

# Shapley Values for Databases and Machine Learning

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LINKS seminar, October 22th 2021

*Inria*

The Shapley value

Shapley values in databases: explaining query results

Shapley values in ML: SHAP-score

# The Shapley value

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## Cooperative games

Notion from **cooperative game theory**. Let  $X$  be a set of **players** and  $\mathcal{G} : 2^X \rightarrow \mathbb{R}$  be a **game on  $X$** . We wish to assign to every player  $p \in X$  a **contribution**  $s_X(\mathcal{G}, p)$ . Some reasonable axioms:

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1. **Symmetry**: For every game  $\mathcal{G}$  on  $X$  and players  $p_1, p_2 \in X$ , if we have  $\mathcal{G}(S \cup \{p_1\}) = \mathcal{G}(S \cup \{p_2\})$  for every  $S \subseteq X \setminus \{p_1, p_2\}$ , then  $s_X(\mathcal{G}, p_1) = s_X(\mathcal{G}, p_2)$

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2. **Null player**: A player  $p$  is null for  $\mathcal{G}$  if  $\mathcal{G}(S \cup \{p\}) = \mathcal{G}(S)$  for every  $S \subseteq X$ . For every null player for  $\mathcal{G}$  we have  $s_X(\mathcal{G}, p) = 0$

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4. **Efficiency**: For every game  $\mathcal{G}$  on  $X$  we have  $\sum_{p \in X} s_X(\mathcal{G}, p) = \mathcal{G}(X) - \mathcal{G}(\emptyset)$



# The Shapley value

## Theorem [Shapley, 1953]

There is a unique function  $s_X(\cdot, \cdot)$  that satisfies all four axioms.

$$\text{Shapley}_X(\mathcal{G}, p) \stackrel{\text{def}}{=} \sum_{S \subseteq X \setminus \{p\}} \frac{|S|!(|X| - |S| - 1)!}{|X|!} (\mathcal{G}(S \cup \{p\}) - \mathcal{G}(S))$$

## Shapley values in databases: explaining query results

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This part of the talk is based on joint work with Daniel Deutch, Nave Frost and Benny Kimelfeld.

(Paper in revision phase of SIGMOD'22)

## Shapley values for databases

- Framework introduced by Livshits, Bertossi, Kimelfeld, and Sebag [LBKS'20]
- Let  $q$  be a Boolean query and  $D = D_n \cup D_x$  be a relational database, partitioned into endogenous facts  $D_n$  and exogenous facts  $D_x$ .

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- We want to define the “contribution” to every endogenous fact  $f \in D_n$  for the (non-)satisfaction of  $q$ . We use the Shapley value where the players = the endogenous facts of  $D$ , the game =  $E \subseteq D_n \mapsto q(D_x \cup E)$

$$\text{Shapley}(q, D_n, D_x, f) \stackrel{\text{def}}{=}$$

$$\sum_{E \subseteq D_n \setminus \{f\}} \frac{|E|!(|D_n| - |E| - 1)!}{|D_n|!} (q(D_x \cup E \cup \{f\}) - q(D_x \cup E)).$$

# Complexity?

When can it be computed efficiently? We will consider **data complexity**:

**Definition: problem**  $\text{Shapley}(q)$

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**Theorem [LBKS'20]**

Let  $q$  be a self-join-free conjunctive query. If  $q$  is **hierarchical** then  $\text{Shapley}(q)$  is PTIME, otherwise it is  $\text{FP}^{\#P}$ -hard

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**Theorem [LBKS'20]**

Let  $q$  be a union of conjunctive queries. Then  $\text{Shapley}(q)$  has a Fully Polynomial-time Randomized Approximation Scheme (**FPRAS**)



## Link to probabilistic databases?

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Is there a more general connection?

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Is there a more general connection?

**Answer:** yes, we show that  $\text{Shapley}(q)$  reduces to probabilistic query evaluation, for every Boolean query  $q$ !

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# Probabilistic databases

*Tuple-independent probabilistic database (TID)*

$D$			$\pi$
Likes			
Charles	monoids		0.9
Claire	turtle programs		0.5
Florent	d-DNNFs		0.7
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$$\Pr(D') = (1 - 0.9) \times 0.5 \times (1 - 0.7) \times 0.2$$

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$q = \llcorner$  there are two people who like the same thing  $\gg$

$$\Pr((D, \pi) \models q) = \sum_{\substack{D' \subseteq D \\ D' \models q}} \Pr(D')$$



## PQE( $q$ ) and Shapley( $q$ )

**Definition: problem PQE( $q$ )**

**Input:** A tuple-independent database  $(D, \pi)$

**Output:** The probability  $\Pr((D, \pi) \models q)$  that  $(D, \pi)$  satisfies  $q$

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## Theorem (ours)

For every Boolean query  $q$ , Shapley( $q$ ) reduces in PTIME to PQE( $q$ )

→ In particular, this implies that Shapley( $q$ ) is PTIME whenever PQE( $q$ ) is PTIME (and we know a lot about this!)

