The Graph Isomorphism Problem and coherent configurations. I, II.

Ilya Ponomarenko

St. Petersburg Department of V.A. Steklov Institute of Mathematics, Russia

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The Graph Isomorphism Problem (ISO).

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**Definition.**

Graphs \( G_1 = (\Omega_1, E_1) \) and \( G_2 = (\Omega_2, E_2) \) are called isomorphic, \( G_1 \cong G_2 \), if there is a bijection \( f : \Omega_1 \rightarrow \Omega_2 \) such that

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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.
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Such a bijection is called the isomorphism from \( G_1 \) to \( G_2 \); the set of all of them is denoted by \( \text{Iso}(G_1, G_2) \).
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$\text{ISO}(G_1, G_2)$: given graphs $G_1$ and $G_2$ test whether or not $G_1 \cong G_2$. 
Current state of the ISO.

Given graphs $G_1$ and $G_2$ with $n$ vertices, and a bijection $f : \Omega_1 \rightarrow \Omega_2$ one can test in time $O(n^2)$ whether or not $f \in \text{Iso}(G_1, G_2)$. 

Theorem (L. Babai, E. Luks and W. Kantor, 1984).
The isomorphism of $n$-vertex graphs can be tested in time $\exp(O(\sqrt{n \log n}))$. 

Therefore $\text{ISO} \in \text{NP}$. An exhaustive search of all the possible bijections runs in exponential time $O(n!)$. At present it is not known whether $\text{ISO} \in \text{P}$. The proof of the time bound of the best algorithm (up to now) for the ISO depends on the Classification of Finite Simple Groups.
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The class of undirected graphs is isomorphism complete:

A directed edge \( \alpha \rightarrow \beta \) is replaced by an undirected graph

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![Undirected graph representation]

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A number of classes of undirected graphs are known to be isomorphism complete: connected, bipartite, of diameter 2, regular, etc.
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A pair \((G, c)\) where \(G = (\Omega, E)\) is a graph and \(c : \Omega \to \{1, \ldots, m\}\) is a surjection, is called a colored graph with the color function \(c\) and color classes \(c^{-1}(i), i = 1, \ldots, m\).
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Isomorphism problem for other categories. Geometry.

Notation.

Denote by $\mathcal{K}$ the category of finite incidence structures $\mathcal{G} = (P, B, I)$ with the point set $P$, the block set $B$ and the incidence relation $I \subseteq P \times B$. 
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- Set $G(\mathcal{G}) = (P \cup B, I)$ to be a graph with two color classes $P$ and $B$. It is known that the isomorphism of finite projective planes of order $n$ can be tested in time $n^{O(\log \log n)}$. 

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Let $\mathcal{K}$ be the category of finite groups (given by the Cayley tables).

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```
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  |        |        |        |
  |        |        |        |
  |        |        |        |
  |        |        |        |
  k -------> k -------> k -------> (k, l)
  |
  l -------> l -------> l
  |
  k\l -------> k\l -------> k\l
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Some problems equivalent to the ISO (R. Mathon, 1979).

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- **APART**: given $G$ find $\Omega / \text{Aut}(G)$. 

Vertex individualization. Given $G$ and $\alpha_1, \ldots, \alpha_i \in \Omega$ set:

$G_{\alpha_1, \ldots, \alpha_i}$ to be the colored graph in which each $\{\alpha_j\}$ is a color class.

**IMAP $\propto$ ISO**: recursively find $\alpha_1, \ldots, \alpha_i \in \Omega$, $\beta_1, \ldots, \beta_i \in \Xi$ and $f : \alpha_i \mapsto \beta_i$ so that $G \cong H$ iff $G_{\alpha_1, \ldots, \alpha_i} \cong H_{\beta_1, \ldots, \beta_i}$.

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**Vertex partition by valences.**

Denote by $d_G(\alpha)$ the **valency** of the vertex $\alpha$ in the graph $G$;
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Denote by $d_G(\alpha)$ the *valency* of the vertex $\alpha$ in the graph $G$; the valency of $\alpha$ in a color class $C$ is denoted by $d_G(\alpha, C)$.
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Denote by $d_G(\alpha)$ the valency of the vertex $\alpha$ in the graph $G$; the valency of $\alpha$ in a color class $C$ is denoted by $d_G(\alpha, C)$.

- To find $\Omega/\text{Aut}(G)$ put vertices $\alpha$ and $\beta$ in the same class iff $d_G(\alpha) = d_G(\beta)$. 

Comments.

The algorithm correctly finds $\Omega/\text{Aut}(G)$ for the class of trees (G. Tinhofer, 1985), for almost all graphs (L. Babai, P. Erdős, S. Selkow, 1980).

