Homomorphism Counts, Logics & Query Algorithms

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ILLC, University of Amsterdam

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Based on joint work with Victor Dalmau, Phokion Kolaitis, and Wei-Lin Wu

Many slides borrowed from a recent presentation by Phokion Kolaitis

What Mathematicians Do

Mathematicians study not objects, but relations between objects; the replacement of these objects by others is therefore indifferent to them, provided the relations do not change. The matter is for them unimportant, the form alone interests them.

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Science and Hypothesis - 1902

Henri Poincaré

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Definition:
Let $G = (V(G), E(G))$ and $H = (V(H), E(H))$ be two graphs.
An isomorphism from G to H is a function $h : V(G) \to V(H)$ such that

1. h is 1-1 and onto;
2. for all $u, v \in V(G)$,
$$(u, v) \in E(G) \text{ if and only if } (h(u), h(v)) \in E(H).$$

- Analogously for isomorphism between relational structures.

Algorithmic Aspects of Graph Isomorphism

The Graph Isomorphism Problem:
Given two finite graphs G and H, are they isomorphic?

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Open Problem:
What is the exact computational complexity of the Graph Isomorphism Problem?

Algorithmic Aspects of Graph Isomorphism

The Graph Isomorphism Problem

- is in NP;
- is unlikely to be NP-complete (else, PH collapses);
- is not known to be solvable in polynomial time;
- is solvable in quasi-polynomial time $2^{O((\log n)^c)}$, for some fixed $c > 0$ (Babai - 2017);
- is solvable in polynomial time on restricted classes of graphs:
  - planar graphs (Hopcroft and Wong - 1974);
  - graphs of bounded degree (Lucs - 1982);
  - ...

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The Graph Isomorphism Disease

Brief digression: Graph Classification

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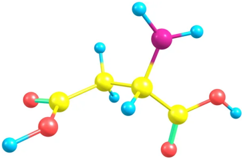

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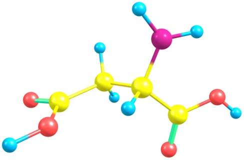

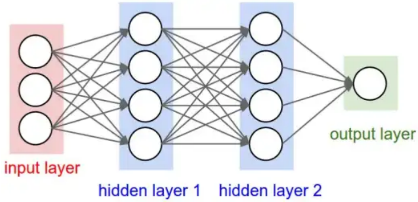

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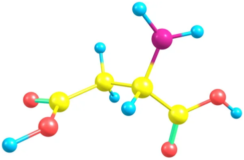

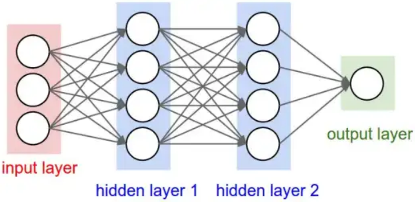

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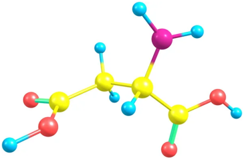

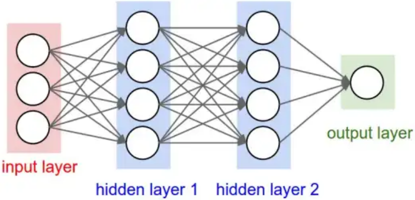

We need to encode a graph G as a "embedding vector" $v_G \in \mathbb{R}^k$.

We would like isomorphic graphs to be indistinguishable for the ML model.

Beyond Isomorphism

- In mathematics, we also study objects up to some other equivalence relation.

Examples:

1. Homeomorphism in Topology
2. Diffeomorphism in Differential Geometry
3. Logical Equivalence in First-Order Logic
4. ...

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- Here, we will focus on equivalence relations that arise from homomorphisms.

Homomorphism

Definition:

Let $G = (V(G), H(E))$ and $H = (V(H), E(H))$ be two graphs.
A homomorphism from G to H is a function $h : V(G) \to V(H)$ such that for all $u, v \in V(G)$,

$$\text{if } (u, v) \in E(G), \text{ then } (h(u), h(v)) \in E(H).$$

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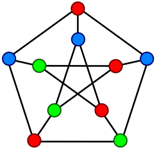
$$\text{if } (u, v) \in E(G), \text{ then } (h(u), h(v)) \in E(H).$$

Example: Let G be a graph and let K_3 be the triangle graph.

