The homomorphism lattice of finite structures, unique characterization, and exact learnability

Balder ten Cate

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About me

Career path:

 $\mathsf{ILLC} \to \mathsf{IvI} \to \mathsf{INRIA} / \mathsf{ENS} \mathsf{ de Cachan} \to \mathsf{UC} \mathsf{ Santa} \mathsf{ Cruz} \to \mathsf{LogicBlox} \to \mathsf{Google} \to \mathsf{ILLC}$

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Past research topics:

- Extended modal languages; well-behaved fragments of first-order logic and fixpoint logic
- XML query languages; automata and logics for finite trees
- Data management and data interoperability (schema mappings, access constraints)
- Knowledge representation and reasoning (ontology-based data access)
- Declarative languages for data analysis and machine learning
- And, conversely, techniques for learning declarative representations

European reintegration fellowship LLAMA (Logic and Learning - an Algebraic and Model-theoretic Approach)

Outline

- 1. Conjunctive queries (CQs)
- 2. Main technical content: Homomorphism lattice of finite structures
- 3. Applications of the above to some problems regarding learning CQs (and other declarative specification languages)

Main reference:

• Balder ten Cate, Victor Dalmau (2020). Conjunctive Queries: Unique Characterizations and Exact Learnability. <u>arxiv.org/abs/2008.06824</u>

Conjunctive Queries

A conjunctive query (CQ) is a positive-existential-conjunctive FO formula (that is, CQs form the fragment of FO that uses only \exists and \land)

A **union of conjunctive queries (UCQ)** is a disjunction of CQs (that is, UCQs form the fragment of FO that uses only \exists , \land , and \lor --- suitably normalized).

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Why are CQs (and UCQs) interesting?

- CQs are of fundamental importance in databases as they capture the core SELECT-FROM-WHERE construct in SQL.
- They arise naturally in numerous other areas of computer science as well.

Brief digression

Recall that

- Modal logic can be viewed as a fragment of FO, and
- In fact, it is the bisimulation-invariant fragment of FO
 - ("Van Benthem Characterization Theorem")

Similarly,

- **UCQ** is a fragment of FO logic, and
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A **homomorphism** is a map $h : dom(A) \rightarrow dom(B)$ that preserves structure (more precise definition will come later in this talk).

Brief digression (ct'd)

Many classic results of model theory "fail in the finite" (restricted to finite structures)

- Examples: Compactness, Craig interpolation, Los-Tarski Theorem, ...
- Failure-in-the-finite appears to be the rule rather than the exception.

What is an example of a model-theoretic result that *does* hold in the finite?

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What is an example of a model-theoretic result that *does* hold in the finite?

- 1. Van Benthem Characterization Theorem (as shown by Rosen, 1997)
- 2. Homomorphism Preservation Theorem (as shown by Rossman, 2008)

World of modal logic

World of database theory



Modal mu-calculus Monadic Datalog

Bisimulations ------ Homomorphisms





End of the Brief digression

(Ask me later if you are interested in this.)

Example-Driven Query Discovery

Scenario: we are trying to construct a database query from data examples.

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- The database schema S and the arity *k* of the query are known.
- A *data example* is a triple: (I, **a**, s)
 - I is a database instance (for schema S)
 - **a** is a k-tuple
 - s in {+, -} indicates if this is a positive or a negative example.
- A query Q ...
 - ... *fits* data example (I,**a**,+) if **a** \in Q(I)
 - ... fits data example (I,a, -) if $a \in Q(I)$



Remainder of this talk

- 1. Some aspects of the Homomorphism Lattice of Finite Structures
- 2. Applications to Example-Driven Query Discovery for CQs.
- 3. (Time permitting:) Schema Mappings and Description Logics

Structures and Homomorphisms

Fix a finite schema S consisting of relation symbols and constants symbols.

By a *structure* we will mean a finite relational structure over **S**.

