

Markov Entanglement Networks

Pierfrancesco La Mura and Lukasz Swiatczak

HHL-Leipzig Graduate School of Management
Jahnallee 59, 04109 Leipzig, Germany

Abstract

Graphical models of probabilistic dependencies have been extensively investigated in the context of classical uncertainty. However, in some domains (most notably, in computational physics and quantum computing) the nature of the relevant uncertainty is non-classical, and the laws of classical probability theory are superseded by those of quantum mechanics. In this paper we introduce Markov Entanglement Networks (MEN), a novel class of graphical representations of quantum-mechanical dependencies in the context of such non-classical systems. MEN are the quantum-mechanical analogue of Markovian Networks, a family of undirected graphical representations which, in the classical domain, exploit a notion of conditional independence among subsystems.

After defining a notion of conditional independence appropriate to our domain (*conditional separability*), we prove that the conditional separabilities induced by a quantum-mechanical wave function are effectively reflected in the graphical structure of MEN. Specifically, we show that for any wave function there exists a MEN which is a *perfect map* of its conditional separabilities. Next, we show how the graphical structure of MEN can be used to effectively classify the pure states of three-qubit systems. We also demonstrate that, in large systems, exploiting conditional independencies may dramatically reduce the computational burden of various inference tasks. In principle, the graph-theoretic representation of conditional independencies afforded by MEN may not only facilitate the classical simulation of quantum systems, but also provide a guide to the efficient design and complexity analysis of quantum algorithms and circuits.

Introduction

Probabilistic inference in large systems is a topic of great interest in computer science. In contexts where the underlying uncertainty is of classical nature, the graphical representation of probabilistic dependencies and independencies has proved to be a valuable tool in order to reduce the computational burden of various inference tasks (Pearl 1988). Two main classes of graphical representations are of special interest in the classical domain. Bayesian Networks (BN) are based on directed, acyclic graphs which capture causal dependencies among variables of interest. By contrast, Marko-

vian Networks¹ (MN) are non-causal representations based on undirected graphs, which encode mutual symmetric dependencies among the variables of interest. Whereas the BN formalism is especially convenient at the modeling stage, as causal dependencies among variables of interest are more easily identified, the structure of MN is particularly advantageous from a computational viewpoint. In particular, several algorithms for probabilistic inference in BN require as a first step the transformation of the original BN into a corresponding MN (*e.g.*, the junction tree algorithm).

Recently, there has been some interest in the graphical representation of non-classical uncertain domains, most notably in the context of computational physics and quantum computing. (Tucci 1997) introduced Quantum Bayesian Networks (QBN), which provide a structured representation of quantum-mechanical wave functions along the lines of classical BN.

Missing a quantum-mechanical generalization of MN, the algorithmic toolbox of QBN is significantly more limited than that of BN. Also motivated by such limitations, we introduce a novel class of undirected networks, Markov Entanglement Networks (MEN), which extends the formalism and computational gains of MN to quantum-mechanical systems.

We also introduce a novel notion of conditional independence appropriate to the context of entangled systems (*conditional separability*), which generalizes the classical notion of conditional probabilistic independence, and provides a rigorous semantics for our graphical framework.

While in applications which only involve classical uncertainty the computational performance of MEN is equivalent to that of MN, many of the computational benefits of the modular structure of MN carry over to MEN even in applications characterized by non-classical uncertainty. In particular, the graphical structure of MEN can in principle be exploited in the context of classical simulations of quantum-mechanical systems (*e.g.*, protein folding), and as a guide

¹The word *Markovian* in graphical representations does not relate directly to Markov processes (a family of stochastic processes in which the probability distribution of future states for a given history only depends upon the current state, *i.e.*, future states are conditionally independent of past states given the present state) but rather to the Markovian property of conditional independence of a random variable from all other variables given its neighbors.

to the efficient design and complexity analysis of quantum algorithms and circuits.

The paper is organized as follows. In the second section we introduce conditional separability, and relate it with both separability and the classical notion of conditional probabilistic independence. In the third section we formally introduce MEN, and discuss some of their structural properties. In particular, we show that the conditional separabilities induced by any wave function are precisely characterized by the graphical structure of an appropriately selected MEN. In the fourth section we address the issue of probabilistic inference, showing how marginal and conditional probabilities can be effectively recovered from the structural elements of MEN, and discussing the computational performance of MEN in the context of some typical inference tasks. The fifth section provides a classification of 3-qubit states based on their network topologies, while the last section concludes.