- There is a homomorphism from K_3 to G if and only if G contains a triangle.
- There is a homomorphism from G to K_3 if and only if G is 3-colorable.



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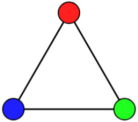
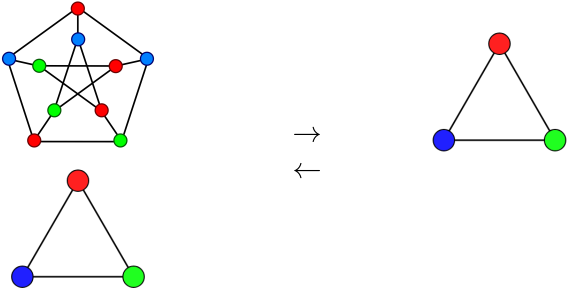
$\not\leftarrow$





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Two graphs G and H are homomorphically equivalent if there is a homomorphism from G and H, and a homomorphism from H and G.

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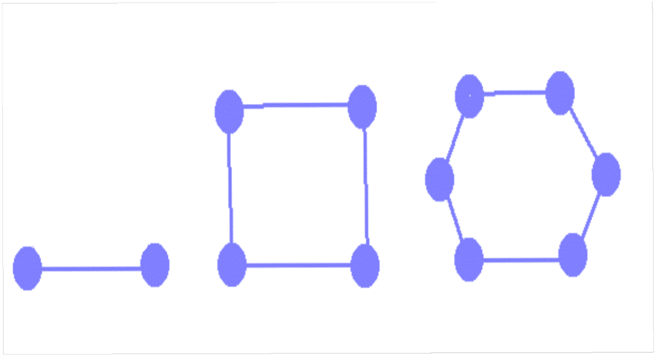
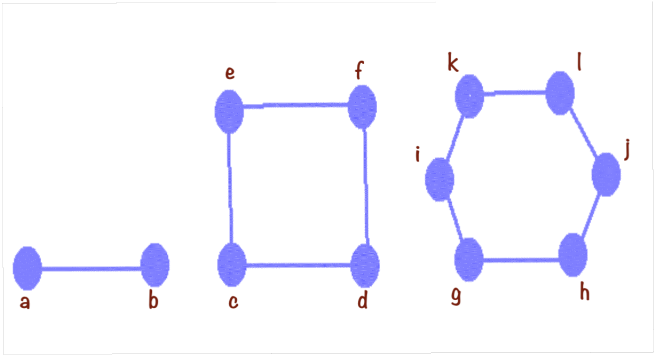
Example:

- If G and H are 2-colorable graphs with at least one edge each, then G and H are homomorphically equivalent.
- In particular, C_4 and C_6 are homomorphically equivalent (where C_n is the cycle with n nodes).

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Complexity of Homomorphism Equivalence

Fact:

- Homomorphism Equivalence is an equivalence relation that is coarser than isomomorphism.

- Homomorphism Equivalence is NP-complete.

  Proof: Reduction from 3-Colorability:
  G is 3-colorable if and only if $G \oplus K_3$ is homomorphically equivalent to K_3.

Homomorphism Counts

Notation:

Let G and H be two graphs.

$\hom(G, H)$ = the number of homomorphisms from G to H.

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Example:

Let G be a graph and let K_3 be the triangle graph.

- $\hom(K_3, G)$ = the number of triangles in G.
- $\hom(G, K_3)$ = the number of 3-colorings of G (times 6).

Two Interpretations of Homomorphism Counts

- Each H, gives rise to the constraint satisfaction problem

  $\mathrm{CSP}(H) = \{G : \text{there is a homomorphism from } G \text{ to } H\}$

  Thus,
  $\hom(G, H) = \#$ solutions of $\mathrm{CSP}(H)$ on input G.

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- Each G, gives rise to a conjunctive query Q^G

  Example: $Q^{K_3} : \exists x, y, z(E(x, y) \wedge E(y, z) \wedge E(z, x))$

  Thus,
  $\hom(G, H) = \#$ satisfying assignments from Q^G to input H.
  (this is the bag semantics of SQL)

Visualization of Homomorphism Counts

$\mathscr{G} = \{G_1, G_2, \dots\}$ is the class of all graphs (up to isomorphism).

