Quantum-inspired relaxations of graph isomorphism[1]

During the last 50 years, the study of equivalence for relational structures has developed into a vast theory embracing combinatorics, optimization, algebra, and mathematical logic. In this context, graph isomorphism (GI) and its hierarchy of relaxations constitute a central topic, not only for its elusive complexity, but also for its mathematical richness. We develop two frameworks which not only provide a new and unifying perspective of well-known relaxations of GI such as fractional isomorphism and graph equivalence but also allow us to define new relaxations of GI. For instance, using our nonlocal games-based framework we can introduce and study variants of GI inspired by different physical postulates. This leads us to notions of quantum and non-signaling graph isomorphism. In the second part of our investigation, we consider conic relaxations of GI.

For all of the considered relaxations we investigate whether they coincide with existing relations. For example, we were surprised to find that our notion of non-signaling isomorphism is equivalent to fractional isomorphism and $\mathcal{DNN}$-isomorphism coincides with graph equivalence. We show that all of the introduced isomorphism relations form a strict hierarchy nested between GI and non-signalling isomorphism. The complexity of testing these relations ranges from linear time (non-signalling isomorphism) to undecidable (quantum isomorphism).The techniques and ideas employed span across quantum information, algebra, combinatorics, and complexity theory.

1 Quantum and non-signalling isomorphism

Our investigation began with our curiosity to see if there is reasonable and mathematically interesting quantum version of GI. To this end, we reformulated GI in terms of a nonlocal game where two players, Alice and Bob, aim to convince a verifier that they know of a graph isomorphism, f, between graphs G and H. Here, a graph isomorphism is a bijective map $f : V(G) \to V(H)$ which preserves both adjacency and non-adjacency. Whenever such a map exists the two graphs are said to be *isomorphic* and we denote this by $G \cong H$.

The (G, H)-isomorphism game

Each player is given a vertex of either G or H, and must respond with a vertex of the *other* graph. Thus Alice receives or sends a vertex of each graph, which we denote by g_A and h_A. We define g_B and h_B similarly. The players win if $\mathrm{rel}(g_A, g_B) = \mathrm{rel}(h_A, h_B)$, where rel is a function indicating whether two vertices are equal, adjacent, or distinct and non-adjacent.

It is not difficult to see that Alice and Bob can win the (G, H)-isomorphism game perfectly with a classical strategy if and only if $G \cong H$. We can now consider Alice and Bob with various super-classical powers to obtain different relaxations of GI. For instance, we define quantum and non-signaling isomorphism as the existence of a perfect quantum or non-signaling strategy for the isomorphism game. We write $G \cong_q H$ and $G \cong_{NS} H$ to denote these isomorphisms.

It is easy to see that $G \cong H \Rightarrow G \cong_q H \Rightarrow G \cong_{NS} H$, but seeing that the converses do not hold is much more non-trivial. Just imagine, how would you go about finding a pair of non-isomorphic graphs which are quantum isomorphic[2]. Since directly finding such a pair of graphs proved challenging for us, we took a reductive approach. Our construction is an FGLSS-type reduction [8] and such reductions have been previously used, for instance, to prove inapproximability results for clique number and minimum vertex cover [7].

Quantum-friendly reduction from satisfiability of linear systems to GI

To each linear BCS $\mathcal{F}$, we associate a graph $G(\mathcal{F})$. The vertices of this graph are pairs (c, a) where c is a constraint of $\mathcal{F}$ and a is a *satisfying* assignment of bits to the variables appearing in c. Two such vertices are adjacent if they assign different values to some variable.

Theorem 1. *Let $\mathcal{F}$ be a linear BCS and let $\mathcal{F}_0$ be its homogeneous version. Then we have (1) $G(\mathcal{F}) \cong G(\mathcal{F}_0)$ if and only if $\mathcal{F}$ is satisfiable and (2) $G(\mathcal{F}) \cong_q G(\mathcal{F}_0)$ if and only if $\mathcal{F}$ is quantum satisfiable (as defined in [6]).*

[1] A short version of this work has been published at ICALP'17 [12]. A pre-print of the first part is available as arXiv:1611.09837 and the second part is available here.

