Holographic Transformation for Quantum Factor Graphs

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Abstract—Recently, a general called a holographic transformation, which transforms an expression of the partition function to another form, has been used for polynomial-time algorithms and for improvement and understanding of the belief propagation. In this work, the holographic transformation is generalized to quantum factor graphs.

I. INTRODUCTION

The computation of the partition function is one of the most important problems in statistical physics, machine learning, computer science and information theory [1]. Recently, Valiant invented the holographic transformation for transforming the expression of the partition function in order to obtain polynomial-time algorithms for planar graphs [2]. The idea of the holographic transformation explains many well-known identities, e.g., high-temperature expansion, MacWilliams identity, loop calculus, etc. [3], [4], [5]. In this work, the holographic transformation is generalized to quantum factor graphs, which is restricted quantum graphical model suggested in [6]. Although problems from quantum statistical physics are not included in our setting, a decoding problem of quantum error correcting codes can be represented by a quantum factor graph [6]. Hence, the quantum generalization in this paper may be considered as the first step for generalizing loop calculus for quantum error correcting codes. This paper suggests the generalization of the holographic transformation to quantum factor graphs, but does not include any particular example.

II. FACTOR GRAPHS

A factor graph is a bipartite graph defining a probability measure. A factor graph consists of variable nodes, factor nodes and edges between a variable node and a factor node. Let $V$ be the set of variable nodes and $F$ be the set of factor nodes. Let $E \subseteq V \times F$ be the set of edges. For a variable node $i \in V$, $\partial i \subseteq F$ denotes the set of neighborhoods of $i$. In the same way $\partial a \subseteq F$ is defined for $a \in F$. For each variable node $i \in V$, there is an associated finite set $X_i$ and an associated function $f_i : X_i \rightarrow \mathbb{R}_{\geq 0}$. For each factor node $a \in F$, there is an associated function $f_a : \prod_{i \in \partial a} X_i \rightarrow \mathbb{R}_{\geq 0}$. Let $x_V \in \prod_{i \in V} X_i$ be variables corresponding to a subset $V' \subseteq V$ of variable nodes. Then, the probability measure on $X := \prod_{i \in V} X_i$ associated with the factor graph $G = (V, F, E, (f_i)_{i \in V}, (f_a)_{a \in F})$ is defined as

$$p(x) = \frac{1}{Z(G)} \prod_{a \in F} f_a(x_{\partial a}) \prod_{i \in V} f_i(x_i).$$

Here, the constant $Z(G)$ for the normalization is called the partition function, which plays an important role in statistical physics, machine learning, computer science and information theory [1].

III. HOLOGRAPHIC TRANSFORMATION FOR FACTOR GRAPHS

In this section, we briefly review the holographic transformation for classical factor graphs. Let $X_{i,a} := X_i \times X_{a,i}$ for all $(i, a) \in E$. Let $\phi_{i,a} : X_i \times X_{a,i} \rightarrow \mathbb{R}$ and $\hat{\phi}_{i,a} : X_{i,a} \times X_{i,a} \rightarrow \mathbb{R}$ be mappings for each $(i, a) \in E$ satisfying

$${\sum_{y \in X_i} \phi_{i,a}(x, y) \hat{\phi}_{i,a}(y, z) = \delta(x, z)} \tag{1}$$

where $\delta(x, z)$ takes 1 if $x = z$ and 0 otherwise. Let $Y := \prod_{(i, a) \in E} X_{i,a}$. Then, it holds

$$Z(G) = \sum_{x \in X} \prod_{a \in F} f_a(x_{\partial a}) \prod_{i \in V} f_i(x_i)$$

$$= \sum_{x \in X} \prod_{a \in F} f_a(x_{\partial a}) \prod_{i \in V} f_i(x_i) \prod_{(i, a) \in E} \delta(x_i, z_i,a)$$

$$= \sum_{x \in X} \prod_{a \in F} f_a(x_{\partial a}) \prod_{i \in V} f_i(x_i)$$

$${\cdot \prod_{(i, a) \in E} \phi_{i,a}(x_i, y_{i,a}) \hat{\phi}_{i,a}(y_{i,a}, z_{i,a})}$$

$$= \sum_{y \in Y} \prod_{a \in F} \left( \sum_{z_{\partial a,a} \in Y_{\partial a,a}} f_a(z_{\partial a,a}) \prod_{i \in \partial a} \hat{\phi}_{i,a}(y_{i,a}, z_{i,a}) \right)$$

