

# A logical approach to Isomorphism Testing and Constraint Satisfaction

Oleg Verbitsky

Humboldt University of Berlin, Germany

ESLLI 2016, 15–19 August

Part 2:  
Isomorphism Testing by Color Refinement and  $\text{FO}_{\#}^2$

# Outline

- 1 Graph Isomorphism Problem
- 2 Color Refinement Algorithm
- 3 Relation to  $\text{FO}_{\#}^2$
- 4 References

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## Graph Isomorphism Problem

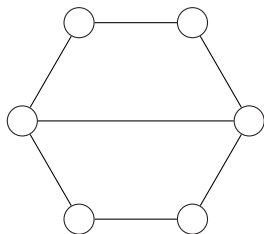
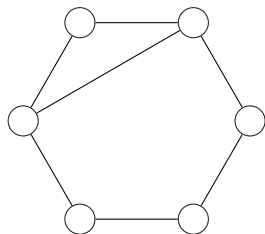
Are two given graphs  $G$  and  $H$  isomorphic?

- the best algorithm takes time  $n^{\log^c n}$  [Babai 2015]
- in NP, but not NP-complete unless the polynomial-time hierarchy collapses [Schöning 1988, Boppana, Håstad, Zachos 1987]
- polynomial time algorithms are known only in particular cases, e.g., for
  - bounded genus [Filotti, Mayer 1980; Miller 1980]
  - bounded degree [Luks 1982]
  - more generally, classes excluding a topological minor [Grohe, Marx 2012]
  - interval graphs [Lueker, Booth 1979]
- in some cases, even logspace algorithms:
  - bounded genus [Elberfeld, Kawarabayashi 2014]
  - bounded treewidth [Elberfeld, Schweitzer 2016]
  - interval graphs [Köbler, Kuhnert, Laubner, V. 2011]

# Outline

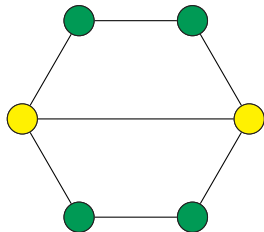
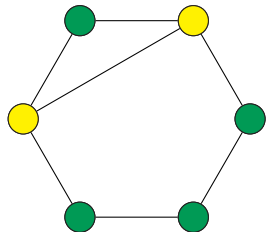
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## Color refinement algorithm: An example



Start with the monochromatic coloring.

## Color refinement algorithm: An example



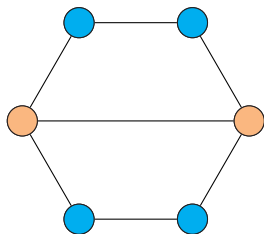
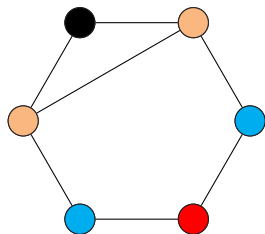
New color of a vertex = old colors of all neighbours.

$$\bullet = \{\circ, \circ\}$$

$$\bullet = \{\circ, \circ, \circ\}$$






## Color refinement algorithm: An example



Next refinement.

 = {, } (absent in the second graph)

 = {, } (absent in the second graph)

 = {, }

 = {, , }

## Color refinement algorithm: Formal definition

$$\begin{aligned}C^1(v) &= \deg v \\C^{i+1}(v) &= \left\{ \left\{ C^i(u) \right\}_{u \in N(v)} \right\}\end{aligned}$$

### Exercise

If  $\phi$  is an isomorphism from  $G$  to  $H$ , then  $C^i(v) = C^i(\phi(v))$ .

Therefore,

$$G \cong H \implies \left\{ \left\{ C^i(v) \right\}_{v \in V(G)} \right\} = \left\{ \left\{ C^i(v) \right\}_{v \in V(H)} \right\}$$

**Color Refinement** accepts  $G$  and  $H$  as isomorphic  
iff  
the equality is true for all  $i$ .

- The output “non-isomorphic” is always true.
- The output “isomorphic” can be wrong.

