

Graph Isomorphism problem, Weisfeiler-Leman algorithm and coherent configurations

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- Graph isomorphism problem and Weisfeiler-Leman algorithm.
- Coherent configurations and coherent (cellular) algebras.
- Association schemes.

References. Coherent configuration and algebras

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Binary relations

Let $R, S \subseteq \Omega^2$ be binary relations. Then

- $S^* := \{(\alpha, \beta) \mid (\beta, \alpha) \in S\}$;
- S is **symmetric** (**antisymmetric**) if $S = S^*$ ($S \cap S^* = \emptyset$ resp.);
- $\alpha S := \{\beta \mid (\alpha, \beta) \in S\}$, $S\alpha := \alpha S^*$;
- $D(S) := \{\alpha \in \Omega \mid \alpha S \neq \emptyset\}$, $R(S) := D(S^*)$;
- $RS = \{(\alpha, \beta) \mid \alpha R \cap S\beta \neq \emptyset\}$;
- $R^+ = \bigcup_{i=1}^{\infty} R^i$ is the transitive closure of R ;
- $1_{\Omega} := \{(\omega, \omega) \mid \omega \in \Omega\}$

Each permutation $g \in \text{Sym}(\Omega)$ is considered as a binary relation.

Thus $\alpha g = \{\alpha^g\}$ and $g^* = g^{-1}$.

Partitions.

- $\mathcal{P} \vdash \Omega$ means that \mathcal{P} is a partition of Ω .
- $\mathcal{P} \sqsubseteq \mathcal{C} \iff \mathcal{C}$ is a refinement of \mathcal{P} ;
- Lattice operations are denoted as $\mathcal{P} \vee \mathcal{C}$ and $\mathcal{P} \wedge \mathcal{C}$;
- if $\mathcal{P} \vdash \Omega$ then \mathcal{P}^{\cup} denotes the set of all possible unions of elements in \mathcal{P} ;
- $\mathcal{C} \vdash \Omega^2 \implies \mathcal{C}^* := \{C^* \mid C \in \mathcal{C}\}$;

Graphs.

In what follows **graph** is a pair $\Gamma = (\Omega, E)$ where Ω is a finite set of **vertices** and $E \subset \Omega \times \Omega$ is the set of (directed) **edges/arcs**.

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$$\forall \alpha_1, \beta_1 \in \Omega_1 : (\alpha_1^f, \beta_1^f) \in E_2 \Leftrightarrow (\alpha_1, \beta_1) \in E_1.$$

Such a bijection is called an **isomorphism** from Γ_1 to Γ_2 ; the set of all of them is denoted by $\text{Iso}(\Gamma_1, \Gamma_2)$. The set $\text{Iso}(\Gamma_1, \Gamma_1)$ is known as the **automorphism group** of Γ_1 , notation $\text{Aut}(\Gamma_1)$.

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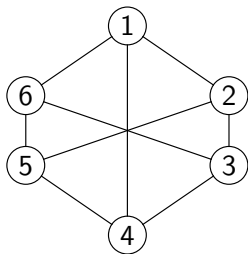
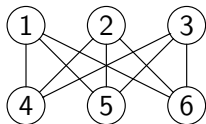
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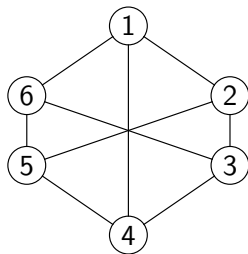
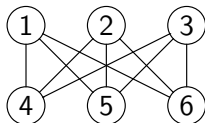
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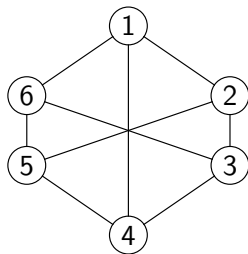
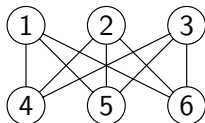
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$$\text{Aut}(\Gamma) = (S_3 \times S_3).S_2.$$

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Theorem (L.Babai, E.Luks and W.Kantor, 1984).

The isomorphism of n -vertex graphs can be tested in time $\exp(O(\sqrt{n \log n}))$.

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Isomorphism problem for colored graphs.

Definition.

A triple (Ω, Y, c) where $c : \Omega^2 \rightarrow Y$ is a surjection, is called a **colored graph** with the **coloring function** c and **color classes** $c^{-1}(y)$, $y \in Y$. Each colored graph determines a partition $\mathcal{C} := \{c^{-1}(y) \mid y \in Y\}$ of Ω^2 .

