
Identification of Latent Graphs: A Quantum Entropic Approach

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Abstract

Quantum causality is an emerging field of study which has the potential to greatly advance our understanding of quantum systems. In this paper, we put forth a new theoretical framework for merging quantum information science and causal inference by exploiting entropic principles. For this purpose, we leverage the tradeoff between the entropy of hidden cause and conditional mutual information of observed variables to develop a scalable algorithmic approach for inferring causality in the presence of latent confounders (common causes) in quantum systems. As an application, we consider a system of three entangled qubits and transmit the second and third qubits over separate noisy quantum channels. In this model, we validate that the first qubit is a latent confounder and the common cause of the second and third qubits. In contrast, when two entangled qubits are prepared and one of them is sent over a noisy channel, there is no common confounder. We also demonstrate that the proposed approach outperforms the results of classical causal inference for Tübingen database when the variables are classical by exploiting quantum dependence between variables through density matrices rather than joint probability distributions. Thus, the proposed approach unifies classical and quantum causal inference in a principled way.

1 Introduction

Motivation. Causal inference lies at the heart of science [Pearl, 2009, Pearl and Mackenzie, 2018]: the conclusions drawn from scientific studies almost always involve extracting causation (cause and effect relationships) from association, even if researchers often refrain from explicitly acknowledging the causal goal of research projects [Hernán, 2018, Hernán et al., 2019]. However, causal inference from observational data is an ambitious and difficult task. Identifying cause and effect relationships from observational data is even more challenging in the presence of *hidden common causes* (*latent confounders*) [Heckerman, 2019]. The broad impact of this phenomena has been studied in multiple domains of science such as epidemiologic studies [Lipsitch et al., 2010], biology and medicine [Skelly et al., 2012, Meinshausen et al., 2016], experiential education [Ewert and Sibthorp, 2009, Kallus et al., 2018], economics and marketing [Varian, 2016, Hünernmund and Bareinboim, 2019], among others.

A similar concept is increasingly appreciated among quantum physicists, namely the inference of *quantum common causes* [Wolfe et al., 2020, Allen et al., 2017, Ried et al., 2015, Chaves et al., 2014a,b, 2015, Hofer-Szabó et al., 1999]. It has been used to provide a satisfactory causal explanation (i.e., non-fine-tuned) of Bell inequality violations [Allen et al., 2017, Hofer-Szabó et al., 1999]. This also has led to a formalization of quantum causal models [Costa and Shrapnel, 2016, Barrett et al., 2019, Chiribella and Ebler, 2019, Shrapnel, 2019]. As shown in [Chaves et al., 2014a,b, 2015], *in*

some cases, (hidden) common causes can be distinguished from direct causation using information theoretical generalization of Bell’s inequalities and causal directed acyclic graphs (DAGs). Also, as shown in [Fitzsimons et al., 2015, Ried et al., 2015], observed quantum correlations alone are *sometimes* enough to imply causation. However, the proposed approach in [Fitzsimons et al., 2015, Ried et al., 2015] depends on the precise knowledge of the physical system and the measurement apparatuses [Gachechiladze et al., 2020]. In this paper, we propose the first tractable algorithmic approach to distinguish between a hidden common cause and direct causal influences among two observed quantum systems without any interventional data.

To show the difficulty of causal structure discovery task even in the simplest classical case, where our observation consists of only two jointly-distributed random variables X and Y that are statically correlated, we recall Reichenbach’s common cause principle [Reichenbach, 1991]: If two random variables X and Y are statistically dependent, then there exists a third variable Z that causally affects both. As a special case, Z may coincide with either X or Y . Furthermore, this variable Z makes X and Y conditionally independent, i.e., $X \perp\!\!\!\perp Y|Z$. So, possible candidates for representing causal relationships between X and Y are: $X \rightarrow Y$, $X \leftarrow Y$, and $X \leftarrow Z \rightarrow Y$, and there is no easy way to determine which one is the right structure based on the observational data alone. The variable Z in the case $X \leftarrow Z \rightarrow Y$ is called *unmeasured (latent) confounder* or *unmeasured (latent) common cause*. So, one of the fundamental questions in causality is to determine how cause-effect relationships can be inferred from statistical information, encoded as a joint probability distribution, obtained under normal, intervention-free experiments.

Co-existence of Quantum Systems. To discover the true cause-effect relationships, scientists normally perform randomized experiments where a sample of units drawn from the population of interest is subjected to the specified manipulation directly. In many cases, however, such a direct approach is not possible due to expense or ethical considerations. Instead, investigators have to rely on observational studies to infer causality. This task is even more challenging in quantum context due to quantum superpositions and entanglement relations. In this work, we are interested in quantum generalizations of causal structures in the presence of latent common causes. These structures can be shown as a directed acyclic graph (DAG), where nodes are quantum systems, and edges are quantum operations. However, the key theoretical distinction between an entirely classical causal structure and a quantum casual structure is the concept of *coexisting*. Because of the impossibility of cloning, the outcomes and the quantum systems that led to them do not exist simultaneously. If a system X is measured to produce Y , then ρ_{XY} is not defined and hence neither is the entropy $S(\rho_{XY})$ [Weilenmann and Colbeck, 2017]. For a given causal structure, a *coexisting set* of systems is one for which a joint state can be defined [Chaves et al., 2015, Weilenmann and Colbeck, 2017, 2020]. If we pick a coexisting set of nodes (e.g., a classical system, or a set of nodes that are created at the same instance of time, i.e., they do enjoy a joint density operator), then we can investigate the identification of quantum causal structures in the presence of latent confounders.