## How many refinement steps are needed on $n$ -vertex graphs?

### Exercise

$$C^{i+1}(v) = C^{i+1}(v') \implies C^i(v) = C^i(v').$$

Regard  $C^i$  as a coloring of the graph  $F = G + H$ .

Let  $\mathcal{P}^i$  be the partition of  $V(F) = V(G) \cup V(H)$  according to  $C^i$ .

$\mathcal{P}^{i+1}$  is a refinement of  $\mathcal{P}^i$  (by Exercise)  $\implies$

$\mathcal{P}^s = \mathcal{P}^{s+1}$  for some  $s < 2n \implies$

For any  $X, Y \in \mathcal{P}^s$ , the induced subgraph  $F[X]$  is regular and the induced bipartite subgraph  $F[X, Y]$  is bi-regular.  $\implies$

$\mathcal{P}^{s+1} = \mathcal{P}^{s+2} = \dots$  (partition stabilization)  $\implies$

For any  $v, v' \in V(G) \cup V(H)$ , if  $C^s(v) = C^s(v')$  then  $C^i(v) = C^i(v')$  for all  $i \geq s$ .  $\implies$

CR distinguishes  $G$  and  $H$  either in  $s < 2n$  steps or never.

## How many refinement steps are needed on $n$ -vertex graphs?

In fact,  $n$  refinement steps are enough.

Indeed, if  $\mathcal{P}^{i+1}$  is a proper refinement of  $\mathcal{P}^i$  and

$$\{\{ C^{i+1}(v) \}\}_{v \in V(G)} = \{\{ C^{i+1}(v) \}\}_{v \in V(H)},$$

then  $\mathcal{P}^{i+1}$  is a proper refinement of  $\mathcal{P}^i$  on both  $V(G)$  and  $V(H)$ .

## Color refinement algorithm: Implementation details

The length of  $C^i(v)$  grows exponentially as  $i$  increases.

Solution: Enumerate (rename) the colors lexicographically after each refinement round!

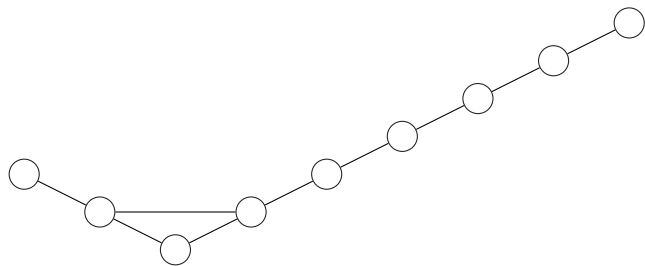
## Graph Canonization Problem

Given: a graph  $G$  on the vertex set  $\{1, \dots, n\}$

Find: a permutation  $\alpha_G$  of  $\{1, \dots, n\}$  such that

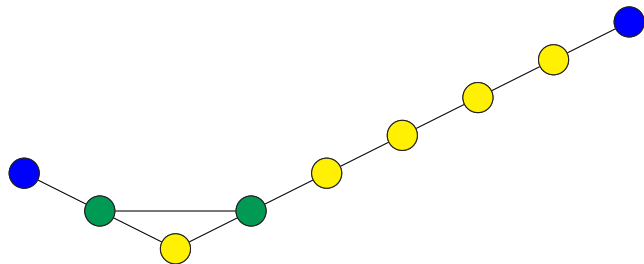
$$\alpha_G(G) = \alpha_H(H) \text{ whenever } G \cong H.$$

## Color refinement algorithm: An example of canonization



An input graph

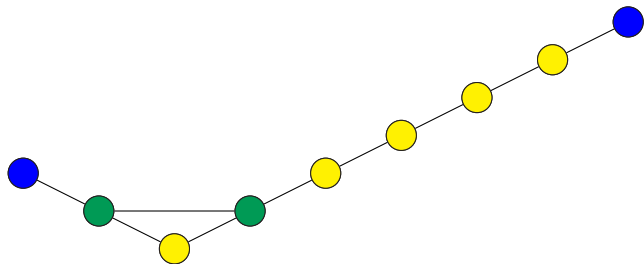
## Color refinement algorithm: An example of canonization



