Isomorphism problem for finite combinatorial objects via coherent configurations

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The Graph Isomorphism Problem is to recognize whether two finite graphs are isomorphic by means of an efficient algorithm.

The naive algorithm for n-vertex graphs takes $O(n!)$ steps.

At present **the best general isomorphism test** makes at least $n^{O(\sqrt{n/\log n})}$ steps in the worst case (Babai-Kantor-Luks, 1983).

The corresponding isomorphism problems for directed graphs, multigraphs, hypergraphs, vertex-colored graphs, edge-colored graphs, ... are **polynomial-time equivalent**.

Proposition 1. *The following three problems are polynomial-time equivalent:*

(1) *the Graph Isomorphism Problem,*

(2) *given a graph* Γ *find a generator set of* $\mathrm{Aut}(\Gamma)$*,*

(3) *given a graph* Γ *find the orbits of* $\mathrm{Aut}(\Gamma)$*.*

The Weisfeiler-Leman approach

Let Γ be a graph with the vertex set V and the edge set E.

The **coherent configuration** or briefly the **scheme** of Γ is defined to be the smallest scheme $\mathcal{C}(\Gamma)$ on V for which E is a union of some basis relations of it:

$$\mathcal{C}(\Gamma) = [E]$$

or equivalently,

$$W(\mathcal{C}(\Gamma)) = [A(\Gamma)]$$

where $W(\mathcal{C}(\Gamma))$ is the adjacency algebra of the scheme $\mathcal{C}(\Gamma)$ and $A(\Gamma)$ is the adjacency matrix of Γ.

Proposition 2. *Let $\mathcal{C} = \mathcal{C}(\Gamma)$. Then*

(1) $\mathrm{Aut}(\mathcal{C}) = \mathrm{Aut}(\Gamma)$*; if $\mathcal{C}$ is Schurian, then the orbits of* $\mathrm{Aut}(\Gamma)$ *are the fibers of $\mathcal{C}$,*

(2) *the scheme $\mathcal{C}$ can be constructed in time $O(n^3 \log n)$ where $n = |V|$.*

Thus if all the schemes were Schurian, then the Graph Isomorphism Problem would solve by means of **the Weisfeiler-Leman algorithm**.

Circulant graphs

A finite graph Γ (resp. a scheme $\mathcal{C}$) is called **circulant** if the group $\mathrm{Aut}(\Gamma)$ (resp. $\mathrm{Aut}(\mathcal{C})$) contains a full cycle:

$$(1, 2, \ldots, n) \in \mathrm{Aut}(\Gamma) \qquad ((1, 2, \ldots, n) \in \mathrm{Aut}(\mathcal{C}))$$

where n is the number of vertices of Γ.

Theorem 3. (EP, (2001)). *There exists an infinite family of non-Schurian circulant schemes.*

For circulant graphs the isomorphism problem is polynomial-time reducible to the recognition problem:

$$\forall \Gamma_1, \Gamma_2 \in \mathcal{K}_n : \quad \Gamma_1 \cong \Gamma_2 \Leftrightarrow \Gamma_1 \cup \Gamma_2 \in \mathcal{K}_{2n}$$

where $\mathcal{K}_n$ is the class of circulant graphs with n vertices and $\Gamma_{\cup}\Gamma_2$ is the disjoint union Γ_1 and Γ_2.

Muzychuk, (2004) found an efficient algorithm to test isomorphism for circulant graphs with *explicitly given* cyclic automorphism group.

The recognition problem for circulant graphs and circulant schemes are **polynomial-time equivalent**.

Theorem 4. (EP, (2003)). *Given a scheme* $\mathcal{C}$ *on a set* V *one can find in polynomial time in* $|V|$ *a set of* $k \leq |V|$ *of binary relations* $R_1, \ldots, R_k \subset V \times V$ *such that the scheme*

$$\mathcal{C}' = [\mathcal{C}, R_1, \ldots, R_k]$$

is circulant iff so is $\mathcal{C}$*. Moreover, the group* $\mathrm{Aut}(\mathcal{C}')$ *is solvable.*

By means of computational group theory technique one can prove that circulant schemes with solvable automorphism groups are polynomial-time recognizable.

A **Cayley representation** of a graph Γ over a group G is a Cayley graph over G isomorphic to Γ; two such representations are called **equivalent** if some isomorphism of the corresponding Cayley graphs belong to $\mathrm{Aut}(G)$.

Theorem 5. (EP, (2003)) *Given a graph* Γ *with* n *vertices, one can find in time* $n^{O(1)}$ *a full system of pairwise nonequivalent Cayley representations of* Γ *over a cyclic group of order* n*.*

Similarities

Two schemes $\mathcal{C} = (V, \mathcal{R})$ and $\mathcal{C}' = (V', \mathcal{R}')$ are called **similar**, if

$$p_{R,S}^{T} = p_{R^\varphi, S^\varphi}^{T^\varphi}, \qquad R, S, T \in \mathcal{R},$$

for some bijection $R \mapsto R^\varphi$ from $\mathcal{R}$ to $\mathcal{R}'$, called a **similarity** (or an **algebraic isomorphism**).

