

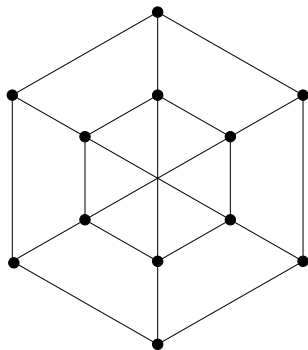
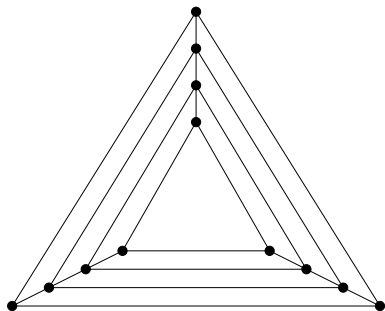
On Continuous and Combinatorial Relaxations of Graph Isomorphism

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Based on joint work with
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Indistinguishability



Overview of the talk

Overview:

1. Iterated degree sequences and Weisfeiler-Lehman algorithm
2. Fractional isomorphisms and Sherali-Adams relaxations
3. Transfer Lemma
4. Indistinguishability in counting logics
5. Applications

Part I

ITERATED DEGREE SEQUENCES

Iterated degree sequences

Let $G = (V, E)$ be a **graph**.

Use u to denote a vertex, and $N_G(u)$ for its **neighborhood**.

Start at the degree sequence:

$$d_1(u) := |N_G(u)|,$$

$$d_1(G) := \{ \{ d_1(u) : u \in V \} \}.$$

Iterate:

$$d_{i+1}(u) := \{ \{ d_i(v) : v \in N_G(u) \} \},$$

$$d_{i+1}(G) := \{ \{ d_{i+1}(u) : u \in V \} \}.$$

Take the limit:

$$D(G) := (d_1(G), d_2(G), d_3(G), \dots).$$

Indistinguishability by iterated degree sequences

Definition:

$$G \cong_D H \text{ iff } D(G) = D(H).$$

Indistinguishability by iterated degree sequences

\cong_D is strong...

Theorem [Babai-Erdős-Selkow 80]:

Let $G = G(n, 1/2)$ be drawn randomly. Then, a.s. as $n \rightarrow \infty$,
for every H with n vertices we have $G \cong_D H$ iff $G \cong H$.

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for **every** H with n vertices we have $G \cong_D H$ iff $G \cong H$.

But also **weak**...

Fact [Obvious]:

If G and H are both d -regular, **then** $G \cong_D H$.

Types of k -tuples

For a k -tuple of vertices $\bar{u} = (u_1, \dots, u_k) \in V^k$,

Define:

$\text{tp}_G(\bar{u}) =$ “complete information about **adjacencies**,
non-adjacencies, **equalities** and **non-equalities**
between the components u_1, \dots, u_k ”.

Example:

$$\begin{aligned} \text{tp}_G(u_1, u_2, u_3) = & \{ \overline{E(1,1)}, E(1,2), E(1,3), \\ & E(2,1), \overline{E(2,2)}, \overline{E(3,2)}, \\ & E(3,1), \overline{E(3,2)}, \overline{E(3,3)}, \\ & 1 \neq 2, 1 \neq 3, 2 = 3 \} \end{aligned}$$

k -dimensional Weisfeiler-Lehman algorithm

Start at the type sequence:

$$\begin{aligned} \ell_0(\bar{u}) &:= \text{tp}_G(\bar{u}), \\ \ell_0(G) &:= \{ \{ \ell_0(\bar{u}) : \bar{u} \in V^k \} \}. \end{aligned}$$

Iterate:

$$\begin{aligned} \ell_{i+1}(\bar{u}) &:= \{ \{ (\text{tp}_G(\bar{u}v), \ell_i(\bar{u}[1/v]), \dots, \ell_i(\bar{u}[k/v])) : v \in V \} \}, \\ \ell_{i+1}(G) &:= \{ \{ \ell_{i+1}(\bar{u}) : \bar{u} \in V^k \} \}. \end{aligned}$$

Take the limit:

$$D^k(G) := (\ell_0(G), \ell_1(G), \dots).$$

Definition:

$$G \cong_{\text{WL}}^k H \text{ iff } D^k(G) = D^k(H).$$

Indistinguishability by k -dim WL

\cong_{WL}^k is strong...

At least as strong as vertex-refinement:

$$G \not\cong_D H \implies G \not\cong_{\text{WL}}^1 H$$

Theorem [Kucera 87]:

Let $G = G_{\text{reg}}(n, d)$ be drawn randomly. Then, a.s. as $n \rightarrow \infty$,
for **every** H with n vertices we have $G \cong_{\text{WL}}^2 H$ iff $G \cong H$.

