MATH 846 Final Presentation:
Quantum Isomorphism of Graphs from Association Schemes

Austen Z. Fan   Ashwin Maran   Ben Young

1 Preliminary

Recall the definition of graph isomorphism.

Definition 1.1. *The graphs $G = (V, E)$ and $H = (V', E')$ are called* isomorphic*, denoted as $G \cong H$, if there exists a 1-1 mapping between V and V' which induces a 1-1 mapping between E and E'.*

This means that up to relabelling of the vertices, G and H are exactly the same graph. The following lemma formalizes this statement.

Lemma 1.2. *Two graphs G and H are isomorphic if and only if there exists a permutation matrix P such that $PA_G = A_H P$, where A_G and A_H are the adjacency matrices of G and H respectively.*

To introduce the notion of quantum isomorphism, we first define the algebraic structure called C^*-algebra.

Definition 1.3. *A C^*-algebra $\mathcal{A}$ is a unital Banach algebra over $\mathbb{C}$ together with a map $x \mapsto x^*$ for any $x \in \mathcal{A}$, called involution, satisfying the following properties:*

1. *For any $x \in \mathcal{A}$, $x^{**} = (x^*)^* = x$.*
2. *For any $x, y \in \mathcal{A}$, $(x + y)^* = x^* + y^*$ and $(xy)^* = y^* x^*$.*
3. *For any $\lambda \in \mathbb{C}$ and $x \in \mathcal{A}$, $(\lambda x)^* = \bar{\lambda} x^*$.*
4. *For any $x \in \mathcal{A}$, $||xx^*|| = ||x||^2$.*

The first three identities are the requirement for being a $*$-algebra and the last identity is called the C^*-identity.

Example 1.4. *The algebra of n-by-n complex matrices $M(n, \mathbb{C})$ equipped with the operator norm $||\cdot||$ and the involution as the conjugate transpose.*

Example 1.5. *The algebra of bounded linear operators $B(\mathcal{H})$ defined on a complex Hilbert space $\mathcal{H}$ equipped with the operator norm $||\cdot||$ and the involution as the adjoint operator.*

Let $\mathcal{A}$ be a C^*-algebra with unit $\mathbb{1}$ and $\mathcal{U} = (u_{i,j})$ be an n-by-n matrix with entries in $\mathcal{A}$. We are now ready to define what's called a quantum permutation matrix.

Definition 1.6. *$\mathcal{U}$ is a* quantum permutation matrix *if*

1. *$u_{i,j}^* = u_{i,j} = u_{i,j}^2$ for any $1 \leq i, j \leq n$.*
2. *$\sum_{k=1}^{n} u_{i,k} = \mathbb{1} = \sum_{k=1}^{n} u_{k,j}$ for any $1 \leq i, j \leq n$.*

3. $\mathcal{U}\mathcal{U}^T = \mathcal{U}^T\mathcal{U} = \begin{pmatrix} \mathbb{1} & 0 & \dots & 0 \\ 0 & \mathbb{1} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & \mathbb{1} \end{pmatrix}$.

Note that when $\mathcal{A} = \mathbb{C}$, this definition recovers the classical permutation matrices.

Example 1.7.
$$\begin{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \\ \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} & \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \\ \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \end{pmatrix}$$

We are now ready to define the notion of quantum isomorphism.

Definition 1.8. *Two graphs G and H are called* quantum isomorphic*, denoted as $G \cong_q H$, if there exists a quantum permutation matrix $\mathcal{U}$ such that $\mathcal{U}A_G = A_H\mathcal{U}$.*

It is not clear from the definition that there exists a pair of graphs that are quantum isomorphic to each other but not isomorphic. The paper shows there are infinitely pairs of graphs that are quantum isomorphic but not classically isomorphic. The authors do this by considering association schemes that are similar to each other in a sense that we will explain.

Before going into association schemes, we introduce another way to characterize classical isomorphism and quantum isomorphism. This will be used later in the proof.

Definition 1.9. *A map $\phi : V(F) \to V(G)$ is a* graph homomorphism from F to G *if for any $\{v_1, v_2\} \in E(F)$, we have $\{\phi(v_1), \phi(v_2)\} \in E(G)$.*

One can consider the total number of homomorphisms from one graph to another.

Definition 1.10. *Given two graphs F and G, we denote* $\hom(F, G) :=$ *# of graph homomorphisms from F to G.*

A celebrated theorem by Lovász [6] sates that two graphs are isomorphic if and only if they admit the same number of homomorphisms from any other graphs.

Theorem 1.11 (Lovász, 67'). *$G \cong H$ if and only if $\hom(F, G) = \hom(F, H)$ for any graph F.*

A remarkable result given by Mančinska and Roberson [7] characterizes quantum isomorphism by homomorphism counts from planar graphs.

Theorem 1.12 (Mančinska & Roberson, 19'). *$G \cong_q H$ if and only if $\hom(F, G) = \hom(F, H)$ for any planar graph F.*

The paper uses this theorem to show the quantum isomorphism between any Hadamard graphs with the same number of vertices.

