Inference on diagrams in the category of Markov kernels (Extended abstract)

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Graphical models are widely used families of probability distributions that capture conditional independence relations between a collection of variables $X_i, i \in I$; celebrated examples are Hidden Markov models and Bayesian Networks [1]. Graphical models are built from directed and undirected graphs $G = (I, A)$ where nodes $i \in I$ are uniquely identified with the variables X_i. Inference in graphical models ultimately boils down to inference for an undirected graphical model, achieved through the Belief Propagation algorithm [2]. Such Inference constitutes a specific instance of variational inference as it revolves around a free energy termed the Bethe free energy [2]. Adopting a variational inference perspective for graphical models has facilitated the extension of the Belief Propagation algorithm to encompass broader classes of probability distributions, enabling the accommodation of interactions among more than 2 variables in contrast to traditional graphical models (factor graphs [3]); this is achieved through the introduction of the Kikuchi free energies [4]. Let us denote $\mathbf{Mes}^f, \mathbf{Kern}^f$, the categories with objects finite measurable spaces and respectively with morphisms measurable maps and the second Markov Kernels (stochastic matrices). $\mathbf{Mes}^f$ can be seen as a subcategory of $\mathbf{Kern}^f$. As exhibited in [5–7], what underlies variational inference for those classes of probability distributions are presheaves from a finite poset to $\mathbf{Mes}^f$, which morphisms are epimorphisms. We will call them the 'graphical' presheaves. Our contribution is to extend the Generalized Belief Propagation [5] to any presheaf from a finite poset to $\mathbf{Kern}^f$. This work is contained in Chapter 9 of [8] and Appendix 1 of unpublished [9], where we consider the more general problem of optimizing a collection of cost functions over a presheaf of signals.

1. Motivation and related work

Consider a collection of agents represented by vertices $i \in I$ that can communicate their beliefs to neighboring vertices ∂i through undirected edges $e \in A$. Each agent has its own representation of its environment, denoted by E_i. They can share their beliefs with neighboring nodes $j \in \partial i$ through a measurable map $f_e^i : E_i \to E_e$. Graphical models and their extensions do not allow us to account for such heterogeneity in the way each agent models their environment. Such setting is better captured by cellular sheaves [10] and applications [11], important examples of which are Sheaf Neural Networks [12], are limited to functors from the poset associated to a graph ($i \le e \iff i \in e$) to the category of finite vector spaces $\mathbf{Vect}^f$. We are interested in the more general case where beliefs transfer through a hierarchy, i.e. a poset, and we provide an algorithm for inference in such case where Sheaf Neural Networks can't be used; by convention, we consider presheaves instead of functors: 'orders' are given top-down. More generally, cellular sheaves are restricted to the face poset of a cell complex and hence don't apply to all hierarchies and therefore not to our case.

2. Free energy for poset shaped diagrams in $\mathbf{Kern}^f$ and message passing algorithm

Definition 1 (Graphical presheaves). Let I be a finite set and $\mathscr{A} \subseteq \mathscr{P}(I)$ be a sub-poset of the powerset of I. Let $E_i, i \in I$ are finite sets. For $a \in \mathscr{A}$ $E_a := \prod_{i \in a} E_i$, let $F(a) := E_a$, and for $b \subseteq a$, let $F_b^a : E_a \to E_b$

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be the projection map from $\prod_{i\in a} E_i$ to $\prod_{i\in b} E_i$. F is called a graphical presheaf from $\mathscr{A}$ to $\mathbf{Mes}^f$.

For $\mathscr{A}$ a finite poset, the 'zeta-operator' of $\mathscr{A}$, denoted ζ, from $\bigoplus_{a\in\mathscr{A}}\mathbb{R}$ to $\bigoplus_{a\in\mathscr{A}}\mathbb{R}$ is defined as, for any $\lambda \in \bigoplus_{a\in\mathscr{A}}\mathbb{R}$ and any $a \in \mathscr{A}$, $\zeta(\lambda)(a) = \sum_{b\leq a}\lambda_b$. ζ is invertible [13], we denote μ its inverse; its matrix expression $(\mu(a,b), b \leq a)$ defines the Möbius function of $\mathscr{A}$. Let F be a presheaf from $\mathscr{A}$ to $\mathbf{Kern}^f$; $F_b^a : F(a) \to F(b)$ is denoted element-wise as $F_b^a(\omega_b|\omega_a)$, with $\omega_b \in F(b), \omega_a \in F(a)$. It induces a presheaf $\tilde{F}$ from $\mathscr{A}$ to $\mathbf{Vect}^f$, where $\tilde{F}_b^a : \mathbb{P}(F(a)) \to \mathbb{P}(F(b))$ is the linear map that sends probability distributions $p \in \mathbb{P}(F(a))$ to $F_b^a \circ p$. Following [5], we introduce a free energy $\mathscr{F}(Q) = \sum_{a\in\mathscr{A}} c(a)\,(\mathbb{E}_{Q_a}[H_a] - S(Q_a))$; $c(a) = \sum_{b\geq a}\mu(b,a)$ is the generalization of the inclusion-exclusion formula associated to $\mathscr{A}$. $S(Q_a) = -\sum_{\omega_a\in F(a)} Q_a(\omega_a)\ln Q_a(\omega_a)$ is the entropy of Q_a. We propose to solve $\inf_{Q\in\lim\tilde{F}}\mathscr{F}(Q)$. $\tilde{F}^*$ is the functor obtained by dualizing the morphisms $\tilde{F}_b^a$, i.e. $\tilde{F}_a^{*,b} : \tilde{F}(b)^* \to \tilde{F}(a)^*$ sends linear maps $l_b : \tilde{F}(b) \to \mathbb{R}$ to $l_b \circ \tilde{F}_b^a : \tilde{F}(a) \to \mathbb{R}$.