The algorithm fails when $G$ is a regular graph and the group $\text{Aut}(G)$ is intransitive.
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Denote by $d_G(\alpha)$ the **valency** of the vertex $\alpha$ in the graph $G$; the valency of $\alpha$ in a color class $C$ is denoted by $d_G(\alpha, C)$.

- To find $\Omega/Aut(G)$ put vertices $\alpha$ and $\beta$ in the same class iff $d_G(\alpha) = d_G(\beta)$.
- Iteratively, put vertices $\alpha$ and $\beta$ in the same class iff $c(\alpha) = c(\beta)$, and $d_G(\alpha, C) = d_G(\beta, C)$ for all color classes $C$.

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The algorithm correctly finds $\Omega/Aut(G)$ for the class of trees (G. Tiňoň, 1985), for almost all graphs (L. Babai, P. Erdős, S. Selkow, 1980). The algorithm fails when $G$ is a regular graph and the group $Aut(G)$ is intransitive.
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No automorphism takes a dushed edge to an undashed one.

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\begin{array}{c}
  \text{\includegraphics[width=0.5\textwidth]{diagram.png}}
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The output partition of the Weisfeiler-Leman algorithm is a coherent configuration, i.e. a pair $\mathcal{X} = (\Omega, S)$ such that:

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$(r, f) = (3, 1)$: $s_0 = \bullet \bullet \bullet$, $s_1 = \downarrow \downarrow \uparrow$

$(r, f) = (5, 2)$: $s_0 = \bullet \bullet \bullet \bullet \bullet$, $s_1 = \downarrow \downarrow \uparrow \uparrow \uparrow$

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Let \((P, B)\) be a symmetric design with the point set \(P\) and the block set \(B\) (in particular, any pair of distinct points is contained in \(\lambda\) blocks for some integer \(\lambda > 0\)).
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Proposition. Set \(X = (\Omega, S)\). Then \(S\) is a partition of \(\Omega \times \Omega\), \(X\) is a coherent configuration (e.g. if \(r = I_P B\) and \(s = P \setminus 1 P\), then \(c_{\star r} = \lambda\)), \(\Phi(X) = \{P, B\}\); in particular \(X\) is non-homogeneous.
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Proposition. The graph $\Gamma$ is distance-regular iff $X = (\Omega, S)$ is a coherent configuration. If it is so, then $X$ is an association scheme; it is the output of the Weisfeiler-Leman algorithm applied to $G$. $X$ is symmetric, i.e. $n_s = n_s^*$ for all $s \in S$. The intersection numbers of $X$ are uniquely determined by the numbers $c_{r_i - 1 r_i}$ and $c_{r_i r_i - 1}$ for $i = 1, \ldots, d$ (that are the parameters of $G$).
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- Set $r_i = \{(\alpha, \beta) \in \Omega^2 : d(\alpha, \beta) = i\}$ where $i = 0, \ldots, d$ and $d(\alpha, \beta)$ is the distance between $\alpha$ and $\beta$ in $G$.
- Then $r_0 = 1_{\Omega}$ and $r_1 = E$.
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Proposition. The graph $\Gamma$ is distance-regular iff $\mathcal{X} = (\Omega, S)$ is a coherent configuration. If it is so, then

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

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Definition.

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

Isomorphisms of coherent configurations.

Definition.

Coherent configurations $\mathcal{X} = (\Omega, S)$ and $\mathcal{X}' = (\Omega', S')$ are **isomorphic** if there is a bijection $f: \Omega \to \Omega'$, the isomorphism from $\mathcal{X}$ to $\mathcal{X}'$, such that $S^f = S'$. 

Notation.

The coherent configuration constructed from a graph $G = (\Omega, E)$ by the Weisfeiler-Leman algorithm is denoted by $\langle\langle G \rangle\rangle$.

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Let $G = (\Omega, E)$ and $G' = (\Omega', E')$ be graphs, and $X = \langle\langle G \rangle\rangle$ and $X' = \langle\langle G' \rangle\rangle$.

Then $f \in \text{Iso}(G, G')$ iff $f \in \text{Iso}(X, X')$ and $E^f = E'$. 

Proof. On each step of the Weisfeiler-Leman algorithm $c(\alpha, \beta; r, s) = c(\alpha^f, \beta^f; r^f, s^f)$ for all $\alpha, \beta, r, s$. 
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The automorphism group and schurian closure.

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For any graph $G$: $\text{Aut}(G) = \text{Aut}(\mathcal{X})$ where $\mathcal{X} = \langle G \rangle$.

In particular, $\Omega / \text{Aut}(G) = \Phi(\text{Sch}(\mathcal{X}))$.

Theorem. The ISO is polynomially equivalent to the problem of finding the schurian closure of a coherent configuration.

