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

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Joint work with Christoph Berkholz

k-Variable Fragments of First-Order Logic

Two vertices are connected by a path of length 4:

$$\varphi_{\textsf{dist-4}}(x, y) = \exists z_1 \exists z_2 \exists z_3 \left(Exz_1 \wedge Ez_1z_2 \wedge Ez_2z_3 \wedge Ez_3y \right)$$

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Vertex has degree ≥ 7:

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Equivalent $\mathcal{C}^2$ formula:

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

Finite Relational Structures

- Structure $\mathcal{A}$
- Domain $V(\mathcal{A}) = \{u_1, u_2, \ldots, u_n\}$
- Relations R_ℓ of arity r_ℓ
- Interpretation $R_\ell^{\mathcal{A}} = \left\{(u_{j_1}, \ldots, u_{j_\ell}) \middle| \text{relation } R_\ell u_{j_1}, \ldots, u_{j_\ell} \text{ holds}\right\}$
- $\mathcal{A} \models \varphi$ if sentence φ true in structure $\mathcal{A}$
- Running example: graphs
  - Elements: vertices
  - Relations: edges

Why Bounded Variable Fragments of First Order Logic?

Numerous applications in finite model theory and related areas [Gro98]

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Model checking problem

Given finite relational structure $\mathcal{A}$ and sentence φ, does $\mathcal{A}$ satisfy φ?

Decidable in polynomial time [Imm82, Var95]

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Equivalence problem

Given two finite relational structures $\mathcal{A}$ and $\mathcal{B}$, do they satisfy the same $\mathcal{L}^k$ or $\mathcal{C}^k$ sentences?

Decidable in time $n^{O(k)}$ [IL90] (i.e., polynomial for constant k)

Connections to Weisfeiler–Leman

- Equivalence problem for $\mathcal{C}^{k+1}$ closely related to k-dimensional Weisfeiler–Leman algorithm (k-WL) for testing non-isomorphism of
  - graphs
  - more general relational structures

- $\mathcal{A}$ and $\mathcal{B}$ distinguished by k-dimensional Weisfeiler–Leman $\Leftrightarrow$ $\exists\ \mathcal{C}^{k+1}$ sentence differentiating between $\mathcal{A}$ and $\mathcal{B}$ [CFI92]

- Quantifier depth of distinguishing $\mathcal{C}^{k+1}$ sentence $=$
  $=$ #iterations k-WL needs to tell $\mathcal{A}$ and $\mathcal{B}$ apart

The Weisfeiler–Leman Algorithm

- Introduced by Babai in 1979 and Immerman and Lander [IL90]
- Iteratively refines colouring of element set
- Ends with canonical stable colouring classifying similar elements
- For parameter k, runs in time $n^{O(k)}$
- Reduces search space (isomorphisms preserve similar elements)
- In particular: different stable colourings $\Rightarrow$ non-isomorphic structures

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Babai's general graph isomorphism algorithm [Bab16]

Applies k-dimensional Weisfeiler–Leman for polylogarithmic k
$\Rightarrow$ quasipolynomial running time

Quantifier Depth of $\mathcal{C}^k$

Definition

$\mathrm{D}^k(\mathcal{A}, \mathcal{B})$: minimal quantifier depth of $\mathcal{C}^k$ sentence distinguishing two n-element structures $\mathcal{A}$ and $\mathcal{B}$ (with $\mathcal{A} \not\equiv_{\mathcal{C}^k} \mathcal{B}$)

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- $\mathrm{D}^n(\mathcal{A},\mathcal{B}) \leq n$

$$\exists x_1 \cdots \exists x_n \left(\bigwedge_{i \neq j} x_i \neq x_j \ \wedge \bigwedge_{\substack{R \in \sigma, \\ (v_{i_1},\ldots,v_{i_r}) \in R^{\mathcal{A}}}} R x_{i_1} \cdots x_{i_r} \ \wedge \bigwedge_{\substack{R \in \sigma, \\ (v_{i_1},\ldots,v_{i_r}) \notin R^{\mathcal{A}}}} \neg R x_{i_1} \cdots x_{i_r} \right)$$