2 Vertex Model and Scaffold

Let's stare at this equation and see why it is true.

$$\hom(F,G) = \sum_{\phi:V(F)\to V(G)} \prod_{\{a,b\}\in E(F)} (A_G)_{\phi(a),\phi(b)} \tag{2.1}$$

Indeed, for any mapping $\phi : V(F) \to V(G)$, we have

$$\prod_{\{a,b\}\in E(F)} (A_G)_{\phi(a),\phi(b)} = \begin{cases} 1 & \text{if } \phi \text{ is a graph homomorphism from } F \text{ to } G, \\ 0 & \text{otherwise.} \end{cases}$$

In statistical physics and the classification program of the complexity of counting problems, this formulation is called the *vertex (coloring) model*. The name is due to the following. Given any graph F, imagine you place A_G on every edge of F, and think of A_G as a binary function which takes its two adjacent vertices as arguments. Then imagine the vertices in F take values as vertices in G which can be thought of as colors. Take the product of all the result of those functions and sum over all possible "colorings" gives us exactly Equation 2.1.

Remark: There is a provably more expressive model called *edge (coloring) model*, where one colors the edges instead of vertices and think of vertices as functions that take arguments from its adjacent edges.

Let $(X, \mathcal{R})$ be an association scheme with Bose-Mesner algebra $\mathbb{A} = \text{span}(\{A_0, A_1, \ldots, A_d\})$. They act on the standard module $V = \mathbb{C}^X$ in the obvious way. Think about $V = \mathbb{C}^X$ as all complex-valued functions on X with standard basis of column vectors $\{\hat{x} \mid x \in X\}$. For a graph $F = (V, E)$, fix an ordered set $R = \{r_1, r_2, \ldots, r_m\}$ of vertices in F called *roots* and a function $w : E \to \text{Mat}_X(\mathbb{C})$ assigning each edge in F with a binary function. The *scaffold* $S(F, \mathcal{R}; w)$ is defined to be the tensor

$$\mathrm{S}(F,R;w) = \sum_{\phi:V(G)\to X} \left(\prod_{\substack{e\in E(G)\\ e=(a,b)}} w(e)_{\phi(a),\varphi(b)} \right) \widehat{\phi(r_1)} \otimes \widehat{\phi(r_2)} \otimes \cdots \otimes \widehat{\phi(r_m)} \tag{2.2}$$

Note that we can associate different binary functions to different edges in F. In fact, two families scaffolds are particularly important in this paper.

(a) Delta shape (b) Wye shape

Figure 1: Delta shape and Wye shape

Finally, consider the vector space spanned by all scaffolds in the above form. Formally, define $\mathbf{W}^D_{\mathbb{A}}$ (*resp.* $\mathbf{W}^Y_{\mathbb{A}}$) to be the vector space spanned by all scaffolds in the Delta shape (*resp.* Wye shape) where $A_i, A_j, A_k \in \mathbb{A}$.

3 Exactly Triply Regular & Main Theorem

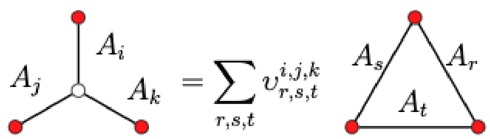
We start with the definition of a triply regular association scheme.

Definition 3.1. *An association scheme* $(X, \mathcal{R})$ *with Bose-Mesner algebra* $\mathbb{A}$ *is called* triply regular *if for any* $x, y, z \in X$ *and all* $0 \le i, j, k \le d$*, we have* $v(x, y, z) := |\{u \in X : x \overset{i}{\sim} u, y \overset{j}{\sim} u, z \overset{k}{\sim} u\}|$ *depends only on* i, j, k *and the three relations joining* x, y, z*, but not on the choice of* x, y, z *themselves.*

A Theorem by Jaeger [4] characterizes when an association scheme is triply regular.

Theorem 3.2 (Jaeger, 95'). $(X, \mathcal{R})$ *is triply regular if and only if* $\mathbf{W}_{\mathbb{A}}^{Y} \subseteq \mathbf{W}_{\mathbb{A}}^{D}$.

When $(X, \mathcal{R})$ is triply regular, denote $v(x, y, z) = v_{r,s,t}^{i,j,k}$ where $x \overset{r}{\sim} z, x \overset{s}{\sim} y, y \overset{t}{\sim} z$, then the scaffold equations



hold for all i, j, k. As one of the themes in this course, we continue with the definition of a dually triply regular association scheme.

Definition 3.3. *An association scheme* $(X, \mathcal{R})$ *is called* dually triply regular *if* $\mathbf{W}_{\mathbb{A}}^{D} \subseteq \mathbf{W}_{\mathbb{A}}^{Y}$.

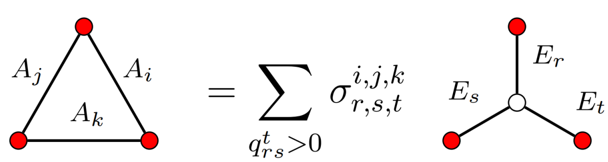
Definition 3.4. *An association scheme* $(X, \mathcal{R})$ *is called* exactly triply regular *if it is both triply regular and dually triply regular.*

Let's finish by stating the main theorem of this paper.

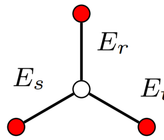
Theorem 3.5. *Let* $(X, \mathcal{R})$ *and* $(Y, \mathcal{S})$ *be exactly triply regular symmetric association schemes that have the same Delta-Wye parameters. Let* G' *be a graph in* $(Y, \mathcal{S})$ *corresponding to* G *in* $(X, \mathcal{R})$*. Then* G *and* G' *are quantum isomorphic.*

4 Delta-Wye parameters

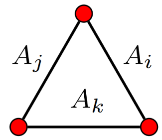
Theorem 4.1. *Let* $(X, \mathcal{R})$ *be an exactly triply regular* d*-class association scheme with Bose-Mesner algebra having an ordered basis* $A_0, \ldots, A_d$ *of adjacency matrices and an ordered basis* $E_0, \ldots, E_d$ *of primitive idempotents. Then there exist unique constants* $\{\sigma_{r,s,t}^{i,j,k} : p_{ij}^{k} > 0, q_{rs}^{t} > 0\}$ *and* $\{\tau_{i,j,k}^{r,s,t} : p_{ij}^{k} > 0, q_{rs}^{t} > 0\}$ *such that*



(4.3)



$$= \sum_{p_{ij}^k > 0} \tau_{i,j,k}^{r,s,t}$$



(4.4)

A proof of Theorem 4.1 can be found in Williams[8]. These values are called the Delta-Wye parameters of $(X, \mathcal{R})$.

