The Algebra of Homomorphism Counts

Martin Grohe

Graph Homomorphisms

A homomorphism from a graph F to a graph G is a mapping $h : V(F) \to V(G)$ that preserves edges, that is,

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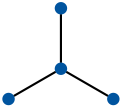

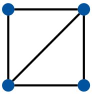

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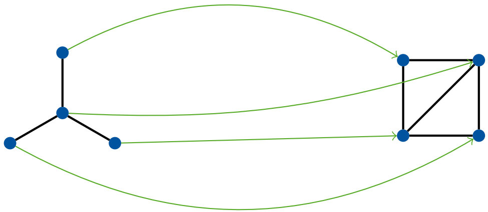

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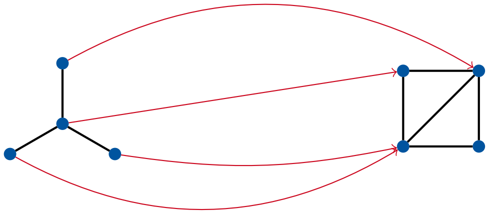

Counting Homomorphisms

For all graphs F, G, we let

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In particular,

$$\mathrm{hom}(\bullet, G) = |V(G)|,$$

$$\mathrm{hom}(\bullet\!\!-\!\!\bullet, G) = 2|E(G)|.$$

What information about G do we get from the numbers $\hom(F, G)$ for a range of Fs?

For every class $\mathscr{F}$ we can define a vector embedding $\mathsf{Hom}_{\mathscr{F}} : \mathscr{All} \to \mathbb{R}^{\mathscr{F}}$ by $\mathsf{Hom}_{\mathscr{F}}(G) := \big(\hom(F, G) \;\big|\; F \in \mathscr{F}\big)$.

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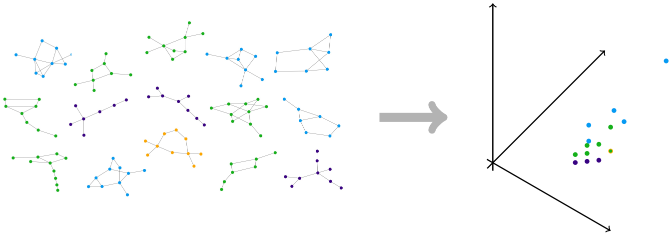

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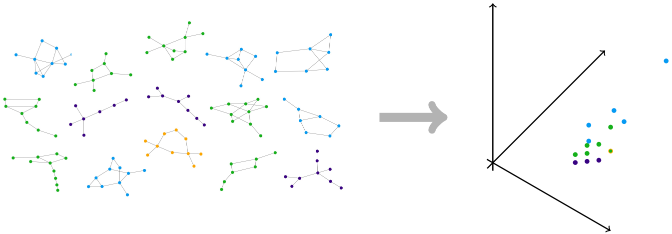

The embedding $\mathrm{Hom}_{\mathscr{F}}$ for $\mathscr{F} = \{\bullet, \bullet\!\!-\!\!\bullet, \triangle\}$

Vector embeddings are the basis for machine learning on graphs.

M. Grohe. word2vec, node2vec, graph2vec, X2vec: Towards a Theory of Vector Embeddings of Structured Data. Proc. PODS'20.

Homomorphism Indistinguishability

G, H are homomorphism indistinguishable over a class $\mathscr{F}$ of graphs (we write $G \equiv_{\mathscr{F}} H$) if

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Observation

Let $\mathscr{S}t$ be the class of all stars. Then

$$G \equiv_{\mathscr{S}t} H \iff G \text{ and } H \text{ have the same degree sequence.}$$

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Let $\mathscr{St}$ be the class of all stars. Then

$$G \equiv_{\mathscr{St}} H \iff G \text{ and } H \text{ have the same degree sequence.}$$

Theorem (Lovász 1967)

$$G \equiv_{\mathscr{All}} H \quad \iff \quad G \cong H.$$

That is, G and H are homomorphism indistinguishable over the class of all graphs if and only if they are isomorphic.