Contributions. In this paper, we consider causality between two coexisting quantum subsystems. As a part of the evaluation framework, we provide a model of such a coexisting system, where two entangled qubits are used, and one of the qubit is transmitted over a quantum channel. Similarly, three entangled qubits are used, and two of them are transmitted over two separate quantum channels. The models can be further generalized, while note that the subsystems which are being considered for quantum causality relationships have to coexist, unlike in the classical case where it is not necessary for the sub-systems to coexist. To address this problem, we introduce a theoretical framework to merge quantum information science with causal inference using entropic principles. Classically, it has been proposed and tested that minimization of the trade-off between the entropy of the (hidden) common cause Z (i.e., $H(Z)$) and the conditional mutual information of observed variables X and Y given Z (i.e., $I(X; Y|Z)$) can be used to distinguish the *latent graph* $X \leftarrow Z \rightarrow Y$ (Z is an unmeasured confounder) from the directed graphs $X \rightarrow Y$ and $X \leftarrow Y$ based on observational data alone under certain assumptions [Kocaoglu et al., 2020] (a brief review is given in [Javidian et al., 2021]). We will provide the first generalization of this approach to the quantum domain.

Even though the paper considers an approach for quantum causal inference, we also apply the proposed approach to a classical setup, where two bits are transmitted over a binary symmetric channel (to illustrate the case of no confounder), or two bits are transmitted over two separate channels (to illustrate the case of latent confounder). We note that finding the optima over a quantum density matrix rather than over the probability distribution function provides larger degrees of

freedom thus resulting in improved results. This example is used to select the hyperparameters for our framework, and these hyperparameters are used in the rest of the paper. This demonstrates that the proposed approach can also be used for classical causal inference with improved results. Our main contributions are as follows:

- Inferring causality in the presence of latent confounders from observational data alone is one of the most important and challenging problems in statistical inference. We propose an iterative algorithm, called QInferGraph, for identifying *latent confounders* in Section 2. Our method leverages the concept of quantum conditional matrices to unify the solution for classical and quantum (latent) common cause problem in a principled way.
- We evaluate the proposed approach for classical causal inference. By leveraging optimization over density matrices, the proposed approach is shown to outperform the results of classical causal inference in [Kocaoglu et al., 2020] for Tübingen database [Mooij et al., 2016] in Section 4.
- We put forth an experimental scheme that can be used to confront our theoretical framework. We consider a minimalistic model of an unknown message (possibly encrypted) with unknown origin in a two-node quantum network with the possibility of the presence of a latent common cause, where nodes are a *coexisting set* of quantum systems for which a joint density matrix can be defined. Entangled quantum subsystems are used, where subsystems are communicated over noisy channels (e.g., optical fiber) to create such coexisting set of quantum systems. We show that only using the joint density matrix of the observed two quantum systems, we can identify the originator of the message (i.e., the sub-system that did not encounter the noisy channel). To verify the validation of QInferGraph, we use realistic quantum noisy links such as quantum symmetric channel and depolarizing channel (valid for quantum networking and quantum communications) (Section 3).

The rest of the paper is organized as follows. In the supplementary material documents [Javidian et al., 2021], we review the classical causal inference approach proposed in [Kocaoglu et al., 2020] for the identification of causal structures in the presence of hidden common causes. In Section 2, we generalize the classical approach to the quantum domain. In Section 3, we put forward an experimental scheme that can be used to validate our proposed approach using a minimalistic model of an unknown message (possibly encrypted) with unknown origin in a two-node/three-node classical/quantum network, respectively. Also, we evaluate the performance of QInferGraph on the real dataset (Section 4) with cause-effect pairs [Mooij et al., 2016], and show that QInferGraph outperforms in identification of latent confounders as compared to the classical approach. In Section 5, we explain and show why should we not map quantum to classical directly.

2 Entropic Approach for Confounder Discovery in Quantum Systems

In this section, we provide an approach for identifying latent graphs in quantum systems, where we assume the Assumptions 1, with the entropy replaced by the von-Neumann entropy, $S(X) = -\text{tr}(\rho_X \log \rho_X)$. We first briefly review the formalism of *quantum conditional density matrices*, which provides a solid framework for adapting classical iterative algorithms (see [Javidian et al., 2021] for details) to the quantum domain. Then, the proposed algorithm to identify latent graphs is described which uses the concept of the quantum conditional density matrix.

Assumption 1 Consider any causal model with observed variables X and Y . Let Z represents the variable that captures all latent confounders between X and Y . Then $H(Z) < \theta$, where $H(Z) = -\sum_{i=1}^n P(x_i) \log(P(x_i))$ and θ is the entropy threshold.