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- $\mathrm{D}^k(\mathcal{A},\mathcal{B}) \leq n^{k-1}$ $\qquad \mathrm{D}^3(\mathcal{A},\mathcal{B}) \leq \mathcal{O}\big(n^2/\log n\big)$ [KS16]
- k constant: $\mathrm{D}^k(\mathcal{A},\mathcal{B}) \geq \Omega\big(n\big)$ [Gro99, Für01, KV15]

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Theorem [BN16a]

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

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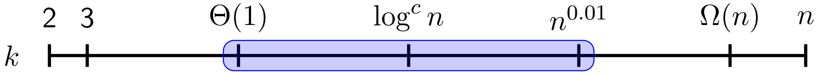
$\mathrm{D}^k(\mathcal{A},\mathcal{B}) = $ #refinement steps $(k-1)$-dimensional Weisfeiler–Leman needs to distinguish $\mathcal{A}$ and $\mathcal{B}$

$\mathcal{C}^k$ and Weisfeiler–Leman



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Application for non-constant k

- Babai's quasipolynomial graph isomorphism test uses $k = \log^c n$ on $(k-1)$-ary relational structures [Bab16]
- Our result implies $\Omega\left(n^{\log^{c-1} n}\right)$ lower bound in this setting

Overview of proof

Essence of Proof

In one sentence, a novel combination of methods from

Descriptive complexity **Proof complexity**

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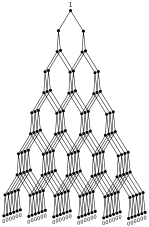

pyramid construction
Immerman [Imm81]

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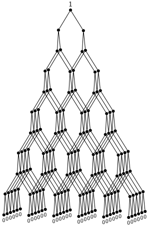

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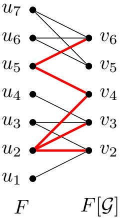

hardness condensation
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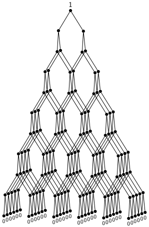

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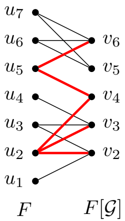

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Connection made via XOR formulas as source of hard instances

Spoiler-Duplicator Game for $\mathcal{L}^k$

- Spoiler and Duplicator play on structures $\mathcal{A}$ and $\mathcal{B}$

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Characterization of $\mathcal{L}^k$ [Bar77, Imm82]

Spoiler wins this game for size-k mappings in R rounds $\Leftrightarrow$
$\exists$ sentence $\varphi \in \mathcal{L}^k$ of quantifier depth R such that $\mathcal{A} \models \varphi$ and $\mathcal{B} \not\models \varphi$

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    1. Spoiler chooses $p' \subseteq p$ with $|p'| < k$
    2. Duplicator selects global bijection $f : V(\mathcal{A}) \to V(\mathcal{B})$
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XOR Formulas

s-XOR formula F over Boolean variables $x_1, \ldots, x_n$:
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

- 2 vertices x_i^0, x_i^1 for every $x_i \in \mathrm{Vars}(F)$
- relations

$$X_i^{\mathcal{A}} = X_i^{\mathcal{B}} = \{x_i^0, x_i^1\}$$
$$R_r^{\mathcal{A}} = \left\{(x_{i_1}^{a_1}, \ldots, x_{i_r}^{a_r}) \middle| (x_{i_1} \oplus \cdots \oplus x_{i_r} = a) \in F,\ \bigoplus_i a_i = 0\right\}$$
$$R_r^{\mathcal{B}} = \left\{(x_{i_1}^{a_1}, \ldots, x_{i_r}^{a_r}) \middle| (x_{i_1} \oplus \cdots \oplus x_{i_r} = a) \in F,\ \bigoplus_i a_i = a\right\}$$