Setting, a -Independence, Separability, Conditional Separability

Let us first introduce the notion of a *quantum bit (qubit)*, the fundamental unit of quantum information, which can be thought of as a quantum mechanical analogue of a classical data bit. A *state* of a quantum bit is represented by a vector in a two-dimensional complex Hilbert space. The two computational basis states are conventionally written as $|0\rangle$ and $|1\rangle$, and form an orthonormal basis² for the Hilbert space. A qubit state is a superposition of those basis states:

$$|\psi\rangle = a(|0\rangle)|0\rangle + a(|1\rangle)|1\rangle,$$

where $a(|0\rangle)$ and $a(|1\rangle)$ are complex numbers denoting probability amplitudes in the directions given by $|0\rangle$ and $|1\rangle$, respectively. These amplitudes are normalized so that their Euclidean norm is unitary, *i.e.* $|a(|0\rangle)|^2 + |a(|1\rangle)|^2 = 1$. The reason is that the probabilities that the qubit will be observed in states $|0\rangle$ and $|1\rangle$, respectively, are represented by the square moduli $|a(|0\rangle)|^2$ and $|a(|1\rangle)|^2$, so with normalized amplitudes the total probability that the qubit is observed to be in either state $|0\rangle$ or $|1\rangle$ is 1. For notational convenience, in the remainder of this paper we shall give up the bra-ket notation $|\cdot\rangle$ and always write x in place of $|x\rangle$.

A general state (*wave function*) of an n -qubit system takes the following form:

$$\psi_N = \sum_{x \in X} a(x)x,$$

where:

²An orthonormal basis of a vector space V equipped with inner product $\langle \cdot, \cdot \rangle$ is a subset $\{v_1, \dots, v_k\}$ of V which spans the whole space, and is such that $(\forall i, j) [\langle v_i, v_j \rangle = \delta_{ij}]$, where δ_{ij} is the Kronecker Delta.

- $N = \{1, \dots, n\}$ is a set of n qubits,
- $x = x_1 \otimes \dots \otimes x_n$ is a vector in an orthonormal basis X of the n -qubit system, while each $x_i \in \{0, 1\}$ is an orthonormal basis of the i -th qubit, $i = 1, \dots, n$, and³
- $a(x)$ is a complex number denoting the probability amplitude of the n -qubit system in the direction given by x

A state of a quantum system is said to be *pure* if the squared moduli of the probability amplitudes sum up to one; formally, $\sum_{x \in X} |a(x)|^2 = 1$. In this paper we deal only with pure states, while deferring the case of mixed states⁴ to future work.

A composite system is said to be *separable* (or *not entangled*) if its states can be written as tensor products of pure states of the component systems (Nielsen and Chuang 2000). Intuitively, the subsystems do not interact with each other, so they can be considered separately. This implies probabilistic independence between subsets of random variables across such non-interacting subsystems. Formally,

$$\psi_N = \psi_{M, N-M} = \psi_M \otimes \psi_{N-M}.$$

Let $\{X_i\}_{i \in N}$ be a finite, ordered set of Boolean random variables representing the possible realizations of the n qubits, and let $x_N^0 = (x_1^0, \dots, x_n^0)$, where x_i^0 is a given realization of the i -th random variable, be an arbitrary reference point.⁵ A joint realization $x_N = (x_1, \dots, x_n)$ corresponds to a *basis state* of the composite n -qubit system. For any $M \subset N$ we denote by \overline{M} the set $N - M$, and by X_M the set $\{X_i\}_{i \in M}$.

Finally, we define a notion of a -independence which, as we shall see, is equivalent to separability.

Two sets of qubits, M and \overline{M} , are said to be a -independent if the following condition is satisfied for all x_M and $x_{\overline{M}}$:

$$a(x_M, x_{\overline{M}})a(x_M^0, x_{\overline{M}}^0) = a(x_M^0, x_{\overline{M}})a(x_M, x_{\overline{M}}^0).$$

Theorem 1 *Two subsystems M and \overline{M} are a -independent if and only if they are separable. Formally,*

$$\forall (x_N) \left[a(x_M, x_{\overline{M}})a(x_M^0, x_{\overline{M}}^0) = a(x_M^0, x_{\overline{M}})a(x_M, x_{\overline{M}}^0) \right] \\ \Leftrightarrow \psi_N = \psi_M \otimes \psi_{\overline{M}}.$$

Proof. We prove *Theorem 1* through a two-step procedure. We first show that separability of the two subsystems implies their a -independence. Next we show the converse,

³The notation $v \otimes u$ stands for the tensor product of two vectors v and u .

⁴A mixed state is a classical probability distribution over pure states. Mixed states are conventionally represented by a density matrix ρ (*i.e.*, a self-adjoint, positive-semidefinite matrix of trace one) with $\text{Tr}(\rho^2) < 1$.