For a functor G from $\mathscr{A}$ to $\mathbb{R}$-vector spaces, we define μ_G as, for any $a \in \mathscr{A}$ and $v \in \bigoplus_{a\in\mathscr{A}} G(a)$, $\mu_G(v)(a) = \sum_{b\leq a}\mu(a,b)G_a^b(v_b)$. Let us define the function $FE : \prod_{a\in\mathscr{A}}\mathbb{P}(E_a) \to \prod_{a\in\mathscr{A}}\mathbb{R}$ as $FE(Q) = (\mathbb{E}_{Q_a}[H_a] - S_a(Q_a), a \in \mathscr{A})$, which sends a collection of probability measures over $\mathscr{A}$ to their Gibbs free energies. For any $Q \in \prod_{a\in\mathscr{A}}\mathbb{P}(E_a)$, let us denote $d_Q FE$ as the differential of FE at the point Q.

Theorem 1. *Let $\mathscr{A}$ be a finite poset, let F be a presheaf from $\mathscr{A}$ to $\mathbf{Kern}^f$. Let $H_a : F(a) \to \mathbb{R}$ be a collection of (measurable) functions. The critical points of $\mathscr{F}$ are the $Q \in \lim\tilde{F}$ such that,*

$$\mu_{\tilde{F}^*} d_Q FE|_{\lim\tilde{F}} = 0 \tag{1}$$

The message-passing algorithm we consider is Algorithm 1; it specializes to the General Belief Propagation for graphical presheaves. For two elements $a, b \in \mathscr{A}$, such that $b \leq a$, two types of messages are considered: top-down messages $m_{a\to b} \in \mathbb{R}^{F(b)}$ and bottom-up messages $n_{b\to a} \in \mathbb{R}^{F(a)}$.

Algorithm 1: Message passage algorithm for presheaves from $\mathscr{A}$ to $\mathbf{Kern}^f$

Data: Initialization: $(m_{a\to b}^0 \in \mathbb{R}^{F(b)}, b, a \in \mathscr{A}$ s.t. $b \leq a)$, a poset $\mathscr{A}$, a presheaf $F : \mathscr{A} \to \mathbf{Kern}^f$;

1 **for** $t \leq T$ **do**
2   **for** $a \in \mathscr{A}, b \in \mathscr{A}$ *such that* $b \leq a$ **do**
3         $\forall \omega_a \in F(a), \quad n_{b\to a}(\omega_a) \leftarrow \prod_{\substack{c:b\leq c \\ c\not\leq a}} \sum_{\omega_b'\in F(b)} m_{c\to b}(\omega_b') \cdot F_b^a(\omega_b'|\omega_a)$
4   **end**
5   **for** $a \in \mathscr{A}, b \in \mathscr{A}$ *such that* $b \leq a$ **do**
6         $b_a = e^{-H_a}\prod_{\substack{b\in\mathscr{A}:\\ b\leq a}} n_{b\to a}$
7         $p_a = \frac{b_a}{\sum_{\omega_a} b_a(\omega_a)}$
8         $m_{a\to b} \leftarrow m_{a\to b} \cdot \frac{\tilde{F}_b^a(p_a)}{p_b}$
9   **end**
10 **end**

A criterion to stop the algorithm is when the beliefs do not change, i.e., when $p_a^{t+1} \approx p_a^t$. The fixed points of the previous message-passing algorithm correspond to critical points of $\mathscr{F}$ over $\lim F$ (Corollary of Theorem 2.2 [9]v2). Theorem 1 differs from a similar characterization of critical points of a free energy for specifications in [14] by the fact that the $\mu_{\tilde{F}^*}$ and $\lim\tilde{F}$ are applied to the same presheaf $\tilde{F}$ and not two different presheaves/functors (G, F).

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