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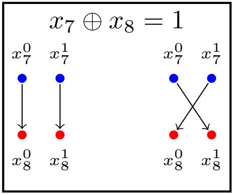
Isomorphism $I : \mathcal{A}(F) \to \mathcal{B}(F)$ corresponds to satisfying assignment α for F via

$$\alpha(x_i) = 0 \iff I(x_i^0) = x_i^0 \Leftrightarrow I(x_i^1) = x_i^1$$
$$\alpha(x_i) = 1 \iff I(x_i^0) = x_i^1 \Leftrightarrow I(x_i^1) = x_i^0$$



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In round i starting from α_{i-1}:

- Player 1 chooses $\alpha \subseteq \alpha_{i-1}$, $|\alpha| < k$
- Player 1 asks for value of variable x
- Player 2 answers with $a \in \{0, 1\}$
- $\alpha_i = \alpha \cup \{x \mapsto a\}$

A Pebble Game on XOR Formulas

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

- Positions: partial assignments α, $|\alpha| \leq k$
- Starting position $\alpha_0 = \emptyset$

In round i starting from α_{i-1}:

- Player 1 chooses $\alpha \subseteq \alpha_{i-1}$, $|\alpha| < k$
- Player 1 asks for value of variable x
- Player 2 answers with $a \in \{0, 1\}$
- $\alpha_i = \alpha \cup \{x \mapsto a\}$

Player 1 wins game in R rounds if α_R falsifies some XOR-constraint

Equivalent Characterizations of the Pebble Game

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- $R, k \in \mathbb{N}^+,\ k > s$

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(d) The s-CNF-formula $\mathrm{cnf}(F)$ has a resolution refutation of
  - depth R
  - width $k - 1$ [AD08]

Outline of Proof

[Imm81]

There are $\mathcal{A}$, $\mathcal{B}$ such that $\mathrm{D}^k(\mathcal{A}, \mathcal{B}) = \Omega\left(2^{\sqrt{\log n}}\right)$ 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

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Part II (hardness condensation):

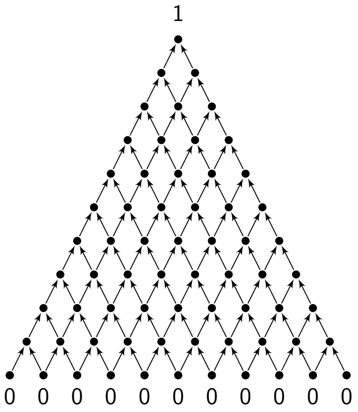
Reduce the number of variables without destroying the lower bound

Transform n-variable 3-XOR into m-variable k-XOR for $m \approx n^{1/k}$

Lower bound remains $n^{\Omega(1/\log k)} = m^{\Omega(k/\log k)}$

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

A 2-Dimensional Pyramid



XORs from DAGs

Let $\mathcal{G}$ directed acyclic graph with unique sink z

XOR-formula $\mathrm{xor}(\mathcal{G})$ over variables $v \in V(\mathcal{G})$ contains constraints:

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

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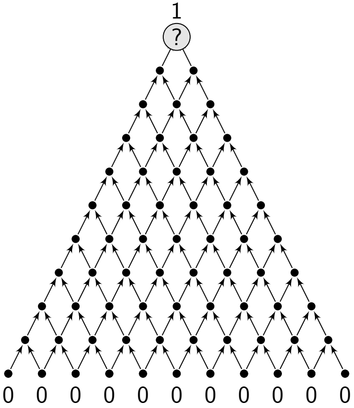

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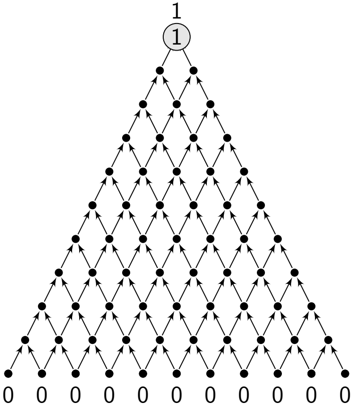

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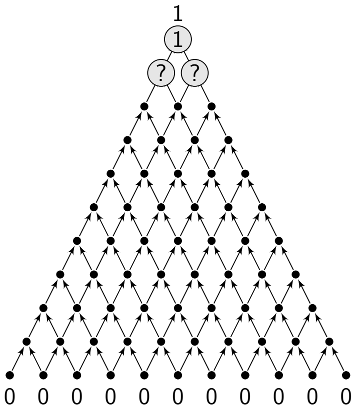