A *homomorphism* from A to B is a function h: $dom(A) \rightarrow dom(B)$ such that

- 1. For every fact of A, its image (under h) is a fact of B.
- 2. $h(c^A) = c^B$ for each constant symbol c

The Homomorphism Lattice

The *Homomorphism Lattice* is the partial order (Str, \leq_{hom})

- Str is the set of all structures
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Two structures are *homomorphically equivalent* if $A \leq_{hom} B$ and $B \leq_{hom} A$. We will not distinguish between homomorphically equivalent structures.



 A^{\perp} : structure with no facts; each constant symbol denotes a different element.

 A^{T} : single-element structure (all constants denote the same element); all facts.





 $A \otimes B$ = direct product of A and B

A ⊕ B ~= disjoint union of A and B (in the case with constants the precise construction is a bit more tedious)

The Homomorphism Lattice

Algebra (Str, \oplus , \otimes , \top , \bot , ...)

The Homomorphism Lattice

Algebra (Str, ⊕, ⊗, ⊤, ⊥, …)

One more relevant operation:

for every A and B there is a structure A^{B} satisfying:

 $C \leq_{hom} A^B$ iff $(C \otimes B) \leq_{hom} A$

Small digression

Product Homomorphism Problem (PHP):

Given A_1, \ldots, A_n and B, decide whether $(A_1 \otimes \ldots \otimes A_n) \leq_{hom} B$

Theorem (Willard 2010; tC and Dalmau 2015) :

PHP is NExpTime-complete (even for a fixed schema).

Density

Let **S** = { R } with R a binary relation. Let $A_1 = \{ R(a,b) \}$ and let $A_2 = \{ R(a,b) , R(b,a) \}$.

Fact 1: $A^{\perp} <_{hom} A_1 <_{hom} A_2$

Density

Let **S** = { R } with R a binary relation. Let $A_1 = \{ R(a,b) \}$ and let $A_2 = \{ R(a,b) , R(b,a) \}$.

Fact 1: $A^{\perp} <_{hom} A_1 <_{hom} A_2$

Fact 2: There is *no* B such that $A^{\perp} < B < A_{1}$.

Fact 3: For every $B <_{hom} A_2$ there is a structure B' such that $B <_{hom} B' <_{hom} A_2$.

Follows from an extension (due to Nesetril and Rodl 1989) of Erdos (1959)'s celebrated theorem on the existence of graphs of high girth and chromatic number

Frontiers

Definition; a *frontier* for A is a finite set of structures { $F_1, ..., F_n$ }, such that

1. each $F_i <_{hom} A$, and 2. whenever $B <_{hom} A$ then $B \leq_{hom} F_i$ for some F_i

The frontier separates A from the structures strictly below A.

Not every structure has a frontier. A_2 has no frontier.



Dualities

Def 1: A pair of structure (F,D) is a *duality pair* if:

$$\{A \mid F \leq_{hom} A\} = \{A \mid A \leq_{hom} D\}$$



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Def 2: A pair of finite sets $({F_1, ..., F_n}, {D_1, ..., D_m})$

is a generalized homomorphism duality if:

 $\{A \mid F_i \leq_{hom} A \text{ for some } i \leq n\} = \{A \mid A \leq_{hom} D_i \text{ for all } i \leq m\}$



Example 1 (duality pair)

Let

- P_{k+1} be the directed path with k+1 elements.
- T_k be the linear order with k elements.

Gallai-Hasse-Roy-Vitaver Theorem (~01965) for directed graphs:

 (P_{k+1}, T_k) is a duality pair,

i.e., for every directed graph G, it holds that $P_{k+1} \rightarrow G$ if and only if $G \rightarrow T_k$

Example 2 (infinitary homomorphism duality)

A graph is 2-colorable if and only if it does not have a cycle of odd length.

$$G \to \mathbf{K_2}$$
 if and only if $\mathbf{C_{2n+1}} \xrightarrow{-}{\to} G$ for all n

where \mathbf{K}_2 is the 2-element clique and \mathbf{C}_n is the a cycle of length n.