Proof Sketch

$aut(G)$:= number of automorphisms of G

$I(F, G)$:= number of injective homomorphisms from F to G

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Observation 2

$\hom(F, H) = \sum_G S(F, G) \cdot \frac{1}{aut(G)} \cdot I(G, H)$.

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Hence the columns of hom are linearly independent and thus mutually distinct.

The Structure of Homomorphorphism Indistinguishability Relations

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There uncountably many homomorphism indistinguishability relations.

Complexity

Theorem

1. *(follows from Dvorák 2010, Dell, G., Rattan 2018, G. 2020, G., Rattan, Seppelt 2022)*
   For every k, homomorphism indistinguishability over the class of graphs of tree width k, the class of graphs of tree depth k, the class of graphs of path with k is decidable in polynomial time.

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2. *(follows from Babai 2016)*
   Homomorphism indistinguishability over the class of all graphs is decidable in quasipolynomial time.

Complexity (cont'd)

Theorem (Böker, Chen, G., Rattan 2019)

There is a polynomial time decidable class $\mathscr{F}$ *of graphs of tree width* 2 *such that homomorphism indistinguishability over* $\mathscr{F}$ *is undecidable.*

Complexity (cont'd)

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Theorem (Atserias, Mančinska, Roberson, Šámal, Severini, Varvitsiotis 2019; Mančinska, Roberson 2020)

Homomorphism indistinguishability over the class of planar graphs is undecidable.

Logical and Algebraic Characterisations

Theorem (Dvorák 2010)

Let $k \geq 1$. For all graphs G, H, the following are equivalent.

1. *G, H are homomorphism indistinguishable over the class $\mathscr{T}w_k$ of graphs of tree width at most k:*

$$G \equiv_{\mathscr{T}w_k} H.$$

2. *The k-dimensional Weisfeiler-Leman algorithm does not distinguish G, H.*
3. *G and H are C_{k+1}-equivalent, where C_{k+1} is the $(k+1)$-variable fragment of first-order logic with counting quantifiers $\exists^{\geq n}$.*

Theorem (G. 2020)

Let $q \geq 1$. For all graphs G, H, the following are equivalent.

1. *G, H are homomorphism indistinguishable over the class $\mathscr{T\!d}_q$ of graphs of tree depth at most q:*
$$G \equiv_{\mathscr{T\!d}_q} H.$$
2. *G and H are $\mathsf{C}^{(q)}$-equivalent, where $\mathsf{C}^{(q)}$ is the quantifier-rank-q fragment of first-order logic with counting quantifiers $\exists^{\geq n}$.*

Notation

- F, G, H will always be graphs with vertex sets $U := V(F), V := V(G), W := V(H)$;

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G, H are isomorphic if and only if there is a permutation matrix X such that

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G, H are fractionally isomorphic if there is a doubly-stochastic matrix X such that $AX = XB$.

Theorem (Tinhofer 1990)

G, H are fractionally isomorphic if and only if the 1-dimensional WL algorithms does not distinguish G, H.

Algebraic Characterisation of Tree and Path Homomorphism Counts

$\mathscr{T}$ and $\mathscr{P}$ denote the classes of trees and paths, respectively.