2.1 Conditional Density Matrix

Quantum theory can be understood as a non-commutative generalization of classical probability theory wherein probability measures are replaced by density operators [Leifer and Spekkens, 2013]. The density matrix describes the quantum state of a physical system, and allows for the calculation of the probabilities of the outcomes of any measurement performed upon this system. The density matrix is a positive semi-definite, Hermitian matrix of trace one. The density matrix can be written as $\sum_j p_j |\psi_j\rangle\langle\psi_j|$ for some states $|\psi_j\rangle$ and coefficients p_j that are non-negative and add up to one. As a generalization of classical probabilities, the density matrix corresponding to a probability distribution can be obtained where p_j corresponds to the probability that the random variable is j and the state

$|\psi_j\rangle$ is given as a column vector with 1 at j^{th} element and zero otherwise¹. Analogies between the classical theory of Bayesian inference and the conditional states formalism for quantum theory are listed in Table 1.

Table 1: Analogies between classical and quantum formalism

Classical Probability	Quantum Theory
probability distribution $p(X)$	density operator (matrix) ρ_X
joint distribution $p(X, Y)$	joint density ρ_{XY}
marginal distribution $p(X) = \sum_Y p(X, Y)$	partial trace $\rho_X = \text{Tr}_Y(\rho_{XY})$
conditional probability	conditional density [Leifer and Spekkens, 2013]
$p(X Y) = p(X, Y)/p(Y)$	$\rho_{X Y} = (\rho_Y^{-1/2} \otimes I_X)\rho_{XY}(\rho_Y^{-1/2} \otimes I_X)$

Quantum conditional densities are a generalization of classical conditional probability distributions. However, to generalize conditional probabilities to the quantum case, several approaches have been proposed in the literature. The three following generalizations are the best known in the literature of quantum information: (1) quantum conditional expectation [Umegaki, 1962], (2) quantum conditional amplitude operator [Cerf and Adami, 1997, 1999], and (3) quantum conditional states [Leifer, 2007, Leifer and Spekkens, 2013]. Arguably, quantum conditional states are the most useful generalization of conditional probability from the point of view of practical applications. For example, quantum conditional states have been used in [Leifer and Spekkens, 2013] to build a quantum theory of Bayesian inference. Since quantum conditional states provides a closer analogy between quantum theory and classical probability theory, we choose this formalism to define quantum conditional density matrices. We will see that this formalism plays a significant role in the design and success of our entropic quantum causal inference algorithm. Following [Leifer, 2007, Leifer and Spekkens, 2013], the conditional density matrix of X given Y is defined as follows:

$$\rho_{X|Y} = (\rho_Y^{-1/2} \otimes I_X)\rho_{XY}(\rho_Y^{-1/2} \otimes I_X).$$

Also, note that this relates the conditional density matrix and the joint density matrix, and thus the joint density matrix can also be written as

$$\rho_{XY} = (\rho_Y^{1/2} \otimes I_X)\rho_{X|Y}(\rho_Y^{1/2} \otimes I_X) = (\rho_X^{1/2} \otimes I_Y)\rho_{Y|X}(\rho_X^{1/2} \otimes I_Y).$$

2.2 QLatentSearch: An Algorithm for Computing Exact Quantum Common Entropy

In this section, we propose an iterative algorithm (Algorithm 1) that discovers the trade-off between the entropy of the unmeasured confounder and the quantum conditional mutual information of two observed quantum systems given the unmeasured confounder. This is fundamental for designing an algorithm for the identification of latent confounders in quantum systems, as we show in the next subsection. This trade-off is formally defined as follows:

$$L = I_Q(X; Y|Z) + \beta S(Z) \quad (1)$$

Note that $I_Q(X; Y|Z) = 0$ implies that the quantum conditional independence of X and Y given Z [Allen et al., 2017, Theorem 3]. Having low von Neumann entropy of hidden common cause Z , i.e., $S(Z)$ under the quantum version of Assumption 1 enable us to identify latent graphs from direct/triangle graphs in practice, as we show in section 4 (see [Javidian et al., 2021] for more details). For this purpose, rather than searching over ρ_{XYZ} and enforcing the constraint $\rho_{XY} = \text{Tr}_Z(\rho_{XYZ})$, we can search over $\rho(Z|X, Y)$ and set $\rho_{XYZ} = (\rho_{XY}^{-1/2} \otimes I_Z)\rho(Z|X, Y)(\rho_{XY}^{-1/2} \otimes I_Z)$ because:

$$\begin{aligned} L &= I_Q(X; Y|Z) + \beta S(Z) \\ &= S(XZ) + S(YZ) - S(Z) - S(XYZ) + \beta S(Z) \\ &= S(XZ) + S(YZ) - S(XYZ) + (\beta - 1)S(Z) \\ &= S(X) + S(Z|X) + S(Y) + S(Z|Y) - S(XY) - S(Z|X, Y) + (\beta - 1)S(Z) \\ &= S(Z|X) + S(Z|Y) - S(Z|X, Y) + (\beta - 1)S(Z) + I_Q(X; Y) \end{aligned}$$

¹Note that this is not a unique method of relating the classical probabilities to quantum density matrix [Bradley and Vlassopoulos, 2020].