$\hom(\cdot,\cdot)$	G_1	G_2	$\cdots$
G_1	$\hom(G_1, G_1)$	$\hom(G_1, G_2)$	$\cdots$
G_2	$\hom(G_2, G_1)$	$\hom(G_2, G_2)$	$\cdots$
$\vdots$	$\vdots$	$\vdots$	$\ddots$

Left and Right Profiles

Definition: Let G be a graph.

- The left profile of G is the vector $\hom(\mathscr{G}, G) := (\hom(G_1, G), \hom(G_2, G), \dots)$.
- The right profile of G is the vector $\hom(G, \mathscr{G}) := (\hom(G, G_1), \hom(G, G_2), \dots)$.

$\hom(\cdot,\cdot)$	G_1	G_2	$\cdots$	G	$\cdots$
G_1	$\hom(G_1, G_1)$	$\hom(G_1, G_2)$	$\cdots$	$\hom(G_1, G)$	$\cdots$
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$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\ddots$
G	$\hom(G, G_1)$	$\hom(G, G_2)$	$\cdots$	$\hom(G, G)$	$\cdots$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\ddots$

Left/Right Profiles and Isomorphism

Lovász's Theorem (1967):

For all graphs G and H:

$$G \text{ and } H \text{ are isomorphic} \quad \text{iff} \quad \hom(\mathscr{G}, G) = \hom(\mathscr{G}, H).$$

- No two columns are equal.

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Chaudhuri-Vardi Theorem (1993):

For all graphs G and H:

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Graph Classification Again

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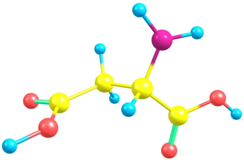

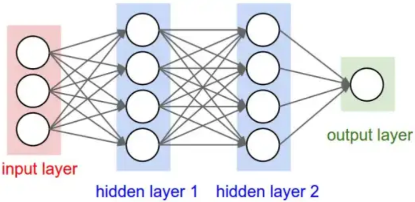

We need to encode a graph G as a embedding vector.

We would like isomorphic graphs to be indistinguishable for the ML model.

The left profile of G (i.e., $\mathrm{hom}(\mathscr{G}, G)$) provides an embedding vector which captures precisely the isomorphism type of G. The only problem is that it is infinite (and expensive to compute).

Restricted Profiles

Definition:

Let $\mathscr{F} = \{F_1, F_2, \ldots\}$ be a class of graphs and let G be a graph.

- The left profile of G restricted to $\mathscr{F}$ is the vector $\hom(\mathscr{F}, G) := (\hom(F_1, G), \hom(F_2, G), \ldots)$ (keep only the rows arising from graphs in $\mathscr{F}$).
- The right profile of G restricted to $\mathscr{F}$ is the vector $\hom(G, \mathscr{F}) := (\hom(G, F_1), \hom(G, F_2), \ldots)$ (keep only the columns arising from graphs in $\mathscr{F}$).

Equivalence Relations from Profiles

Each class $\mathscr{F}$ of graphs gives rise to two equivalence relations:

- $G \equiv^{L}_{\mathscr{F}} H$ if G and H have the same left profile restricted to $\mathscr{F}$.
- $G \equiv^{R}_{\mathscr{F}} H$ if G and H have the same right profile restricted to $\mathscr{F}$.

Note:
These equivalence relations are relaxations of isomorphism.

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Question:

- Which equivalence relations $\equiv$ on graphs are of the form $\equiv^{L}_{\mathscr{F}}$ or of the form $\equiv^{R}_{\mathscr{F}}$?

Counting Logics with Finitely Many Variables

Definition: Let k be a positive integer.

- FO^k: First-order logic FO with at most k distinct variables.
- C^k: FO^k + Counting Quantifiers $(\exists i\ y)$, $i \geq 2$

$(\exists i\ y)\varphi(y)$: there are are at least i nodes y such that $\varphi(y)$ holds.

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Theorem (Cai, Fürer, Immerman - 1992):
For every two graphs G and H, and for every $k \geq 2$, TFAE:

1. $G \equiv_{\mathrm{C}^k} H$ (i.e., G and H satisfy the same C^k-sentences).
2. G and H are indistinguishable by the $(k-1)$-dimensional Weisfeiler-Leman algorithm.