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Relevant note:

\cong_{WL}^k is decidable in time $n^{O(k)}$.

Is k -dim WL weak at all?

Truth is:

For years no two \cong_{WL}^{37} -indistinguishable graphs were known...
It was even **conjectured** that no such graphs existed...

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Theorem [Cai-Fürer-Immerman 92]:

There exists **explicitly defined** graphs G_n and H_n ,
with n vertices each and maximum degree 3, such that

$$G_n \cong_{\text{WL}}^{\Omega(n)} H_n \quad \text{yet} \quad G_n \not\cong H_n.$$

Note:

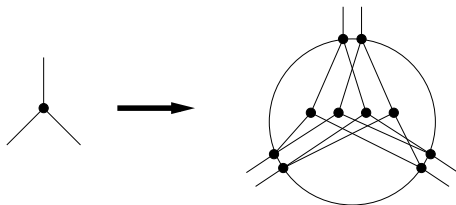
Reasoning about \cong_{WL}^k requires an excursion
into finite model theory (more on this later).

CFI-construction

1. Start with a 3-regular graph G without $\Omega(n)$ -separators.

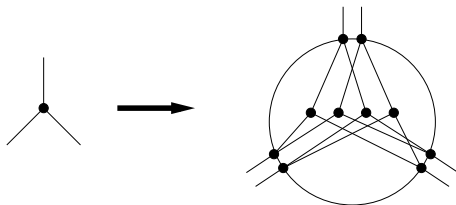
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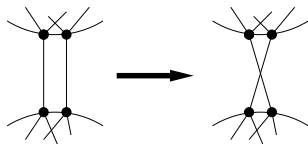


CFI-construction

1. Start with a 3-regular graph G without $\Omega(n)$ -separators.
2. Replace each vertex by gadget:



3. Let G_n be the result and let $H_n = G_n +$ "one flip".



Part II

SHERALI-ADAMS RELAXATIONS

Adjacency matrices

Let $G = (V^G, E^G)$ and $H = (V^H, E^H)$ be graphs.

Say $V^G = V^H = \{1, \dots, n\}$.

Let A and B be their **adjacency matrices**.

$$A = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 \end{pmatrix} \quad B = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{pmatrix}$$

Permutation matrices and isomorphisms

A **permutation matrix** P is a real matrix such that

$$\begin{aligned}\sum_{j=1}^n P_{ij} &= 1 && \text{for every } i \in \{1, \dots, n\}, \\ \sum_{i=1}^n P_{ij} &= 1 && \text{for every } j \in \{1, \dots, n\}, \\ P_{ij} &\in \{0, 1\} && \text{for every } i, j \in \{1, \dots, n\}.\end{aligned}$$

Properties:

- $P^T P = I$,
- $A \mapsto AP$: permutes the columns of A ,
- $A \mapsto P^T A$: permutes the rows of A ,
- $A \mapsto P^T AP$: permutes the vertices.

Fact: The following are equivalent:

1. $G \cong H$,
2. there exists $P \in \mathcal{P}_n$ such that $P^T AP = B$,
3. there exists $P \in \mathcal{P}_n$ such that $AP = PB$.

Doubly stochastic matrices and fractional isomorphisms

A **doubly stochastic** matrix S is a real matrix such that:

$$\begin{aligned}\sum_{j=1}^n S_{ij} &= 1 && \text{for every } i \in \{1, \dots, n\}, \\ \sum_{i=1}^n S_{ij} &= 1 && \text{for every } j \in \{1, \dots, n\}, \\ S_{ij} &\geq 0 && \text{for every } i, j \in \{1, \dots, n\}.\end{aligned}$$

Relaxation of isomorphism:

- **Replace** “there exists $P \in \mathcal{P}_n$ such that $AP = PB$ ”
- **by this** “there exists $S \in \mathcal{S}_n$ such that $AS = SB$ ”.

In other words, let $I(G, H)$ be the LP for \mathcal{S}_n plus

$$\sum_{i=1}^n A_{ui} S_{iv} = \sum_{j=1}^n S_{uj} B_{jv}$$

for every $u, v \in V^G \times V^H$.

Indistinguishability by fractional isomorphisms

Definition:

$$G \cong_F H \text{ iff } I(G, H) \neq \emptyset.$$

Indistinguishability by fractional isomorphisms

Suppose $G \cong_F H$. Then:

- $|E^G| = |E^H|$,
- actually $d_1(G) = d_1(H)$,
- and even $D(G) = D(H)$.

Indistinguishability by fractional isomorphisms

Suppose $G \cong_F H$. Then:

- $|E^G| = |E^H|$,
- actually $d_1(G) = d_1(H)$,
- and even $D(G) = D(H)$.

