Belief propagation algorithm and graph zeta function

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Loopy Belief Propagation (LBP), or BP in short, is a successful method for approximating marginal distributions and partition functions of graphical models. For example, given a graphical model of the form

$$p(\boldsymbol{x}) \propto \prod_{ij \in E} \psi_{ij}(x_i, x_j) \prod_{i \in V} \psi_i(x_i), \quad G = (V, E)\text{: undirected graph,} \tag{1}$$

BP often gives good approximations of $p_{ij}(x_i, x_j) := \sum_{\boldsymbol{x} \setminus \{x_i, x_j\}} p(\boldsymbol{x})$, $p_i(x_i) := \sum_{\boldsymbol{x} \setminus \{x_i\}} p(\boldsymbol{x})$ and $Z := \sum_{\boldsymbol{x}} p(\boldsymbol{x})$.

BP is a message passing algorithm that has message vectors associated with the all directed edges of the graph. Roughly speaking, each messages are updated by those of neighboring edges at each step. These updates are repeated until the messages converge to a fixed point. If the graph G is a tree, the algorithm has the unique fixed point and gives exact marginals. However, if G has cycles, the algorithm may have multiple fixed points.

The well known property of BP is that the set of fixed points corresponds to the set of stationary points of the Bethe free energy (BFE) function [1]. The BFE function F is defined by

$$\begin{aligned} F(b) := &- \sum_{ij \in E} \sum_{x_i x_j} b_{ij}(x_i, x_j) \log \psi_{ij}(x_i, x_j) - \sum_{i \in V} \sum_{x_i} b_i(x_i) \log \psi_i(x_i) \\ &+ \sum_{ij \in E} \sum_{x_i x_j} b_{ij}(x_i, x_j) \log b_{ij}(x_i, x_j) + \sum_{i \in V} (1 - d_i) \sum_{x_i} b_i(x_i) \log b_i(x_i) \end{aligned} \tag{2}$$

on a convex set, called local polytope:

$$L(G) = \left\{ \{b_{ij}, b_i\} \middle| b_{ij}(x_i, x_j) > 0, \sum_{x_i, x_j} b_{ij}(x_i, x_j) = 1, \sum_{x_j} b_{ij}(x_i, x_j) = b_i(x_i) \right\}. \tag{3}$$

Note that d_i is the degree (number of neighboring vertices) of $i \in V$. The above correspondence tells us that, to understand the fixed points of BP, we can investigate on the BFE instead.

BFE is a computationally tractable approximation of the Gibbs free energy $F_{Gibbs}(\hat{p}) = \sum_{\boldsymbol{x}} \hat{p} \log(\hat{p}/p) - \log Z$, which is a convex function on the marginal polytope of G. $L(G)$ is a tractable relaxation of the marginal polytope. When G is a tree, BFE and $L(G)$ coincide with the Gibbs free energy and marginal polytope, but when G has cycles, these are just approximations.

We found the following formula which connects BP, BFE and graph zeta function. This formula shows that the breakdown of the convexity of BFE, which is described by the Hessian $\nabla^2 F$, is related to the graph zeta function. For the proof we derive and utilize the multivariate version of the Ihara-Bass formula [2].

Theorem 1 (Main Formula [2])**.** *The following equality holds at any point of $L(G)$:*

$$\zeta_G(\boldsymbol{u})^{-1} = \det(\nabla^2 F) \prod_{ij \in E} \prod_{x_i, x_j = \pm 1} b_{ij}(x_i, x_j) \prod_{i \in V} \prod_{x_i = \pm 1} b_i(x_i)^{1 - d_i} \; 2^{2N + 4M}, \tag{4}$$

where $\zeta_G(\boldsymbol{u})$ is the edge zeta function (multivariate graph zeta function) and $u_{i \to j}$ is the correlation coefficient of b_{ij}.

References

[1] J. S. Yedidia, W. T. Freeman, and Y. Weiss. Constructing free-energy approximations and generalized belief propagation algorithms. *IEEE Trans. on Info. Theo.*, 51(7):2282–2312, 2005.

[2] Y. Watanabe and K. Fukumizu. Graph zeta function in the Bethe free energy and loopy belief propagation. *Advances in Neural Information Processing Systems 23*, pages 2017–2025, 2009.

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