Available online at www.sciencedirect.com

ScienceDirect

Annals of Physics 323 (2008) 1899–1946

ANNALS of PHYSICS

www.elsevier.com/locate/aop

Quantum Graphical Models and Belief Propagation

M.S. Leifer [a,b], D. Poulin [c,*]

[a] *Institute for Quantum Computing, University of Waterloo, 200 University Avenue West, Waterloo Ont., Canada N2L 3G1*

[b] *Perimeter Institute for Theoretical Physics, 31 Caroline Street North, Waterloo Ont., Canada N2L 2Y5*

[c] *Center for the Physics of Information, California Institute of Technology, 1200 E. California Boulevard, 107-81, Pasadena, CA 91125, USA*

Received 21 September 2007; accepted 7 October 2007
Available online 12 October 2007

Abstract

Belief Propagation algorithms acting on Graphical Models of classical probability distributions, such as Markov Networks, Factor Graphs and Bayesian Networks, are amongst the most powerful known methods for deriving probabilistic inferences amongst large numbers of random variables. This paper presents a generalization of these concepts and methods to the quantum case, based on the idea that quantum theory can be thought of as a noncommutative, operator-valued, generalization of classical probability theory. Some novel characterizations of quantum conditional independence are derived, and definitions of Quantum n-Bifactor Networks, Markov Networks, Factor Graphs and Bayesian Networks are proposed. The structure of Quantum Markov Networks is investigated and some partial characterization results are obtained, along the lines of the Hammersley–Clifford theorem. A Quantum Belief Propagation algorithm is presented and is shown to converge on 1-Bifactor Networks and Markov Networks when the underlying graph is a tree. The use of Quantum Belief Propagation as a heuristic algorithm in cases where it is not known to converge is discussed. Applications to decoding quantum error correcting codes and to the simulation of many-body quantum systems are described.

Keywords: Quantum information; Markov Networks; Bayesian Networks; Factor Graphs; Graphoids; Belief Propagation; Sum–product; Quantum error correction; Quantum many-body systems

* Corresponding author. Fax: +1 626 568 2764.
E-mail addresses: matt@mattleifer.info (M.S. Leifer), dpoulin@ist.caltech.edu (D. Poulin).

0003-4916/$ - see front matter
doi:10.1016/j.aop.2007.10.001

1. Introduction

Quantum theory is first and foremost a calculus for computing the probabilities of outcomes of measurements made on physical systems. Therefore, the generic problem in quantum theory is one of probabilistic inference, i.e. given a specified class of quantum states, compute the predicted probabilities of measurement outcomes and their correlations. For example, computing the correlation functions of a system in the ground state of a Hamiltonian, or computing the probabilities for the possible measurement outcomes after implementing a quantum circuit, are problems of this general type. Such quantum inferences present a formidable computational challenge as the number of subsystems becomes large, since the number of parameters needed to specify a quantum state grows exponentially with the number of subsystems, and the formulas for quantities of interest typically also involve an exponentially large number of terms.

A similar problem arises in classical probabilistic inference, since the number of terms required to specify a general probability distribution also grows exponentially with the number of random variables involved. A variety of algorithms for classical probabilistic inference have been discovered, of which Belief Propagation algorithms on Graphical Models are amongst the most powerful. Such algorithms are particularly interesting for two reasons. Firstly, they are highly parallelizable in the sense that they can be implemented by associating each random variable with a separate processor. Messages are received and sent by the processors along the links of a network corresponding to the edges of a graph and, importantly, the order in which the messages arrive does not matter. Secondly, Belief Propagation performs remarkably well as a heuristic algorithm, even in cases where it is not guaranteed to converge to the exact solution. Important examples include the near optimal decoding of low density [14] and turbo [8] error correction codes, spin glass models [33], and random satisfiability problems [34]. Understanding the reasons for this is currently an active area of research, but it is understood [58] to be related to a hierarchy of approximation schemes commonly used in statistical physics.

Due to the similarity between the classical and quantum problems, one might hope to leverage the power of Belief Propagation in the quantum case also, especially since quantum theory can be regarded as a noncommutative generalization of classical probability theory. This is indeed the case, and in this paper we develop the necessary theory of Quantum Belief Propagation and its associated Graphical Models.

This paper should be of interest to researchers in Graphical Models and Belief Propagation, as well as to researchers in quantum theory, particularly in quantum information and the simulation of quantum many-body systems. As such, it is intended to be as self-contained as possible, although we do assume familiarity with the basic formalism of quantum theory on finite dimensional Hilbert spaces, including the theory of density matrices, generalized measurements and completely positive maps, as used in quantum information theory. These are covered in detail in the textbook of Nielsen and Chuang [38], as well as in Preskill's lecture notes [43]. For further background on classical Graphical Models and Belief Propagation, we suggest the texts of Lauritzen [24], MacKay [31], and Neapolitan [36,37], as well as the review articles by Yedida et al. [58,59] and Aji and McEliece [6].

The remainder of this paper is structured as follows. In Section 2, the generic classical and quantum probabilistic inference problems are defined. In Section 3, we review the notions of classical and quantum conditional independence, which are crucial for the