Note that $\rho(Z|Y) = \text{Tr}_X((\rho^{1/2}(X|Y) \otimes I_Z)\rho(Z|X, Y)(\rho^{1/2}(X|Y) \otimes I_Z))$, $\rho(Z|X) = \text{Tr}_Y((\rho^{1/2}(Y|X) \otimes I_Z)\rho(Z|X, Y)(\rho^{1/2}(Y|X) \otimes I_Z))$, and $\rho_Z = \text{Tr}_{X, Y}((\rho_{XY}^{1/2} \otimes I_Z)\rho(Z|X, Y)(\rho_{XY}^{1/2} \otimes I_Z))$. So, we have $L = L(\rho(Z|X, Y))$, which is the counterpart of the classical loss function with the following differences: (i) rather than using (conditional) probability distributions, we use (conditional) density matrices, and (ii) rather than using Rényi entropy, we use the von Neumann entropy.

We aim to optimize the objective L over $\rho(Z|X, Y)$. Although first order methods (e.g., gradient descent) or genetic algorithm (GA)² can be used to find a stationary point of the optimization problem in (1), as we empirically observed the convergence is unattainable/slow and the performance is very sensitive to the tuning parameters such as step size and the mutation probability. This optimization problem is difficult to perform numerically because the boundary of the space of positive semidefinite matrices is hard to compute. In order to provide a scalable algorithm for this optimization, we extend the iterative algorithm that was proposed for classical version of the problem in [Kocaoglu et al., 2020]. The proposed iterative algorithm for the optimization of L is described in Algorithm 1, and is called QLatentSearch. This algorithm starts from a random initialization $\rho_1(Z|X, Y)$, and then at each iteration i does the following two phases to update $\rho_{i+1}(Z|X, Y)$ from $\rho_i(Z|X, Y)$ to finally minimize the loss function L in (1):

- **Calculate Phase:** In this phase we use partial trace to get $\rho_i(Z|X)$ (line 3-5), $\rho_i(Z|Y)$ (line 6-8), and ρ_Z^i (line 9) from ρ_{XYZ}^i .
- **Update Phase:** In this phase we update $\rho_{i+1}(Z|X, Y)$ to get ρ_{XYZ}^{i+1} (line 10) for the next iteration.

Algorithm 1: QLatentSearch, An Iterative Algorithm for Computing Exact Quantum Common Entropy

Input: Joint density matrix ρ_{XYZ} ; Number of iterations N ; β parameter in the loss function $L = I_Q(X; Y|Z) + \beta S(Z)$,
Initialization of $\rho_1(Z|X, Y)$.
Output: Joint density matrix ρ_{XYZ} .

```

1 for  $i = 1 : N$  do
  /* Form the joint density matrix: */
2   $\rho_{XYZ}^i = (\rho_{XY}^{1/2} \otimes I_Z)\rho_i(Z|X, Y)(\rho_{XY}^{1/2} \otimes I_Z)$ ;
  /* Calculate Phase: */
  /* (i) Calculate  $\rho_i(Z|X)$ : */
3   $\rho_{XZ}^i = \text{Tr}_Y(\rho_{XYZ}^i)$  // Then, compute  $\rho_{X^i I_Y Z}^i$  by reordering the entries of  $\rho_{XZ}^i$ 
4   $\rho_X^i = \text{Tr}_Z(\rho_{XZ}^i)$ ;
5   $\rho_i(Z|X) \leftarrow ((\rho_X^i)^{-1/2} \otimes I_{YZ})\rho_{X^i I_Y Z}^i((\rho_X^i)^{-1/2} \otimes I_{YZ})$ ;
  /* (ii) Calculate  $\rho_i(Z|Y)$ : */
6   $\rho_{YZ}^i = \text{Tr}_X(\rho_{XYZ}^i)$  // Then, compute  $\rho_{I_X Y Z}^i = I_X \otimes \rho_{YZ}^i$ 
7   $\rho_Y^i = \text{Tr}_Z(\rho_{YZ}^i)$ ;
8   $\rho_i(Z|Y) \leftarrow (I_X \otimes (\rho_Y^i)^{-1/2} \otimes I_Z)\rho_{I_X Y Z}^i(I_X \otimes (\rho_Y^i)^{-1/2} \otimes I_Z)$ ;
  /* (iii) Calculate  $\rho_Z^i$ : */
9   $\rho_Z^i = \text{Tr}_{XY}(\rho_{XYZ}^i)$ ;
  /* Update Phase: */
10  $\rho_{i+1}(Z|X, Y) \leftarrow \exp(\log(\rho_i(Z|X)) + \log(\rho_i(Z|Y)) + (\beta - 1) \log(\rho_Z^i))$ ;
11 end
12 return  $\rho_{XYZ} := (\rho_{XY}^{1/2} \otimes I_Z)\rho_{N+1}(Z|X, Y)(\rho_{XY}^{1/2} \otimes I_Z)$ .

```

Formally, to prove the correctness of QLatentSearch, the following theorem shows that QLatentSearch converges to a stationary point of the loss function L in Equation 1. The proof is available at [Javidian et al., 2021].