Restricted Left Profiles and Counting Logics

Theorem (Dvořák - 2010):

For every two graphs G and H, and for every $k \geq 2$, TFAE:

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2. $\hom(\mathscr{T}_k, G) = \hom(\mathscr{T}_k, H)$, where $\mathscr{T}_k$ is the class of all graphs of treewidth < k.

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Note: The treewidth of a graph is a positive integer that measures how far from being a tree the graph is.

- Every tree has treewidth 1
- Every cycle has treewidth 2
- The clique K_n with n nodes has treewidth $n - 1$

In particular, $G \equiv_{\mathrm{C}^2} H$ iff $\hom(\textit{trees}, G) = \hom(\textit{trees}, H)$.

Restricted Left Profiles and Co-Spectrality

Definition:
Two graphs G, H are co-spectral if their adjacency matrices have the same spectrum, i.e., the same multiset of eigenvalues.

Example: $C_4 \oplus K_1$ and the star S_5 have spectrum $\{-2, 0^3, 2\}$.

Restricted Left Profiles and Co-Spectrality

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Theorem (Dell-Grohe-Rattan 2018):
For every two graphs G and H, the following are equivalent:

1. G and H are co-spectral.
2. $\hom(\mathscr{C}, G) = \hom(\mathscr{C}, H)$, where $\mathscr{C}$ is the class of all cycles.

Restricted Left Profiles vs. Restricted Right Profiles

- Restricted left profiles can capture interesting relaxations of isomorphism, such as C^k-equivalence and co-spectrality.
- Atserias-Kolaitis-Wu (2021): what about restricted right profiles?

Restricted Left Profiles vs Restricted Right Profiles

$\mathscr{G}$: all graphs $\mathscr{T}_k$: all graphs of treewidth $< k$ ($k \geq 2$)
$\mathscr{C}$: all cycles $\mathscr{K}$: all cliques

$\equiv$	$\hom(\mathscr{F}, \cdot)$	$\hom(\cdot, \mathscr{F})$
isomorphism	$\mathscr{G}$	$\mathscr{G}$
C^k-equivalence ($k \geq 2$)	$\mathscr{T}_k$	none
co-spectrality	$\mathscr{C}$	none
chromatic equivalence	none	$\mathscr{K}$
FO^k-equivalence ($k \geq 1$)	none	none
QD^k-equivalence ($k \geq 1$)	none	none

Note:

- FO^k: first-order sentences with at most k variables.
- QD^k: first-order sentences of quantifier depth at most k.

Modal Equivalence Relations

Jesse Comer (MSc Thesis 2023):

- Performed a similar analysis for modal equivalence relations between pointed labeled transition systems M_a
- Considers both $\hom_{\mathbb{B}}(\cdot,\cdot)$ and $\hom_{\mathbb{N}}(\cdot,\cdot)$ — following Atserias-Kolaitis-Wu (2021)

$$\hom_{\mathbb{B}}(F,G) = \begin{cases} 1, & \text{if } F \to G \\ 0, & \text{if } F \not\to G. \end{cases}$$

Language	Invariance Relation	Characterizing Vector
$\mathrm{ML}^{+}_{\Diamond}$	Simulation Equivalence	$\hom_{\mathbb{B}}(\mathcal{T}, M_a)$
ML^{+}	Directed Simulation Equivalence	None for $\mathbb{B}$ or $\mathbb{N}$
BML	Bisimulation	None for $\mathbb{B}$ or $\mathbb{N}$
$\mathrm{ML}_{\#}$	Graded Bisimulation	$\hom_{\mathbb{N}}(\mathcal{T}, M_a)$
$\mathrm{ML}^{+,B}_{\Diamond}$	Back-and-Forth Simulation Equivalence	$\hom_{\mathbb{B}}(\mathcal{A}, M_a)$
$\mathrm{ML}^{+,G}_{\Diamond}$	Global Simulation Equivalence	$\hom_{\mathbb{B}}(\mathcal{F}, M_a)$
$\mathrm{ML}^{B}_{\#}$	Back-and-Forth Graded Bisimulation	$\hom_{\mathbb{N}}(\mathcal{A}, M_a)$
$\mathrm{ML}^{G}_{\#}$	Global Graded Bisimulation	$\hom_{\mathbb{N}}(\mathcal{F}, M_a)$

See also: Barceló et al (2020). The logical expressiveness of graph neural networks.