Corollary

$$G \equiv_{\mathscr{T}} H \iff G \text{ and } H \text{ are fractionally isomorphic.}$$

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A matrix X is pseudo-stochastic if its row- and column sums are 1:

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Theorem (Dell, G. Rattan 2018)

$$G \equiv_{\mathscr{P}} H \iff \textit{there is a pseudo-stochastic } X \textit{ such that } AX = XB.$$

Observation

$$A \left\{ \begin{array}{c} \textit{pseudo-stochastic} \\ \textit{doubly-stochastic} \\ \textit{permutation} \end{array} \right\} \textit{matrix } X = (X_{vw})_{\substack{v \in V \\ w \in W}} \textit{ such that}$$

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Equational Characterisation

Observation

A $\left\{\begin{array}{c}\textit{pseudo-stochastic}\\ \textit{doubly-stochastic}\\ \textit{permutation}\end{array}\right\}$ *matrix* $X = (X_{vw})_{\substack{v\in V\\ w\in W}}$ *such that*

$$AX = XB$$

is a $\left\{\begin{array}{c}\textit{real}\\ \textit{nonnegative real}\\ \textit{nonnegative integer}\end{array}\right\}$ *solution to the following system of linear equations:*

$$L(G,H) \qquad \sum_{w\in W} X_{vw} = \sum_{v\in V} X_{vw} = 1$$

$$\sum_{v'\in V} A_{vv'}X_{v'w} = \sum_{w'\in W} X_{vw'}B_{w'w} \quad \textit{for all } v\in V, w\in W.$$

For $k \geq 2$, we define a a system of equations in variable X_π for $\pi \in \binom{V \times W}{\leq k}$. Essentially, this is the Sherali-Adams lift of $L(G, H)$.

$L^k(G, H)$

$$X_\emptyset = 1,$$

$$\sum_{w \in W} X_{\pi \cup vw} = \sum_{v \in V} X_{\pi \cup vw} = X_\pi \quad \text{for } \pi \in \binom{V \times W}{< k},\ v \in V, w \in W$$

$$X_\pi = 0 \quad \text{for } \pi \text{ that are not partial isomorphisms.}$$

Higher Dimensions

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Theorem (Atserias, Maneva 2013, G., Otto 2015)

For all $k \geq 1$, the following are equivalent.

1. *G and H are not distinguished by the k-dimensional WL algorithm.*
2. *$L^{k+1}(G, H)$ has a non-negative real solution.*

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Theorem (Dell, G., Rattan 2018, G., Rattan, Seppelt 2022)

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$G \equiv_{\mathscr{P}\!w_k} H \iff L^{k+1}(G,H)$ *has a real solution.*

Remark

There is also a logical characterisation of $\equiv_{\mathscr{P}\!w_k}$ (Montacute and Shah 2021).

For $q \geq 2$, we define a a system of equations in variables $X_{\boldsymbol{p}}$ for $\boldsymbol{p} \in \bigcup_{\ell=0}^{q} (V \times W)^{\ell}$.

$D^q(G, H)$

$$X_{()} = 1,$$

$$\sum_{w \in W} X_{\boldsymbol{p}vw} = \sum_{v \in V} X_{\boldsymbol{p}vw} = X_{\boldsymbol{p}} \quad \text{for } \boldsymbol{p} \in \bigcup_{\ell=0}^{q-1} (V \times W)^{\ell},\ v \in V, w \in W$$

$$X_{\boldsymbol{p}} = 0 \quad \text{for } \boldsymbol{p} \text{ that are not partial pseudo isomorphisms.}$$

Here $\boldsymbol{p} = (v_1 w_1, \ldots, v_\ell w_\ell)$ is a partial pseudo isomorphism if $v_i = v_{i+1} \iff w_i = w_{i+1}$ and $v_i v_j \in E(G) \iff w_i w_j \in E(H)$ for all $i < j \leq \ell$.

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Theorem (G., Rattan, Seppelt 2022)

$$G \equiv_{\mathcal{T}\!d_q} H \iff D^q(G, H) \text{ has a real solution.}$$

Planar Graphs

Quantum isomorphism is an equivalence relation on graphs based on a similar system of equations, but now we are looking for solutions in an arbitrary C*-algebra.

$\mathscr{P}\ell$ is the class of planar graphs.

