

Graph Isomorphism problem, Weisfeiler-Leman algorithm and coherent configurations

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Coherent algebras (D. Higman) = Cellular algebras (Weisfeiler-Leman)

Notation.

Let $A, B \in M_{\Omega}(\mathbb{F})$ be arbitrary matrices. We denote by

- AB (or $A \cdot B$) the usual matrix product;
- $A \circ B$ the Schur-Hadamard (component-wise) product, i.e. $(A \circ B)_{\alpha\beta} := A_{\alpha\beta} B_{\alpha\beta}$;
- A^{\top} the transposed of A ;
- I_{Ω} the identity matrix;
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Proposition

The algebra $(M_{\Omega}(\mathbb{F}), \circ)$ is a commutative associative algebra with identity J_{Ω} . It is isomorphic to \mathbb{F}^n where $n = |\Omega|^2$.

Idempotents

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Exercise. Prove that a symmetric matrix is \cdot and \circ idempotent iff it's $(0, 1)$ -diagonal matrix.

Coherent (cellular) algebras.

Definition.

A subspace $\mathcal{A} \leq M_\Omega(\mathbb{F})$ is called a **coherent** (or **cellular**) algebra if it contains I_Ω, J_Ω and is closed with respect to \cdot, \circ, \top . The numbers $\dim(\mathcal{A})$ and $|\Omega|$ are called the **rank** and the **degree** of \mathcal{A} .

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Proposition

Let $\mathcal{X} = (\Omega, \mathcal{C})$ be a coherent configuration. Then the linear span $\mathbb{F}[\mathcal{C}] := \langle A(C) \rangle_{C \in \mathcal{C}}$ is a coherent algebra of dimension $|\mathcal{C}|$. It is called the **adjacency** (or **Bose-Mesner**) algebra of \mathcal{X} .

Adjacency algebra of a coherent configuration.

The basis $A(C)$, $C \in \mathcal{C}$ is called the **standard** basis of $\mathbb{F}[\mathcal{C}]$. The structure constants of the algebra $\mathbb{F}[\mathcal{C}]$ with respect to the standard basis coincide with the intersection numbers of \mathcal{X} , i.e.

$$A(S)A(T) = \sum_{R \in \mathcal{C}} c_{ST}^R A(R)$$

Notice that the standard basis matrices $A(S)$, $S \in \mathcal{C}$ are $(0, 1)$ -matrices, or, equivalently, they are minimal \circ -idempotents.

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Theorem

Every coherent algebra $\mathcal{A} \leq M_{\Omega}(\mathbb{F})$ has a unique basis consisting of minimal \circ -idempotents which are pairwise orthogonal. If $\text{char}(\mathbb{F}) = 0$ then \mathcal{A} is the adjacency algebra of a uniquely determined coherent configuration.

Proof of the Theorem

Since \mathcal{A} is a \circ -subalgebra of $(M_\Omega(\mathbb{F}), \circ) \cong (\mathbb{F}^n, \circ)$, $n = |\Omega|^2$, we start with the following

Lemma

Let \mathcal{A} be a k -dimensional subalgebra of (\mathbb{F}^n, \circ) . Then there exists a unique basis A_1, \dots, A_k of \mathcal{A} consisting of minimal, pairwise orthogonal, \circ -idempotents. Each \circ -idempotent of \mathcal{A} is a $(0, 1)$ -linear combination of A_1, \dots, A_k and $A_1 + \dots + A_k$ is the unit of \mathcal{A} .

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- $(A_i A_j)_{\alpha\beta} = c_{ij}^k$ where k is defined by $(\alpha, \beta) \in R_k$;
- if $\text{char}(\mathbb{F}) = 0$, then
$$(A_i A_j)_{\alpha\beta} = |\alpha R_i \cap R_j \beta| \implies |\alpha R_i \cap R_j \beta| = c_{ij}^k.$$

Isomorphisms between coherent algebras

Definition

Given two coherent algebras $\mathcal{A} \leq M_{\Omega}(\mathbb{F})$, $\mathcal{A}' \leq M_{\Omega'}(\mathbb{F})$, a linear bijection $L : \mathcal{A} \rightarrow \mathcal{A}'$ is called an **(algebraic) isomorphism** iff