Homomorphism Counts and Query Algorithms

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Definition: A class $\mathcal{C}$ of structures admits a left query algorithm over $\mathbb{N}$, if for some $k \geq 1$, there are structures $F_1, F_2, \ldots, F_k$ and a set $X \subseteq \mathbb{N}^k$ such that for every structure G,

$$G \in \mathcal{C} \iff (\hom(F_1, G), \hom(F_2, G), \ldots, \hom(F_k, G)) \in X.$$

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Fact: The following are equivalent:

1. $\mathcal{C}$ admits a left query algorithm over $\mathbb{N}$.
2. There is a finite class $\mathcal{F} = \{F_1, \ldots, F_k\}$ such that for all structures G and H, if $\hom(\mathcal{F}, G) = \hom(\mathcal{F}, H)$, then
$$G \in \mathcal{C} \iff H \in \mathcal{C}.$$

Homomorphism Counts and Query Algorithms

Definition: A class $\mathcal{C}$ of structures admits a left query algorithm over $\mathbb{N}$, if for some $k \geq 1$, there are structures $F_1, F_2, \ldots, F_k$ and a set $X \subseteq \mathbb{N}^k$ such that for every structure G,

$$G \in \mathcal{C} \iff (\hom(F_1, G), \hom(F_2, G), \ldots, \hom(F_k, G)) \in X.$$

Theorem: (Chen, Flum, Liu, and Xun - 2022)

- Every class of graphs definable by a Boolean combination of universal FO-sentences admits a left query algorithm over $\mathbb{N}$.
- The class of all K_3-free graphs does not admit a right query algorithm over $\mathbb{N}$.

Homomorphism Counts and Query Algorithms

tC-Dalmau-Kolaitis-Wu (to appear in ICDT 2024):

- studied query algorithms over the Boolean semiring $\mathbb{B}$;
- compared query algorithms over $\mathbb{B}$ to those over $\mathbb{N}$.

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$$\hom_{\mathbb{B}}(F, G) = \begin{cases} 1, & \text{if } F \to G \\ 0, & \text{if } F \not\to G. \end{cases}$$

Definition: A class $\mathcal{C}$ of structures admits a left query algorithm over $\mathbb{B}$, if for some $k \geq 1$, there are structures $F_1, F_2, \ldots, F_k$ and a set $X \subseteq \{0, 1\}^k$ such that for every structure G,

$$G \in \mathcal{C} \iff (\hom_{\mathbb{B}}(F_1, G), \hom_{\mathbb{B}}(F_2, G), \ldots, \hom_{\mathbb{B}}(F_k, G)) \in X.$$

Left Query Algorithms over $\mathbb{B}$

Theorem (tCDKW - 2023) Let $\mathcal{C}$ be a class of structures. TFAE:

1. $\mathcal{C}$ admits a left query algorithm over $\mathbb{B}$.
2. $\mathcal{C}$ is definable by a Boolean combination of conjunctive queries.
3. $\mathcal{C}$ is FO-definable and closed under homomorphic equivalence.

Proof Hint: (3) $\Longrightarrow$ (1) use tools by Rossman to prove the Homomorphism Preservation Theorem in the finite.

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Corollary: If $\mathcal{C}$ is closed under homomorphism equivalence, then TFAE:

1. $\mathcal{C}$ admits a left query algorithm over $\mathbb{B}$.
2. $\mathcal{C}$ is FO-definable.

Special Cases: $\mathrm{CSP}(H)$ and $[H]_{\leftrightarrow}$, for every structure H.

Existence vs. Counting ($\mathbb{B}$ vs. $\mathbb{N}$)

Fact: Let $\mathcal{C}$ be a class of structures.

- If $\mathcal{C}$ admits a left query algorithm over $\mathbb{B}$, then $\mathcal{C}$ admits a left query algorithm over $\mathbb{N}$.
- $\mathcal{C}$ may admit a left query algorithm over $\mathbb{N}$, but not over $\mathbb{B}$. For example, take $\mathcal{C}$ to be the class of all graphs with at least 7 edges.