⁵We always use capital letters to denote random variables, and small letters to denote their realizations.

namely that a -independence implies separability. The two steps are sufficient to conclude the proof.

Step 1. separability $\implies a$ -independence

If the two subsystems, X_M and $X_{\overline{M}}$, are separable then we know that $\psi_N = \psi_M \otimes \psi_{\overline{M}}$. Let us write each of these wave functions in vector form

$$\psi_F = \begin{pmatrix} a(x_F^1) \\ \vdots \\ a(x_F^{2^{|F|}}) \end{pmatrix}$$

where $|F|$ is the cardinality of set F , and $2^{|F|}$ is the number of basis states of the $|F|$ -qubit system.

Next, we rewrite the separability condition in the following form

$$\begin{pmatrix} a(x_N^1) \\ \vdots \\ a(x_N^{2^{|N|}}) \end{pmatrix} = \begin{pmatrix} a(x_M^1) \\ \vdots \\ a(x_M^{2^{|M|}}) \end{pmatrix} \otimes \begin{pmatrix} a(x_{\overline{M}}^1) \\ \vdots \\ a(x_{\overline{M}}^{2^{|M|}}) \end{pmatrix}$$

or, equivalently,

$$\begin{pmatrix} a(x_M^1, x_{\overline{M}}^1) \\ \vdots \\ a(x_M^1, x_{\overline{M}}^{2^{|M|}}) \\ \vdots \\ a(x_M^{2^{|M|}}, x_{\overline{M}}^{2^{|M|}}) \end{pmatrix} = \begin{pmatrix} a(x_M^1)a(x_{\overline{M}}^1) \\ \vdots \\ a(x_M^1)a(x_{\overline{M}}^{2^{|M|}}) \\ \vdots \\ a(x_M^{2^{|M|}})a(x_{\overline{M}}^{2^{|M|}}) \end{pmatrix}$$

It is straightforward to verify that the following condition must then hold:

$$a(x_M^i, x_{\overline{M}}^j)a(x_M^{i'}, x_{\overline{M}}^{j'}) = a(x_M^{i'}, x_{\overline{M}}^j)a(x_M^i, x_{\overline{M}}^{j'})$$

for all $x_M^i, x_M^{i'}, x_{\overline{M}}^j$ and $x_{\overline{M}}^{j'}$. In particular, the condition must hold true when $x_M^{i'} = x_M^0$ and $x_{\overline{M}}^{j'} = x_{\overline{M}}^0$. It follows that separability implies a -independence.

Step 2. a -independence \implies separability

Let us define the two following functions: $\alpha(x_M) = a(x_M, x_M^0)$ for all x_M , and $\beta(x_{\overline{M}}) = a(x_M^0, x_{\overline{M}})$ for all $x_{\overline{M}}$. In order to prove that a -independence implies separability one needs to show that the state of a composite system can be factorized into appropriate states of the component systems. We show that if two systems are a -independent then the state of its composite system can be factorized in the following way:

$$\psi_N = \frac{1}{a(x_N^0)} \alpha \otimes \beta \quad (\spadesuit)$$

where $a(x_N^0)$ stands for the amplitude of the arbitrary reference point x_N^0 , which without loss of generality we assume

to be non-zero, and α (*resp.* β) is a vector of $\alpha(x_M)$ (*resp.* $\beta(x_{\overline{M}})$) for all x_M (*resp.* $x_{\overline{M}}$).

In vector notation, the right-hand side of equation (\spadesuit) assumes the form

$$\frac{1}{a(x_N^0)} \begin{pmatrix} \alpha(x_M^1) \\ \vdots \\ \alpha(x_M^{2^{|M|}}) \end{pmatrix} \otimes \begin{pmatrix} \beta(x_{\overline{M}}^1) \\ \vdots \\ \beta(x_{\overline{M}}^{2^{|M|}}) \end{pmatrix}$$

which can be rearranged as

$$\psi_N = \frac{1}{a(x_N^0)} \begin{pmatrix} \alpha(x_M^1)\beta(x_{\overline{M}}^1) \\ \vdots \\ \alpha(x_M^1)\beta(x_{\overline{M}}^{2^{|M|}}) \\ \vdots \\ \alpha(x_M^{2^{|M|}})\beta(x_{\overline{M}}^{2^{|M|}}) \end{pmatrix} \quad (\clubsuit)$$

Utilizing the definitions of $\alpha(\cdot)$ and $\beta(\cdot)$, we obtain

$$\forall(i, j) \left[\alpha(x_M^i)\beta(x_{\overline{M}}^j) = a(x_M^i, x_{\overline{M}}^0)a(x_M^0, x_{\overline{M}}^j) \right].$$