- $L(XY) = L(X)L(Y)$;
- $L(X \circ Y) = L(X) \circ L(Y)$;
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Proposition

Let $L : \mathbb{F}[\mathcal{C}] \rightarrow \mathbb{F}[\tilde{\mathcal{C}}]$ be an algebraic isomorphism between the adjacency algebras of co.co.s \mathcal{C} and $\tilde{\mathcal{C}}$. Then there exists a bijection $\varphi : \mathcal{C} \rightarrow \tilde{\mathcal{C}}$ such that $L(A(C)) = A(C^\varphi)$ and $c_{RS}^T = \tilde{c}_{R^\varphi S^\varphi}^T$. Vice versa, any bijection $\varphi : \mathcal{C} \rightarrow \tilde{\mathcal{C}}$ satisfying the above equations extends uniquely up to an algebraic isomorphism between $\mathbb{F}[\mathcal{C}]$ and $\mathbb{F}[\tilde{\mathcal{C}}]$. We'll call it an **algebraic isomorphism** between the co.co.s.

Properties of algebraic isomorphisms

Proposition

Let $\varphi : \mathcal{C} \rightarrow \tilde{\mathcal{C}}$ be an algebraic isomorphism between the co.co.s $\mathcal{X} = (\Omega, \mathcal{C})$ and $\tilde{\mathcal{X}} = (\tilde{\Omega}, \tilde{\mathcal{C}})$. Then

- $(RS)^\varphi = R^\varphi S^\varphi$ for any $R, S \in \mathcal{C}^\cup$
- for each fiber Δ of \mathcal{X} there exists a unique fiber Δ' of $\tilde{\mathcal{X}}$ such that $(1_\Delta)^\varphi = 1_{\Delta'}$, that is φ induces a bijection between fibres;
- $S \in \mathcal{C} \implies D(S^\varphi) = D(S)^\varphi, R(S^\varphi) = R(S)^\varphi$;
- $|n_{\mathcal{C}^\varphi}| = |n_{\mathcal{C}}|$ for each $C \in \mathcal{C}$;
- $|\Delta^\varphi| = |\Delta|$ for any $\Delta \in \Phi(\mathcal{X})$;

Isomorphisms between coherent algebras

Proposition

For each $f \in \text{Iso}(\mathcal{X}, \mathcal{X}')$ the mapping f^* is an algebraic isomorphism between the configurations. In this case we say that f^* is an algebraic isomorphism induced by a combinatorial one.

All algebraic automorphisms of a co.co. $\mathcal{X} = (\Omega, \mathcal{C})$ form a group (a subgroup of $\text{Sym}(\mathcal{C})$) denoted as $\text{Alg}(\mathcal{X})$ or $\text{Alg}(\mathcal{C})$. Notice that $\text{Iso}(\mathcal{X}) / \text{Aut}(\mathcal{X}) \hookrightarrow \text{Alg}(\mathcal{X})$.

Proposition

Let $A \leq \text{Alg}(\mathcal{X})$. Then the subspace

$$\mathbb{Q}[\mathcal{C}]^A := \{x \in \mathbb{Q}[\mathcal{C}] \mid \forall_{a \in A} x^a = x\}$$

is a coherent algebra. The corresponding coherent congruence is denoted as \mathcal{C}^A . It is called an **algebraic fusion** of \mathcal{C} .

Coherent closure.

Proposition. Let $\mathcal{X} = (\Omega, \mathcal{C})$ and $\mathcal{X}' = (\Omega, \mathcal{C}')$ be coherent configurations. Then

- $\mathbb{F}[\mathcal{C}] \subseteq \mathbb{F}[\mathcal{C}'] \iff \mathcal{C} \sqsubseteq \mathcal{C}'$;
- $\mathbb{F}[\mathcal{C}] \cap \mathbb{F}[\mathcal{C}'] = \mathbb{F}[\mathcal{C} \wedge \mathcal{C}'] \implies \mathcal{C} \wedge \mathcal{C}'$ is a coherent configuration.

Notice that the sum of coherent algebras is not necessarily coherent algebra.