[2] Keep in mind that there is no algorithmic way to determine if a nonlocal game admits a perfect quantum strategy.

Since there exist infinite families of unsatisfiable linear BCSs which are quantum satisfiable [6, 10, 1], Theorem 1 supplies infinitely many examples of pairs of non-isomorphic graphs (G, H) which are quantum isomorphic. For instance, the BCS based on Mermin's magic square [13], yields two vertex-transitive graphs on 24 vertices providing one such example. From a computational perspective Theorem 1, in combination with the results of [15], implies that quantum isomorphism is undecidable.

"Matrix-based" formulation of quantum isomorphism. A common reformulation of GI says that $G \cong H$ if and only if there exists a permutation matrix P such that $A_G P = P A_H$, where A_X is the adjacency matrix of a graph X. Fractional isomorphism [14] is obtained as a linear relaxation of GI. More precisely, we say that G and H are *fractionally isomorphic* ($G \cong_f H$) if $A_G S = S A_H$ for some doubly stochastic matrix S[3]. It turns out that quantum isomorphism also admits such a "matrix reformulation". In particular, we show that

$$G \cong_q H \quad \Longleftrightarrow \quad (A_G \otimes I_d)\mathcal{P} = \mathcal{P}(A_H \otimes I_d) \tag{1}$$

for some d and some *projective permutation matrix* (PPM) $\mathcal{P}$ of block size d. Here, a PPM is a unitary block matrix, where each of the blocks is an orthogonal projector. A PPM of block size 1 is exactly a permutation matrix and so our notion of PPMs generalizes permutation matrices.

One easy consequence of (1) is that quantum isomorphic graphs are cospectral. More generally, due to the analogy with the matrix formulations of GI and fractional isomorphism, it suggests that our definition of quantum isomorphism is natural and mathematically rich.

Non-signalling isomorphism. Initially we turned to non-signalling isomorphism in hopes of better understanding quantum isomorphism. To our surprise, we found that our operationally defined non-signalling isomorphism coincides with fractional isomorphism.

Theorem 2. *For any graphs G and H, $G \cong_{NS} H$ if and only if $G \cong_f H$.*

Babai, Erdős, and Selkow [2] showed that for almost all graphs G, if $G \cong_f H$ then $G \cong H$ for any graph H. Therefore, non-signalling isomorphism distinguishes almost all graphs. In addition to lending a physical interpretation to fractional isomorphism, Theorem 2 also creates interesting connections to descriptive complexity. For instance, it implies that $G \cong_{NS} H$ if and only if the two graphs cannot be distinguished by any formula in two-variable counting first-order logic [5]. Furthermore, we get that $G \cong_{NS} H$ if and only if the two graphs cannot be distinguished by the 1-dimensional Weisfeiler-Leman (1-WL) algorithm [14]. Since 1-WL has linear average runtime, this implies that non-signalling isomorphism can be tested in linear time on average.

2 Conic relaxations of GI

In the second part of this investigation our starting point was to think of the probabilities $p(yy'|xx')$ coming from a strategy for the isomorphism game as entries in a matrix and require that this matrix belongs to a specific cone.

$\mathcal{K}$-isomorphism

Given a matrix cone $\mathcal{K}$, we say that graphs G and H are $\mathcal{K}$-isomorphic, denoted $G \cong_{\mathcal{K}} H$, if there exists a matrix $M \in \mathcal{K}^{V \times V}$, with $V := V(G) \times V(H)$, such that

$$\begin{aligned} &\sum_{h,h' \in V(H)} M_{gh,g'h'} = 1 \text{ for all } g, g' \in V(G) \\ &\sum_{g,g' \in V(G)} M_{gh,g'h'} = 1 \text{ for all } h, h' \in V(H) \\ &M_{gh,g'h'} = 0 \text{ if } \operatorname{rel}(g,g') \neq \operatorname{rel}(h,h'). \end{aligned} \tag{2}$$

The last condition imposes that the entries corresponding to losing the isomorphism game are zero.

[3]Recall that by Birkhoff's theorem the set of doubly stochastic matrices is the convex hull of permutation matrices.

First, we show that both GI and quantum isomorphism can be expressed as $\mathcal{K}$-isomorphisms for properly chosen convex cones.