Theorem 1 (Correctness of QLatentSearch) *The stationary points of the algorithm QLatentSearch are also stationary points of the loss function L in Equation 1 for $0 < \beta < 1$.*

2.3 QInferGraph: An Algorithm for the Identification of Latent Confounders

In this section, we propose a quantum entropic approach to causal inference that can discern the difference between causation and correlation. Specifically, under Assumption 1, extended to quantum,

²Genetic algorithm (GA) is a metaheuristic method inspired by the process of natural selection.

Algorithm 1 can be used to distinguish causation from spurious correlation between two observed quantum systems. This enables us to distinguish latent graph in Figure 1(a) from the triangle or direct graphs in Figure 1(b)-(c). Our main assumption is that the latent confounders, if they exist, have small von Neumann entropy. Formally, we have:

Assumption 2 Consider any causal model with observed quantum subsystems X and Y . Let Z represents the quantum system that captures all latent confounders between X and Y . Then $S(Z) < \theta$, where $S(Z) = -\text{tr}(\rho \log \rho)$.

In other words, in Figure 1(a), $S(Z) \leq \theta$ for some θ . Similar to the classical version of this problem, we conjecture that $\theta = \alpha \min\{S(X), S(Y)\}$ for some $\alpha < 1$. Considering Assumption 2 along with QLatentSearch (Algorithm 1), we propose an algorithm, called QInferGraph (Algorithm 2), to identify latent graphs.

Algorithm 2: QInferGraph: Identifying the Latent Graph

Input: Joint density matrix ρ_{XY} ; Number of iterations N ; $I_Q(X; Y|Z)$ threshold T ; $S(Z)$ threshold that is determined by $\theta = \alpha \min\{S(X), S(Y)\}$; $\{\beta_i\}_{i=1}^N$; The number of rows (or equivalently, columns) of X , Y , and Z , i.e., r , m , and n , respectively.

Output: "Latent Graph" if Z is an unmeasured confounder for X and Y , otherwise, returns "Triangle or Direct Graph".

```

1 for  $i = 1 : N$  do
2    $\rho_{XYZ}^i \leftarrow \text{QLatentSearch}(\rho_{XY}, \alpha, \beta_i, r, m, n)$ ;
3   Calculate  $I_Q^i(X; Y|Z)$  and  $S_i(Z)$  from  $\rho_{XYZ}^i$ ;
4 end
5  $S = \{i : I_Q^i(X; Y|Z) \leq T\}$ ;
6 if  $\min\{S_i(Z) : i \in S\} > \theta$  or  $S = \emptyset$  then
7   return Triangle or Direct Graph;
8 else
9   return Latent Graph;
10 end

```

In short, QInferGraph calls QLatentSearch N times to figure out if there exist a W , for which $I_Q(X; Y|W) < T$, i.e., W makes X and Y conditionally independent. Also, the von Neumann entropy of W is enough small such that $S(W) < \alpha \min\{S(X), S(Y)\}$ for some α in practice. If there exist such a W , the algorithm declares W is a latent confounder. In other words,

latent graph represents correlation without causation relationship between observed quantum systems X and Y . Otherwise, very likely such a W that minimizes the loss function L does not exist, and QInferGraph declares that a triangle graph or a direct graph represents the connection between X and Y better than a latent graph in this case. In the next section we conduct experiments to verify this procedure in practice.

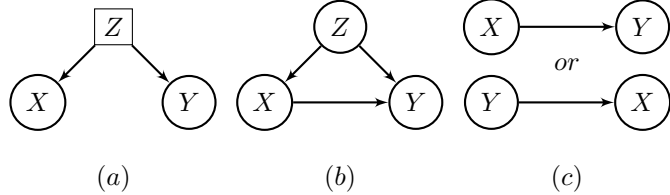


Figure 1: (a) Latent Graph, (b) Triangle Graph, and (c) Direct Graph.

3 Evaluation on Quantum Causal Synthetic Data

Since there is no quantum cause-effect repository to verify the validity of our proposed algorithm, we put forward an experimental scheme that can be used to confront our theoretical framework. To show the effectiveness of the proposed approach in section 2, we use quantum noisy links, where it is validated that the input before noise, as a latent confounder (hidden source), is the cause of the noisy outputs. We first apply our proposed approach on a quantum (non-classical) model, where mixed entangled quantum subsystems are used for which subsystems are communicated over noisy channels (e.g., optical fiber) to create a coexisting set of quantum systems.

Model 1 (Depolarizing Quantum Channel: Latent Graph and Direct Graph)

Part I: Latent Graph. Assume that there are real numbers $\gamma_1, \gamma_2, \lambda_1$, and λ_2 such that $\gamma_1^2 + \lambda_1^2 = 1$ and $\gamma_2^2 + \lambda_2^2 = 1$. We consider a joint entangled system (of three qubits) as the mixture of the following pure density matrices:

$$\begin{cases} [(\gamma_1|0\rangle + \lambda_1|1\rangle)(\gamma_1|0\rangle + \lambda_1|1\rangle)(\gamma_1|0\rangle + \lambda_1|1\rangle)] [(\gamma_1|0\rangle + \lambda_1|1\rangle)(\gamma_1|0\rangle + \lambda_1|1\rangle)(\gamma_1|0\rangle + \lambda_1|1\rangle)]^\dagger & q \\ [(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)] [(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)]^\dagger & 1 - q \end{cases}$$