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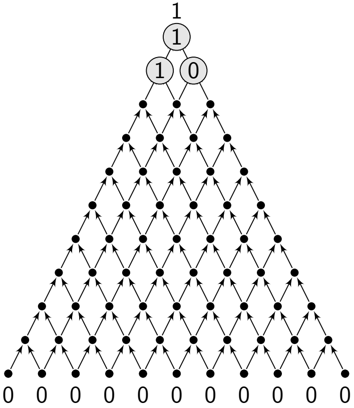

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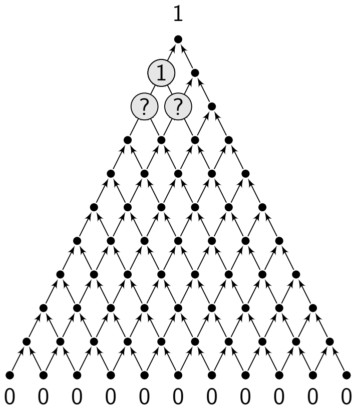

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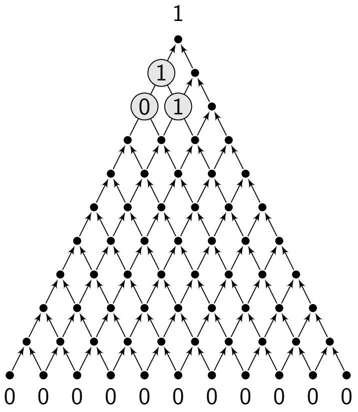

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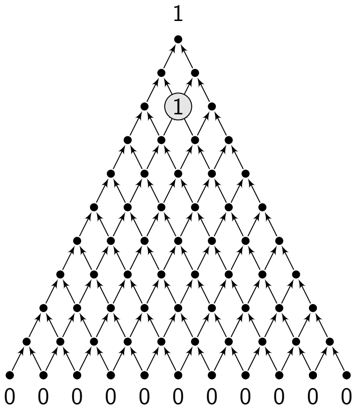

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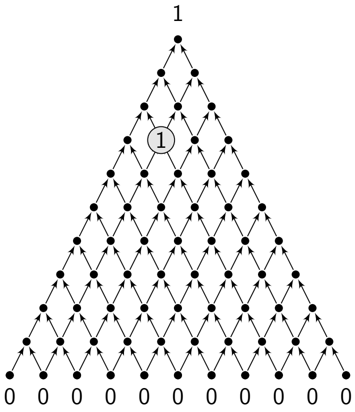

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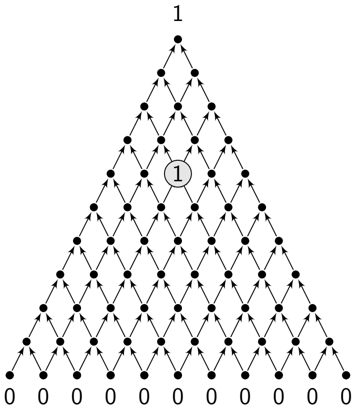

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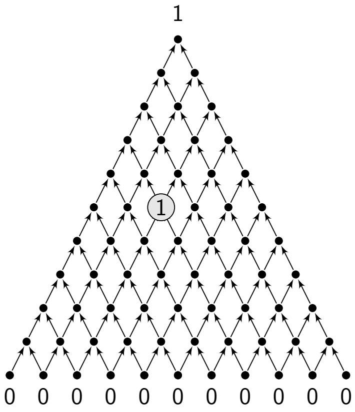

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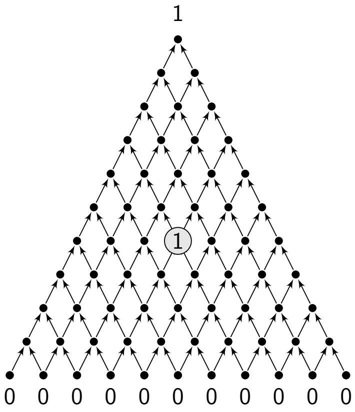