Indeed:

Theorem [Ramana-Scheinerman-Ullman 94]

$$G \cong_F H \text{ iff } G \cong_D H.$$

Sherali-Adams relaxations

Let

$$P = \{x \in \mathbb{R}^n : Ax \geq b\},$$

$$P^{\mathbb{Z}} = \text{convexhull}\{x \in \{0, 1\}^n : Ax \geq b\}.$$

The **Sherali-Adams levels** are nested polytopes:

$$P = P^0 \supseteq P^1 \supseteq P^2 \supseteq \dots \supseteq P^n = P^{\mathbb{Z}}$$

and the **SA-rank** of P is:

$$\min\{k : P^k = P^{\mathbb{Z}}\}.$$

Definition of P^k in four steps

Let

$$P = \left\{ x \in \mathbb{R}^n : \begin{bmatrix} a_1^T x \geq b_1 \\ \vdots \\ a_m^T x \geq b_m \end{bmatrix} \right\}.$$

be the LP.

Definition of P^k in four steps

Step 1: Multiply each $a_i^T x \geq b_i$ by all multipliers of the form

$$\prod_{i \in I} x_i \prod_{j \in J} (1 - x_j)$$

for $I, J \subseteq [n]$, $|I \cup J| \leq k - 1$, $I \cap J = \emptyset$.

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Step 1 leaves an equivalent system of **polynomials** of degree k .

Definition of P^k in four steps

Step 2: Expand the products and replace each square x_i^2 by x_i .

Definition of P^k in four steps

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Step 2 leaves a system of multi-linear polynomials of degree k .
This is the **integrality** step: valid on $\{0, 1\}^n$ only.

Definition of P^k in four steps

Step 3: Linearize each monomial $\prod_{i \in I} x_i$ by introducing a new variable y_I .

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Step 3 leaves a linear program Q^k on the y_I -variables in \mathbb{R}^{n^k} .
This is the **relaxation** step.

Definition of P^k in four steps

Step 4: Define

$$P^k := \{x \in \mathbb{R}^n : \exists y \in Q^k \text{ s.t. } y_{\{i\}} = x_i \text{ for every } i\}.$$

Definition of P^k in four steps

Step 4: Define

$$P^k := \{x \in \mathbb{R}^n : \exists y \in Q^k \text{ s.t. } y_{\{i\}} = x_i \text{ for every } i\}.$$

Step 4 takes us back to \mathbb{R}^n .

It's the **projection** step: from \mathbb{R}^{n^k} to \mathbb{R}^n .

Solving P^k

Note:

The polytope P^k is definable by an LP on n^k variables and $m \cdot n^k$ inequalities.

Therefore:

Feasibility and optimization of linear functions over P^k can be solved in time $m^{O(1)} n^{O(k)}$.

Indistinguishability by SA-levels of fractional isomorphisms

Definition:

$$G \cong_{\text{SA}}^k H \text{ iff } I(G, H)^k \neq \emptyset.$$

Part III

TRANSFER LEMMA

Statement of the transfer lemma

Transfer Lemma:

$$G \cong_{\text{WL}}^k H \implies G \cong_{\text{SA}}^{k-1} H \implies G \cong_{\text{WL}}^{k-1} H.$$

Interpretation:

A **geometric** concept is captured by purely **combinatorial** means.

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Proof of the transfer lemma

Intermediate notions of indistinguishability:

$$G \cong_{\text{WL}}^k H \Rightarrow G \cong_{\text{C}}^k H \Rightarrow G \cong_{\text{CS}}^{k-1} H \Rightarrow G \cong_{\text{EP}}^{k-1} H \Rightarrow G \cong_{\text{SA}}^{k-1} H$$

and

$$G \cong_{\text{SA}}^{k-1} H \Rightarrow G \cong_{\text{C}}^{k-1} H \Rightarrow G \cong_{\text{WL}}^{k-1} H.$$

Proof of the transfer lemma

Intermediate notions of indistinguishability:

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and

$$G \cong_{\text{SA}}^{k-1} H \Rightarrow G \cong_{\text{C}}^{k-1} H \Rightarrow G \cong_{\text{WL}}^{k-1} H.$$

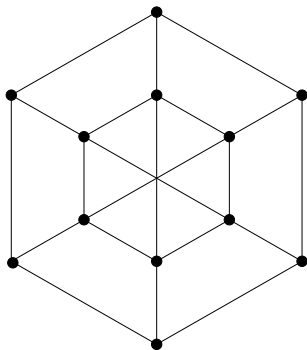
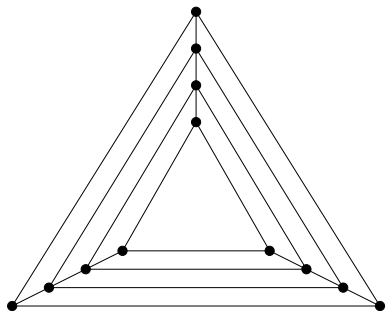
Here:

\cong_{C}^k is indistinguishability by properties definable in first-order logic with counting quantifiers and width k .