In other words, the system considered has density matrix $q[(\gamma_1|0\rangle + \lambda_1|1\rangle)(\gamma_1|0\rangle + \lambda_1|1\rangle)(\gamma_1|0\rangle + \lambda_1|1\rangle)] [(\gamma_1|0\rangle + \lambda_1|1\rangle)(\gamma_1|0\rangle + \lambda_1|1\rangle)(\gamma_1|0\rangle + \lambda_1|1\rangle)]^\dagger + (1 - q)[(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)] [(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)]^\dagger$. The system is a mixture of two pure density matrices. This quantum system has entanglement among the three quantum bits. Let the second quantum bit is transmitted over a *quantum depolarizing channel* with error probability p_1 , and the third quantum bit is transmitted over a *quantum depolarizing channel* with error probability p_2 . Note that the depolarizing channel with error probability p has no error with probability $1 - p$, and each of the phase-flip, bit-flip, or the combination of phase-flip and bit-flip errors with probability $p/3$ [Nielsen and Chuang, 2002]. With this setup, the joint density matrix is given as $\rho_{ZXY} = q\rho_{ZXY}^{\gamma_1, \lambda_1} + (1 - q)\rho_{ZXY}^{\gamma_2, \lambda_2}$, where $\rho_{ZXY}^{\gamma, \lambda}$ is given as the mixture of the following pure density matrices:

$$\left\{ \begin{array}{l} [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)]^\dagger \\ [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)]^\dagger \\ [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)]^\dagger \\ [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)]^\dagger \\ [(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)]^\dagger \\ [(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)]^\dagger \\ [(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)]^\dagger \\ [(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)]^\dagger \\ [(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)]^\dagger \\ [(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)]^\dagger \\ [(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)]^\dagger \\ [(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)]^\dagger \\ [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)]^\dagger \\ [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)]^\dagger \\ [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)]^\dagger \\ [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)] [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)]^\dagger \end{array} \right. \begin{array}{l} (1 - p_1)(1 - p_2) \\ (1 - p_1)(p_2/3) \\ (1 - p_1)(p_2/3) \\ (1 - p_1)(p_2/3) \\ (p_1/3)(1 - p_2) \\ (p_1/3)(p_2/3) \\ (p_1/3)(p_2/3) \\ (p_1/3)(p_2/3) \\ (p_1/3)(1 - p_2) \\ (p_1/3)(p_2/3) \\ (p_1/3)(p_2/3) \\ (p_1/3)(p_2/3) \\ (p_1/3)(1 - p_2) \\ (p_1/3)(p_2/3) \\ (p_1/3)(p_2/3) \\ (p_1/3)(p_2/3) \\ (p_1/3)(p_2/3) \end{array}$$

We note that X and Y coexist, thus we can find joint density matrix of X and Y by tracing out Z in ρ_{ZXY} . Then, we apply `QInferGraph` (Algorithm 2) on ρ_{XY} to verify that X and Y are confounded by a latent confounder. For this purpose, we use the same parameters specification as explained in [Javidian et al., 2021] with $\alpha = 0.2$, $\beta \in (0, 1)$, $T = 0.005$, and $q = 0.4$. Table 2 summarizes the results, where $\alpha = 0.2$. T means that `QInferGraph` (Algorithm 2) identifies the latent graph correctly. But, F means that the algorithm fails to identify the latent graph. In this case, for $\alpha = 0.2$ we have: true positive rate (recall) = 1, false positive rate (fall-out) = 0, false negative rate (miss rate) = 0, accuracy = 1.

Table 2: Validation of Latent Graph in Model 1 (Part I) for $\alpha = 0.2$, and $\beta \in (0, 1)$ via `QInferGraph`, and with the density matrix obtained from $0.6\rho_{ZXY}^{1/\sqrt{2}, 1/\sqrt{2}} + 0.4\rho_{ZXY}^{0.6, 0.8}$ via tracing out Z .

		p_2										
		0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99
p_1	0.01	T	T	T	T	T	T	T	T	T	T	T
	0.1	T	T	T	T	T	T	T	T	T	T	T
	0.2	T	T	T	T	T	T	T	T	T	T	T
	0.3	T	T	T	T	T	T	T	T	T	T	T
	0.4	T	T	T	T	T	T	T	T	T	T	T
	0.5	T	T	T	T	T	T	T	T	T	T	T
	0.6	T	T	T	T	T	T	T	T	T	T	T
	0.7	T	T	T	T	T	T	T	T	T	T	T
	0.8	T	T	T	T	T	T	T	T	T	T	T
	0.9	T	T	T	T	T	T	T	T	T	T	T
	0.99	T	T	T	T	T	T	T	T	T	T	T

Table 3: Classical Approach to Identify Direct Graph for Model 1 does not work.

		p										
		0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99
α	0.7	F	F	F	F	F	F	F	F	F	F	F
	0.8	F	F	F	F	F	F	F	F	F	F	F
	0.9	F	F	F	F	F	F	F	F	F	F	F
	1	F	F	F	F	F	F	F	F	F	F	F