If all coherent configurations were schurian, then the Weisfeiler-Leman algorithm solves the ISO.
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When a class $\mathcal{K}$ consists of graphs $G$ for which $\langle \langle G \rangle \rangle$ is schurian, then usually $\text{ISO}_\mathcal{K}$ is solved by the W-L algorithm.
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Coherent configurations $\mathcal{X} = (\Omega, S)$ and $\mathcal{X}' = (\Omega', S')$ are algebraically isomorphic if there is a bijection $\varphi : S \to S'$ such that

$$c_{rs}^t = c_{r\varphi s\varphi}^{t\varphi}, \quad r, s, t \in S;$$

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The canonical modification of the Weisfeiler-Leman algorithm. 

At the first step $S = \{ s_0, s_1, s_2 \}$ where $s_0 = 1_\Omega$ and $s_1 = E$. 

At each iteration $S = \{ s_0, \ldots, s_i \}$ where the indices are chosen according to the lex. order of $\{ c(\alpha, \beta; r, s) \}$. 

If $X = \langle \langle G \rangle \rangle$ and $X' = \langle \langle G \rangle \rangle$ are obtained by the canonical W-L algorithm, then $G \cong G'$ only if $|S| = |S'|$ and the bijection $s_i \mapsto s_i'$ is an algebraic isomorphism.
Algebraic isomorphisms. II.

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Algebraic isomorphisms. II.

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If $\mathcal{X} = \langle \langle G \rangle \rangle$ and $\mathcal{X}' = \langle \langle G \rangle \rangle$ are obtained by the canonical W-L algorithm, then $G \cong G'$ only if $|S| = |S'|$ and the bijection $s_i \mapsto s'_i$ is an algebraic isomorphism.
Proposition.

The ISO is polynomially equivalent to the following problem: given an algebraic isomorphism \( \varphi: \mathcal{X} \to \mathcal{X}' \) test whether \( \text{Iso}(\mathcal{X}, \mathcal{X}', \varphi) \) is not empty.
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Any algebraic isomorphism $\varphi : \langle\langle G \rangle\rangle \to \langle\langle G' \rangle\rangle$ where $G$ and $G'$ are algebraic forests, is induced by isomorphism. Thus ISO for algebraic forests is solved by the canonical modification of the W-L algorithm.
Bases of coherent configurations.

There is a natural partial order \( \sqsubseteq \) on the set of all coherent configurations on \( \Omega \): if \( \mathcal{X} = (\Omega, S) \) and \( \mathcal{Y} = (\Omega, T) \), then
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$b(\text{Aut}(\mathcal{X})) \leq b(\mathcal{X})$; in particular, $|\text{Aut}(\mathcal{X})| \leq n^{b(\mathcal{X})}$. 

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Theorem.

Let $G$ be a graph on $n$ vertices and $b = b(X')$ where $X' = \langle\langle G\rangle\rangle$. Then for any $G'$ the set $\text{Iso}(G, G')$ can be found in time $n^{O(b)}$. 

Let $H = G_{\alpha_1, \ldots, \alpha_b}$ where $\{\alpha_1, \ldots, \alpha_b\}$ is a base of $X$. Then the coherent configuration $X = \langle\langle H\rangle\rangle$ is complete. So $|\text{Iso}(X, X', \phi)| \leq 1$ for any algebraic isomorphism $\phi: X \to X'$: the unique possible isomorphism in $\text{Iso}(X, X', \phi)$ is induced by the bijection $\Phi(X) \to \Phi(X')$. Thus $\text{Iso}(G, G') = \bigcup \text{Iso}(\langle\langle H\rangle\rangle, \langle\langle H'\rangle\rangle, \phi_{H'})$ where $H'$ runs over all colored graphs $H_{\alpha'_1, \ldots, \alpha'_b}$ for which there is the algebraic isomorphism $\phi_{H'}: \langle\langle H\rangle\rangle \to \langle\langle H'\rangle\rangle$ found by the canonical W-L algorithm.
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Let $\mathcal{X}$ be the coherent configuration of a projective plane (resp. group, skew Hadamard matrix, Latin square) of order $n$.
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Let $\mathcal{X}$ be the coherent configuration of a projective plane (resp. group, skew Hadamard matrix, Latin square) of order $n$. Then $b(\mathcal{X})$ is at most $O(\log \log n)$ (resp. $O(\log n)$). This gives the isomorphism test running in time $n^{O(\log \log n)}$ (resp. $n^{O(\log n)}$).

A homogeneous coherent configuration $\mathcal{X}$ is called primitive if the only equivalence relations in $S^\cup$ are $1_\Omega$ and $\Omega \times \Omega$.

- $\text{Inv}(\Gamma)$ is primitive iff so is $\Gamma$.
- $b(\mathcal{X}) < 4\sqrt{n} \log n$ for primitive $\mathcal{X}$ of rank $\geq 3$ (L.Babai, 1981).

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- If the Babai problem has a positive answer, then probably the Luks algorithm for graphs of bounded valency can be reformulated in terms of bases.