Frontiers and Dualities

Theorem (from Nesetril and Tardiff 2000, cf. also tC and Dalmau 2020):

• If $\{B_1, ..., B_n\}$ is a frontier for A, then

({A}, { A^{B1} , ..., A^{Bn} }) is a generalized homomorphism duality

• If $({A}, {B_1, ..., B_n})$ is a generalized homomorphism duality,

then $\{(A \otimes B_1), \dots, (A \otimes B_1)\}$ is a frontier for A

(*Statement assumes no constants but naturally extends to the case with constants)

C-acyclicity

A structure is *c*-acyclic if it does not have cycles except for cycles that involve an element named by a constant symbol.

More precise definition:

- The *incidence graph* of a structure A is the bi-partite multi-graph where
 - The nodes of the graph are the elements and facts of A
 - There is an edge between an element and a fact if the element occurs in the fact.
 - If an element occurs multiple times in a fact, each occurrence generates an edge.
- A structure is *c-acyclic* if every cycle in the incidence graph goes through at least one element named by a constant symbol.

Examples

Т R S R S R Т R R R С С С cyclic acyclic c-acyclic

S

Frontiers: existence and how to construct them

Thm 1: For all structures A, the following are equivalent:

- 1. A has a frontier
- 2. A is homomorphically equivalent to a **c-acyclic** structure.

Thm 2: For c-acyclic structures, a frontier can be computed in polynomial time.

Thm 3: Testing whether a given set of structures { F1,, Fn } is a frontier for a structure A is **NP-complete**.

Foniok, Nesetril and Tardiff (2008), tC and Dalmau (2020)

Some further results on frontiers

The class of c-acyclic structures is not *"frontier-closed"* (although every c-acyclic structure has a frontier, it does not necessarily consist of c-acyclic structures).

Thm (tC and Dalmau 2020). The class of acyclic connected structures (with a single constant) is polynomial-time frontier-closed.

Thm (from Nešetřil and Ossona de Mendez 2008; cf. tC and Dalmau 2020): Every class of structures that has bounded expansion admits relatized frontiers.

Example-Driven Query Discovery



Conjunctive Queries

Let's restrict attention to conjunctive queries (CQs).

- Every k-ary CQs over a relational schema S can be equivalently viewed as a structure over schema S ∪ {c₁, .., c_k}.
- Every example corresponds to a structure over **S** \cup { $c_1 \dots c_k$ } as well.
- Q fits a (I,a, +) iff there is a homomorphism from q(x) to (I,a)
- Q fits a (I,a, -) iff there is no homomorphism from q(x) to (I,a)

This sets the stage for us to apply results about the homomorphism lattice.

1. The Fitting Problem

Fitting problem:

Input: a finite set E of data examples. Decide whether there is a CQ that fits all data examples in E.

Lemma: let **Q*** be the direct product of the positive examples in E. The following are equivalent:

- 1. There exists a CQ that fits the data examples in E.
- 2. Q* fits the data examples in E.
- 3. Q* does not have a homomorphism to any negative example in E.
- 4. Q* is the *most-specific fitting CQ* for the data examples in E.

Theorem: the fitting problem is coNExpTime-complete. (by reduction from PHP)

Example-Driven Query Discovery



2. The Uniqueness Problem

Definition: E *uniquely characterizes* Q if Q is the only CQ (up to logical equivalence) that fits the examples in E.

Unique characterization problem:

Input: a finite set of data examples E and a most-specific-fitting CQ Q for E. Decide if E uniquely characterizes Q.

Lemma: The following are equivalent:

- 1. E uniquely characterizes Q
- 2. The negative examples in E form a frontier for Q.

Theorem: the unique characterization problem is NP-complete.

Example-Driven Query Discovery



3. Eliciting Further Examples

Will finitely many examples even ever be enough to uniquely characterize the target CQ?

Theorem 1: for all CQs Q, the following are equivalent

- 1. Q is uniquely characterized by a finite set of data examples
- 2. Q has a frontier.
- 3. Q is logically equivalent to a c-acyclic CQ.