Proposition

Let $A_1, \dots, A_m \in M_\Omega(\mathbb{F})$ be an arbitrary sequence of matrices. The intersection of all coherent algebras containing A_1, \dots, A_m is a coherent algebra too, called the **coherent closure** of A_1, \dots, A_m and denoted as $\langle\langle A_1, \dots, A_m \rangle\rangle$.

Computing coherent closure by WL-algorithm.

Definition

Given a sequence $M_1, \dots, M_k \in M_\Omega(\mathbb{F})$ of matrices. We define a partition $\mathcal{P}(M_1, \dots, M_k)$ of Ω^2 via the following equivalence relation

$$(\alpha, \beta) \sim (\gamma, \delta) \iff \forall_{1 \leq i \leq k} (M_i)_{\alpha\beta} = (M_i)_{\gamma\delta}$$

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Proposition. Let $\mathcal{X} = (\Omega, \mathcal{C})$ be a co.co. and $\mathcal{S} \vdash \Omega^2$. Then

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$\mathcal{S} \sqsubseteq \mathcal{C} \implies \text{bl}(\mathcal{S}) \sqsubseteq \mathcal{C}$ (follows from $\text{bl}(\mathcal{S}) \sqsubseteq \text{bl}(\mathcal{C})$ and $\text{bl}(\mathcal{C}) = \mathcal{C}$)

Computing coherent closure by WL algorithm.

- **Input:** $A_1, \dots, A_k \in M_\Omega(\mathbb{F})$,
- **Output:** the coherent closure $\langle\langle A_1, \dots, A_k \rangle\rangle$;
- Compute $\mathcal{S}_0 := \mathcal{P}(A_1, \dots, A_k, A_1^\top, \dots, A_k^\top, I_\Omega)$;
- Starting from $\mathcal{S} := \mathcal{S}_0$ apply WL-stabilization procedure $\mathcal{S} \rightarrow \text{bl}(\mathcal{S})$ until $\mathcal{S} = \text{bl}(\mathcal{S})$.

Theorem

The WL-algorithm produces the coherent closure of the matrices A_1, \dots, A_k .

Proof. Let \mathcal{C} denote the underlying coherent configuration of $\langle\langle A_1, \dots, A_k \rangle\rangle$, i.e. $\langle\langle A_1, \dots, A_k \rangle\rangle = \mathbb{Q}[\mathcal{C}]$. Then

- $A_1, \dots, A_k, A_1^\top, \dots, A_k^\top, l_\Omega \in \mathbb{Q}[\mathcal{C}] \implies \mathcal{S}_0 \sqsubseteq \mathcal{C}$
- Let $\mathcal{S}_i := \text{bl}(\mathcal{S}_{i-1}), i = 1, \dots, m$ be the sequence of partitions generated by WL-algorithm (thus $|\mathcal{S}_{m+1}| = |\mathcal{S}_m|$);
- since $\mathcal{S}_{i-1}^* = \mathcal{S}_{i-1}$ and $1_\Omega \in \mathcal{S}_{i-1}^\cup$, we obtain

$$\mathcal{S}_i^* = \mathcal{S}_i, \mathcal{S}_{i-1} \sqsubseteq \mathcal{S}_i \implies 1_\Omega \in \mathcal{S}_i^\cup, \mathcal{S}_{m+1} = \mathcal{S}_m;$$

- $\mathcal{S}_{i-1} \sqsubseteq \mathcal{C} \implies \mathcal{S}_i \sqsubseteq \mathcal{C}$;
- $\mathcal{S}_m \sqsubseteq \mathcal{C} \implies \mathcal{S}_m = \mathcal{C}. \quad \square$

Canonical ordering

Proposition

Let $\vec{S} = (S_1, \dots, S_m)$ and $\vec{T} = (T_1, \dots, T_m)$ be ordered partitions of Ω^2 and Δ^2 resp. Let $\langle\langle \vec{S} \rangle\rangle = (P_1, \dots, P_k)$ and $\langle\langle \vec{T} \rangle\rangle = (Q_1, \dots, Q_\ell)$ be the canonical ordering of the coherent closures produced by WL-algorithm. If there exists an isomorphism $f : \Omega \rightarrow \Delta$ such that $S_i^f = T_i$, then $k = \ell$ and $P_i^f = Q_i, i = 1, \dots, k$. In particular, the mapping $P_i \mapsto Q_i$ is an algebraic isomorphism between the co.co.s $\langle\langle \vec{S} \rangle\rangle$ and $\langle\langle \vec{T} \rangle\rangle$.