Theorem (Mančinska and Roberson 2020)

$$G \equiv_{\mathscr{P}\ell} H \iff G \textit{ and } H \textit{ are quantum isomorphic.}$$

The Algebra of Graph Homomorphisms

A *k-labelled graph* is a pair

$$\boldsymbol{F} = (F; \boldsymbol{u}) = (F; u_1, \ldots, u_k)$$

where F is a graph (with $V(F) = U$) and $\boldsymbol{u} = (u_1, \ldots, u_k) \in U^k$.

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- $\overset{1}{\bullet}\!-\!\bullet\!-\!\overset{2}{\bullet} = \big((\{u_1, u_2, u_3\}, \{u_1u_2, u_2u_3\}); u_1, u_3\big)$ is a 2-labelled graph.

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We have natural operations linking these classes.

Example (Disjoint Union)

For k-labelled $\boldsymbol{F} = (F, \boldsymbol{u})$ and ℓ-labelled $\boldsymbol{F}' = (F', \boldsymbol{u})$, we obtain $(k+\ell)$-labelled $\boldsymbol{F} \otimes \boldsymbol{F}' = (F \uplus F'; \boldsymbol{u}\boldsymbol{u}')$.

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We usually assume $\mathscr{F}$ to be closed under disjoint union. Then

$$\otimes : \mathscr{F}^{(k)} \times \mathscr{F}^{(\ell)} \to \mathscr{F}^{(k+\ell)}$$

for all k, ℓ.

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Other basic operations are permuting labels, merging labels, dropping labels. We can combine these to obtain operations like series composition and parallel composition.

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$$\sum_{i=1}^{n} a_i \boldsymbol{F}_i$$

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$$\mathbb{C}\mathscr{F}^{(k)}.$$

We can linearly extend operations like disjoint union.

Homomorphisms from Labelled Graphs

For every G, we let $\hom(\boldsymbol{F}, G) \in \mathbb{C}^{V^k}$ to be the tensor (or vector or mapping $V^k \to \mathbb{C}$) defined by

$$\hom(\boldsymbol{F}, G)(\boldsymbol{v}) \coloneqq \text{number of homomorphisms } h \text{ from } F \text{ to } G \text{ with } h(\boldsymbol{u}) = \boldsymbol{v}$$

for $\boldsymbol{v} \in V^k$.

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$$\hom(\boldsymbol{F}, G)(\boldsymbol{v}) := \begin{array}{l}\text{number of homomorphisms } h \text{ from } F \text{ to } G \\ \text{with } h(\boldsymbol{u}) = \boldsymbol{v}\end{array}$$

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- $(\bullet\!-\!\bullet)_G \in \mathbb{C}$ is the number of edges of G.

Homomorphism Tensors as Representations

For each k and every graph G, we have

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The operations on the spaces $\mathbb{C}\mathscr{F}^{(k)}$ correspond to natural algebraic operations on the spaces $\mathbb{C}^{V^k}$:

- Disjoint union corresponds to tensor product.
- Dropping labels corresponds to aggregation of a coordinate: for all k-labelled $(F; u_1, \dots, u_k)$ and G we have

$$\big((F; u_1, \dots, u_{k-1})\big)_G(v_1, \dots, v_{k-1}) = \sum_{v \in V} \big((F; u_1, \dots, u_k)\big)_G(v_1, \dots, v_{k-1}, v).$$

Schur Product and Matrix Product

- For k-labelled $\boldsymbol{F} = (F; u_1, \ldots, u_k)$, $\boldsymbol{F'} = (F', u'_1, \ldots, u'_k)$, let $\boldsymbol{F} \odot \boldsymbol{F'}$ be the graph obtained from $\boldsymbol{F} \otimes \boldsymbol{F'}$ by identifying u_i with u'_i, for all i.

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  We can easily generalise this to $2k$-labelled graphs.

