## A logical approach to Isomorphism Testing and Constraint Satisfaction

Oleg Verbitsky

Humboldt University of Berlin, Germany

ESSLLI 2016, 15-19 August

# Part 4: $FO_{\#}^2$ and linear-programming techniques.

### Outline



- The graph canonization problem
- 2 Fractional isomorphism and compactness
- (3)  $FO_{\#}^2$ -definable graphs are compact
- Tinhofer's canonization algorithm

### 6 References

### Outline



### The graph canonization problem

- 2 Fractional isomorphism and compactness
- $3 \text{ FO}_{\#}^2$ -definable graphs are compact

### Canonizing almost all graphs

All graphs on n vertices Efficiently canonizable graphs

Discrete graphs

Almost all graphs

### Canonizing almost all graphs

All graphs on n vertices Efficiently canonizable graphs

Graphs definable in  $FO_{\#}^2$ Discrete graphs

Almost all graphs

# Canonizing almost all graphs

All graphs on $n$ vertices	
Efficiently canonizable grap	hs
Compact graphs	
Graphs definable in ${ m FO}_{\#}^2$	
Discrete graphs	
Almost all graphs	



### Practional isomorphism and compactness

- (3)  $FO_{\#}^2$ -definable graphs are compact
  - 4 Tinhofer's canonization algorithm

### 5 References

### Fractional isomorphism and equivalent concepts

Consider graphs G and H with adjacency matrices A and B resp.  $G \cong H$  iff there is a permutation matrix X such that

$$AX = XB. \tag{1}$$

### Fractional isomorphism and equivalent concepts

Consider graphs G and H with adjacency matrices A and B resp.  $G \cong H$  iff there is a permutation matrix X such that

$$AX = XB. \tag{1}$$

 $X = (x_{ij})$  is doubly stochastic (d.s.) if  $x_{ij} \ge 0$ ,  $\sum_i x_{ij} = 1$  for all j, and  $\sum_j x_{ij} = 1$  for all i.

#### Definition

G and H are fractionally isomorphic if (1) is true for some d.s. X.

### Fractional isomorphism and equivalent concepts

Consider graphs G and H with adjacency matrices A and B resp.  $G \cong H$  iff there is a permutation matrix X such that

$$AX = XB. \tag{1}$$

 $X = (x_{ij})$  is doubly stochastic (d.s.) if  $x_{ij} \ge 0$ ,  $\sum_i x_{ij} = 1$  for all j, and  $\sum_j x_{ij} = 1$  for all i.

#### Definition

G and H are fractionally isomorphic if (1) is true for some d.s. X.

#### Theorem [Ramana, Scheinerman, Ullman 94; Immerman, Lander 90]

The following three conditions are equivalent:

- G and H are fractionally isomorphic,
- $\bullet$  G and H are indistinguishable by Color Refinement,
- G and H are indistinguishable in  $FO_{\#}^2$ .

Let  $S(G) = \{ X - d.s. : AX = XA \}$ , the set of all fractional automorphisms of G.

Let  $S(G) = \{ X - d.s. : AX = XA \}$ , the set of all fractional automorphisms of G.

```
• This is a polytope in \mathbb{R}^{n^2}.
```

Let  $S(G) = \{X - \mathsf{d.s.} : AX = XA\},\$ 

the set of all fractional automorphisms of G.

- This is a polytope in  $\mathbb{R}^{n^2}$ .
- Automorphisms of G (permutation matrices) are extreme points of S(G).

Let  $S(G) = \{X - \mathsf{d.s.} : AX = XA\},\$ 

the set of all fractional automorphisms of G.

- This is a polytope in  $\mathbb{R}^{n^2}$ .
- Automorphisms of G (permutation matrices) are extreme points of S(G).

```
Definition (Tinhofer 1991)
```

G is compact if S(G) has no other extreme points.

Let  $S(G) = \{X - \mathsf{d.s.} : AX = XA\},\$ 

the set of all fractional automorphisms of G.

- This is a polytope in  $\mathbb{R}^{n^2}$ .
- Automorphisms of G (permutation matrices) are extreme points of S(G).

```
Definition (Tinhofer 1991)
```

G is compact if S(G) has no other extreme points.

#### Equivalently,

- ullet all extreme points of S(G) are integral, or
- every fractional automorphism of G is a convex combination of automorphisms of G.

Let  $S(G) = \{X - \mathsf{d.s.} : AX = XA\},\$ 

the set of all fractional automorphisms of G.

- This is a polytope in  $\mathbb{R}^{n^2}$ .
- Automorphisms of G (permutation matrices) are extreme points of S(G).

#### Definition (Tinhofer 1991)

G is compact if S(G) has no other extreme points.

#### Equivalently,

- ullet all extreme points of S(G) are integral, or
- every fractional automorphism of G is a convex combination of automorphisms of G.

If G is known to be compact, then  $G \cong H$  can be tested by computing an extreme point of  $S(G, H) = \{X - d.s. : AX = XB\}$ :

- If  $G \cong H$ , then all extreme points of S(G, H) are integral;
- If  $G \not\cong H$ , then S(G, H) has no integral point.

Complete graphs are compact.

Every  $n \times n$  d.s. matrix is a fractional automorphism of  $K_n$ . Indeed, let J and I be the all-ones and the identity matrices. Then

$$X \text{ is d.s.} \implies JX = XJ \implies (J-I)X = X(J-I) \implies X \in S(K_n).$$

#### Birkhoff's theorem

Every doubly stochastic matrix is a convex combination of permutation matrices.