Two colored graphs (Ω, Y, c) and (Δ, Z, d) are isomorphic iff there exist bijections $f : \Omega \rightarrow \Delta, \phi : Y \rightarrow Z$ s.t.

$$d(\alpha^f, \beta^f) = c(\alpha, \beta)^\phi.$$

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Notice that ϕ is uniquely determined by f . For this reason we define $f^* := \phi$.

Isomorphism problem for colored graphs.

We also set $\text{Iso}(\Omega, Y, c)$ for the group of all isomorphisms from (Ω, Y, c) to itself and $\text{Aut}(\Omega, Y, c)$ for the normal subgroup of $\text{Iso}(\Omega, Y, c)$ which does not interchange the colors (that is $f^* = 1_Y$).

Proposition

Let (Ω, Y, c) be a colored graph and $\mathcal{C} := \{c^{-1}(y) \mid y \in Y\}$ be the corresponding partition. Then

$$\begin{aligned}\text{Iso}(\Omega, Y, c) &= \{g \in \text{Sym}(\Omega) \mid \mathcal{C}^g = \mathcal{C}\}, \\ \text{Aut}(\Omega, Y, c) &= \{g \in \text{Sym}(\Omega) \mid \forall C \in \mathcal{C} \ C^g = C\}.\end{aligned}$$

Theorem.

Isomorphism problem for colored graphs is polynomially equivalent to ISO.

Cayley Graphs and their Isomorphisms.

A **Cayley** graph over a finite group H defined by a **connection set** $S \subseteq H$ has H as a set of nodes and arc set

$$\text{Cay}(H, S) := \{(x, y) \mid xy^{-1} \in S\}$$

A **circulant** graph is a Cayley graph over a cyclic group.

Definition

Two Cayley graphs $\text{Cay}(H, S)$ and $\text{Cay}(K, T)$ are **Cayley isomorphic** if there exists a group isomorphism $f : H \rightarrow K$ which is a graph isomorphism too, that is

$$\text{Cay}(H, S)^f = \text{Cay}(K, T) \iff S^f = T.$$

Cayley representations of graphs.

An automorphism of a Cayley graph $\text{Cay}(H, S)$ contains a regular subgroup H_R consisting of right translations $h_R, h \in H$:

$$x^{h_R} = xh, x \in H.$$

Theorem (Sabidussi)

A graph $\Gamma = (\Omega, E)$ is isomorphic to a Cayley graph over a group H iff $\text{Aut}(\Gamma)$ contains a regular subgroup isomorphic to H .

Isomorphism problems for Cayley graphs.

Given $\Gamma = \text{Cay}(H, S)$ and $\Gamma' = \text{Cay}(H, S')$:

- **IMAP**: find $f \in \text{Iso}(\Gamma, \Gamma')$ (if it exists),
- **ICOUNT**: find $|\text{Iso}(\Gamma, \Gamma')|$,
- **ACOUNT**: find $|\text{Aut}(\Gamma)|$,
- **AGEN**: find generators of the group $\text{Aut}(\Gamma)$,
- **CGR**: given a graph Θ find whether it's a Cayley graph over a group H .

Isomorphism problem for finite groups.

Construction. Let K be a finite group.

Define a graph $\Gamma(K)$ with vertex set $K \times K$ and edges:

$$(a, b) \sim (c, d) \iff a = c \vee b = d \vee ab = cd.$$

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Exercise. Prove that $\Gamma(\mathbb{Z}_4) \not\cong \Gamma(\mathbb{Z}_2 \times \mathbb{Z}_2)$.

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|---|---|---|---|
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The isomorphism of groups of order n can be tested in time $n^{O(\log n)}$.

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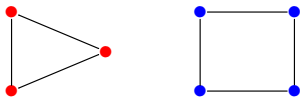
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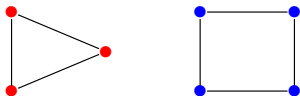
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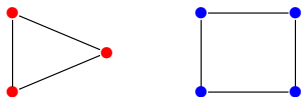
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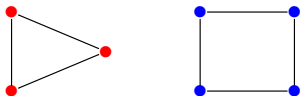


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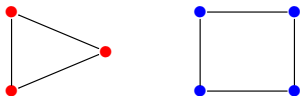
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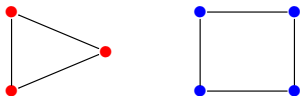
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- Repeat the procedure till $|\mathcal{C}|$ stops to increase.

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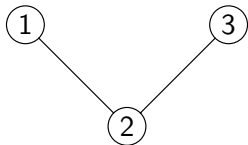
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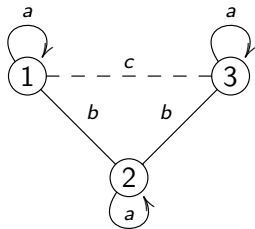
$$c(\alpha, \beta; R, S) = |\alpha R \cap S \beta|.$$

- Build a new partition $\text{bl}(\mathcal{C})$ by putting (α, β) and (α', β') to the same class of $\text{bl}(\mathcal{C})$ if $|\alpha R \cap S \beta| = |\alpha' R \cap S \beta'|$ for all $R, S \in \mathcal{C}$.
- Repeat the procedure till $|\mathcal{C}|$ stops to increase.