Part IV

COUNTING LOGICS

Indistinguishability



Counting quantifiers

Counting witnesses:

$\exists^{\geq i} x(\phi(x))$: there are at least i vertices x that satisfy $\phi(x)$.

Example:

$$\psi_d(x) := \exists^{\geq d} y(E(x, y)) \wedge \neg \exists^{d+1} y(E(x, y)),$$

$$\phi := \neg \exists^{\geq 1} x(\neg \psi_d(x)).$$

Note:

We used only **two** first-order variables (x and y) where $d + 1$ are required in pure first-order logic.

Bounded width formulas

Example: First paths

$$P_1(x, y) := E(x, y)$$

$$P_2(x, y) := \exists z_1 (E(x, z_1) \wedge P_1(z_1, y))$$

$$P_3(x, y) := \exists z_2 (E(x, z_2) \wedge P_2(z_2, y))$$

\vdots

$$P_{i+1}(x, y) := \exists z_i (E(x, z_i) \wedge P_i(z_i, y)).$$

and then

$$\forall x (\neg P_3(x, x) \wedge \neg P_5(x, x) \wedge \cdots \wedge \neg P_{2\lceil n/2 \rceil - 1}(x, x)).$$

Counting logic with k variables:

C^k : collection of formulas for which
all subformulas have at most k free variables.

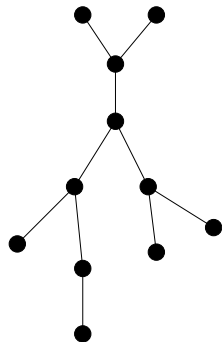
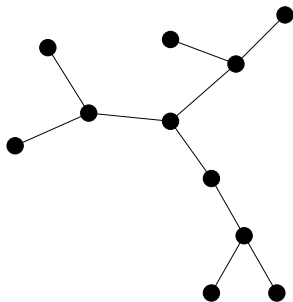
Indistinguishability by C^k

Definition:

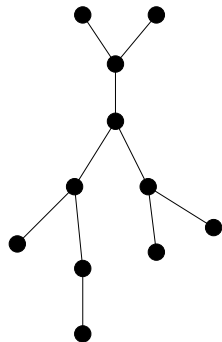
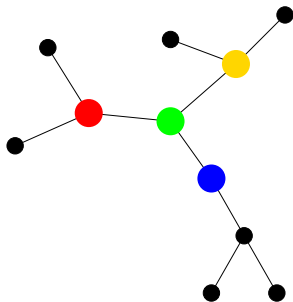
$G \cong_C^k H$ iff for every $\phi \in C^k$ we have $G \models \phi \Leftrightarrow H \models \phi$.

Pebble game (without counting moves)

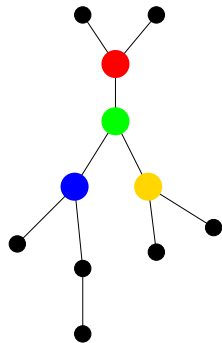
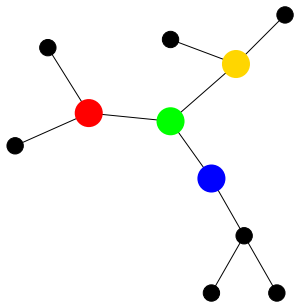
Forced win for Spoiler.



