Near-Optimal Lower Bounds on Quantifier Depth and Weisfeiler-Leman Refinement Steps

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Joint work with Jakob Nordström (KTH Stockholm).

Two vertices are connected by a path of length 4:

$$\varphi_{\mathsf{dist-4}}(x,y) = \exists z_1 \exists z_2 \exists z_3 \left( \mathsf{Ex} z_1 \land \mathsf{E} z_1 z_2 \land \mathsf{E} z_2 z_3 \land \mathsf{E} z_3 y \right)$$

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Equivalent  $\mathcal{L}^3$  formula:

$$\varphi'_{\mathsf{dist-4}}(x,y) = \exists z \left( \mathsf{Exz} \land \exists x \left( \mathsf{Ezx} \land \exists z \left( \mathsf{Exz} \land \mathsf{Ezy} \right) \right) \right)$$

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Equivalent  $\mathcal{L}^3$  formula:

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Vertex has degree  $\geq 7$ :  $\varphi_{deg-7}(x) = \exists y_1 \cdots \exists y_7 \ \bigwedge_{i \neq j} y_i \neq y_j \bigwedge_i Exy_i$ 

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$$\varphi'_{\mathsf{deg-7}}(x) = \exists^{\geq 7} y \, \mathsf{Exy}$$

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$$\mathsf{D}^{k}(\mathcal{A},\mathcal{B}) \leq n^{k-1}$$

$$\begin{aligned} \mathbf{D}^{n}(\mathcal{A},\mathcal{B}) &\leq n \\ \exists x_{1} \cdots \exists x_{n} \left( \bigwedge_{i \neq j} x_{i} \neq x_{j} \land \bigwedge_{\substack{R \in \sigma, \\ (v_{i_{1}}, \dots, v_{i_{r}}) \in R^{\mathcal{A}}} Rx_{i_{1}} \cdots x_{i_{r}} \land \bigwedge_{\substack{R \in \sigma, \\ (v_{i_{1}}, \dots, v_{i_{r}}) \notin R^{\mathcal{A}}} \neg Rx_{i_{1}} \cdots x_{i_{r}} \right) \\ \mathbf{D}^{k}(\mathcal{A},\mathcal{B}) &\leq n^{k-1} \quad \mathbf{D}^{3}(\mathcal{A},\mathcal{B}) \leq \mathbf{O}(n^{2}/\log n) \text{ [Kiefer, Schweitzer 2016]} \end{aligned}$$

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- ▶  $k ext{ const.: } \mathsf{D}^k(\mathcal{A},\mathcal{B}) \geq \Omegaig(nig)$  [Grohe 1996] [Fürer 2001] [Krebs, Verbitsky 2015]

**Definition**  $D^{k}(\mathcal{A}, \mathcal{B})$  is the minimal quantifier depth of a  $\mathcal{C}^{k}$  sentence that distinguishes two *n*-element structures  $\mathcal{A}$  and  $\mathcal{B}$  (with  $\mathcal{A} \not\equiv_{\mathcal{C}^{k}} \mathcal{B}$ ).

- $\mathsf{D}^{n}(\mathcal{A},\mathcal{B}) \leq n$   $\exists x_{1} \cdots \exists x_{n} \left( \bigwedge_{i \neq j} x_{i} \neq x_{j} \land \bigwedge_{\substack{R \in \sigma, \\ (v_{i_{1}}, \dots, v_{i_{r}}) \in R^{\mathcal{A}}}} Rx_{i_{1}} \cdots x_{i_{r}} \land \bigwedge_{\substack{R \in \sigma, \\ (v_{i_{1}}, \dots, v_{i_{r}}) \notin R^{\mathcal{A}}}} \neg Rx_{i_{1}} \cdots x_{i_{r}} \right)$
- ►  $\mathsf{D}^k(\mathcal{A},\mathcal{B}) \leq n^{k-1}$   $\mathsf{D}^3(\mathcal{A},\mathcal{B}) \leq \mathrm{O}\big(n^2/\log n\big)$  [Kiefer, Schweitzer 2016]
- ▶  $k ext{ const.: } \mathsf{D}^k(\mathcal{A},\mathcal{B}) \geq \Omega(n)$  [Grohe 1996] [Fürer 2001] [Krebs, Verbitsky 2015]

#### Theorem [B., Nordström 2016a]

For every  $k \leq n^{0.01}$  there are *n*-element relational structures  $\mathcal{A}$ ,  $\mathcal{B}$  of arity k - 1 such that  $D^k(\mathcal{A}, \mathcal{B}) \geq n^{\Omega(k/\log k)}$ .