Idea

- To understand homomorphism indistinguishability over $\mathscr{F}$ we need to understand finite dimensional representations of the spaces $\mathbb{C}\boldsymbol{\mathscr{F}}^{(k)}$ for a family $\boldsymbol{\mathscr{F}}$ of labelled graphs over $\mathscr{F}$.

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- Representation theory tells us a lot about finite dimensional representations of algebras.

Application: Graphs of Bounded Path Width

Theorem (Dell, G., Rattan 2018, G., Rattan, Seppelt 2022)

Graph G, H are homomorphism indistinguishable over the class of graphs of path width at most k if only if the system $L^{k+1}(G, H)$ of linear equations has a solution.

The Algebra of Graphs of Pathwidth k

- We consider $2(k+1)$-labelled graphs of pathwidth k with $(k+1)$ labels on the first and last bag of a path decomposition of width k. Let $\mathscr{P}$ be the set of all such graphs and $\mathbb{C}\mathscr{P}$ the corresponding vector space.

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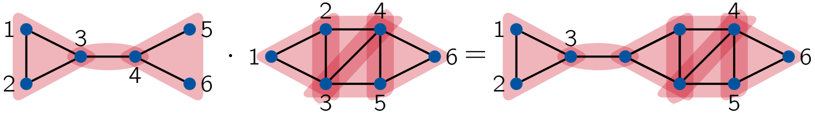
- $(k+1)$-dimensional series composition (that is, concatenation of the path decompositions) gives us a binary product on this space, resulting in an algebra $\mathbb{P}$.



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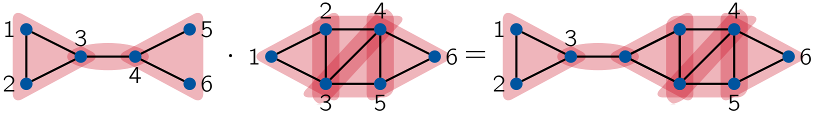

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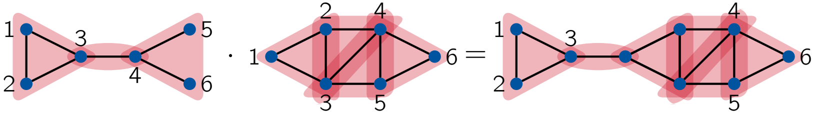

- This algebra is generated by a finite set of basal graphs (single-bag path decompositions).
- Reverting the paths gives us an involution operation, which turns $\mathbb{P}$ into a *-algebra.

Proof of the Theorem (Sketch)

- In the representations $(\cdot)_G$, series composition corresponds to matrix multiplication and reverting the paths to matrix transposition.

  Thus the image of the pathwidth-k graph algebra $\mathbb{P}$ under $(\cdot)_G$ is a finite-dimensional *-algebra.

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- We relate equivalence of characters to homomorphism indistinguishability.
- Equivalence of representations can be described by a finite system of linear equations involving the finitely many generators of our algebra.
- We massage this system to turn it into $L^{k+1}(G, H)$.

Concluding Remarks

Where We Stand

- Homomorphism counts extract interesting information from graphs that characterise many natural equivalence relations on graphs and pull together combinatorics, logic, and algebra.

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- When generalised to rooted graphs, they induce a rich algebraic structure.
- Homomorphism counts are also useful and expressive graph features in practice (Master's thesis of Pascal Kühner).

Homomorphism Indistinguishability and Graph Minors—Roberson's Conjecture

Conjecture (Roberson 2022)

Let $\mathscr{F}$ and $\mathscr{F}'$ be graph classes closed under taking minors and under taking disjoint unions. Then homomorphism indistinguishability over $\mathscr{F}$ and $\mathscr{F}'$ coincide if and only if the classes are equal, that is:

$$\equiv_{\mathscr{F}} = \equiv_{\mathscr{F}'} \quad \iff \quad \mathscr{F} = \mathscr{F}'.$$

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- Jan Böker obtained results for trees and graphs of bounded tree width.