Initial coloring:  $C^1(v) = \deg v$



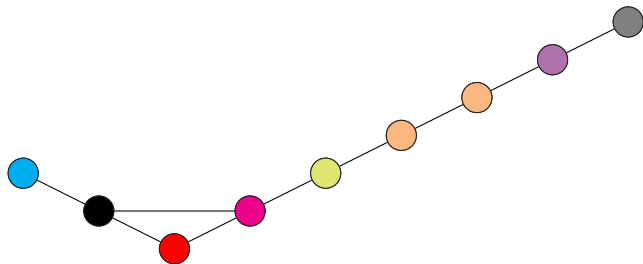
## Color refinement algorithm: An example of canonization



Initial coloring:  $C^1(v) = \deg v$

A color refinement step:  $C^{i+1}(v) = \{ \{ C^i(u) \} \}_{u \in N(v)}$

# Color refinement algorithm: An example of canonization



1st refinement step:  $C^2(v) = \{ \{ C^1(u) \} \}_{u \in N(v)}$

$$\text{Red} = \{ \{ \text{Green}, \text{Green} \} \}$$

$$\text{Black} = \{ \{ \text{Green}, \text{Yellow}, \text{Blue} \} \}$$

$$\text{Pink} = \{ \{ \text{Green}, \text{Yellow}, \text{Yellow} \} \}$$

$$\text{Blue} = \{ \{ \text{Green} \} \}$$

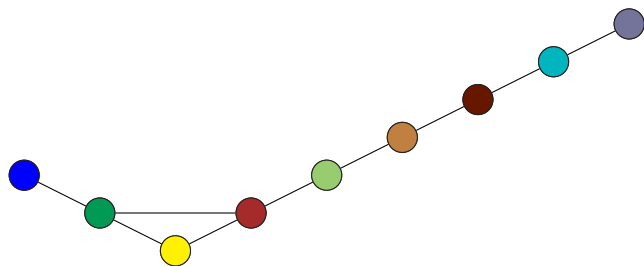
$$\text{Light Green} = \{ \{ \text{Green}, \text{Yellow} \} \}$$

$$\text{Orange} = \{ \{ \text{Yellow}, \text{Yellow} \} \}$$

$$\text{Purple} = \{ \{ \text{Yellow}, \text{Blue} \} \}$$

$$\text{Grey} = \{ \{ \text{Yellow} \} \}$$

## Color refinement algorithm: An example of canonization



2nd refinement step:  $C^3(v) = \{ \{ C^2(u) \} \}_{u \in N(v)}$

● =  $\{ \{ \text{orange}, \text{light green} \} \}$

● =  $\{ \{ \text{orange}, \text{purple} \} \}$

...

# CR canonizes almost all graphs

## Definition

We call  $G$  **discrete** if its stable partition consists of singletons.

## Theorem (Babai, Erdős, Selkow 1980)

$G_{n,1/2}$  is discrete with high probability.

## Proof-scheme

Let  $m = o(\sqrt[4]{n/\log n})$  and  $U$  be the set of vertices with the  $m$  largest degrees. Then, with high probability,

- vertices in  $U$  have pairwise distinct degrees, cf. [Bollobás 1981]
- vertices not in  $U$  have pairwise distinct sets of neighbors in  $U$ , assuming also that  $m > 3 \log_2 n$ .

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## Color Refinement and $\text{FO}_{\#}^2$

Lemma (Immerman and Lander 1990)

For any possible  $C^i$ -color  $c$  there is  $\Phi(x) \in \text{FO}_{\#}^2$  such that

$$G, v \models \Phi(x) \quad \text{iff} \quad C^i(v) = c$$

for every  $G$  and  $v \in V(G)$ .

Corollary

Discrete graphs are definable in  $\text{FO}_{\#}^2$ .

# Proof of the Immerman-Lander lemma

Base case  $i = 1$ .

$\deg v = d$  can be expressed by

$$\Phi(x) \stackrel{\text{def}}{=} \exists^{\geq d} y (y \sim x) \wedge \neg \exists^{\geq d+1} y (y \sim x)$$

(shorter:  $\exists^{=d} y (y \sim x)$ ).