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#### Theorem [Cai, Fürer, Immerman 1992]

 $D^k(\mathcal{A}, \mathcal{B})$  agrees with the number of refinement steps (k-1)-dimensional Weisfeiler-Leman needs to distinguish  $\mathcal{A}$  and  $\mathcal{B}$ .

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#### An application for non-constant $\boldsymbol{k}$

- Babai's quasipolynomial graph isomorphism test uses
   k = log<sup>c</sup> n on (k 1)-ary relational structures. [Babai 2016]
- Our result implies an  $\Omega(n^{\log^{c-1} n})$  lower bound in this setting.

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u<sub>2</sub> u<sub>1</sub> F

The link between both areas is made via XOR formulas as a source of hard instances.

## XOR formulas

An *s*-XOR formula *F* over Boolean variables  $x_1, \ldots, x_n$  is a set of parity constraints  $x_{i_1} \oplus \cdots \oplus x_{i_r} = a$ ,  $r \leq s$ ,  $a \in \{0, 1\}$ .

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Let  $\mathcal{A}(F)$  and  $\mathcal{B}(F)$  relational structures with two vertices  $x_i^0$ ,  $x_i^1$  for every  $x_i \in Vars(F)$  and relations

$$\begin{aligned} X_{i}^{\mathcal{A}} &= X_{i}^{\mathcal{B}} = \{x_{i}^{0}, x_{i}^{1}\} \\ R_{r}^{\mathcal{A}} &= \{(x_{i_{1}}^{a_{1}}, \dots, x_{i_{r}}^{a_{r}}) \mid (x_{i_{1}} \oplus \dots \oplus x_{i_{r}} = a) \in F, \ \bigoplus_{i} a_{i} = 0\} \\ R_{r}^{\mathcal{B}} &= \{(x_{i_{1}}^{a_{1}}, \dots, x_{i_{r}}^{a_{r}}) \mid (x_{i_{1}} \oplus \dots \oplus x_{i_{r}} = a) \in F, \ \bigoplus_{i} a_{i} = a\} \end{aligned}$$

Isomorphism  $I : \mathcal{A}(F) \to \mathcal{B}(F)$  corresponds to satisfying assignment  $\alpha$  for F via

$$\begin{aligned} \alpha(x_i) &= 0 \iff I(x_i^0) = x_i^0 \Leftrightarrow I(x_i^1) = x_i^1\\ \alpha(x_i) &= 1 \iff I(x_i^0) = x_i^1 \Leftrightarrow I(x_i^1) = x_i^0 \end{aligned}$$



# A pebble game on XOR formulas

The k-pebble game on F is played by two players.

- Positions are partial assignments  $\alpha$ ,  $|\alpha| \leq k$ .
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In each round starting from  $\alpha_i$ :

- ▶ Player 1 chooses  $\alpha \subseteq \alpha_i$ ,  $|\alpha| < k$ ,
- Player 1 asks for the value of a variable x,
- Player 2 answers with  $a \in \{0, 1\}$ ,

$$\triangleright \ \alpha_{i+1} = \alpha \cup \{ \mathbf{x} \mapsto \mathbf{a} \}.$$

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Player 1 wins the game, if  $\alpha_i$  falsifies an XOR-constraint.

#### Equivalent characterizations of the pebble game

Let *F* be an *s*-XOR formula and R > 0, k > s be integers. Then the following statements are equivalent:

(a) Player 1 wins the R-round k-pebble game on F.