Definition 4.2. *Let $(X, \mathcal{R})$ and $(Y, \mathcal{S})$ be exactly triply regular d-class association schemes. We say that they have the same Delta-Wye parameters, if there exists an ordering $A_0, \dots, A_d$ and $A'_0, \dots, A'_d$ of the respective adjacency matrices and an ordering $E_0, \dots, E_d$ and $E'_0, \dots, E'_d$ of their respective primitive idempotents such that $\sigma_{r,s,t}^{i,j,k} = (\sigma')_{r,s,t}^{i,j,k}$, and $\tau_{i,j,k}^{r,s,t} = (\tau')_{i,j,k}^{r,s,t}$.*

Lemma 4.3. *Let $(X, \mathcal{R})$ and $(Y, \mathcal{S})$ be exactly triply regular d-class association schemes with the same Delta-Wye parameters. Then, the association schemes $(X, \mathcal{R})$ and $(Y, \mathcal{S})$ have the same intersection numbers, Krein parameters, eigenvalues, and dual eigenvalues. Moreover, the bijective map $A_i \mapsto A'_i$ extends to a linear isomorphism $\kappa : \mathbb{A} \to \mathbb{A}'$, such that $\kappa(MN) = \kappa(M)\kappa(N)$ and $\kappa(M \circ N) = \kappa(M) \circ \kappa(N)$.*

Proof. We consider Equation 4.3, for a fixed i, j, k. We sum up all coefficients of all the tensors on both the LHS and the RHS. We will first consider the RHS. We see that

$$\text{RHS} = \sum_{q_{rs}^t > 0} \sigma_{r,s,t}^{i,j,k} \sum_{x,y,z,u \in X} (E_r)_{xu}(E_s)_{yu}(E_t)_{zu} = \sum_{q_{rs}^t > 0} \sigma_{r,s,t}^{i,j,k} \sum_{y \in X} \sum_{x,z \in X} (E_r A_s^* E_t)_{xz}$$

where each A_s^* in the sum is with respect to y [10].

It is known that $\{E_r A_r^* E_t : 0 \leq r, s, t \leq d, q_{rs}^t > 0\}$ is an orthogonal basis of $\mathbb{A}\mathbb{A}^*\mathbb{A}$ [11]. We note that when $r = s = t = 0$, $E_0 A_0^* E_0 = E_0 = \frac{1}{|X|} J$, where J is the all-ones matrix. Since every other matrix of the form $E_r A_s^* E_t$ is orthogonal to this matrix, it follows that for all $(r, s, t) \neq (0, 0, 0)$,

$$\sum_{x,z \in X} (E_r A_s^* E_t)_{xz} = 0.$$

Therefore, we see that

$$\text{RHS} = \sigma_{0,0,0}^{i,j,k}(|X|).$$

Now, when $i = j$ and $k = 0$, we see that the sum of coefficients on the LHS is

$$\text{LHS} = \sum_{x,y,z \in X} (A_i)_{x,y}(A_i)_{y,z}(A_0)_{z,x} = \sum_{x,y \in X} (A_i)_{x,y} = |X| p_{ii}^0.$$

This proves that $p_{ii}^0 = \sigma_{0,0,0}^{i,i,0}$. For any other choice of i, j, k, we see that the sum of coefficients on the LHS is $|X| p_{ij}^k p_{ii}^0$.

This proves that the Delta-Wye parameters determine the intersection numbers. The remaining association scheme parameters are then recoverable from the intersection numbers.

Since $\kappa(A_i) = A'_i$ is a $0-1$ matrix and both $A_i \circ A_j = \delta_{ij} A_i$ and $A'_i \circ A'_j = \delta_{ij} A'_i$ holds for this pair of bases, we have $\kappa(M \circ N) = \kappa(M) \circ \kappa(N)$ by linearity. Also,

$$\kappa(A_i A_j) = \kappa\left(\sum_{k=0}^{d} p_{ij}^k A_k\right) = \sum_{k=0}^{d} p_{ij}^k A'_k = A'_i A'_j = \kappa(A_i)\kappa(A_j).$$

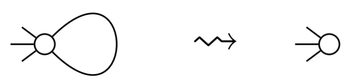
□

5 Main Theorem

Theorem 5.1 (Main Theorem)**.** *Let $(X, \mathcal{R})$ and $(Y, \mathcal{S})$ be exactly triply regular symmetric association schemes that have the same Delta-Wye parameters. Let G be a graph whose adjacency matrix M lies in the Bose-Mesner algebra of $(X, \mathcal{R})$. Then, $\kappa(M)$ is the adjacency matrix of a graph G', and the two graphs G and G' are quantum isomorphic.*

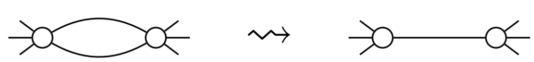
5.1 Epifanov's theorem

Given an embedding of a planar graph, we consider the following local operations:

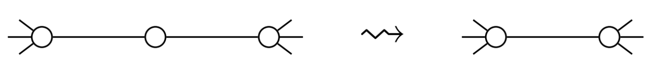


Local Transformation 1: **loop**

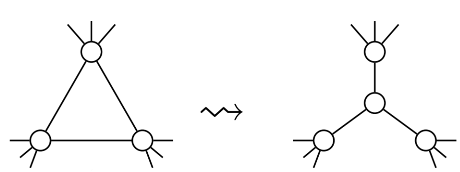
Local Transformation 2: **pendent**



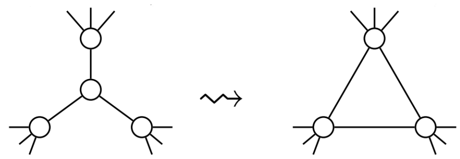
Local Transformation 3: **parallel**



Local Transformation 4: **series**



Local Transformation 5: **Delta**



Local Transformation 6: **Wye**

Theorem 5.2 (Epifanov's Theorem)**.** *Let F be a connected planar graph. There exist a sequence of planar graphs $(F_0, \dots, F_l)$ such that*

1. *$F_0 = F$ and F_l is a graph with a single vertex and no edges.*
2. *F_{h+1} is obtained from F_h using one of the local transformations above, for $0 \leq h < l$.*

Proofs of Epifanov's Theorem can be found in Feo and Provan[3] and Truemper[12].

5.2 Main Lemma

We consider the problem of computing $\mathrm{S}(F, \emptyset; w)$ for planar F and $w : E(F) \to \mathbb{A}$. Recall that

$$\mathrm{S}(F, \emptyset; w) = \sum_{\phi : V(F) \to X} \left(\prod_{\substack{e \in E(F) \\ e=(u,v)}} w(e)_{\phi(u), \varphi(v)} \right).$$

If F has connected components $F^1, \dots, F^k$, then it can be seen that

$$\mathrm{S}(F, \emptyset; w) = \prod_{i=1}^{k} \mathrm{S}(F^i, \emptyset; w|_{F_i}). \tag{5.5}$$

Therefore, we can restrict our attention to connected, planar F. We know from Epifanov's Theorem, that there exists a sequence of planar graphs $(F_0, \dots, F_l)$.

The main technical lemma used in the proof of the Main Theorem is as follows:

Lemma 5.3 (Main Lemma)**.** *Let $(X, \mathcal{R})$ and $(Y, \mathcal{S})$ be an exactly triply regular symmetric association schemes with the same Delta-Wye parameters. Let κ be the isomorphism from Theorem 4.3, and let $\kappa \bullet w$ represent the function composition. For any $0 \leq h < l$, there exists a positive integer m_h, constants $\{\alpha_{h,m}\}_{m=1}^{m_h}$, and weight functions $\{w_{h,m}\}_{m=1}^{m_h}$ where each $w_{h,m} : E(F_{h+1}) \to \mathbb{A}$, such that*

$$\mathrm{S}(F_h, \emptyset; w) = \sum_{m=1}^{m_h} \alpha_{h,m} \mathrm{S}(F_{h+1}, \emptyset; w_{h,m}); \qquad \mathrm{S}(F_h, \emptyset; \kappa \bullet w) = \sum_{m=1}^{m_h} \alpha_{h,m} \mathrm{S}(F_{h+1}, \emptyset; \kappa \bullet w_{h,m}). \tag{5.6}$$

Before proving Theorem 5.3, we will quickly see how it implies the Main Theorem. By repeated application of Theorem 5.3, we see that there exists a positive integer M, constants $\{\beta_m\}_{m=1}^{M}$ and weight functions $\{w_m\}_{m=1}^{M}$ such that

$$\mathrm{S}(F_0, \emptyset; w) = \sum_{m=1}^{M} \beta_m \mathrm{S}(F_l, \emptyset; w_m); \qquad \mathrm{S}(F_0, \emptyset; \kappa \bullet w) = \sum_{m=1}^{M} \beta_m \mathrm{S}(F_l, \emptyset; \kappa \bullet w_m).$$

Then, we note that F_l is the graph with just one vertex and no edges. Therefore, for any weight function $w : \emptyset \to \mathrm{Mat}_X(\mathbb{C})$, we have that $\mathrm{S}(F_l, \emptyset; w) = |X|$. This implies that $\mathrm{S}(F, \emptyset; w) = \mathrm{S}(F, \emptyset; \kappa \bullet w)$. If we let w be the function such that $w(e) = M$ for all $e \in E(F)$, then we see that for any planar F,

$$\hom(F, G) = \mathrm{S}(F, \emptyset; w) = \mathrm{S}(F, \emptyset; \kappa \bullet w) = \hom(F, G').$$

This implies that G and G' are quantum isomorphic.