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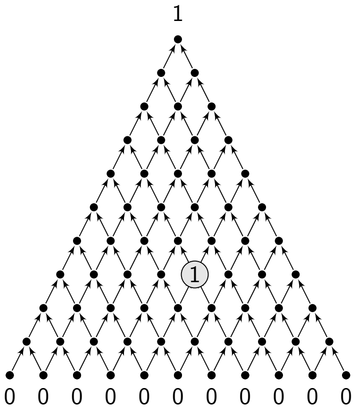

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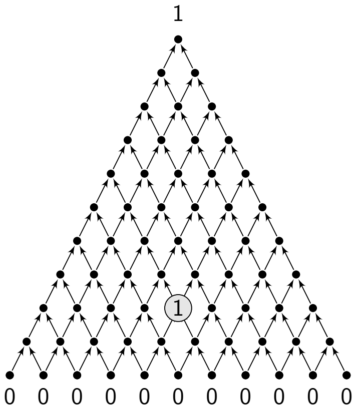

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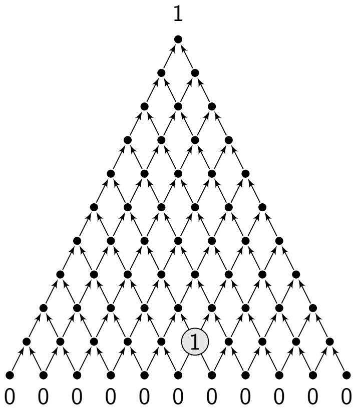

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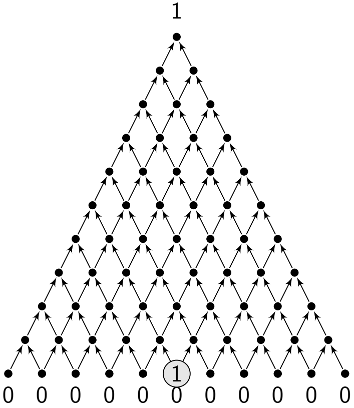

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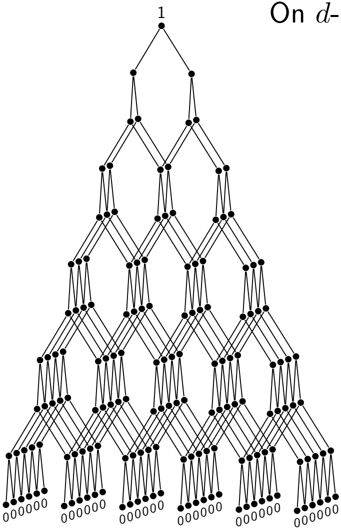

On d-dimensional pyramid of height h

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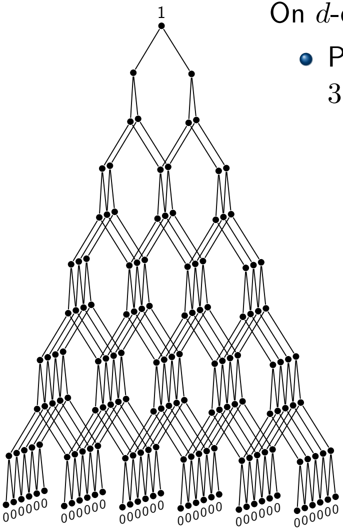

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- Player 1 wins the k-pebble game, $3 \leq k \leq 2^{d-1}$, in $\Theta(h)$ rounds

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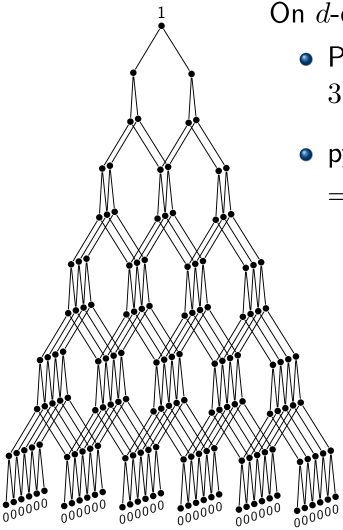