By a -independence of systems M and \overline{M} , one has that

$$\forall(i, j) \left[a(x_M^i, x_{\overline{M}}^0)a(x_M^0, x_{\overline{M}}^j) = a(x_M^i, x_{\overline{M}}^j)a(x_M^0, x_{\overline{M}}^0) \right],$$

which can then be rewritten as

$$\forall(i, j) \left[\alpha(x_M^i)\beta(x_{\overline{M}}^j) = a(x_M^i, x_{\overline{M}}^j)a(x_N^0) \right].$$

Applying this condition to equation (\clubsuit) one arrives at

$$\begin{pmatrix} a(x_M^1, x_{\overline{M}}^1) \\ \vdots \\ a(x_M^1, x_{\overline{M}}^{2^{|M|}}) \\ \vdots \\ a(x_M^{2^{|M|}}, x_{\overline{M}}^{2^{|M|}}) \end{pmatrix}$$

which is the state of the composite system, ψ_N . \blacksquare

The above characterization of separability via a -independence makes it possible to introduce in a natural way a notion of *conditional separability*, defined as follows. Let $\{A, B, C\}$ be a partition of N into non-empty subsets. We say that A and B are *conditionally separable* given C if

$$\begin{aligned} \forall(x_N) [a(x_A, x_B, x_C)a(x_A^0, x_B^0, x_C) \\ = a(x_A^0, x_B, x_C)a(x_A, x_B^0, x_C)]. \end{aligned}$$

Theorem 2 *Conditional separability implies conditional probabilistic independence.*

Proof. Observe that conditional probabilistic independence of X_A and X_B given X_C can be expressed as

$$\forall(x_N) [p(x_A|x_B, x_C) = p(x_A|x_B^0, x_C)],$$

where

$$p(x_A|x_B, x_C) = \frac{p(x_A, x_B, x_C)}{\sum_{x_A} p(x_A, x_B, x_C)}.$$

In terms of probability amplitudes, this condition takes the following form:

$$p(x_A|x_B, x_C) = \frac{|a(x_A, x_B, x_C)|^2}{\sum_{x_A} |a(x_A, x_B, x_C)|^2}.$$

By multiplying the above fraction's numerator and denominator by $|a(x_A^0, x_B^0, x_C)|^2$ and by the fact that $|c_1||c_2| = |c_1 c_2|$, where $c_1, c_2 \in \mathbb{C}$, we obtain

$$p(x_A|x_B, x_C) = \frac{|a(x_A, x_B, x_C)a(x_A^0, x_B^0, x_C)|^2}{\sum_{x_A} |a(x_A, x_B, x_C)a(x_A^0, x_B^0, x_C)|^2}$$

Next, from conditional separability of A and B given C , one obtains that

$$\begin{aligned} p(x_A|x_B, x_C) &= \frac{|a(x_A^0, x_B, x_C)a(x_A, x_B^0, x_C)|^2}{\sum_{x_A} |a(x_A^0, x_B, x_C)a(x_A, x_B^0, x_C)|^2} \\ &= \frac{|a(x_A^0, x_B, x_C)|^2 |a(x_A, x_B^0, x_C)|^2}{|a(x_A^0, x_B, x_C)|^2 \sum_{x_A} |a(x_A, x_B^0, x_C)|^2} \\ &= \frac{|a(x_A, x_B^0, x_C)|^2}{\sum_{x_A} |a(x_A, x_B^0, x_C)|^2} \end{aligned}$$

Observing that the latter term is equal to $p(x_A|x_B^0, x_C)$ concludes the proof. ■

Finally, we introduce a potential function that we shall utilize in defining Markov Entanglement Networks. Following the approach of (La Mura and Shoham 1999), we define the *amplitude potential function* (q -function) as follows:

$$q(x_M|x_{\overline{M}}) = \frac{a(x_M, x_{\overline{M}})}{a(x_M^0, x_{\overline{M}})}.$$

The q -function, whenever it is well defined, can be interpreted in terms of *ceteris paribus* comparisons: it describes how the probability amplitude changes when the qubits in M are shifted away from the reference point, while the values of those in \overline{M} are held unchanged at $x_{\overline{M}}^0$.

Note that, whenever q is well defined, the condition $\forall(x_N)[q(x_A|x_B, x_C) = q(x_A|x_B^0, x_C)]$ exactly corresponds to conditional separability of A and B given C , in which case we shall simply write $q(x_A|x_C)$ in place of $q(x_A|x_B, x_C)$.