5.3 Proof of the Main Lemma

We will focus on the weight function w. Consider an edge $e_1 = (u_1, v_1) \in E(F)$. We can represent w as $w = a_0 w_0 + \cdots + a_d w_d$, where $\{a_i\}_{i=0}^d$ are constants, and each w_i is defined as:

$$w_i(e) = \begin{cases} A_i & \text{if } e = e_1 \\ w(e) & \text{if } e \neq e_1 \end{cases}$$

Lemma 5.4.

$$\mathrm{S}(F, \emptyset; w) = \sum_{i=0}^{d} a_i \cdot \mathrm{S}(F, \emptyset; w_i).$$

Proof. By definition, we see that

$$\begin{aligned} \mathrm{S}(F, \emptyset; w) &= \sum_{\phi: V(F) \to X} \left((a_0 w_0 + \cdots + a_d w_d)(e_1)_{\phi(u_1), \phi(v_1)} \cdot \prod_{\substack{e \in E(F) \setminus \{e_1\} \\ e = (u,v)}} w(e)_{\phi(u), \varphi(v)} \right) \\ &= \sum_{i=0}^{d} a_i \sum_{\phi: V(F) \to X} \left(w_i(e_1)_{\phi(u_1), \phi(v_1)} \cdot \prod_{\substack{e \in E(F) \setminus \{e_1\} \\ e = (u,v)}} w(e)_{\phi(u), \varphi(v)} \right) \\ &= \sum_{i=0}^{d} a_i \cdot \mathrm{S}(F, \emptyset; w_i). \end{aligned}$$

□

By repeated application of Theorem 5.4 on each edge of $E(F)$, we can assume that the range of the weight function w is $\{A_0, \ldots, A_d\}$.

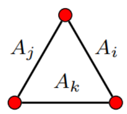
Now, we consider the local transformation $F_h \mapsto F_{h+1}$. We will consider each of the local transformations possible.

1. **loop**: Let e be the loop that is deleted. We may assume that $w(e) = A_r$. In this case, $m_h = 1$, $\alpha_{h,1} = \delta_{r,0}$, and $w_{h,1} = w|_{E(F) \setminus \{e\}}$.
2. **pendent**: Let e be the edge that is deleted. We may assume that $w(e) = A_r$. In this case, $m_h = 1$, $\alpha_{h,1} = p^0_{r,r}$, and $w_{h,1} = w|_{E(F) \setminus \{e\}}$.
3. **parallel**: Let e be the edge that is deleted, and let e' be its parallel edge. We may assume that $w(e) = A_r$ and $w(e') = A_s$. In this case, $m_h = 1$, $\alpha_{h,1} = \delta_{s,r}$, and $w_{h,1} = w|_{E(F) \setminus \{e\}}$.

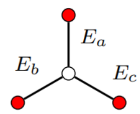
4. **series**: Let e and e' be the edges in series, that are replaced with the single edge e'' in F_{h+1}. We may assume that $w(e) = A_r$ and $w(e') = A_s$. In this case, $m_h = d + 1$, $\alpha_{h,m} = p^m_{r,s}$, and $w_{h,m}$ is defined as

$$w_{h,m}(e) = \begin{cases} A_m & \text{if } e = e'' \\ w(e) & \text{if } e \neq e'' \end{cases}$$

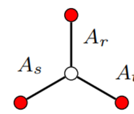
5. **Delta**: Let e_1, e_2, e_3 be the edges that are replaced with the edges e'_1, e'_2, e'_3 in F_{h+1} (with e'_i being the edge that is not incident on any of the endpoints of the edge e_i). We may assume that $w(e_1) = A_i, w(e_2) = A_j$, and $w(e_3) = A_k$. Now, we note that from Equation 4.3, we have that



$$= \sum_{q^c_{ab}>0} \sigma^{i,j,k}_{a,b,c}$$



$$= \frac{1}{|X|^3} \sum_{q^c_{ab}>0} \sigma^{i,j,k}_{a,b,c} \sum_{r,s,t} Q_{ra} Q_{sb} Q_{tc} \tag{5.7}$$



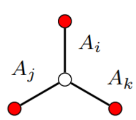
Consequently, we may let $m_h = (d+1)^3$, and for each $m = (r, s, t) \in [d]^3$, we let

$$\alpha_{h,(r,s,t)} = \frac{1}{|X|^3} \sum_{a,b,c:\ q^c_{ab}>0} \sigma^{i,j,k}_{a,b,c} Q_{ra} Q_{sb} Q_{tc},$$

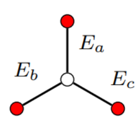
and we define $w_{h,(r,s,t)}$ as

$$w_{h,(r,s,t)}(e) = \begin{cases} A_r & \text{if } e = e'_1 \\ A_s & \text{if } e = e'_2 \\ A_t & \text{if } e = e'_3 \\ w(e) & \text{if } e \notin \{e'_1, e'_2, e'_3\} \end{cases}$$

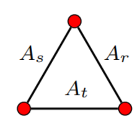
6. **Wye**: Let e_1, e_2, e_3 be the edges that are replaced with the edges e'_1, e'_2, e'_3 in F_{h+1} (with e'_i being the edge that is incident on the two vertices that e_i is not incident on). We may assume that $w(e_1) = A_i, w(e_2) = A_j$, and $w(e_3) = A_k$. Now, we note that from Equation 4.4, we have that



$$= \sum_{a,b,c} P_{ai} P_{bj} P_{ck}$$



$$= \sum_{a,b,c} P_{ai} P_{bj} P_{ck} \sum_{p^t_{rs}>0} \tau^{a,b,c}_{r,s,t} \tag{5.8}$$



Consequently, we may let $m_h = (d+1)^3$, and for each $m = (r, s, t) \in [d]^3$, we let

$$\alpha_{h,(r,s,t)} = \sum_{a,b,c=0}^{d} \tau^{a,b,c}_{r,s,t} P_{ai} P_{bj} P_{ck},$$

and we define $w_{h,(r,s,t)}$ as

$$w_{h,(r,s,t)}(e) = \begin{cases} A_r & \text{if } e = e'_1 \\ A_s & \text{if } e = e'_2 \\ A_t & \text{if } e = e'_3 \\ w(e) & \text{if } e \notin \{e'_1, e'_2, e'_3\} \end{cases}$$

We see that Equation 5.6 holds true for each of the transformations above.