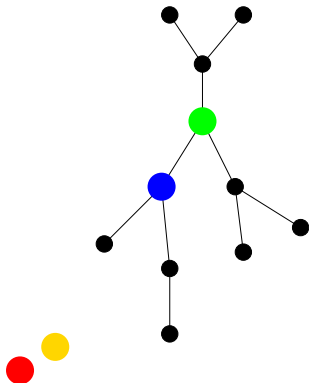
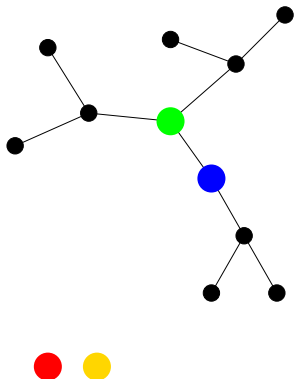
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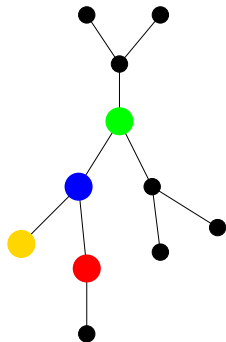
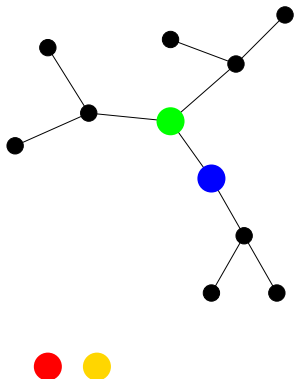
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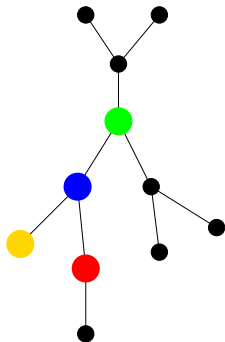
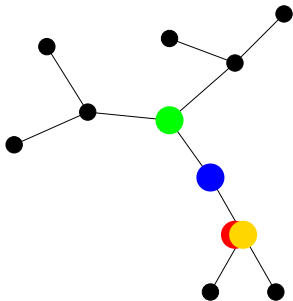
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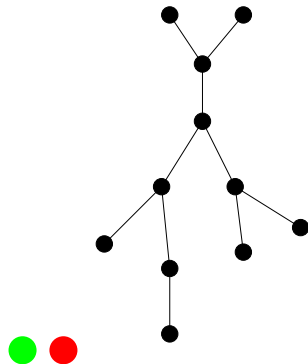
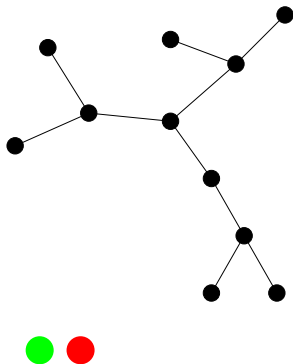


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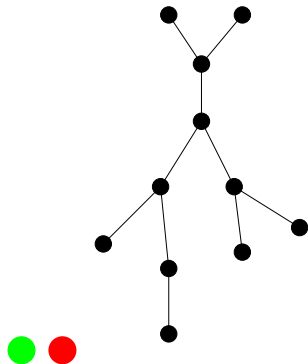
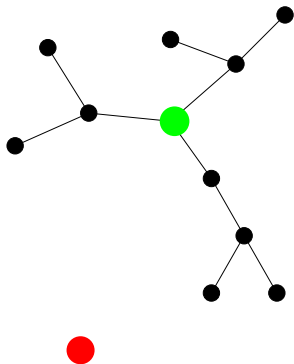


Pebble game WITH counting moves

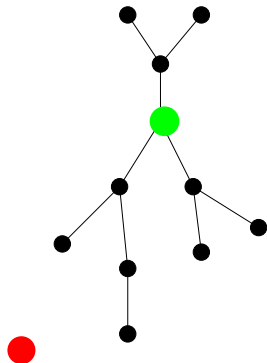
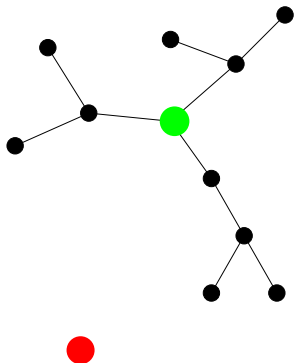
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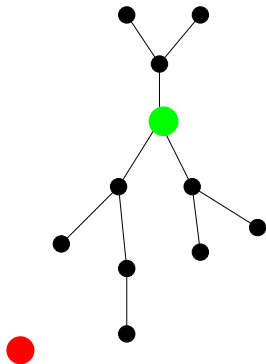
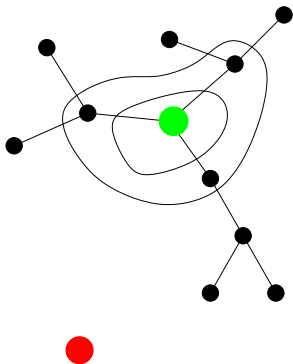
Pebble game with counting moves