Theorem 2: the class of c-acyclic CQs is efficiently exactly learnable with membership queries.

Theorem 2 means that, if the "target CQ" is c-acyclic, then there is a PTIME algorithm that, after asking for the label of one or more examples, terminates and identifies it correctly (modulo logical equivalence).



Unions of Conjunctive Queries

The situation for UCQs is a little different:

- Unique characterizations for UCQs ~ generalized homomorphism dualities
- A UCQ is uniquely characterized by a finite set of examples iff if is logically equivalent to a c-acyclic UCQ.
- For c-acyclic UCQs, a uniquely characterizing set of examples can be effectively constructed but (provably) not in polynomial time.
- The class of c-acyclic UCQs is *not* efficiently exactly learnable with membership queries (but is efficiently exactly learnable with membership and equivalence queries).

Schema Mappings

A schema mapping $M=(S,T,\Sigma)$ is a high-level declarative specifications of the relationships between two database schemas.

Two of the most well-studied schema mapping specification languages are LAV ("Local-as-View") and GAV ("Global-as-View") schema mappings.

Schema Mappings

A schema mapping $M=(S,T,\Sigma)$ is a high-level declarative specifications of the relationships between two database schemas.

Two of the most well-studied schema mapping specification languages are LAV ("Local-as-View") and GAV ("Global-as-View") schema mappings.

Alexe, tC, Kolaitis, and Tan (2011) studied the question when a schema mapping be uniquely characterized by a finite set of data examples.

tC, Dalmau, and Kolaitis (2013) studied efficient exact learnability for GAV schema mappings.

Schema Mappings

Corr. Fix a source schema S and a target schema T.

- A LAV schema mapping M=(S,T,Σ) is uniquely characterizable by a finite set of positive and negative schema-mapping examples if and only if M is logically equivalent to a c-acyclic LAV schema mapping.
- 2. If M is c-acyclic, then a uniquely characterizing set of positive and negative schema-mapping examples can be constructed in PTIME.
- 3. The class of c-acyclic LAV schema mappings over S, T is efficiently exactly learnable with membership queries.

Question: what happens in the presence of integrity constraints?

Description logics

Description logics (DLs) are formal specification languages used to represent domain knowledge.

The DL concept language *ELI* can be characterized as a notational variant of acyclic connected unary CQs (over a schema with unary and binary relations only).

For example, the ELI concept

```
logician \sqcap \exists HasParent. \exists HasParent.logician
```

corresponds to $q(x) = \exists y, z$. (logician(x) \land HasParent(x,y) \land HasParent(y,z) \land logician(z))

Description logics

Corr.

- 1. Every ELI concept expression is uniquely characterizable by a finite collection of positive and negative QA examples, which is PTIME-computable.
- 2. Furthermore, the class of ELI concept expressions is efficiently exactly learnable with membership queries.

Question: does this hold also in the presence of an ontology (background theory)?

One recent result

Assume a schema **S** consisting of unary and binary relations only.

A DL-Lite ontology is a FO theory consisting of

- Inclusion constraints $\alpha(x) \rightarrow \beta(x)$ and/or
- Disjointness constraints of the form $\alpha(x) \rightarrow \neg \beta(x)$, R(x,y) $\rightarrow \neg S(x,y)$, and/or R(x,y) $\rightarrow \neg S(y,x)$

where $\alpha(x)$, $\beta(x)$ are unary projections of relations, i.e., of the form P(x), $\exists y.R(x,y)$ or $\exists y.R(y,x)$

Thm (Funk, Jung and Lutz, DL 2021): Acyclic, connected, unary CQs over **S** (in other words, ELI description logic concepts) are efficiently exactly learnable in the presence of DL-Lite ontologies.

Outlook (LLAMA)

- Unique characterizations and exact learnability for modal formulas
- Unique characterizations and exact learnability in the presence of a background theory

Collaboration with Raoul Koudijs, ... (room for more collaborations!)

Thank you!