6 Extending to #CSP

6.1 #CSP preliminaries

Recall the vertex coloring model definition of (2.1), which we repeat below.

$$\hom(F,G) = \sum_{\phi:V(F)\to V(G)} \prod_{\{a,b\}\in E(F)} (A_G)_{\phi(a),\phi(b)}$$

Consider the following slightly different formulation (closer to the edge coloring model mentioned earlier): subdivide each of F's edges with a new degree-2 vertex, assigned function A_G. Call the resulting graph, or *signature grid*, Ω_F. See Figure 7.

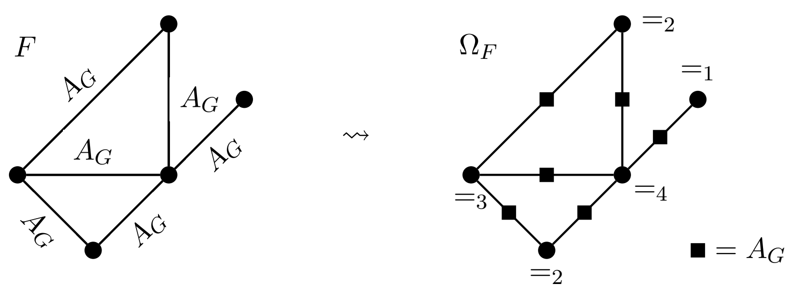


Figure 7: Converting an vertex-coloring model input graph F to an equivalent edge-coloring model input signature grid Ω_F.

Let $V_{\mathcal{EQ}}(\Omega_F) \subset V(\Omega_F)$ denote the original vertices of F (drawn as circles), and $V_{\mathcal{C}}(\Omega_F) \subset V(\Omega_F)$ denote the new degree-2 vertices (drawn as squares) Then Ω_F is bipartite, with $V(\Omega_F) = V_{\mathcal{EQ}}(\Omega_F) \sqcup V_{\mathcal{C}}(\Omega_F)$. Now

$$\hom(F,G) = \sum_{\phi:V_{\mathcal{EQ}}(\Omega_F)\to V(G)} \prod_{v\in V_{\mathcal{C}}(\Omega_F)} (A_G)_{\phi(\Omega_F(v))}, \tag{6.9}$$

where $\Omega_F(v) \subseteq V_{\mathcal{EQ}}(\Omega_F)$ denotes the set of vertices adjacent to v.

Observe that nothing in the formulation (6.9) limits any vertices to have degree 2, as the A_G vertices have in the case of graph homomorphism. Instead of a binary function A_G, we may consider a *constraint function* G on n inputs from a *domain* X or equivalently a tensor $G \in \mathbb{C}^{X^n}$. For a set $\mathcal{G}$ of functions on common domain X (but possibly of different arities) , define the *counting constraint satisfiability problem* (#CSP) for $\mathcal{G}$ as follows: given a bipartite signature grid Ω with vertices partitioned into *equality* and *constraint* vertices as $V(\Omega) = V_{\mathcal{EQ}}(\Omega) \sqcup V_{\mathcal{C}}(\Omega)$ and each constraint vertex $v \in V_{\mathcal{C}}(\Omega)$ assigned a constraint function $g_v \in \mathcal{G}$, the problem is to compute the partition function

$$\#\mathrm{CSP}(\Omega,\mathcal{G}) = \sum_{\phi:V_{\mathcal{EQ}}(\Omega)\to X} \prod_{v\in V_{\mathcal{C}}(\Omega)} g_v(\phi(\Omega(v))).$$

We similarly extend Theorem 1.2 and Theorem 1.8 to definitions of classical and quantum isomorphism of constraint functions:

Definition 6.1. *Constraint functions $F, G \in \mathbb{C}^{X^n}$ are* isomorphic *($F \cong G$) if there is a permutation matrix P, indexed by X, satisfying $P^{\otimes n} f = g$, where $f, g \in \mathbb{C}^{d^n}$ are the natural vectorizations of F and G, respectively ($F(x_1,\dots,x_n) = f_{x_1\dots x_n}$, where $x_1\dots x_n$ is a base-d integer).*

Constraint function sets $\mathcal{F} = \{F_i\}_{i=1}^t$ and $\mathcal{G} = \{G_i\}_{i=1}^t$ are isomorphic if there is a single permutation matrix P satisfying $Pf_i = g_i$ for all $i \in [t]$.

Definition 6.2. *Constraint functions $F, G \in \mathbb{C}^{X^n}$ are* quantum isomorphic *($F \cong_q G$) if there is a $d \times d$ quantum permutation matrix $\mathcal{U}$ satisfying $\mathcal{U}^{\otimes n} f = g$.*

Constraint function sets $\mathcal{F} = \{F_i\}_{i=1}^t$ and $\mathcal{G} = \{G_i\}_{i=1}^t$ are quantum isomorphic if there is a single quantum permutation matrix $\mathcal{U}$ satisfying $\mathcal{U} f_i = g_i$ for all $i \in [t]$.

The study of #CSP in this context is motivated by the following two results, which by the above discussion are generalizations of Theorem 1.11 and Theorem 1.12, respectively.