On d-dimensional pyramid of height h

- Player 1 wins the k-pebble game, $3 \leq k \leq 2^{d-1}$, in $\Theta(h)$ rounds
- pyramid has $n \approx h^d$ vertices $\Rightarrow n^{\Theta(\frac{1}{\log k})}$ rounds in k-pebble game

PART II: Hardness condensation

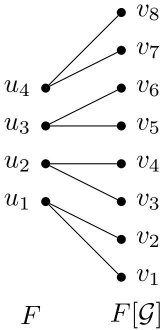
XOR Substitution with Recycling (1/2)

Suppose

- F XOR formula over variables U
- $\mathcal{G} = (U \,\dot\cup\, V, E)$ bipartite graph

Substituted formula $F[\mathcal{G}]$ over variables V:

- replace every $u \in U$ by $\bigoplus_{v \in N(u)} v$



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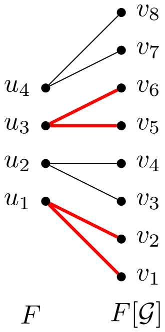

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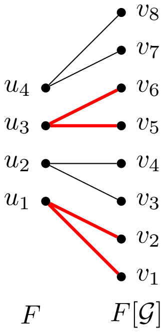

$$u_1 \oplus u_3 = 1 \quad \longrightarrow \quad (v_1 \oplus v_2) \oplus (v_5 \oplus v_6) = 1$$

Player 2 survives R-round k-pebble game on F
$\Rightarrow$ survives $2R$-round $2k$-pebble game on $F[\mathcal{G}]$

But #variables in instance goes up

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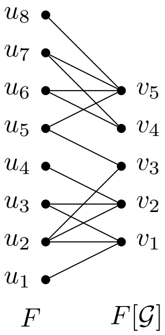

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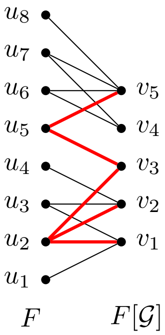
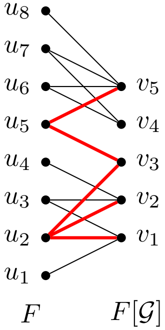


$$u_2 \oplus u_5 = 0 \quad \longrightarrow \quad (v_1 \oplus v_2 \oplus v_3) \oplus (v_3 \oplus v_5) = 0$$

Now #variables in instance goes down

Possible to maintain hardness?

XOR Substitution with Recycling (2/2)



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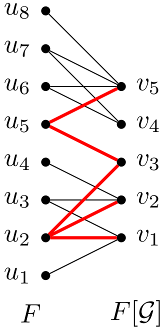

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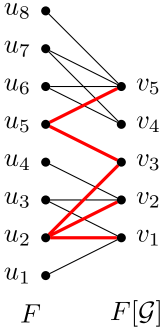

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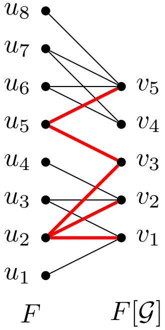

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  - Player 1 wins with k pebbles on $F[\mathcal{G}]$

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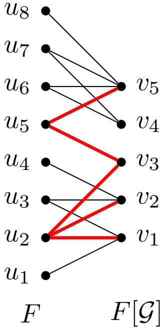

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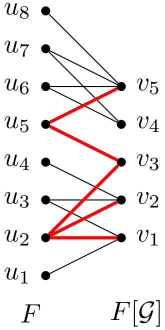

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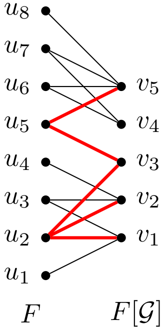
  - #rounds needed for $F[\mathcal{G}] \gtrapprox$
    #rounds needed for $F = \Omega\left(|U|^{1/\log k}\right) = \Omega\left(|V|^{k/\log k}\right)$

XOR Substitution with Recycling (2/2)



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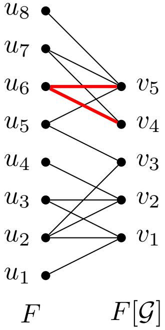

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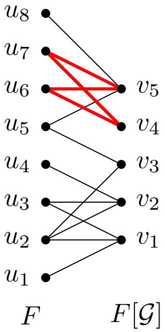

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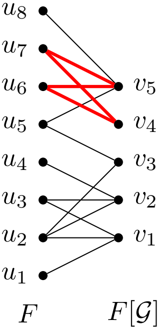

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Solution: Use expander graphs!