Markov Entanglement Networks: a formal definition

We define a Markov Entanglement Network as an undirected graph $G(V, E)$ with vertices $v \in V$ representing quantum-mechanical subsystems,⁶ and edges $\{v, u\} \in E$ representing quantum entanglement between vertices v and u . Each node is associated with a non-zero function $q(x_i|x_{U(i)})$ (as defined in the previous section), where $U(i)$ denotes the set of nodes directly connected to v_i (i.e., i) via entanglement edges (or *neighbors*). Figure 1 depicts a simple MEN.

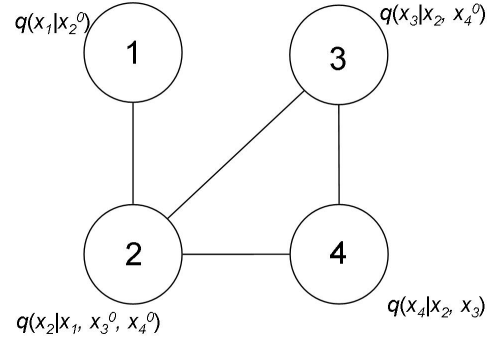


Figure 1: A simple MEN. Nodes represent qubits, and edges the fact that two qubits are entangled.

If the q -functions are specified directly, then any arbitrary assignment of non-zero complex-valued functions $q(x_i|x_{U_-(i)}, x_{U_+(i)}^0)$ for all i (where $U_+(i)$ denotes the set of all qubits in $U(i)$ whose index is greater than i , and $U_-(i) = U(i) - U_+(i)$) uniquely identifies a corresponding wave function, up to the phase of the reference point. In fact, once all the q -functions are specified, the relative amplitudes $a(x_N)/a(x_N^0)$ are determined as follows:

$$\begin{aligned} \frac{a(x_N)}{a(x_N^0)} &= \frac{a(x_1, x_R)}{a(x_1^0, x_R)} \frac{a(x_N)}{a(x_1, x_R^0)} \\ &= q(x_1|x_{U_-(1)}, x_{U_+(1)}^0) \frac{a(x_1, x_2, x_{R'})}{a(x_1, x_2^0, x_{R'}^0)} \frac{a(x_N)}{a(x_1, x_2, x_{R'}^0)} \\ &= q(x_1|x_{U_-(1)}, x_{U_+(1)}^0) q(x_2|x_1, x_{U_+(2)}^0) \frac{a(x_N)}{a(x_1, x_2, x_{R'}^0)} \\ &= \dots = \prod_i q(x_i|x_{U_-(i)}, x_{U_+(i)}^0), \end{aligned}$$

where $x_R, x_{R'}$ denote the realizations of the remaining qubits in the appropriate context.

Since the state of the composite n -qubit system is pure, we obtain the following condition:

$$\sum_{x_N} \left| \prod_i q(x_i|x_{U_-(i)}, x_{U_+(i)}^0) a(x_N^0) \right|^2 = 1.$$

⁶For simplicity of exposition, we proceed under the assumption that each node represents a single quantum bit.

Performing some elementary algebra, we conclude that

$$|a(x_N^0)| = \frac{1}{\sqrt{\sum_{x_N} \left| \prod_i q(x_i | x_{U-(i)}, x_{U+(i)}^0) \right|^2}}.$$

From the last condition follows that only the the modulus, but not the phase, of the reference amplitude $a(x_N^0)$ is identified, which means that the corresponding wave function is only identified up to the phase of the reference point. Conversely, any wave function in a given computational basis can be represented by an appropriately selected MEN, as long as all the amplitudes are non-zero.

We remark that, if $q(x_i | x_{N-\{i\}})$ only depends on $x_{U(i)}$, then fixing $x_{U(i)}$ completely specifies the behavior of the wave function along the i -th coordinate (up to the phase of the reference point), and that such behavior does not depend on the specific values taken by the remaining variables.

It turns out that node separation with respect to MEN characterizes all the implied conditional separabilities. More precisely, for any wave function there exists an undirected graph G such that, for any partition of N into three non-empty sets of quantum bits A , B , and C , A is conditionally separable from B given C if, and only if, C separates A from B in graph G , i.e., every path from a node in A to a node in B passes through some node in C . In the terminology of (Pearl and Paz 1987), such a graph is said to be a *perfect map* of the independence structure.

Theorem 3 *The set of conditional separabilities generated by any wave function has a perfect map.*

Proof. We appeal to a necessary and sufficient condition in (Pearl and Paz 1987). Specifically, we check whether conditional separability satisfies the following five properties: symmetry, decomposition, intersection, strong union and transitivity.

Let A, B, C, D, R, R', R'' be subsets of qubits, where R, R', R'' denote the subset of remaining qubits in the appropriate context.