Theorem 6.3 ([13]). *Constraint function sets $\mathcal{F} \cong \mathcal{G}$ if and only if $\#\mathrm{CSP}(\Omega, \mathcal{F}) = \#\mathrm{CSP}(\Omega, \mathcal{G})$ for every signature grid Ω.*

Theorem 6.4 ([1]). *Constraint function sets $\mathcal{F} \cong_q \mathcal{G}$ if and only if $\#\mathrm{CSP}(\Omega, \mathcal{F}) = \#\mathrm{CSP}(\Omega, \mathcal{G})$ for every planar signature grid Ω.*

However, there are currently no known examples of constraint function sets $\mathcal{F}$ and $\mathcal{G}$ containing a signature of arity greater than 2 such that $\mathcal{F} \cong_q \mathcal{G}$ but $\mathcal{F} \not\cong \mathcal{G}$. To work towards constructing such an example, we turn to superschemes.

6.2 Superschemes

Just as #CSP is a generalization of binary graph homomorphism to higher-arity tensors, a superscheme is a generalization of association schemes from binary to higher-arity relations. For $n \in \mathbb{N}$ and finite set X with $|X| = d$, call $R \subset X^n$ an "n-ary relation". For $j \in [n]$, define $\pi_j^n : X^n \to X^{n-1}$ by $\pi_j^n(x_1, \ldots, x_n) = (x_1, \ldots, x_{j-1}, x_{j+1}, x_n)$.

Definition 6.5 ([5],[9]). *Let $\Pi = \{\Pi^1, \ldots, \Pi^t\}$, with each $\Pi^n \subset \mathcal{P}(X^n)$. Then (X, Π) is a t-*superscheme *if*

1. *For each $n \in [t]$, Π^n is a partition of X^n.*
2. *For each $n \in [t]$, every $R_i \in \Pi^n$, and every permutation $\sigma \in S_n$, $\sigma(R_i) \in \Pi^n$ (where $\sigma(x_1, \ldots, x_n) = (x_{\sigma(1)}, \ldots, x_{\sigma(n)})$).*
3. *For each $2 \le n \le t$, $j \in [n]$, and $R_i \in \Pi^n$, $\pi_j^n(R_i) \in \Pi^{n-1}$.*
4. *For each $2 \le n \le t$, $j \in [n]$, $R_i \in \Pi^n$, and $x = (x_1, \ldots, x_{j-1}, x_{j+1}, x_n) \in \pi_j^n(R_i)$, $|(\pi_j^n)^{-1}(x) \cap R_i| = p_{i,j}$, where $p_{i,j}$ is a constant that does not depend on the choice of $x \in R_i$.*

For example, let $\Pi^2 = \{R_0, \ldots, R_d\}$ with $R_0 = \{(x, x) \mid x \in X\}$, $R_i = R_i^t$ for each i, and Π^3 consist of the nonempty

$$R_{ijk} = \{(x, y, z) \mid (x, y) \in R_i, (x, z) \in R_j, (y, z) \in R_k\} \tag{6.10}$$

for $i, j, k \in [d]$. Then property 1 for $n = 2$ and property 4 for $n = 3$ imply that Π^2 is a symmetric association scheme. Indeed, for $(x, y) \in R_i$ and $j, k \in [d]$, apply property 4 to $R_{ijk} \in \Pi^3$ and $j = 3$ to get

$$p_{ijk,3} = |(\pi_3^3)^{-1}((x, y)) \cap R_{ijk}| = |\{z \mid (x, z) \in R_j, (z, y) \in R_k\}| = p_{jk}^i,$$

a constant that does not depend on the choice of $(x, y) \in R_i$.

Now suppose we start with a symmetric association scheme $\Pi^2 = \{R_0, \dots, R_d\}$, and let Π^3 consist of the ternary relations defined in (6.10). Extend this idea as follows: let Π^4 consist of the nonempty 4-ary relations

$$\begin{aligned} R_{ijkrst} = \{(w, x, y, z) \mid\ & (w, x) \in R_i \\ & (w, y) \in R_j \\ & (w, z) \in R_k \\ & (x, y) \in R_r \\ & (x, z) \in R_s \\ & (y, z) \in R_t\}. \end{aligned}$$

Observe that, for $(x, y, z) \in R_{rst}$,

$$|(\pi_1^4)^{-1}((x, y, z)) \cap R_{ijkrst}| = |\{w \mid (w, x) \in R_i, (w, y) \in R_j, (w, z) \in R_k\}|.$$

Similar identities hold for (π_j^4) for $j > 1$. Thus Π^2 and Π^3 define a superscheme if and only if the base association scheme is triply regular, with $p_{ijkrst,j} = v_{rst}^{ijk}$.

For a tuple $x = (x_1, \dots, x_n)$, for $i \in [n]$, let

$$x^2|_i = \{(x_i, x_1), (x_i, x_2), \dots, (x_i, x_n)\} \setminus (x_i, x_i)$$

denote the set of all pairs of distinct elements from x containing x_i. Then define

$$x^2 \setminus i = x^2 \setminus (x^2|_i)$$

to be the set of all pairs of distinct elements from x not containing x_i. For appropriately sized multisets $\alpha, \beta \subset [d]$, write $x^2|_i \in R_\alpha$ and $x^2 \setminus i \in R_\beta$ to mean that the pairs in $x^2|_i$ and $x^2 \setminus i$ are contained in the binary relations specified by α and β, respectively (e.g. above $(w, x, y, z)^2|_1 \in R_{i,j,k}$ and $(w, x, y, z)^2 \setminus 1 \in R_{r,s,t}$). Then, for $x^2 \setminus i \in R_\beta$, define

$$v_\beta^\alpha = |\{x_i \mid x^2|_i \in R_\alpha\}|.$$

Definition 6.6. *An association scheme (X, R) is* t-super-regular *if all constants v_β^α exist for X^ℓ, for each $\ell \in [t]$. Call these constaints v_β^α the* regularity parameters *of the scheme.*

Equivalently, (X, R) is t-super-regular if $(X, \Pi^1, \dots, \Pi^t)$, with Π^n consisting of n-ary relations partitioning X^n, and each such relation defined by a size-$\binom{n}{2}$ multiset of $[d]$ dictating the relationship between each pair of elements in a tuple of X^n, is a superscheme.