$${\cdot \prod_{i \in V} \left( \sum_{x_i \in X_i} f_i(x_i) \prod_{a \in \partial i} \phi_{i,a}(x_i, y_{i,a}) \right)}$$

where $z_{\partial a,a} := (z_{i,a})_{i \in \partial a}$. By letting

$$\hat{f}_a(y_{\partial a,a}) := \sum_{z_{\partial a,a} \in Y_{\partial a,a}} f_a(z_{\partial a,a}) \prod_{i \in \partial a} \hat{\phi}_{i,a}(y_{i,a}, z_{i,a})$$

$$\hat{f}_i(y_{i,\partial i}) := \sum_{x_i \in X_i} f_i(x_i) \prod_{a \in \partial i} \phi_{i,a}(x_i, y_{i,a})$$

$$f_a(x_{\partial a}) := \prod_{i \in \partial a} f_a(x_i)$$

$$f_i(x_i) := \prod_{a \in \partial i} f_i(x_i)$$

$$(f_i)_{i \in V}, (f_a)_{a \in F}$$
where \( \mathbf{y}_{i, \partial i} := (y_{i,a})_{a \in \partial i} \), one obtains
\[
Z(G) = \sum_{y \in \mathcal{Y}} \prod_{a \in F} \hat{f}_a(y_{\partial a, a}) \prod_{i \in V} \hat{f}_i(y_{i, \partial i}). \tag{2}
\]
This equality is called the Holant theorem \([2, 7]\), which explains many known equalities \([3]\).

IV. QUANTUM FACTOR GRAPHS

There are several quantum graphical models understood as generalizations of classical factor graphs. In quantum physics, quantum state is expressed by a positive semidefinite trace-1 matrix, called a density matrix. The conventional matrix product cannot be used for factor graph directly since a product of two positive semidefinite matrices is not necessarily positive semidefinite. By considering the conditional independence, the most natural generalization \( \odot \) of the products in the classical factor graph would be
\[
(\Lambda \odot \Lambda')|\psi\rangle := \begin{cases} 0, & \text{if } |\psi\rangle \notin S \\ \exp\{\log \Lambda S + \log \Lambda'_S\}|\psi\rangle, & \text{if } |\psi\rangle \in S
\end{cases}
\]
where \( S \) is the intersection of the supports of \( \Lambda \) and \( \Lambda' \), and where \( \Lambda S \) and \( \Lambda'_S \) are the restriction of \( \Lambda \) and \( \Lambda' \), respectively, to \( S \). Here, \( \Lambda \) and \( \Lambda' \) must be positive semidefinite. Obviously \( \Lambda \odot \Lambda' \) is also positive semidefinite. While the product \( \odot \) is commutative and associative, the product \( \odot \) is not distributive with the partial trace in general \([6]\). Hence, in this paper, we do not deal with the quantum graphical model using the product \( \odot \) although it includes problems from quantum statistical physics.

The Suzuki-Trotter approximation for \( \odot \) gives a set of definitions of products \( \star^{(n)} \) as
\[
\Lambda \star^{(n)} \Lambda' := \left( \Lambda^{\frac{1}{n}} \odot \Lambda' \star \Lambda^{\frac{1}{n}} \right)^n.
\]
The product \( \odot \) is obtained as the limit of \( \star^{(n)} \)
\[
\Lambda \odot \Lambda' = \lim_{n \to \infty} \Lambda \star^{(n)} \Lambda'.
\]
While \( \Lambda \star^{(n)} \Lambda' \) is positive semidefinite if \( \Lambda \) and \( \Lambda' \) are positive semidefinite, \( \star^{(n)} \) is neither commutative nor associative. However, \( \star := \star^{(1)} \) is useful for guaranteeing the distributive law with the partial trace, i.e.,
\[
\text{Tr}(\Lambda_{AB} \star \Lambda_{BC}) = \text{Tr}_{HB}(\text{Tr}_{HA}(\Lambda_{AB}) \star \text{Tr}_{HC}(\Lambda_{BC}))
\]
where \( \Lambda_{AB} \) and \( \Lambda_{BC} \) are positive semidefinite operators acting on Hilbert spaces \( \mathcal{H}_A \otimes \mathcal{H}_B \) and \( \mathcal{H}_B \otimes \mathcal{H}_C \), respectively. Hence, in this paper, we deal with the quantum factor graph using the product \( \star \) defined in \([6]\).