For the purpose of this proof, let us say that A is conditionally independent of B given C , and write $I(A, B|C)$ if and only if

$$(\forall x_N) [a(x_A, x_B, x_C, x_R) a(x_A^0, x_B^0, x_C, x_R) = a(x_A^0, x_B, x_C, x_R) a(x_A, x_B^0, x_C, x_R)]$$

Then the following properties hold.

Symmetry: $I(A, B|C) \Rightarrow I(B, A|C)$.

This follows trivially from the definition of conditional independence. Specifically, $I(A, B|C) \Leftrightarrow I(B, A|C)$.

Decomposition: $I(A, B \cup D|C) \Rightarrow I(A, B|C) \wedge I(A, D|C)$.

This is equivalent to

$$[a(x_A, x_B, x_C, x_D, x_R) a(x_A^0, x_B^0, x_C, x_D^0, x_R) = a(x_A^0, x_B, x_C, x_D, x_R) a(x_A, x_B^0, x_C, x_D^0, x_R)] \Rightarrow$$

$$\begin{aligned} & [a(x_A, x_B, x_C, x_{R'}) a(x_A^0, x_B^0, x_C, x_{R'}) = a(x_A^0, x_B, x_C, x_{R'}) a(x_A, x_B^0, x_C, x_{R'})] \wedge \\ & [a(x_A, x_C, x_D, x_{R''}) a(x_A^0, x_C, x_D^0, x_{R''}) = a(x_A^0, x_C, x_D, x_{R''}) a(x_A, x_C, x_D^0, x_{R''})]. \end{aligned}$$

This follows trivially, since $R' = (D, R)$ and $R'' = (B, R)$.

Intersection:

$$I(A, B|C \cup D) \wedge I(A, D|B \cup C) \Rightarrow I(A, B \cup D|C).$$

Equivalently,

$$\begin{aligned} & [a(x_A, x_B, x_C, x_D, x_R) a(x_A^0, x_B^0, x_C, x_D, x_R) = a(x_A^0, x_B, x_C, x_D, x_R) a(x_A, x_B^0, x_C, x_D, x_R)] \wedge \\ & [a(x_A, x_B, x_C, x_D, x_R) a(x_A^0, x_B, x_C, x_D^0, x_R) = a(x_A^0, x_B, x_C, x_D, x_R) a(x_A, x_B, x_C, x_D^0, x_R)] \Rightarrow \\ & [a(x_A, x_B, x_C, x_D, x_R) a(x_A^0, x_B^0, x_C, x_D^0, x_R) = a(x_A^0, x_B, x_C, x_D, x_R) a(x_A, x_B^0, x_C, x_D^0, x_R)]. \end{aligned}$$

This follows quite easily by algebraic manipulation.

Strong union: $I(A, B|C) \Rightarrow I(B, A|C \cup D)$.

Equivalently,

$$\begin{aligned} & [a(x_A, x_B, x_C, x_R) a(x_A^0, x_B^0, x_C, x_R) = a(x_A^0, x_B, x_C, x_R) a(x_A, x_B^0, x_C, x_R)] \Rightarrow \\ & [a(x_A, x_B, x_C, x_D, x_{R'}) a(x_A^0, x_B^0, x_C, x_D, x_{R'}) = a(x_A^0, x_B, x_C, x_D, x_{R'}) a(x_A, x_B^0, x_C, x_D, x_{R'})]. \end{aligned}$$

This follows by symmetry, and the fact that $R = (D, R')$.

Transitivity: $I(A, B|C) \Rightarrow I(A, V|C) \vee I(B, V|C)$

where V is one qubit. This is equivalent to

$$\begin{aligned} & [a(x_A, x_B, x_C, x_R) a(x_A^0, x_B^0, x_C, x_R) = a(x_A^0, x_B, x_C, x_R) a(x_A, x_B^0, x_C, x_R)] \Rightarrow \\ & [a(x_A, x_C, x_V, x_{R'}) a(x_A^0, x_C, x_V^0, x_{R'}) = a(x_A^0, x_C, x_V, x_{R'}) a(x_A, x_C, x_V^0, x_{R'})] \vee \\ & [a(x_B, x_C, x_V, x_{R''}) a(x_B^0, x_C, x_V^0, x_{R''}) = a(x_B^0, x_C, x_V, x_{R''}) a(x_B, x_C, x_V^0, x_{R''})]. \end{aligned}$$

which follows by observing that V is either an element of A , or B , or R .

Thus, we appeal to Pearl and Paz's result to conclude the proof. ■

The relevance of this result lies in the fact that one can represent and reason about conditional separabilities graphically (i.e., one can exploit the graphical structure of the perfect map to reason about conditional separabilities).