6.3 Constraint functions from superschemes

Given a t-super-regular association scheme with corresponding superscheme $(X, \Pi^1, \dots, \Pi^t)$, for $R_\alpha \in \Pi^n$, let $A_\alpha \in \{0, 1\}^{X^n}$ be the characteristic tensor of R_α. View $\mathcal{F} = \bigcup_{n=1}^t \{A_\alpha \mid R_\alpha \in \Pi^n\}$ as a set of constraint functions. We would like to show that any two constraint function sets $\mathcal{F}$ and $\mathcal{G}$ constructed in this way from t-super-regular association schemes with the same delta-wye and regularity parameters are quantum isomorphic. The first step in this direction is a generalization of the series transformation in the proof of Lemma 5.4.

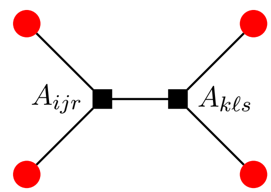


Figure 8: A scaffold in the context of #CSP, with two incident constraint vertices.

The scaffold in Figure 8 has value

$$\begin{aligned}
&\sum_{w,x,y,z\in X}\sum_{a\in X} A_{ijr}(a,w,x)A_{k,\ell,s}(a,y,z)\hat{w}\otimes\hat{x}\otimes\hat{y}\otimes\hat{z}\\
&=\sum_{w,x,y,z\in X}\sum_{a\in X} A_i(a,w)A_j(a,x)A_r(w,x)A_k(a,y)A_\ell(a,z)A_s(y,z)\hat{w}\otimes\hat{x}\otimes\hat{y}\otimes\hat{z}\\
&=\sum_{q,t,u,v\in[d]}\sum_{(w,x,y,z)\in R_{rqtuvs}} v^{ijk\ell}_{rqtuvs}\hat{w}\otimes\hat{x}\otimes\hat{y}\otimes\hat{z}\\
&=\sum_{q,t,u,v\in[d]} v^{ijk\ell}_{rqtuvs}A_{rqtuvs}.
\end{aligned}$$

A_{rqtuvs} is the characteristic tensor of a 4-ary relation, so is a 4-ary constraint function, which we can view as the result of contracting the edge between the constraint vertices in Figure 8. Hence, similar to the series reduction in the proof of Lemma 5.4, if two t-super-regular association schemes have the same regularity parameters, we can reduce the above scaffold to a linear combination of two scaffolds with an edge contracted, with the linear combinations for the two schemes having the same coefficients. Analogous, but somewhat more complicated, reasoning yields a similar reduction for two adjacent constraint vertices of arity higher than 3, or for multiple parallel edges between the two constraint vertices.

Next, we consider delta-wye transformations. We have two types of delta-wye transformations, as the center of the wye can be either a constraint or equality vertex. The first transformation is shown in Figure 9. Note that this is not a 'true' delta-wye transformation, since the delta

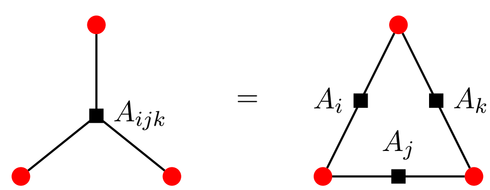


Figure 9: Equivalence between a delta and wye scaffold, with a constraint vertex at the center of the wye.

has extra degree-2 constraint vertices on each edge. However, recall that, in the #CSP view of graph homomorphism, these degree-2 constraint vertices were implicitly present when we applied Epifanov's theorem. Hence we may ignore them in this context as well.

Let A_α, A_β, and A_γ be binary, ternary, and 4-ary constraint functions, respectively. Define

$$R_{\alpha'} = \{(a, x, y) : (a, x), (a, y) \in R_\alpha, (x, y) \in R_0\}$$
$$R_{\beta'} = \{(b, c, x, z) : (b, c, x), (b, c, z) \in R_\beta, (x, z) \in R_0\}$$
$$R_{\gamma'} = \{(d, e, f, y, z) : (d, e, f, y), (d, e, f, z) \in R_\gamma, (y, z) \in R_0\}.$$

Since $R'_\alpha, R'_\beta, R'_\gamma$ define all binary relationships between the entries of their tuples, they are indeed members of Π^3, Π^4, and Π^5, respectively. Observe that the scaffold equation in Figure 10 holds: The transformation in Figure 10 is a 'true' delta-wye transformation, but the delta violates the

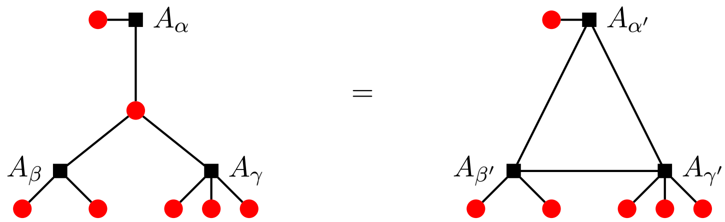


Figure 10: Equivalence between a delta and wye scaffold, with an equality vertex at the center of the wye.

signature grid bipartiteness. Thankfully, this is not an issue, as we can apply the edge contraction procedure in Figure 8.

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