V. NON-COMMUTATIVE HOLOANTHROPIAN TRANSFORMATION FOR QUANTUM FACTOR GRAPHS

In this section, the holographic transformation and the Holant theorem in \([2, 7, 5]\) for classical factor graphs is generalized to quantum factor graphs. Let \( \mathcal{H}'_{i,a} \) and \( \mathcal{H}_{i,a} \) be new Hilbert spaces which are isomorphic to \( \mathcal{H}_i \). Let \( q_i \) be the dimension of \( \mathcal{H}_i \) and \( (|\hat{e}_i| \mathcal{H}_i)_{j=1,\ldots,q_i} \) be a basis for \( \mathcal{H}_i \) for all \( i \in V \). For any linear map \( f_a \) acting on \( \mathcal{H}'_i := \bigotimes_{a \in \partial i} \mathcal{H}'_{i,a} \) for all \( a \in F \). Let \( \mathcal{B}(\mathcal{H}) \) be the set of linear operators acting on a Hilbert space \( \mathcal{H}_i \). The set \( \mathcal{B}(\mathcal{H}_A) \) of linear operators can also be regarded as a linear space with respect to the conventional summation and scalar multiplication. Let \( \Phi_{i,a} \) and \( \hat{\Phi}_{i,a} \) be linear maps from \( \mathcal{B}(\mathcal{H}_{i,a}) \) to \( \mathcal{B}(\mathcal{H}_i) \) and from \( \mathcal{B}(\mathcal{H}'_{i,a}) \) to \( \mathcal{B}(\mathcal{H}_{i,a}) \), respectively, for all \( (i,a) \in E \). For any linear map \( T: \mathcal{B}(\mathcal{H}_A) \to \mathcal{B}(\mathcal{H}_B) \), there is the Choi-Jamiolkowski representation \( T \in \mathcal{B}(\mathcal{H}_B \otimes \mathcal{H}_A) \) of \( T \), i.e.,
\[
T := \sum_{k,l} T(|e_k\rangle \mathcal{H}_A \langle e_l| \mathcal{H}_A) \otimes |e_k\rangle \mathcal{H}_A \langle e_l| \mathcal{H}_A
\]
which satisfies
\[
T(G) = \text{Tr}_{HA} (T(I_{\mathcal{H}_B} \otimes G^T))
\]
for any \( G \in \mathcal{B}(\mathcal{H}_A) \) where \( I_{\mathcal{H}_B} \) denotes the identity operator on \( \mathcal{H}_B \) and \( T \) denotes the transpose of linear map \([8]\). Let \( \hat{\Phi}_{i,a} \in \mathcal{B}(\mathcal{H}_{i,a} \otimes \mathcal{H}_{i,a}^\prime) \) be the Choi-Jamiolkowski representations for \( \Phi_{i,a} \) and \( \hat{\Phi}_{i,a} \), respectively, for all \( (i,a) \in E \).

We assume that \( (\Phi_{i,a})_{a \in \partial i} \) are mutually commute with respect to the conventional matrix product for all \( (i,a) \in E \) where
\[
\text{id}_{\mathcal{H}_i, \mathcal{H}_{i,a}^\prime} \left(|e_k\rangle \mathcal{H}_{i,a} \langle e_l| \mathcal{H}_{i,a}^\prime\right) := |e_k\rangle \mathcal{H}_i \langle e_l| \mathcal{H}_i
\]
Although this condition may not be necessary, we assume it for the simplicity.
for all $k, l \in \{1, 2, \ldots, q_i\}$. It is easy to verify that this condition is equivalent to
\[
\text{Tr}_{\hat{H}_{i,a}} \left( \hat{\phi}_{i,a}^T \hat{\phi}_{i,a} \right) = \sum_{k,l} |e_k \rangle_{\hat{H}_i} \langle e_l|_{\hat{H}_i} \otimes |e_k \rangle_{\hat{H}'_{i,a}} \langle e_l|_{\hat{H}'_{i,a}}.
\]
Let $\hat{H} := \bigotimes_{(i,a) \in E} \hat{H}_{i,a}$ and $\hat{H}' := \bigotimes_{(i,a) \in E} \hat{H}'_{i,a}$. Then, one obtains
\[
Z(G) = \text{Tr}_{\hat{H}} \left( \prod_{a \in F} \text{Tr}_{\hat{H}'_{i,a}} \left( f'_a \bigotimes_{i\in\partial a} F_{i,a} \right) \bigotimes_{i \in V} f_i \right)
= \text{Tr}_{\hat{H} \otimes \hat{H}'_{i,a}} \left( \prod_{a \in F} \left( f'_a \bigotimes_{i\in\partial a} \hat{\phi}_{i,a}^T \hat{\phi}_{i,a} \bigotimes_{i \in V} f_i \right) \right)
= \text{Tr}_{\hat{H}} \left( \bigotimes_{a \in F} \text{Tr}_{\hat{H}'_{i,a}} \left( f'_a \bigotimes_{i\in\partial a} \hat{\phi}_{i,a}^T \hat{\phi}_{i,a} \bigotimes_{i \in V} f_i \right) \right).
\]

