathcal{X}| \times d}} \text{KL}(B \| \exp(-\frac{C}{\epsilon})) \]
\[ \text{s.t.} \quad P_j(B) = \mu_j, \quad \forall j \in \Gamma. \]  
(17)

Plugging (16) into the above and taking \( \epsilon = 1 \) yields exactly the same expression as in (15).

Consequently, we can adopt the Sinkhorn algorithm (Algorithm 2) for MOT problems, which is guaranteed to converge (Franklin & Lorenz, 1989) to solve the aggregate inference problem (15). Thanks to the graphical structure (16) of the cost \( C \), we can further accelerate the algorithm by utilizing standard BP to realize the key projection step \( P_j(K \odot U) \) in the Sinkhorn algorithm; we call this combination of Sinkhorn and BP as Sinkhorn belief propagation (SBP) algorithm.

Before presenting our SBP algorithm, we first characterize the stationary points of the aggregate inference problem (15) in terms of local messages; these will be used to compute the projections in a Sinkhorn scaling step. When the underlying graph is a tree, the objective function of problem (15) is the same as the Bethe free energy (Yedidia et al., 2005)
\[ F_{\text{Bethe}}(n) = \sum_{i,j} \sum_{x_i,x_j} n_{ij}(x_i, x_j) \ln \frac{n_{ij}(x_i, x_j)}{\psi_{ij}(x_i, x_j)} - \sum_{i=1}^{d_n} (d_i - 1) n_i(x_i) \ln n_i(x_i). \]  
(18)

Thus, the aggregate inference problem, with fixed aggregate observations \( y_i, \forall i \in \Gamma \), takes the form
\[ \min_{n_{ij}, n_i} F_{\text{Bethe}}(n) \]
\[ \text{s.t.} \quad n_i(x_i) = y_i(x_i), \quad \forall i \in \Gamma \]  
(19a)
\[ \sum_{x_j} n_{ij}(x_i, x_j) = n_i(x_i), \forall (i, j) \in E \]  
(19b)
\[ \sum_{x_i} n_i(x_i) = 1, \quad \forall i \in V. \]  
(19c)

Here (19b) corresponds to aggregate observation constraints and (19c)-(19d) represent consistency constraints. One can apply Lagrangian duality theory (Boyd & Vandenberghe, 2004) to the constrained convex optimization (19) to obtain the following.

**Theorem 1.** The solution to the aggregate inference problem (19) is characterized by
\[ \hat{n}_i(x_i) \propto \prod_{k \in N(i)} m_{k \to i}(x_i), \quad \forall i \not\in \Gamma \]  
(20)

where \( m_{i \to j}(x_j) \) are fixed points of
\[ m_{i \to j}(x_j) = \sum_{x_i} \psi_{ij}(x_i, x_j) \prod_{k \in N(i) \setminus j} m_{k \to i}(x_i); \]
\[ \forall i \not\in \Gamma, \forall j \in N(i), \]  
(21a)
\[ m_{i \to j}(x_j) = \sum_{x_i} \psi_{ij}(x_i, x_j) \frac{y_i(x_i)}{m_{j \to i}(x_i)}; \]
\[ \forall i \in \Gamma, \forall j \in N(i). \]  
(21b)

The expression \( m_{i \to j} \) in (21) can be viewed as messages between nodes, as in BP. Among the two classes of messages in (21), (21a) resembles that in standard BP while (21b) corresponds to the scaling step (13).

Taking all these components into account, we arrive at the Sinkhorn belief propagation algorithm (Algorithm 3). In the

**Algorithm 3 Sinkhorn Belief Propagation (SBP)**

Initialize the messages \( m_{i \to j}(x_j) \)
Update \( m_{i \to j}(x_j) \) using (21)
while not converged do
for \( i = 1, 2, \ldots, |\Gamma| \) do
    i) Update \( m_{i \to j}(x_j) \) using (21b)
    ii) Update all the messages on the path from \( i \) to \( i + 1 \) according to (21a) (if \( i = |\Gamma| \), then \( i + 1 = 1 \))
end for
end while

language of the Sinkhorn algorithm (Algorithm 2), \( m_{i \to j} \) is associated with \( u_i \), thus step i) corresponds to modifying the PGM potential from \( K \) to \( K \odot U \) with the most recent \( U \). The update ii) then calculates the marginal distribution at node \( i + 1 \) of the PGM with this modified potential. Due to the tree structure of the PGM, it suffices to update only messages from node \( i \) to \( i + 1 \) as in ii).