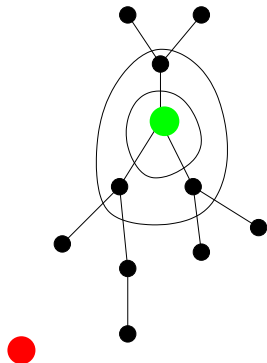
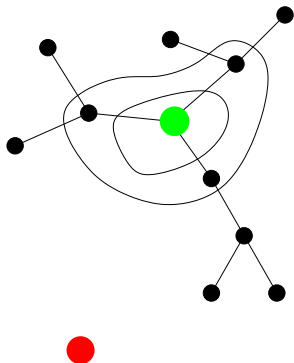
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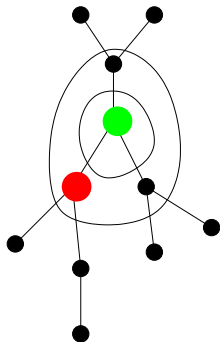
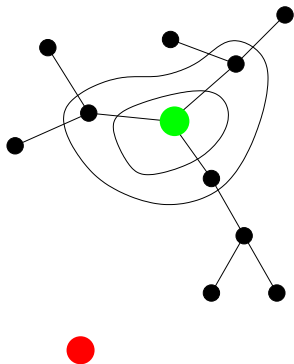
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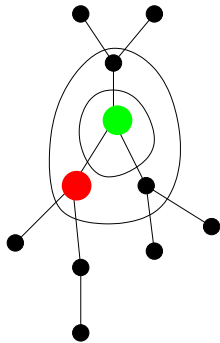
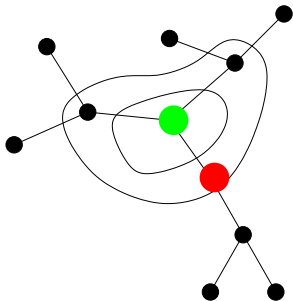
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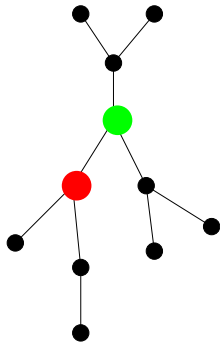
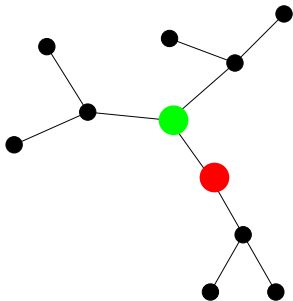
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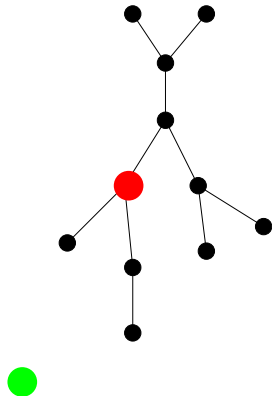
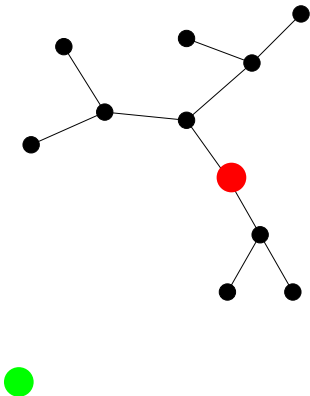
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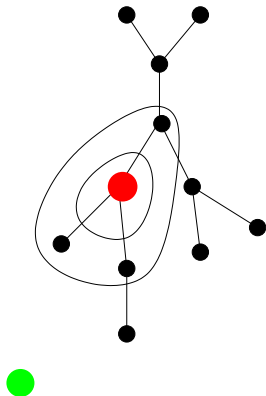
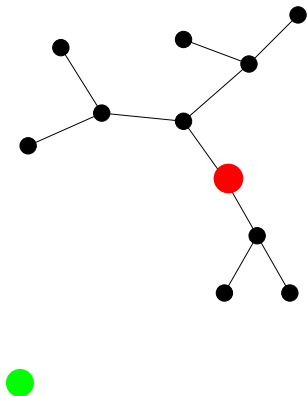
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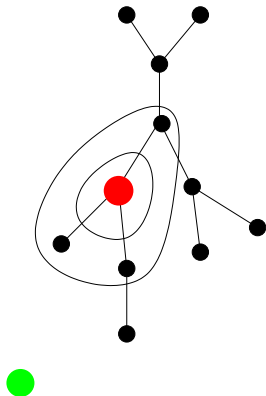
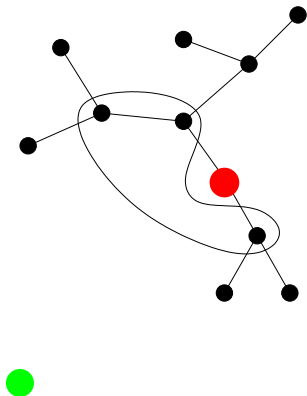
Pebble game with counting moves