Properties of the similarity φ:

(1) $|V| = |V'|$,

(2) $(R^T)^\varphi = (R^\varphi)^T$ for all $R \in \mathcal{R}$,

(3) $W(\mathcal{C}) \to W(\mathcal{C}'), A(R) \mapsto A(R^\varphi),\ R \in \mathcal{R}$ is a matrix algebra isomorphism,

Any isomorphism $f \in \mathrm{Iso}(\mathcal{C}, \mathcal{C}')$ induces a similarity $\varphi_f : \mathcal{C} \to \mathcal{C}'$ such that

$$R^{\varphi_f} = R^f, \qquad R \in \mathcal{R}.$$

However, there exist similar schemes which are not isomorphic. In the class of circulant schemes the smallest known example has 4225 points (EP, (2001)).

Given graphs Γ and Γ' set $\mathcal{C} = \mathcal{C}(\Gamma)$ and $\mathcal{C}' = \mathcal{C}(\Gamma')$. Then

$$\mathrm{Iso}(\Gamma, \Gamma') \subset \mathrm{Iso}(\mathcal{C}, \mathcal{C}')$$

and

$$E^{\varphi_f} = E', \qquad f \in \mathrm{Iso}(\Gamma, \Gamma')$$

where E and E' are the edge sets of Γ and Γ' respectively.

Proposition 6. **(Weisfeiler-Leman)** *Let $\mathcal{C} = [E]$ and $\mathcal{C}' = [E']$ where $E, E' \subset V \times V$. Then in polynomial time one can test whether there exists a similarity $\varphi : \mathcal{C} \to \mathcal{C}'$ such that $E^{\varphi} = E'$ and find it if it does exist.*

Proposition 6 gives a constructive necessary condition for isomorphism of graphs Γ and Γ'.

Algebraic forests

A graph Γ is called an **algebraic forest** if there exists a forest T such that

$$\mathcal{C}(\Gamma) = \mathcal{C}(T)_L$$

where L is the set of leaves of T and $\mathcal{C}(T)_L$ is the restriction of the scheme $\mathcal{C}(T)$ to the set L. (One can prove that L is a union of some fibers of $\mathcal{C}(T)$).

Examples.

1. Any **tree** is an algebraic forest.

2. Any **interval graph** is an algebraic forest. (An interval graph has a set of line segments as the set of vertices and two vertices are adjacent if the corresponding segments have nonempty intersection.)

3. Any **cograph** is an algebraic forest. (A cograph is a graph that contain no induced path on four vertices.)

For all the above classes of graphs there exist polynomial-time algorithms to test isomorphism. However, the corresponding algorithms are different.

Set $\mathcal{F}$ to be the class of all schemes of algebraic forests. One can prove that $\mathcal{F}$ is closed with respect to the **direct sums** and **wreath products**:

The direct sum of schemes $\mathcal{C}_1$ on V_1 and $\mathcal{C}_2$ on V_2 where V_1 and V_2 are disjoint sets, is defined to be

$$\mathcal{C}_1 \boxplus \mathcal{C}_2 = [\mathcal{C}_1, \mathcal{C}_2].$$

The group $\mathrm{Aut}(\mathcal{C}_1 \boxplus \mathcal{C}_2)$ is induced by the natural action of $\mathrm{Aut}(\mathcal{C}_1) \times \mathrm{Aut}(\mathcal{C}_2)$ on $V_1 \cup V_2$.

Let $\mathcal{C}_1 = (V_1, \{R_0, \ldots, R_{m-1}\})$ be a scheme. **The wreath product** of the scheme $\mathcal{C}_1$ and a scheme $\mathcal{C}_2$ on V_2 of rank 2 is defined to be

$$\mathcal{C}_1 \wr \mathcal{C}_2 = [R'_0, \ldots, R'_{m-1}].$$

where R'_i is the disjoint union of $|V_2|$ copies of R_i. The group $\mathrm{Aut}(\mathcal{C}_1 \wr \mathcal{C}_2)$ is induced by the natural action of $\mathrm{Aut}(\mathcal{C}_1) \wr \mathrm{Sym}(V_2)$ on $V_1 \times V_2$.

Theorem 7. **(EPT, (2000))** *Given a scheme $\mathcal{C} \in \mathcal{F}$ one of the following three statements holds:*

(1) $\mathrm{rk}(\mathcal{C}) \leq 2$,

(2) $\mathcal{C} = \mathcal{C}_1 \boxplus \mathcal{C}_2$ *for some schemes* $\mathcal{C}_1, \mathcal{C}_2 \in \mathcal{F}$,

(3) $\mathcal{C} = \mathcal{C}_1 \wr \mathcal{C}_2$ *for some scheme* $\mathcal{C}_1 \in \mathcal{F}$, *and a scheme* $\mathcal{C}_2$ *of rank 2.*

(The direct sum in (2) and the wreath product in (3) are nontrivial.)

From Theorem 7 one can deduce the following statement showing that the Weisfeiler-Leman algorithm solves the isomorphism problem in the class of algebraic forests.

Theorem 8. **(EPT, (2000))** *Let $\mathcal{C}, \mathcal{C}' \in \mathcal{F}$. Then for each similarity $\varphi : \mathcal{C} \to \mathcal{C}'$ there exists an isomorphism $f \in \mathrm{Iso}(\mathcal{C}, \mathcal{C}')$ such that $\varphi = \varphi_f$.*