(b) There is a k-variable sentence  $\varphi \in C^k$  of quantifier rank R such that  $\mathcal{A}(F) \models \varphi$  and  $\mathcal{B}(F) \not\models \varphi$ .

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(c) The s-CNF-formula cnf(F) has a resolution refutation of width k-1 and depth R.

# Outline of the proof



[Immerman 1981]:

There are  $\mathcal{A}$ ,  $\mathcal{B}$  such that  $D^k(\mathcal{A}, \mathcal{B}) = \Omega(2^{\sqrt{\log n}})$  for all  $k \geq 3$ .

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#### Part I (pyramid construction):

For every k there are n-variable 3-XOR formulas such that Player 1 needs  $n^{\Omega(\frac{1}{\log k})}$  rounds to win the  $\ell$ -pebble game for  $3 \le \ell \le k$ .

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#### Part II (hardness condensation):

Reduce the number of variables without destroying the lower bound. Transform *n*-variable 3-XOR into *m*-variable *k*-XOR, for  $m \approx n^{\frac{1}{k}}$ . Lower bound remains  $n^{\Omega(\frac{1}{\log k})} = m^{\Omega(\frac{k}{\log k})}$ .

# PART I: An $n^{\Omega(\frac{1}{\log k})}$ lower bound



#### XORs from DAGs

Let  $\mathcal{G}$  be an acyclic directed graph with a unique sink z. The XOR-formula xor( $\mathcal{G}$ ) over the variables  $v \in V(\mathcal{G})$  contains the following constraints:

(i) 
$$v \oplus \bigoplus_{w \in N^-(v)} w = 0$$

(ii) 
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 for every source  $s$ ,



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• Player 1 wins the *k*-pebble game,

$$3 \le k \le 2^{d-1}$$
, in  $\Theta(h)$  rounds

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#### PART II: Hardness condensation

Let F be an XOR-formula over variables U and  $\mathcal{G} = (U \cup V, E)$  a bipartite graph.

The formula F[G] is defined over variables V with constraints

$$\left(\bigoplus_{v\in N(u_1)} v\right)\oplus\cdots\oplus\left(\bigoplus_{v\in N(u_\ell)} v\right)=\mathsf{a}$$

for all constraints  $u_1 \oplus \cdots \oplus u_\ell = a$  from F.



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 $u_2 \oplus u_5 = 0 \ \longrightarrow \ v_2 \oplus v_3 \oplus v_4 \oplus v_4 \oplus v_6 = 0$ 

▶ We use boundary expander G with left-degree  $\langle k/3, |U| = n$ , and  $|V| \approx n^{\frac{1}{k}}$ .



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#### Remark

This method was introduced in [Razborov 2016a] to show that treelike resolution refutations of bounded width k require doubly exponential length  $2^{n^{\Omega(k)}}$ .



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Later applied to linear programming hierarchies [Razborov 2016b]



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This method was introduced in [Razborov 2016a] to show that treelike resolution refutations of bounded width k require doubly exponential length  $2^{n^{\Omega(k)}}$ . Later applied to linear programming hierarchies [Razborov 2016b],

space/width trade-offs in resolution [B., Nordström 2016b]



 $u_2 \oplus u_5 = 0 \implies v_2 \oplus v_3 \oplus v_4 \oplus v_4 \oplus v_6 = 0$ 

- ▶ We use boundary expander G with left-degree  $\langle k/3, |U| = n$ , and  $|V| \approx n^{\frac{1}{k}}$ .
- Player 1 wins the k-pebble game on F[G].
- If Player 2 survives the *R*-round *k*-pebble game on *F*, then she survives the (≈ *R*)-round *k*-pebble game on *F*[*G*].

#### Remark

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# • $n^{\Omega(\frac{k}{\log k})}$ lower bound on the quantifier depth of $\mathcal{L}^k$ and $\mathcal{C}^k$

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#### **Open Question**

Our examples are k-ary relational structures. Are there similar lower bounds for graphs?

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# Thank you for your attention!