The WL-algorithm. Very small example



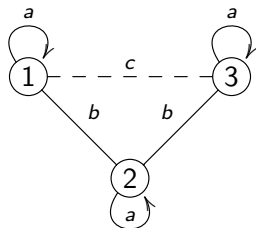
Initial coloring



Adjacency matrix

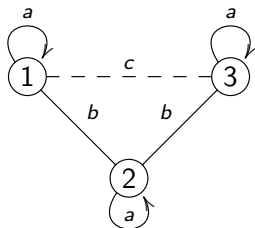
$$A = \begin{pmatrix} a & b & c \\ b & a & b \\ c & b & a \end{pmatrix}.$$

First iteration



$$A^2 = \begin{pmatrix} a^2 + b^2 + c^2 & ab + ba + cb & ac + b^2 + ca \\ ba + ab + bc & 2b^2 + a^2 & bc + ab + ba \\ ca + b^2 + ac & cb + ba + ab & c^2 + b^2 + a^2 \end{pmatrix}.$$

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New matrix A

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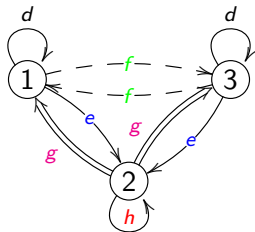
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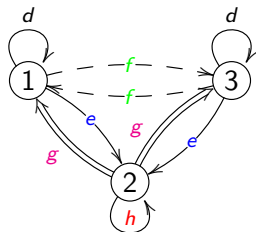
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The matrix A is **stable**, that is A^2 produces the same coloring as A does.

WL-refinement (operation \sqsubseteq)

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Let $f : \Omega \rightarrow \Delta$ be a bijection that maps a partition \mathcal{C} of Ω^2 onto a partition \mathcal{T} of Δ^2 (i.e. $\mathcal{C}^f = \mathcal{T}$). Then $\mathfrak{bl}(\mathcal{C})^f = \mathfrak{bl}(\mathcal{T})$.

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Given an ordered partition $\vec{\mathcal{C}} = (S_1, \dots, S_m)$ of Ω^2 the WL-algorithm produces a unique (**canonical**) ordering of the refinement $\mathfrak{bl}(\mathcal{C})$ (denoted as $\mathfrak{bl}(\vec{\mathcal{C}})$) with the following property:

$$\vec{\mathcal{C}}^f = \vec{\mathcal{T}} \implies \mathfrak{bl}(\vec{\mathcal{C}})^f = \mathfrak{bl}(\vec{\mathcal{T}})$$

Coherent configurations (D. Higman, 1970).

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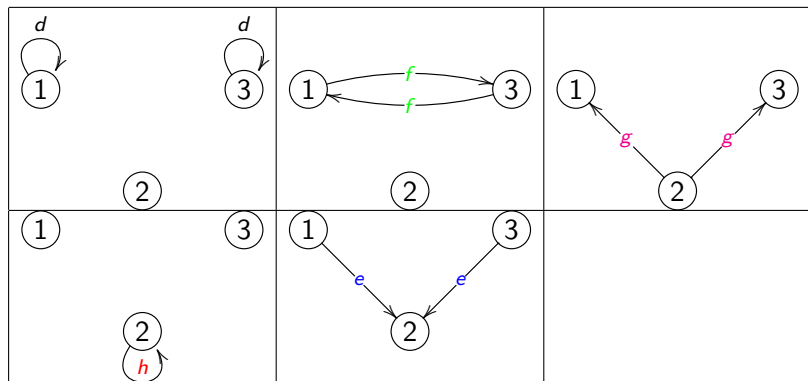
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The configuration \mathcal{X} is **homogeneous** (or **association scheme**, or **scheme**), if $1_\Omega \in \mathcal{C}$.

Coherent configurations: a concrete example.



Coherent configurations. Fibers and relations.

A **fiber** of \mathcal{X} is a set $\Delta \subset \Omega$ such that $1_\Delta \in \mathcal{C}$; the set of all fibers is denoted by $\Phi = \Phi(\mathcal{X})$.

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- for any fiber $\Delta \in \Phi$ the set of relations $\mathcal{C}_\Delta := \{C \in \mathcal{C} \mid D(C) = \Delta, R(C) = \Delta\}$ form a homogeneous co.co. on Δ , called a **homogeneous constituent** of \mathcal{C} .