- Apply to XOR formulas over Immerman's pyramids [Imm81]
  - Player 1 wins with 3 pebbles
  - but needs $n^{\Omega(1/\log k)}$ rounds
- $\mathcal{G}$ expander with left-degree $\leq k/3$, $|U| = n$, and $|V| = n^{\mathcal{O}(1/k)}$
  - Player 1 wins with k pebbles on $F[\mathcal{G}]$ ✓
  - #rounds needed for $F[\mathcal{G}] \gtrapprox$
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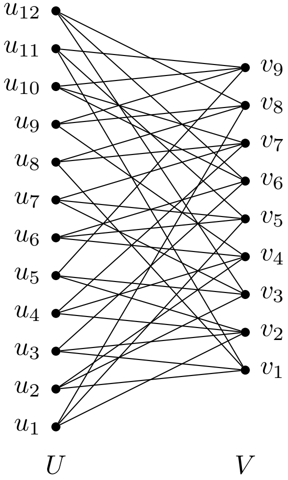
Bipartite Boundary Expander



$\mathcal{G} = (U \,\dot\cup\, V, E)$ is (d, r, c)-boundary expander if

- left-degree $\leq d$
- for every $U' \subseteq U$, $|U'| \leq r$ it holds that $|\partial(U')| \geq c|U'|$

$\partial(U') = \{v \in N(U') : |N(v) \cap U'| = 1\}$

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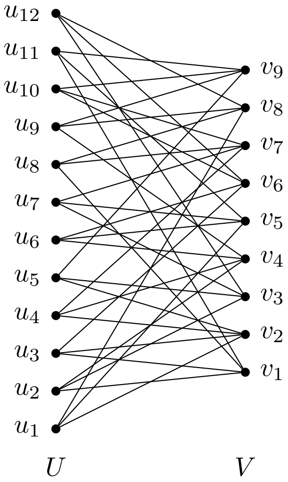

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Example

- left-degree $d = 3$
- expanding set size $r = 3$
- boundary expansion factor $c = 1$

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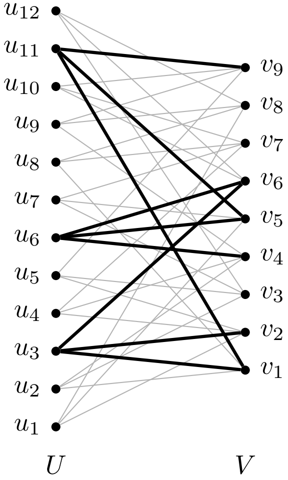

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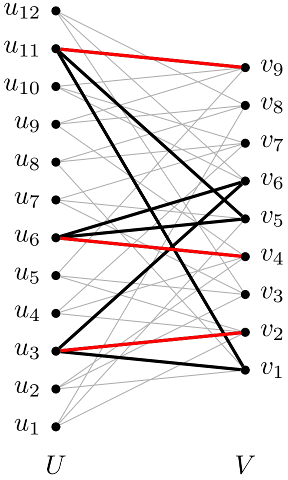

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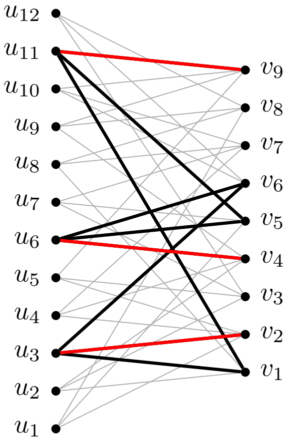