Exact Probabilistic Inference in MEN

Markov entanglement networks contain information about quantum probabilistic dependencies, but the information is not explicit. It is encoded in the potential functions, together with the topological structure of the network. The basic operation of computing marginal probabilities, and hence conditional probabilities, can be reduced to manipulations of the wave potentials. In fact, one readily obtains $p(x_M)/p(x_N^0)$ (where $p(x_M)$ is the marginal probability of obtaining x_M) by summing up the squared moduli of the q -functions:

$$\frac{p(x_M)}{p(x_N^0)} = \sum_{x_{N-M}} \left| \prod_i q(x_i | x_{U-(i)}, x_{U+(i)}^0) \right|^2.$$

The computational performance of MEN in evaluating probabilistic queries is similar to that of MN. In particular, as in the case of MN, exact inference in singly-connected networks⁷ can be performed in time linear in the number of nodes. We provide time-complexity analyses for some basic inference tasks in the simplest singly-connected networks, chains (Figure 2).

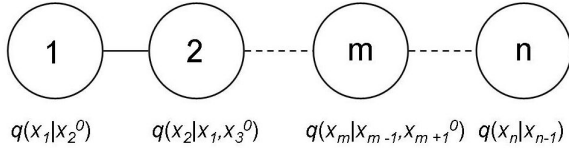


Figure 2: A MEN chain.

Specifically, we consider three types of queries: (i) computing marginal probabilities, (ii) computing conditional probabilities given evidence, and (iii) finding a maximum likelihood instantiation.

(i) Computing marginal probability ratios takes the following form:

$$\frac{p(x_M)}{p(x_N^0)} = \sum_{x_{N-M}} \left| \prod_i q(x_i | x_{i-1}, x_{i+1}^0) \right|^2.$$

The right-hand side of the above formula can be rearranged as follows:

$$\sum_{x_{N-M}} \prod_{i=1}^m q(x_i | x_{i-1}, x_{i+1}^0) q(x_{m+1} | x_m, x_{m+2}^0) \cdots q(x_n | x_{n-1})^2$$

We assume, for simplicity, that $M \subseteq N$ is the set of qubits with indices from 1 to m , whereas in $N - M$ are all the qubits with higher indices. Hence, the following holds:

$$\sum_{x_{m+1}} \cdots \sum_{x_n} \left| \prod_{i=1}^m q(x_i | x_{i-1}, x_{i+1}^0) \cdots q(x_n | x_{n-1}) \right|^2 =$$

⁷A network is said to be *singly connected* if, in the associated graph, there exists at most one path between any two nodes.

$$\prod_{i=1}^m |q(x_i | x_{i-1}, x_{i+1}^0)|^2 \sum_{x_{m+1}} |q(x_{m+1} | x_m, x_{m+2}^0)|^2 \cdots \cdots \sum_{x_n} |q(x_n | x_{n-1})|^2.$$

The above decomposition makes it possible to compute the marginal probability of interest performing $6(n - m) + 2m - 1$ operations. Thus, the time complexity of this task is linear in the number of qubits n .

(ii) Computing conditional probabilities given some evidence x_M takes the form

$$p(x_{N-M} | x_M) = \frac{p(x_M, x_{N-M})}{p(x_M)} = \frac{p(x_M, x_{N-M})/p(x_N^0)}{p(x_M)/p(x_N^0)}.$$

Since the computation of marginal probability ratios has linear time complexity, this is also the case for the computation of conditional probabilities.

(iii) Finding a maximum likelihood instantiation takes the form

$$\begin{aligned} \operatorname{argmax}_{x_N} |a(x_N)|^2 &\Leftrightarrow \operatorname{argmax}_{x_N} \left| \prod_i q(x_i | x_{i-1}, x_{i+1}^0) \right|^2 \\ &= \operatorname{argmax}_{x_1} \cdots \operatorname{argmax}_{x_n} |q(x_1 | x_2^0) \cdots q(x_n | x_{n-1})|^2 \\ &= \operatorname{argmax}_{x_1} |q(x_1 | x_2^0)|^2 \cdots \operatorname{argmax}_{x_n} |q(x_n | x_{n-1})|^2 \end{aligned}$$

Thanks to the exploitation of conditional separabilities, the problem enjoys a decomposition which, once again, allows to find a solution in time linear in the number of qubits. Specifically, a global maximum can be found by solving a sequence of n simpler maximization problems.

MEN for 3-qubit systems

From Theorem 3, we know that all conditional separabilities induced by any given wave function can be encoded in the graphical layer of an appropriately chosen MEN. In the case of a two-qubit system, the dependencies generated are trivial: either the two qubits are entangled, or separable. Hence, for two-qubit systems there are only two classes of MEN topologies: one with connected, and one with unconnected nodes. Since in two-qubit systems conditional separability plays no role, in this section we investigate conditional separabilities in the context of the simplest interesting class: three-qubit systems. First, following (Duer, Vidal, and Cirac 2006), we classify states of such systems into equivalence classes under orthonormal basis changes. Next, we analyze the topological properties of the corresponding MEN, and what structural changes they undergo once we instantiate (measure) a component qubit.