Reformulation of the GI

Given an algebraic isomorphism between the coherent configurations \mathcal{S} and \mathcal{T} . Find whether it is induced by a combinatorial one.

Association schemes.

Association scheme.

A pair (Ω, \mathcal{S}) where $\mathcal{S} \vdash \Omega^2$ is an association scheme
(=homogeneous coherent configuration) iff

- $1_\Omega \in \mathcal{S}$;
- $\mathcal{S}^* = \mathcal{S}$;
- $\text{bl}(\mathcal{S}) = \mathcal{S}$

Recall that the intersection numbers are

$$\forall_{S,R,T \in \mathcal{S}} \forall_{(\alpha,\beta) \in T} |\alpha S \cap R \beta| = c_{RS}^T.$$

The number $n_S := c_{SS}^{1_\Omega} = |\omega S|$ is called the **valency** of S .

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Elementary properties of schemes.

Proposition

- the set \mathcal{S}^U is closed w.r.t. boolean operations;
- $1_\Omega, \Omega^2 \in \mathcal{S}^U$;
- $(\mathcal{S}^U)^* = \mathcal{S}^U$;
- \mathcal{S} is closed w.r.t. relational product $\implies \forall \ell \in \mathbb{N} \forall S \in \mathcal{S} S^\ell \in \mathcal{S}^U$;
- each relation $R \in \mathcal{S}^U$ is regular;
- for any $S \in \mathcal{S}$ there exists m s.t. $1_\Omega \subseteq S^m$;
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- $S \in \mathcal{S}^U \implies S^+ = \bigcup_{i=1}^{\infty} S^i \in \mathcal{S}^U$;
- $S \in \mathcal{S}^U \implies S^+$ is an equivalence relation on Ω

Elementary properties of schemes.

Definition

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- $|\mathcal{S}| = |\Omega| \iff \forall_{S \in \mathcal{S}} n_S = 1$

Primitive and Imprimitive schemes

Definition

A scheme (Ω, \mathcal{S}) is called **imprimitive** if \mathcal{S}^{\cup} contains a non-trivial and non-discrete equivalence relation E . The equivalence classes $\omega E, \omega \in \Omega$ form a partition of Ω called **imprimitivity system** of \mathcal{S} .

Proposition

If $E \in \mathcal{S}^{\cup}$ is an equivalence. Then $|\Omega/E| \cdot n_E = |\Omega|$.

Proposition

The following are equivalent

- \mathcal{S} is imprimitive;
- $\exists S \in \mathcal{S}, S \neq 1_{\Omega}$ s.t $S^+ \neq \Omega^2$;
- $\exists \mathcal{T} \subset \mathcal{S}, 1 < |\mathcal{T}| < |\mathcal{S}|$ s. t. $\langle A(T) \rangle_{T \in \mathcal{T}}$ is a subalgebra of $\mathbb{Q}[\mathcal{S}]$

Schurian schemes

Recall that a scheme (Ω, \mathcal{S}) is **schurian** iff there exists $G \leq \text{Sym}(\Omega)$ s.t. $\mathcal{S} = \text{Inv}(G)$.

- G is transitive on Ω ;
- ωS is an orbit of G_ω for each $\omega \in \Omega$ and $S \in \mathcal{S}$;
- the mapping $S \mapsto \{g \in G \mid \omega^g \in \omega S\}$ is a bijection between the basic relations of \mathcal{S} and double cosets of G_ω .
- a rescaling of the above mapping is an isomorphism between the adjacency algebra $\mathbb{F}[\mathcal{S}]$ and the Hecke algebra $\mathbb{F}(G_\omega \backslash G / G_\omega)$;
- G is primitive iff $\text{Inv}(G)$ is primitive.