Induction step  $i \mapsto i + 1$

Assumption: Each  $C^i$ -color  $c$  is definable by  $\Phi_c(x)$ .

Suppose  $C^{i+1}(v) = c'$  iff  $v$  has  $s_1$  neighbors  $u$  with  $C^i(u) = c_1$ ,  $s_2$  neighbors  $u$  with  $C^i(u) = c_2$  and so on.

Then  $c'$  is definable by

$$\Phi_{c'}(x) \stackrel{\text{def}}{=} \bigwedge_j \exists^{=s_j} y (y \sim x \wedge \Phi_{c_j}(y)) \wedge \exists^{=\deg v} y (y \sim x).$$

## Theorem (Immerman and Lander 1990)

*The following two conditions are equivalent:*

- 1  $G$  and  $H$  are indistinguishable by CR.
- 2  $G$  and  $H$  are indistinguishable in  $\text{FO}_{\#}^2$ .

## Example

$C_6$  is not definable in  $\text{FO}_{\#}^2$  because CR cannot distinguish it from  $2C_3$ .



## Proof of the Immerman-Lander theorem

$\neg(1) \implies \neg(2)$  by the preceding lemma

(1)  $\implies$  (2). The assumption (1) means that

$$\{\{C^i(v)\}\}_{v \in V(G)} = \{\{C^i(v)\}\}_{v \in V(H)} \text{ for all } i.$$

Let  $\mathcal{P}^s$  be the stable partition of  $V(G) \cup V(H)$ .  $\mathcal{P}^s$  consists of unions  $Z \cup Z'$  such that  $Z \subseteq V(G)$ ,  $Z' \subseteq V(H)$ ,  $|Z| = |Z'|$ , and all vertices in  $Z$  have the same  $C^s$ -color as all vertices in  $Z'$ .

We design a winning strategy for Duplicator in the 2-pebble counting game on  $G$  and  $H$ .

*1st round.* If Spoiler marks a set of vertices  $A \subseteq V(G)$ , Duplicator responds with  $B \subseteq V(H)$  such that

$$|A \cap Z| = |B \cap Z'| \text{ for every } Z \cup Z' \in \mathcal{P}^s$$

and ensures pebbling a pair of vertices  $x \in X$  and  $x' \in X'$  for some  $X \cup X' \in \mathcal{P}^s$ .

## Proof of the Immerman-Lander theorem (cont'd)

For any  $X \cup X' \in \mathcal{P}^s$  and  $Y \cup Y' \in \mathcal{P}^s$

- $G[X]$  and  $H[X']$  are regular graphs of the same degree;
- $G[X, Y]$  and  $H[X', Y']$  are bi-regular graphs with the same degrees.

*i*-th round. Suppose that  $x \in X$  and  $x' \in X'$  are pebbled. If Spoiler marks  $A \subseteq V(G)$ , Duplicator responds with  $B \subseteq V(H)$  such that

$$\begin{aligned} |A \cap (Z \cap N(x))| &= |B \cap (Z' \cap N(x'))|, \\ |A \cap (Z \setminus N(x))| &= |B \cap (Z' \setminus N(x'))| \end{aligned}$$

for every  $Z \cup Z'$ . Therewith she ensures pebbling a pair of vertices  $y \in Y$  and  $y' \in Y'$  for some  $Y \cup Y' \in \mathcal{P}^s$  such that

$$y \in N(x) \iff y' \in N(x').$$

## Conclusion

Color Refinement works correctly on  $G$  and every  $H$   
iff  
 $G$  is definable in  $\text{FO}_{\#}^2$ .

## Conclusion

Color Refinement works correctly on  $G$  and every  $H$   
iff  
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### Question

Which graphs are definable in  $\text{FO}_{\#}^2$ ?

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- N. Immerman and E. Lander. Describing graphs: A first-order approach to graph canonization. In *Complexity Theory Retrospective*, Springer, 1990.
- C. Berkholz, P.S. Bonsma, M. Grohe. Tight lower and upper bounds for the complexity of canonical colour refinement. ESA'13.