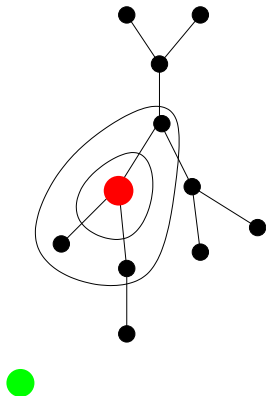
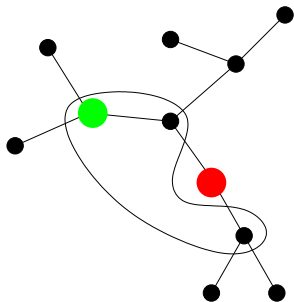
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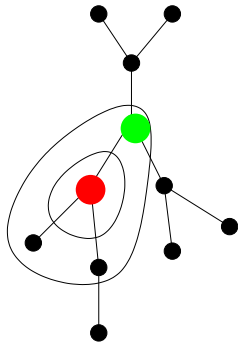
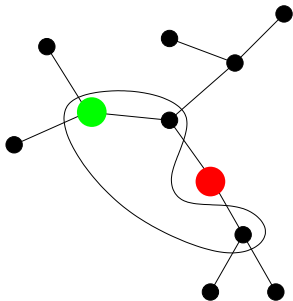
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Systems with the back-and-forth properties

A **winning strategy** for the Duplicator in $G \cong_C^k H$ is a non-empty collection \mathcal{F} of partial isomorphisms from G to H such that for every $f \in \mathcal{F}$ we have:

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for every $X \subseteq V_G$ there exists $Y \subseteq V_H$ with $|Y| = |X|$ s.t.
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Counting pebble game vs. Weisfeiler-Lehman algorithm

Theorem [Immerman-Lander 90, Cai-Fürer-Immerman 92]

$$G \cong_{\text{WL}}^k H \iff G \cong_{\text{C}}^{k+1} H.$$

Relevant note: From its definition, it is not even obvious that $G \cong_{\text{C}}^k H$ is decidable in time $n^{O(k)}$.

From feasible solutions to systems with B&F

Wanted:

$$G \cong_{SA}^k H \implies G \cong_C^k H$$

Ingredient 1:

Birkhoff decomposition theorem: every doubly stochastic matrix is a **convex combination** of permutation matrices.

Ingredient 2:

Permutations preserve sizes of sets.

From systems with B&F to feasible solutions

Wanted:

$$G \cong_C^k H \implies G \cong_{SA}^{k-1} H$$

Ingredient 1:

A sliding game to account for $AS = SB$;
here is where the -1 is lost.

Ingredient 2:

Normalizing winning strategies into uniform ones.

Part V

APPLICATIONS (or what to do of this?)

Isomorphism testing for special graphs

Theorem [Immerman-Lander 90, Grohe 98, ...]

1. If G is a tree, then $G \cong_C^2 H$ iff $G \cong H$, for every H .
2. If G is planar, then $G \cong_C^{15} H$ iff $G \cong H$, for every H .
3. ...

Corollary

For all such graph classes,
an **explicit** and **poly-size** LP
solves graph isomorphism.

SA-rank lower bounds

Consider the standard LP-relaxation of **vertex cover**:

$$\text{minimize } \sum_{u \in V} x_u$$

subject to

$$x_u + x_v \geq 1 \quad \text{for every } (u, v) \in E,$$

$$x_u \geq 0 \quad \text{for every } u \in V.$$

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We expect that the inequality

$$\sum_{u \in V} x_u \geq \text{vc}(G) \tag{1}$$

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Indeed:

Theorem [exercise, also follows Schoenebeck 08]

There exist graphs G for which (2) is not valid over $P^{\Omega(n)}(G)$.

New proof

Sketch:

1. Start with the n -vertex **CFI graphs** $G \cong_C^{\Omega(n)} H$ yet $G \not\cong H$.
2. In particular $(G, G) \cong_C^{\Omega(n)} (G, H)$ yet $G \cong G$ and $G \not\cong H$.
3. Apply the **reduction** from graph isomorphism to vertex cover.
4. Get graphs $A \cong_C^{\Omega(n)} B$ with $\text{vc}(A) \neq \text{vc}(B)$.
5. Apply **transfer lemma** and get $A \cong_{SA}^{\Omega(n)} B$.

Final step:

$$A \cong_{SA}^{2k} B \implies \text{opt}(P^k(A)) = \text{opt}(P^k(B)).$$

SA-rank lower bounds

Consider the standard LP-relaxation of **max-cut**:

$$\text{maximize } \frac{1}{2} \sum_{uv \in E} x_{uv}$$

subject to

$$x_{uv} = x_{vu}$$

$$x_{uw} \leq x_{uv} + x_{vw}$$

$$x_{uv} + x_{vw} + x_{wu} \leq 2$$

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We expect that the inequality

$$\sum_{u \in V} x_u \leq \text{mc}(G) \tag{2}$$

will **not**, in general, be **valid** over $P^k(G)$ for any $k = O(1)$.