Part II: Direct Graph. Assume that there are real numbers γ_1 , γ_2 , λ_1 , and λ_2 such that $\gamma_1^2 + \lambda_1^2 = 1$ and $\gamma_2^2 + \lambda_2^2 = 1$. We consider a joint entangled system (of two qubits) as the mixture of the following pure density matrices:

$$\begin{cases} (\gamma_1^2|00\rangle + \gamma_1\lambda_1|01\rangle + \gamma_1\lambda_1|10\rangle + \lambda_1^2|11\rangle)(\gamma_1^2|00\rangle + \gamma_1\lambda_1|01\rangle + \gamma_1\lambda_1|10\rangle + \lambda_1^2|11\rangle)^\dagger & q \\ (\gamma_2^2|00\rangle + \gamma_2\lambda_2|01\rangle + \gamma_2\lambda_2|10\rangle + \lambda_2^2|11\rangle)(\gamma_2^2|00\rangle + \gamma_2\lambda_2|01\rangle + \gamma_2\lambda_2|10\rangle + \lambda_2^2|11\rangle)^\dagger & 1 - q \end{cases}$$

The system is a mixture of two pure density matrices. This quantum system has entanglement among the two quantum bits. Let the second quantum bit is transmitted over a *quantum depolarizing channel* with error probability p . With this setup, the joint density matrix is given as $\rho_{XY} = q\rho_{XY}^{\gamma_1, \lambda_1} + (1 - q)\rho_{XY}^{\gamma_2, \lambda_2}$, where $\rho_{XY}^{\gamma, \lambda}$ is given as the mixture of the following pure density matrices:

$$\begin{cases} (\gamma^2|00\rangle + \gamma\lambda|01\rangle + \gamma\lambda|10\rangle + \lambda^2|11\rangle)(\gamma^2|00\rangle + \gamma\lambda|01\rangle + \gamma\lambda|10\rangle + \lambda^2|11\rangle)^\dagger & 1 - p \\ (\gamma^2|00\rangle - \gamma\lambda|01\rangle + \gamma\lambda|10\rangle - \lambda^2|11\rangle)(\gamma^2|00\rangle - \gamma\lambda|01\rangle + \gamma\lambda|10\rangle - \lambda^2|11\rangle)^\dagger & p/3 \\ (\gamma\lambda|00\rangle + \gamma^2|01\rangle + \lambda^2|10\rangle + \gamma\lambda|11\rangle)(\gamma\lambda|00\rangle + \gamma^2|01\rangle + \lambda^2|10\rangle + \gamma\lambda|11\rangle)^\dagger & p/3 \\ (-\gamma\lambda|00\rangle + \gamma^2|01\rangle - \lambda^2|10\rangle + \gamma\lambda|11\rangle)(-\gamma\lambda|00\rangle + \gamma^2|01\rangle - \lambda^2|10\rangle + \gamma\lambda|11\rangle)^\dagger & p/3 \end{cases}$$

We note that X and Y coexist in the quantum system, and thus the joint density matrix has been obtained. We already know that X is the cause of Y in this scenario, i.e., $X \rightarrow Y$ is the corresponding directed graph. To verify this, we use Algorithm 1 and 2 as we explained earlier in this model. The results are summarized in Table 4. T means that QInferGraph (Algorithm 2) identifies the direct graph correctly. But, F means that the algorithm fails to identify the direct graph. In all cases the probability of X be in state X_1 is $q = 0.4$.

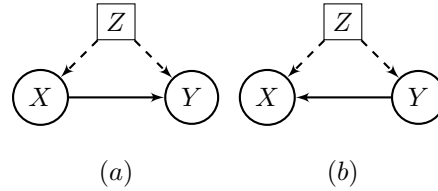
From a combination of Part I and Part II, we note that for this setup, there are no false positive or false negatives. This shows that the choice of hyperparameters is well suited for the problem, and that the proposed framework is efficient in determining if there is a latent confounder.

Table 4: Validation of Direct Graph in Model 1 (Part II) with joint density matrix $\rho_{XY} = 0.4 * \rho_{XY}^{0.6, 0.8} + 0.6 * \rho_{XY}^{1, 0}$.

		p										
		0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99
α	0.2	T	T	T	T	T	T	T	T	T	T	T

4 Cause-Effect Using Observational Data: Tuebingen dataset

Inferring causal relationships from observational data alone is a challenging task even in the most elementary form of such a causal discovery problem, i.e., determining whether X causes Y or, alternatively, Y causes X , given only joint measurements of both variables. Tuebingen dataset is a benchmark database that includes more than 100 different cause-effect pairs selected from various domains (e.g., meteorology, biology, medicine, engineering, economy, etc.) [Mooij et al., 2016]. Here, we only consider the first 41 pairs of cause-effect datasets, available at : <https://webdav.tuebingen.mpg.de/cause-effect/>, to evaluate the performance of QInferGraph on real data. According to the website of Tuebingen database, each datafile contains two variables, where one of them is the cause and the other one is the effect with the possibility of the existence of a latent confounder. So, all cause-effect pairs have a form of a direct/triangle graph, as shown in Figure 2. Here, the goal is to decide whether the correlation between altitude and temperature is only due to a common cause (latent graph) or one of them causes the other one (direct/triangle graph).