For linear maps $T : B(\hat{H}_A) \rightarrow B(\hat{H}_B)$ and $T' : B(\hat{H}_C) \rightarrow B(\hat{H}_B)$, $T \otimes T' : B(\hat{H}_A) \otimes B(\hat{H}_C) \rightarrow B(\hat{H}_B)$ is defined as
\[
(T \otimes T') |e_k \rangle_{\hat{H}_A} |e_l \rangle_{\hat{H}_C} = |e'_k \rangle_{\hat{H}_C} |e'_l \rangle_{\hat{H}_A}.
\]
Let $T^*$ be the adjoint map of $T$, i.e., $\text{Tr}(BT(A)) = \text{Tr}(T^*(B)A)$ [8]. Then, one obtains
\[
Z(G) = \text{Tr}_{\hat{H}} \left( \bigotimes_{a \in F} f'_a \bigotimes_{i \in V} f_i \right) = \text{Tr}_{\hat{H}} \left( \bigotimes_{a \in F} f'_a \bigotimes_{i \in V} f_i \right).
\]

where
\[
f'_a := \text{Tr}_{\hat{H}'_{i,a}} \left( \bigotimes_{i\in\partial a} \hat{\phi}_{i,a} \bigotimes_{i \in V} f_i \right) = \left( \bigotimes_{i\in\partial a} \hat{\phi}_{i,a} \right) \langle f'_a \rangle,
\]
\[
f_i := \text{Tr}_{\hat{H}_i} \left( f_i \bigotimes_{a \in \partial i} \hat{\phi}_{i,a}^T \hat{\phi}_{i,a} \right) = \left( \bigotimes_{a \in \partial i} \hat{\phi}_{i,a} \right)^* \langle f_i \rangle.
\]

The equation (4) can be regarded as a quantum generalization of the Holant theorem (3).

Note that for the classical case, $(f_a)_{a \in F}$ and $(f_i)_{i \in V}$ are diagonal with respect to some basis $\{ | \epsilon_i \rangle_{\hat{H}_i} \}_{\forall \epsilon_i \in V}$, $k_i = 1, \ldots, q_i$. In this case, the condition (3) can be replaced by a different condition
\[
(\hat{\phi}_{i,a}^T \hat{\phi}_{i,a}) |e_k \rangle_{\hat{H}'_{i,a}} |e_l \rangle_{\hat{H}'_{i,a}} := \delta(k,l) |e_k \rangle_{\hat{H}_i} |e_l \rangle_{\hat{H}_i}
\]
for all $k, l \in \{1, 2, \ldots, q_i\}$ or equivalently,
\[
\text{Tr}_{\hat{H}'_{i,a}} (\hat{\phi}_{i,a}^T \hat{\phi}_{i,a}) = \sum_{j=1}^{q_i} |e_j \rangle_{\hat{H}_i} |e_j \rangle_{\hat{H}_i} \otimes |e_j \rangle_{\hat{H}'_{i,a}} |e_j \rangle_{\hat{H}'_{i,a}}.
\]

If $(\hat{\phi}_{i,a}^T \hat{\phi}_{i,a})_{(i,a) \in E}$ and $(\hat{\phi}_{i,a}^T \hat{\phi}_{i,a})_{(i,a) \in E}$ are restricted to be diagonal with respect to the same basis, the above condition corresponds to (1).