Existence vs. Counting ($\mathbb{B}$ vs. $\mathbb{N}$)

Fact: Let $\mathcal{C}$ be a class of structures.

- If $\mathcal{C}$ admits a left query algorithm over $\mathbb{B}$, then $\mathcal{C}$ admits a left query algorithm over $\mathbb{N}$.
- $\mathcal{C}$ may admit a left query algorithm over $\mathbb{N}$, but not over $\mathbb{B}$. For example, take $\mathcal{C}$ to be the class of all graphs with at least 7 edges.

However, this is an unfair comparison:
If $\mathcal{C}$ admits a left query algorithm over $\mathbb{B}$, then $\mathcal{C}$ is closed under homomorphic equivalence.

Existence vs. Counting ($\mathbb{B}$ vs. $\mathbb{N}$)

Question:

- Is there a class $\mathcal{C}$ of structures that is closed under homomorphic equivalence, admits a left query algorithm over $\mathbb{N}$, but it does not admit a left query algorithm over $\mathbb{B}$?

In other words, is counting more powerful than existence as regards homomorphic-equivalence closed classes?

Existence vs. Counting ($\mathbb{B}$ vs. $\mathbb{N}$)

Theorem (tCDKW - 2023) Let $\mathcal{C}$ be a class of structures that is closed under homomorphic equivalence. TFAE:

1. $\mathcal{C}$ admits a left query algorithm of the form $(\mathcal{F}, X)$ over $\mathbb{N}$, for some set $X \subseteq \mathbb{N}^k$.
2. $\mathcal{C}$ admits a left query algorithm of the form $(\mathcal{F}, X')$ over $\mathbb{B}$, for some set $X' \subseteq \{0, 1\}^k$.

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Proof Outline: (1) $\Longrightarrow$ (2)

- Write X as the disjoint union $X = \bigcup_{j=1}^{m} X_j$ of basic sets X_j, i.e.,
  if $\mathbf{t}, \mathbf{t}' \in X_j$, then $\mathbf{t}(i) = 0 \Longleftrightarrow \mathbf{t}'(i) = 0$, for all $i \leq k$.
- Show that if $\mathscr{C}$ is closed under homomorphic equivalence and admits a left query algorithm $(\mathcal{F}, X)$ over $\mathbb{N}$ where X is a basic set, then $\mathcal{C}$ is definable by

$$\psi : \quad (\bigwedge_{\mathbf{t}(i) \neq 0} Q^{F_i}) \wedge (\bigwedge_{\mathbf{t}(i)=0} \neg Q^{F_i}).$$

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Given B such that $B \models \psi$, show $B \in \mathcal{C}$.

- Take $A \in \mathcal{C}$, construct A' and B' such that
  1. A' is a disjoint union of "many" copies of A and a disjoint union of direct products of members of $\mathcal{F}$ and substructures of members of $\mathcal{F}$; similarly for B' and B.
  2. $A' \leftrightarrow A$ and $B' \leftrightarrow B$.
  3. $\hom(\mathcal{F}, A') = \hom(\mathcal{F}, B')$ (this uses an interpolation lemma for multivariate integer polynomials).
- By (2), $A' \in \mathcal{C}$; by (3), $B' \in \mathcal{C}$; by (2), $B \in \mathcal{C}$. $\square$

Synopsis

- Homomorphism counts capture interesting relaxations of isomorphism.
- Sharp differences in expressive power exist between restricted left profiles and restricted right profiles.
- Homomorphism counts give rise to algorithms for testing for membership in a class of structures.
- For left query algorithms and homomorphic-equivalence closed classes, counting homomorphisms is not more powerful than existence of homomorphisms.

Open Problems

- For right query algorithms and homomorphic-equivalence closed classes, is counting homomorphisms more powerful than existence of homomorphisms?

Open Problems

- For right query algorithms and homomorphic-equivalence closed classes, is counting homomorphisms more powerful than existence of homomorphisms?
- Characterize the logics L for which L-equivalence $\equiv_L$ is captured by a restricted left or by a restricted right profile.

  Tarski's Program: Characterize notions of "metamathematical origin" in "purely mathematical terms".