Results over the first 41 pairs of Tubingen database. As we discussed in [Javidian et al., 2021], for the classical InferGraph algorithm, as suggested in [Kocaoglu et al., 2020], the best hyperparameters are $\alpha = 0.8$ and $T = 0.001$; while for QInferGraph the best hyperparamete-

Figure 2: Tuebingen: Database with cause-effect pairs of the form (a) or (b).

ters are $\alpha = 0.2$ and $T = 0.005$. Table 5 summarizes the results for QInferGraph and the classical **InferGraph** algorithm with the above mentioned parameters on Tübingen database. Thus, we see that the proposed approach helps achieve significantly better accuracy (0.83) as compared to lower than 50% in the baseline approach. In addition, the false negative rate of 0.17 in the proposed approach is significantly lower than the baselines which have this rate above 0.5. Thus, we see that the proposed approach outperforms classical approach on Tübingen database.

Table 5: Performance of QInferGraph vs classical **InferGraph** on Tübingen database.

Algorithm	True Positive	False Positive	False Negative	Accuracy
QInferGraph ($\alpha = 0.2, T = 0.005$)	0.83	0	0.17	0.83
Classical InferGraph ($\alpha = 0.8, T = 0.001$)	0.32	0	0.68	0.32
Classical InferGraph ($\alpha = 0.7, T = 0.001$)	0.49	0	0.51	0.49

5 Why Should We Not Map Quantum to Classical Directly?

Here, we show why classical common entropy approach do not directly apply to the quantum case. We emphasize that although a joint density operator (matrix) can be converted to a joint probability distribution (as explained in Example 1), we *lose* some *quantum information* due to the loss of entanglement. We give an example that shows converting a joint density matrix ρ_{XY} directly to a joint probability distribution $p(X, Y)$, and then applying classical common entropy approach on $p(X, Y)$ will not lead to the correct results.

Algorithm 3: Rotational procedure for computing the joint probability distribution of a joint density matrix

Input: Joint density matrix of quantum systems X and Y i.e., ρ_{XY} .

Output: Joint probability distribution $p(X, Y)$ corresponding to the joint density matrix ρ_{XY} .

```

/* Compute eigenvalues and eigenvectors of  $\rho_X$ .          */
1  $[V_1, D_1] = \text{eig}(\rho_X)$ ;                               */
/* Compute eigenvalues and eigenvectors of  $\rho_Y$ .          */
2  $[V_2, D_2] = \text{eig}(\rho_Y)$ ;                               */
/* Rotational procedure                                     */
3  $U = V_1 \otimes V_2$ ;                                       */
4  $\rho'_{XY} = U^\dagger \rho_{XY} U$ ;                             */
5 return  $p(X, Y)$  as the entries on the main diagonal of  $\rho'_{XY}$ .

```

Example 1 (Counter Example) Assume the depolarizing channel as described in Model 1, Part II. We already know that X causes Y in this model. To convert the joint density matrix ρ_{XY} , we use a rotational procedure explained as follows: Assume that ρ_{XY} is rotated using a unitary matrix U . Let us say $\rho_{XY} = U \rho'_{XY} U^\dagger$. So, the joint density matrix ρ'_{XY} is computed as $\rho'_{XY} = U^\dagger \rho_{XY} U$. To compute the unitary matrix U for a given ρ_{XY} we use the eigenspaces of ρ_X and ρ_Y , where $\rho_X = \text{Tr}_Y(\rho_{XY})$ and $\rho_Y = \text{Tr}_X(\rho_{XY})$ are computed by tracing out Y and X , respectively. This simple observation enables us to design a procedure that converts a joint density matrix ρ_{XY} to a joint probability distribution $p(X, Y)$ in a way that it takes into account the rotation. This procedure is formally described in Algorithm 3. By converting the joint density matrix ρ_{XY} directly to a joint probability distribution $p(X, Y)$, using Algorithm 3, and then applying classical entropic causal inference on $p(X, Y)$ we obtain the results represented in Table 3 which are opposite to the expected results in all cases. This confirms that classical statistics are not adequate for identification of cause-effect relations in quantum systems due to accessibility of a richer spectrum of causal relations in quantum scenarios.

Conclusions and Future Work

This paper provides a new approach for quantum entropic causal inference in the presence of hidden common causes. As a part of the approach, an iterative algorithmic solution is provided for the

optimization problem that deals with the trade-off between the entropy of the latent quantum system and the quantum conditional mutual information of the observed quantum systems. We show that the use of quantum density matrix helps achieve significantly better tradeoff even for the classical data. The approach is validated on quantum noisy links, where the approach detects the expected causal relation or correlation without causation. Our experiments on the synthetic and real classical data confirms that our quantum entropic approach takes advantage of quantum dependency between random variables through density matrices, and as a result it outperforms its classical counterpart approach. The extension of the problem to general quantum causality graph relations between multiple quantum systems is an open problem for the future.

Acknowledgments and Disclosure of Funding

This research was supported by the Defense Advanced Research Projects Agency (DARPA) Quantum Causality [Grant No. HR00112010008].

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