Theorem 3. *For any pair of graphs G and H, we have*

$$G \cong H \iff G \cong_{\mathcal{CP}} H \quad \text{and} \quad G \cong_q H \iff G \cong_{\mathcal{CS}_+} H$$

where $\mathcal{CP}$ is the completely positive cone and $\mathcal{CS}_+$ is the completely positive semidefinite cone recently introduced in [11].

In other words, both classical and quantum isomorphisms can be formulated as linear feasibility programs over the $\mathcal{CP}$ and $\mathcal{CS}_+$ cones respectively. (The former has been also independently shown in [9].) At this point we have seen that the same notion of quantum isomorphism can be obtained as a relaxation of GI in three distinct ways (game-based, matrix-based, and as a conic relaxation).

Next, we consider two cones which are usually easy to optimize over. Specifically, we focus on the positive semidefinite cone ($\mathcal{S}_+$) and the doubly nonnegative cone ($\mathcal{DNN}$) which consists of entry-wise nonnegative psd matrices. These cones obey the following:

$$\mathcal{CP}^n \subseteq \mathcal{CS}_+^n \subseteq \mathcal{DNN}^n \subseteq \mathcal{S}_+^n$$

with strict containment everywhere for $n \geq 5$ [11]. The above containments directly imply that

$$G \cong H \;\Rightarrow\; G \cong_q H \;\Rightarrow\; G \cong_{\mathcal{DNN}} H \;\Rightarrow\; G \cong_{\mathcal{S}_+} H \;\Rightarrow\; G \cong_f H, \tag{3}$$

except for the last implication which requires a separate proof. Moreover, we have found examples to show that none of the converses hold and hence all the above isomorphisms are indeed distinct.

Our investigation of $\mathcal{DNN}$- and $\mathcal{S}_+$-isomorphisms revealed that both of them admit surprisingly beautiful algebraic characterizations which in turn imply strong structural similarities between the $\mathcal{DNN}$- or $\mathcal{S}_+$-isomorphic graphs. This investigation falls more naturally within the areas of algebra and graph theory than quantum information. However, many of the key ideas and techniques are inspired by approaches commonly used in quantum information. For instance, one such key idea was to interpret the $\mathcal{K}$-isomorphism matrix as a Choi matrix of some CP map. It was an involved analysis of precisely this CP map that led us to the previously mentioned algebraic characterizations. Hence, the following results might be of interest to quantum community as examples of "quantum proofs of classical results".

Our algebraic characterizations are in terms coherent and partially coherent algebras of graphs. The *coherent algebra* of G, denoted $\mathcal{C}_G$ is the minimal self-adjoint, unital algebra that is closed under entrywise product and contains both A_G and the all ones matrix. Coherent algebras of graphs have been extensively studied in the literature, with relations to areas as varied as k-boson quantum walks on graphs [16], cospectrality [3], and logic [5]. In contrast, the partial coherent algebra, $\mathcal{P}_G$, is a new notion that we introduce.

Theorem 4. *We have that $G \cong_{\mathcal{DNN}} H$ ($G \cong_{\mathcal{S}_+} H$) if and only if $\mathcal{C}_G \cong \mathcal{C}_H$ ($\mathcal{P}_G \cong \mathcal{P}_H$) via an isomorphism that sends A_G to A_H.*

In combination with previous results [18], the above theorem implies that the 2-dimensional Weisfeiler-Leman algorithm provides a poly-time test for $\mathcal{DNN}$-isomorphism. The above theorem also implies that $G \cong_{\mathcal{DNN}} H$ if and only if the two graphs cannot distinguished by any formula in three-variable counting first-order logic [5]. Thus, $\mathcal{DNN}$-isomorphism is in a sense a higher dimensional version of non-signalling isomorphism.

The relationship between cospectrality and GI has generated a lot of interest (see surveys [4, 17]). In particular, it has been asked what fraction and which classes of all graphs are determined by their spectrum. We show that for a large class of graphs $\mathcal{S}_+$-isomorphism is determined solely by the spectra of the two graphs.

Theorem 5. *Let G and H be a connected 1-walk-regular graphs. Then $G \cong_{\mathcal{S}_+} H$ if and only if G and H are cospectral.*

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