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We expect that the inequality

$$\sum_{u \in V} x_u \leq \text{mc}(G) \tag{2}$$

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Indeed:

Theorem [follows from Schoenebeck 08]

There exist graphs G for which (2) is not valid over $P^{\Omega(n)}(G)$.

Sketch:

1. Start with the n -vertex **CFI graphs** $G \cong_C^{\Omega(n)} H$ yet $G \not\cong H$.
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Final step:

$$A \cong_{SA}^{3k} B \implies \text{opt}(P^k(A)) = \text{opt}(P^k(B)).$$

Local LPs

Basic k -local LPs:

1. one **variable** $x_{\mathbf{u}}$ for each k -tuple $\mathbf{u} \in V^k$,
2. one **inequality** $\sum_{\mathbf{u} \in V^k} a_{\mathbf{u}, \mathbf{v}} \cdot x_{\mathbf{u}} \geq b_{\mathbf{v}}$ for every k -tuple $\mathbf{v} \in V^k$,
3. coefficients $a_{\mathbf{u}, \mathbf{v}}$ **depend only** on the type $\text{tp}_G(\mathbf{u}, \mathbf{v})$,
4. coefficients $b_{\mathbf{v}}$ **depend only** on the type $\text{tp}_G(\mathbf{v})$.

Generic k -local LPs:

Unions of generic basic k -local LPs
(with coefficients given as a function of the types).

Instantiation of generic k -local LPs:

Let P is a generic k -local LP.
Then $P(G)$ is the LP associated to G .

Recall the metric polytope:

$$\frac{1}{2} \sum_{uv \in E} x_{uv} \geq W$$

$$x_{uv} = x_{vu}$$

$$x_{uw} \leq x_{uv} + x_{vw}$$

$$x_{uv} + x_{vw} + x_{uw} \leq 2$$

$$0 \leq x_{uv} \leq 1$$

1. Objective function: basic 2-local LP
2. Symmetry constraint: two basic 2-local LPs
3. Triangle inequality: basic 3-local LP
4. Perimetric inequality: basic 3-local LP
5. Unit cube constraint: two basic 2-local LPs

Preservation of local LPs

Theorem: Let P be a generic k -local LP.

If $G \cong_{\text{SA}}^k H$, then $P(G)$ is feasible iff $P(H)$ is feasible.

'Just do it' proof:

1. Let $\{x_u\}$ be a feasible solution for $P(G)$.
2. Let $\{X_{u,v}\}$ be a feasible solution for $I(G, H)^k$.
3. Define:

$$y_v := \sum_{u \in G^k} X_{u,v} \cdot x_u.$$

4. Check that $\{y_v\}$ is a feasible solution for $P(H)$.

More examples of local LPs

More examples:

1. maximum flows (2-local)
2. matchings on bipartite graphs (2-local)
3. relaxation of max-cut via the metric polytope (3-local)
4. relaxation of vertex cover (2-local)
5. r SA-levels of k -local LPs are $O(kr)$ -local LPs.

Expressibility results

Consider the max-flow LP. It is 2-local. It is integral.

Corollary

$$G \cong_C^3 H \Rightarrow \text{mf}(G) = \text{mf}(H).$$

Corollary

There exists a sentence in C^3 that, over st -networks with n vertices, defines those whose maximum flow is at least the out-degree of the source.

Expressibility results

Consider the metric polytope again.

Theorem [Barahona-Majoub 86]:

If G is a K_5 minor-free graph, then $\text{mc}(G) = \text{opt}(P(G))$.

Corollary

If G and H are K_5 minor-free, then $G \cong_C^4 H \Rightarrow \text{mc}(G) = \text{mc}(H)$.

Corollary

There exists a sentence in C^4 that,
over K_5 minor-free n -vertex graphs, defines those
whose max-cut is at least $n/4$.

Part VI

DISCUSSION AND OPEN PROBLEMS

Get new rank lower bounds from inexpressibility results?

Challenging problem:

Prove that an **integrality gap** of $2 - \epsilon$ resists $\Omega(n)$ SA-levels of vertex-cover.

Get new rank lower bounds from inexpressibility results?

Challenging problem:

Prove that an **integrality gap** of $2 - \epsilon$ resists $\Omega(n)$ SA-levels of vertex-cover.

What would be enough?:

Find G and H such that:

1. $\text{mc}(G) \geq (2 - \epsilon) \cdot \text{mc}(H)$
2. $G \cong_C^{\Omega(n)} H$.

New expressibility/inexpressibility results?

Challenging problem:

Is **perfect matching** definable in $C^{O(1)}$?
(answer is YES for bipartite graphs)

New expressibility/inexpressibility results?

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SOLVED! [Anderson-Dawar-Holm 13]:

YES even for general graphs!

TODA!