The Sinkhorn algorithm (Algorithm 2) has a linear convergence rate (Luo & Tseng, 1993), so does SBP. Each iteration in Algorithm 2 requires a projection step \( P_j \), which is realized by belief propagation between neighboring observation nodes. For a graph with \( J \) nodes, each node takes \( d \) possible values, the complexity of operation (21a) is \( O(d^2) \). The update ii) in SBP takes at most \( J \) numbers of operation (21a), thus, the worst case iteration complexity of SBP is \( O(Jd^2) \).

4. Evaluation

We conduct three sets of experiments to evaluate the performance of our algorithm. The first one aims to evaluate
we employ model parameters $w$ which follows $y \propto \text{Poisson}(\beta n)$. In the SBP setting, we use a Gaussian observation model. The probability for an individual bird to be observed by a sensor follows a Gaussian distribution centered at the sensor. In all experiments, we employ model parameters $w = (3, 5, 5, 10)$; the same parameters are used in the estimation algorithms. We set $M = 5000$, and $\beta = 1$. We compare the convergence performance between NLBP and SBP with different $L$ and $T$ values, as depicted in Figure 2. When $T$ is fixed and $L$ varies, SBP is faster than NLBP. When $L$ is fixed and $T$ varies, SBP is also faster than NLBP. Moreover, we find that the run time does not grow much as $T$ increases. This makes SBP suitable for large HMMs. The convergence behaviors of NLBP and SBP are displayed in Figures 2(c) and 2(d). The 1-norm distance between true marginal distributions and estimated distributions decrease monotonically for SBP, whereas some instability occurs for NLBP. To stabilize NLBP, a damping ratio $\alpha$ is needed. However, higher damping rate implies smaller step size which in turn slows down the algorithm. We also find that the convergence property of NLBP is sensitive to the prior distribution and damping ratio when $T$ is large.

4.2. Ensemble Estimation with Sparse Information

Next, we conduct a more challenging experiment wherein the aggregate observations are sparse. The task is to track ensembles over a network with limited number of sensors. The sensors can not tell the exact locations of the agents, such as in the case of Wi-Fi hotspots, or cell phone based stations, which can only tell the number of connected devices. Ensemble estimation is needed in tracking the human group activity without loss of individual privacy. We evaluate the model over a $20 \times 20$ grid network with 16 sensors placed randomly as in Figure 4. At each timestamp, each sensor observes a count, which records the number of agents connected to the sensor. Each agent can only connect with one sensor at a time and the probability of the connection decreases exponentially as the distance between agent and the sensor increases. To demonstrate the performance of SBP in estimating multi-modal distribution, we simulate a population with two clusters: one from left-bottom and one from center-bottom; both aim to the right-top corner of the grid in a $T = 15$ time interval. We model the transition probability as in the bird migration setup discussed in Section 4.1. We run simulations with 100 agents (Figure 3(a)) and 10000 agents (Figure 3(b)). As can be seen from the figures, even with such a sparse observation model, SBP can still infer the population movements to a satisfying accuracy.
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Figure 3. Simulation of the movement of (a) 100 agents and (b) 10000 agents over $20 \times 20$ grid for $T = 15$. In each of the figures, first column depicts the real movement of agents at different time steps, second column represents the aggregate sensor observations, and third column depicts estimated aggregated positions. Here, the size of the circles is proportional to the number of agents.

4.3. Empirical Loopy Graph Validation

Finally, we run a simple toy experiment where the underlying graph has loops as shown in Figure 5. We set $|X_u| = |X_o| = 5$ and generate the aggregate node distributions randomly. Moreover, the edge potential were generated using $\exp(I + Q)$, where $I$ is the identity matrix and $Q$ represents a random matrix generated by a Gaussian distribution. We estimate the marginal distribution by solving (15) using the SBP algorithm and then compare them with exact marginals by solving (15) using generic convex optimization algorithms. The convergence of the estimates for five different random seeds in terms or 1-norm distance is shown in Figure 6. We observe that the SBP algorithm has a good performance on the loopy graph.

Figure 6. Convergence of SBP on the loopy graph shown in Figure 5. Different colors represent different realizations.

5. Conclusion

In this paper, we presented a reliable algorithm for marginal inference from aggregate data based on multi-marginal optimal transport theory. We established that the aggregate inference problem is a special case of the entropic regularized MOT problem when the cost of MOT is structured according to the graphical model. We then combined the Sinkhorn algorithm for the MOT problems and the standard belief propagation algorithm to establish our method. Our algorithm enjoys fast convergence and has a convergence guarantee when the underlying graph structure is a tree. We evaluated the performance of our algorithm on multiple applications involving inference from aggregate data such as bird migration and human mobility based on hidden Markov models. In the future, we plan to extend our current algo-
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Algorithm to cover graphical models with continuous state. We also plan to investigate the parameter learning of CGMs using the MOT framework.

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