The number $n_S = c_{SS^*}^T$ is called the **valency** of S .

Properties of coherent configurations.

Proposition

Let $\mathcal{X} = (\Omega, \mathcal{C})$ be a co.co. Then

- the set \mathcal{C}^{\cup} is closed w.r.t. boolean operations;
- $1_{\Omega}, \Omega^2 \in \mathcal{C}^{\cup}$;
- $(\mathcal{C}^{\cup})^* = \mathcal{C}^{\cup}$;
- \mathcal{C}^{\cup} is closed w.r.t. relational product;

Isomorphisms between coherent configurations

Definition

Two coherent configurations $\mathcal{X} = (\Omega, \mathcal{C})$ and $\mathcal{X}' = (\Omega', \mathcal{C}')$ are called **(combinatorially) isomorphic** iff there exist bijections $f : \Omega \rightarrow \Omega'$, $\phi : \mathcal{C} \rightarrow \mathcal{C}'$ such that

$$\forall_{\alpha, \beta \in \Omega} (\alpha, \beta) \in \mathcal{C} \iff (\alpha^f, \beta^f) \in \mathcal{C}^\phi.$$

The set of all isomorphisms between \mathcal{X} and \mathcal{X}' is denoted as $\text{Iso}(\mathcal{X}, \mathcal{X}')$. Notice that ϕ is uniquely determined by f .

In what follows we set $\text{Iso}(\mathcal{X}) := \text{Iso}(\mathcal{X}, \mathcal{X})$. We call the elements of this group **colored automorphisms** of the configuration.

Coherent configurations generated by a graph.

The mapping $(f, \phi) \mapsto \phi$ is an group homomorphism from $\text{Iso}(\mathcal{X})$ into $\text{Sym}(\mathcal{C})$. The kernel of this homomorphism denoted as $\text{Aut}(\mathcal{X})$ is called the the **automorphism group** of \mathcal{X} :

$$\text{Aut}(\mathcal{X}) = \{f \in \text{Sym}(\Omega) : S^f = S \text{ for all } S \in \mathcal{C}\}$$

Theorem

Let $\langle\langle \Gamma \rangle\rangle$ be the **WL-closure** of a graph $\Gamma = (\Omega, E)$ obtained by applying WL-algorithm to Γ . Then

- $E \in \langle\langle \Gamma \rangle\rangle^{\cup}$;
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Examples. Strongly regular graphs.

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A graph $\Gamma = (\Omega, E)$ is called **strongly regular** if its WL-closure has rank three. In other words, WL-algorithm stops at the first iteration and $\langle\langle\Gamma\rangle\rangle = \{1_\Omega, E, E^c\}$.

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Proposition

A graph $\Gamma = (\Omega, E)$ is strongly regular if and only if there exists non-negative integers k, λ, μ such that

- 1 Γ is k -regular,
- 2 any pair of points connected by an edge have λ common neighbours,
- 3 any pair of points not connected by an edge have μ common neighbours

Examples. Permutation groups.

Let $G \leq \text{Sym}(\Omega)$ be a permutation group. It acts on $\Omega \times \Omega$:

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Definition.

A coherent configuration \mathcal{X} is called **schurian** if $\mathcal{X} = \text{Inv}(G)$ for some group G .

Schurity problem

Given a coherent configuration \mathcal{X} , find whether it is schurian.

Galois correspondence.

Definition

Let $\mathcal{X} = (\Omega, \mathcal{C})$, $\mathcal{X}' = (\Omega, \mathcal{C}')$ be two coherent configurations. We say that \mathcal{X} is a **fusion** of \mathcal{X}' (equivalently \mathcal{X}' is a **fission** of \mathcal{X}), notation $\mathcal{X} \sqsubseteq \mathcal{X}'$ if $\mathcal{C} \sqsubseteq \mathcal{C}'$.

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Proposition

Let $\mathcal{X}, \mathcal{X}'$ be two coherent configurations defined on Ω and $G, H \leq \text{Sym}(\Omega)$ arbitrary subgroups. Then

- $\mathcal{X} \sqsubseteq \mathcal{X}' \implies \text{Aut}(\mathcal{X}) \geq \text{Aut}(\mathcal{X}')$;
- $H \leq G \implies \text{Inv}(H) \supseteq \text{Inv}(G)$;
- $G \leq \text{Aut}(\text{Inv}(G))$;
- $\mathcal{X} \sqsubseteq \text{Inv}(\text{Aut}(\mathcal{X}))$

Galois closed objects.

Definition

The group $G^{(2)} := \text{Aut}(\text{Inv}(G))$ is called a **2-closure** of $G \leq \text{Sym}(\Omega)$. A group is called **2-closed** if $G = G^{(2)}$.

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