### Basic facts: Closure properties

G is compact iff its complement  $\overline{G}$  is compact.

#### Proof:

 $Aut(G) = Aut(\overline{G})$  and  $S(G) = S(\overline{G})$ . Indeed,

$$\begin{aligned} X \in S(\overline{G}) & \iff (J - I - A)X = X(J - I - A) \\ & \iff AX = XA \iff X \in S(G), \end{aligned}$$

where A is the adjacency matrix of G.

### Basic facts: Closure properties

G is compact iff its complement  $\overline{G}$  is compact.

#### Proof:

 $Aut(G) = Aut(\overline{G})$  and  $S(G) = S(\overline{G})$ . Indeed,

$$\begin{array}{rcl} X\in S(\overline{G}) & \Longleftrightarrow & (J-I-A)X=X(J-I-A)\\ & \Leftrightarrow & AX=XA \iff X\in S(G), \end{array}$$

where A is the adjacency matrix of G.

#### Lemma (Tinhofer 91)

If a connected graph G is compact, then the m-fold disjoint union mG is compact.

Example: The matching graph  $mK_2$  and its complement  $\overline{mK_2}$  are compact.

Thus, the cycle graphs  $C_3 = K_3$  and  $C_4 = \overline{2K_2}$  are compact.

 $C_5$  is compact too.

Thus, the cycle graphs  $C_3 = K_3$  and  $C_4 = \overline{2K_2}$  are compact.

 $C_5$  is compact too.

Other examples:

- All cycles [Tinhofer 1986]
- All trees [Tinhofer 1986]
- Many regular graphs [Brualdi 88, Godsil 97, Wang and Li 05]

### A negative example

 $C_3 \cup C_4$  is not compact.

### A negative example

 $C_3 \cup C_4$  is not compact.

#### Lemma (Tinhofer 1991)

A regular compact graph is vertex-transitive.

#### Proof:

- Consider the  $n \times n$  all-ones matrix J, where n is the number of vertices in G.
- If G is regular, then  $\frac{1}{n}J \in S(G)$ .
- If G is compact, then

$$\frac{1}{n}J = \sum_{s} \alpha_{s} P_{s},$$

a convex combination of permutation matrices from Aut(G).

• Therefore, for all i and j there is s such that  $[P_s]_{ij} = 1$ .



2 Fractional isomorphism and compactness

## (3) $FO_{\#}^2$ -definable graphs are compact

Tinhofer's canonization algorithm

#### 5 References

### Theorem (Arvind, Köbler, Rattan, V. 2015) All graphs definable in $FO_{\#}^2$ are compact.

### Proof-scheme

 $\bullet$  The proof is based on our characterization of  $\mathrm{FO}_{\#}^2\text{-definable}$  graphs.

### Proof-scheme

• The proof is based on our characterization of  $\mathrm{FO}_\#^2\text{-definable}$  graphs.

Let G be a definable graph. If  $X, Y \subseteq V(G)$  are vertex classes in the stable coloring of G (cells), then

• G[X] is one of

$$K_s, \overline{K_s}, mK_2, \overline{mK_2}, \text{ and } C_5.$$

 $\bullet \ G[X,Y]$  is one of

 $K_{s,t}, \ \overline{K_{s+t}}, \ sK_{1,t} (s \ge 2), \text{ and its bipartite complement.}$ 

## Proof-scheme (cont'd)

- homogeneous (isotropic) links G[X, Y] can be ignored;
- there is no cycle of non-homogeneous (anisotropic) links;
- each of the corresponding tree-like components of G can be considered separately;
- each such component contains at least one non-homogeneous cell X ( $G[X] \cong mK_2, \overline{mK_2}$ , or  $C_5$ );
- induction on the number of cells is possible because fractional automorphisms respect the stable partition [Ramana, Scheinerman, Ullman 1994];
- the base case is done by the compactness of  $K_s$ ,  $\overline{K_s}$ ,  $mK_2$ ,  $\overline{mK_2}$ , and  $C_5$ .



- Practional isomorphism and compactness
- $\bigcirc \operatorname{FO}^2_{\#}$ -definable graphs are compact
- Tinhofer's canonization algorithm

#### 5 References

### Tinhofer's canonization algorithm for compact graphs

Input: a graph G

- **1** Run Color Refinement on G till color stabilization.
- **2** If all color classes are singletons, terminate.
- If there is a color class with 2 or more vertices, individualize one of them by assigning a new color (the lexicographically first unused one).
- Goto Step 1.

Input: a graph G

- $\blacksquare$  Run Color Refinement on G till color stabilization.
- 2 If all color classes are singletons, terminate.
- If there is a color class with 2 or more vertices, individualize one of them by assigning a new color (the lexicographically first unused one).
- Goto Step 1.

#### Theorem (Tinhofer 1991)

If an input graph G is compact, then the above algorithm produces a canonical labeling of G for any choice of vertices to be individualized.



- Practional isomorphism and compactness
- (3)  $FO_{\#}^2$ -definable graphs are compact
  - 4 Tinhofer's canonization algorithm



### References

- G. Tinhofer. Graph isomorphism and theorems of Birkhoff type. Computing 36, 285–300 (1986).
- G. Tinhofer. A note on compact graphs. Discrete Applied Mathematics 30, 253–264 (1991).
- M.V. Ramana, E.R. Scheinerman, D. Ullman. Fractional isomorphism of graphs. Discrete Mathematics 132, 247–265 (1994).
- V. Arvind, J. Köbler, G. Rattan, O. Verbitsky. On Tinhofer's linear programming approach to Isomorphism Testing. MFCS'15.