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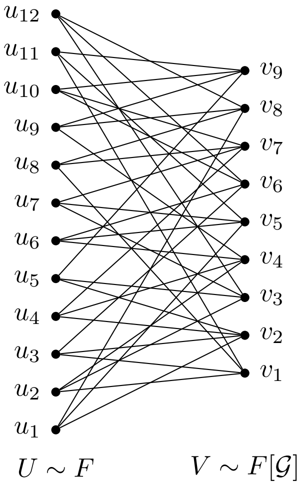
Lemma ([Raz16a])

For $\varepsilon > 0$ and n, d with $|U| = n$, $|V| = n^{\mathcal{O}(1/d)}$, $d \leq |V|^{\frac{1}{2}-\varepsilon}$, there are $(d, r, 2)$-boundary expanders $\mathcal{G}$ with $r = d \log n$

Sketch of Proof Sketch



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$\forall$ position β on $F[\mathcal{G}]$, maintain position α on F

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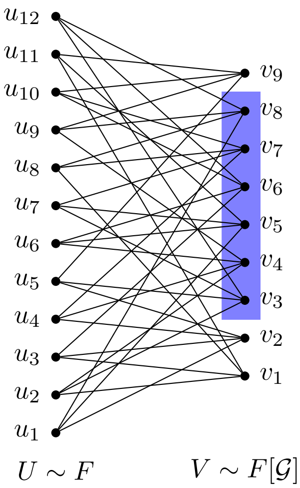

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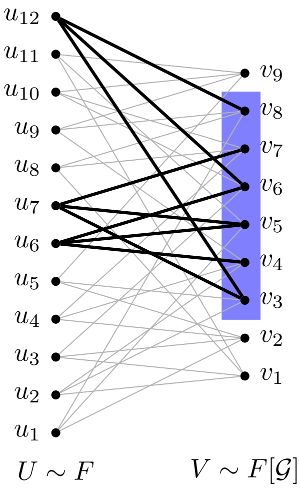

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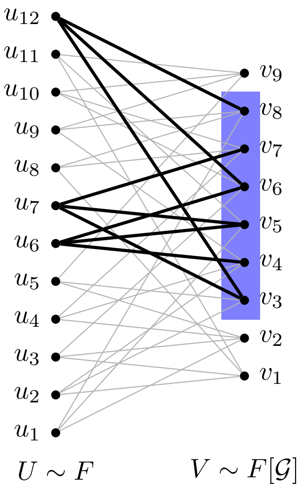

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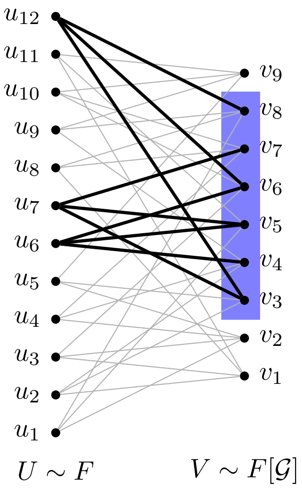

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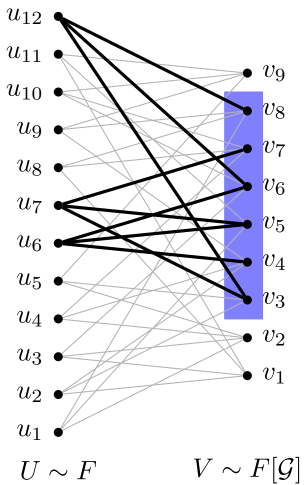

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Locally looks almost like XORification without recycling, so previous approach might work...
And give bound in terms of $|U| \gg |V|$

Hardness Condensation

Actual details more involved, but work out as follows:

Main Technical Lemma

If

- Player 2 survives R of k-game on F
- $\mathcal{G}$ is $(d, 2k, 2)$-boundary expander

then

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More about hardness condensation

- Method introduced in [Raz16a] to show that treelike resolution in bounded width k can require doubly exponential length $2^{n^{\Omega(k)}}$
- Also applied to linear programming hierarchies [Raz16c]
- Space/width trade-offs in resolution [BN16b]
- Variable space/length trade-offs [Raz16b]

Concluding Remarks

Summary

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Thank you for your attention!

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