(Duer, Vidal, and Cirac 2006) classifies three-qubit system states into fully entangled (*i.e.*, states of composite systems, in which no component system is separable) and not fully entangled. Each of these classes is comprised of two subclasses. The first one contains GHZ-like and W -like states, while the second contains completely separable (*i.e.*, there is no entanglement present) and bi-separable states (*i.e.*, two qubits are entangled and separable from the remaining one).

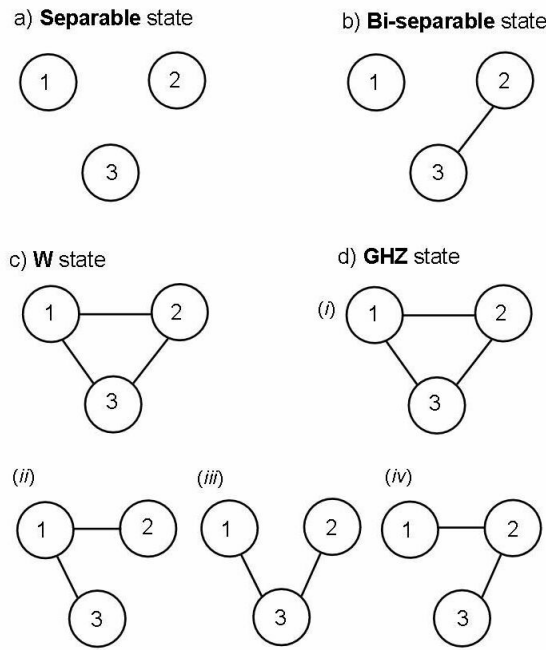


Figure 3: MEN for all states classes of 3-qubit systems.

The classification is robust with respect to local operations: in particular, by means of basis changes no state in one class can be obtained from a state in a different class. It is a natural question whether these four classes of three-qubit states can be characterized purely in terms of their MEN topology.

All possible MEN topologies corresponding to the four classes of three-qubit states are summarized in Figure 3. One can easily see that the MEN topology of all classes except for GHZ is invariant under basis changes. However, in the case of GHZ states, there exist bases in which the MEN graph assumes each of the configurations in Figure 3(d) (i.e. the complete graph, or any permutation of a three-node chain). In passing, we observe that conditional separabilities, unlike unconditional ones, are not preserved under basis changes. We conclude that the four classes of three-qubit system states introduced above are completely characterized by the topology of their associated MEN.

Next, we move on to the issue of measurement and its impact on MEN topology. Measuring (instantiating) a qubit collapses the wave function along one of the qubit's basis states, destroying any entanglement with the remaining qubits. This has an impact on MEN topology: specifically, after measuring a qubit, the MEN graph in the new state is obtained by erasing all the edges which involve the measured qubit. While measurement may destroy edges, it never introduces new ones, as conditional separabilities are always preserved under qubit instantiation.

Conclusions

We introduced Markov Entanglement Networks, a novel class of graphical representations for quantum-mechanical

systems, and argued that the modular representation of quantum-mechanical states gives rise to computational advantages analogous to those afforded by classical Markovian Networks. We also showed that, based on MEN topology alone, one can effectively classify all possible three-qubit system states. The most related approaches in the literature are (Tucci 1997) and (Buzek and Plesch 2003). (Tucci 1997) introduced *Quantum Bayesian Networks (QBN)*, a graphical representation based on directed acyclic graphs. In QBN the emphasis is on modelling, rather than on computation, and QBN cannot be directly used to facilitate computational tasks. (Buzek and Plesch 2003) introduced *Entangled Graphs (EG)*, which capture the distribution of bipartite entanglement in multi-qubit systems. The graphical decomposition EG is based on concurrence (a statistical measure of bipartite entanglement), and cannot directly represent conditional separabilities. Furthermore, missing a modular representation of amplitudes, EG cannot encode all the information contained in a quantum-mechanical state.

Two main areas of application for MEN come to mind: the classical simulation of quantum-mechanical systems, and quantum computing. In particular, we hope that the identification and exploitation of conditional separabilities in quantum-mechanical systems may lead to the design of more efficient classical simulations in a variety of computationally demanding applications, from physical chemistry to quantum optics. Furthermore, in the context of quantum computation, we hope that the graphical structure of MEN may provide a guide for the efficient design and complexity analysis of quantum algorithms and circuits.

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