**Next:** full proof of this result

## Reduction from Shapley( $q$ ) to PQE( $q$ ) (1/4)

We wish to compute  $\text{Shapley}(q, D_n, D_x, f) \stackrel{\text{def}}{=}$

$$\sum_{E \subseteq D_n \setminus \{f\}} \frac{|E|!(|D_n| - |E| - 1)!}{|D_n|!} (q(D_x \cup E \cup \{f\}) - q(D_x \cup E)).$$

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For an integer  $k \in \{0, \dots, |D_n|\}$ , define

$$\#\text{Slices}(q, D_n, D_x, k) \stackrel{\text{def}}{=} |\{E \subseteq D_n \mid |E| = k \text{ and } q(D_x \cup E) = 1\}|.$$

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Regroup the terms by size to obtain  $\text{Shapley}(q, D_n, D_x, f) =$

$$\sum_{k=0}^{|D_n|-1} \frac{k!(|D_n| - k - 1)!}{|D_n|} \left( \#\text{Slices}(q, D_n \setminus \{f\}, D_x \cup \{f\}, k) - \#\text{Slices}(q, D_n \setminus \{f\}, D_x, k) \right).$$

In other words, Shapley( $q$ ) reduces to the problem of computing  $\#\text{Slices}(q)$ , so it suffices to reduce  $\#\text{Slices}(q)$  to PQE( $q$ )

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For  $z \in \mathbb{Q}$ , we define a TID database  $(D_z, \pi_z)$  as follows:  $D_z$  contains all the facts of  $D$ , and for an exogenous fact  $f$  of  $D$  we define  $\pi_z(f) \stackrel{\text{def}}{=} 1$  while for an endogenous fact  $f$  of  $D$  we define  $\pi_z(f) \stackrel{\text{def}}{=} \frac{z}{1+z}$ .

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$$\begin{aligned} \Pr(q, (D_z, \pi_z)) &\stackrel{\text{def}}{=} \sum_{D' \subseteq D_z \text{ s.t. } q(D')=1} \Pr(D') \\ &= \sum_{E \subseteq D_n \text{ s.t. } q(D_x \cup E)=1} \Pr(D_x \cup E) \\ &= \sum_{i=0}^{n \stackrel{\text{def}}{=} |D_n|} \sum_{\substack{E \subseteq D_n \text{ s.t.} \\ |E|=i \text{ and } q(D_x \cup E)=1}} \Pr(D_x \cup E) \end{aligned}$$



## Reduction from Shapley( $q$ ) to PQE( $q$ ) (3/4)

$$\begin{aligned}\Pr(q, (D_z, \pi_z)) &= \sum_{i=0}^n \sum_{\substack{E \subseteq D_n \text{ s.t.} \\ |E|=i \text{ and } q(D_x \cup E)=1}} \Pr(D_x \cup E) \\ &= \sum_{i=0}^n \sum_{\substack{E \subseteq D_n \text{ s.t.} \\ |E|=i \text{ and } q(D_x \cup E)=1}} \left(\frac{z}{1+z}\right)^i \left(1 - \frac{z}{1+z}\right)^{n-i} \\ &= \sum_{i=0}^n \left(\frac{z}{1+z}\right)^i \left(\frac{1}{1+z}\right)^{n-i} \sum_{\substack{E \subseteq D_n \text{ s.t.} \\ |E|=i \text{ and } q(D_x \cup E)=1}} 1 \\ &= \frac{1}{(1+z)^n} \sum_{i=0}^n z^i \# \text{Slices}(q, D_x, D_n, i).\end{aligned}$$

## Reduction from Shapley( $q$ ) to PQE( $q$ ) (3/4)

Hence we have

$$(1+z)^n \Pr(q, (D_z, \pi_z)) = \sum_{i=0}^n z^i \#Slices(q, D_x, D_n, i).$$

This suffices to conclude. Indeed, we now call an oracle to PQE( $q$ ) on  $n+1$  databases  $D_{z_0}, \dots, D_{z_n}$  for  $n+1$  arbitrary distinct values  $z_0, \dots, z_n$ , forming a **system of linear equations** as given by the relation above. Since the corresponding matrix is a **Vandermonde with distinct coefficients**, it is invertible, so we can compute in polynomial time the value  $\#Slices(q, D_x, D_n, k)$ .

So Shapley( $q$ ) reduces in PTIME to PQE( $q$ ).

# Open problem

Do we have **the other direction**? We don't know

## Open problem

For every Boolean query  $q$ , is it the case that  $\text{PQE}(q)$  reduces in PTIME to  $\text{Shapley}(q)$ ?

- (By [LBKS'20], this is true for self-join-free CQs)

# Using provenance and knowledge compilation to solve Shapley( $q$ ) (1/2)

- An approach to probabilistic query evaluation: compute the **provenance** of the query  $q$  on the database  $D$  in a formalism from **knowledge compilation**, and then use this representation to compute the probability.

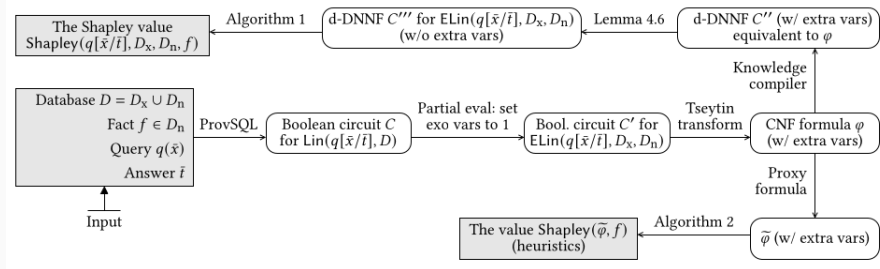
→ We can do the same for computing Shapley values

## Proposition (ours)

Given as input a **deterministic and decomposable circuit**  $C$  representing the provenance, we can compute in time  $O(|C| \cdot |D_n|^2)$  the value  $\text{SHAP}(q, D_n, D_x, f)$ .

# Using provenance and knowledge compilation to solve $\text{Shapley}(q)$ (2/2)

Implementation, experiments on TPC-H and IMDB datasets.



## Shapley values in ML: SHAP-score

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This part of the talk is based on the preprint “On the Complexity of SHAP-Score-Based Explanations: Tractability via Knowledge Compilation and Non-Approximability Results” [Arxiv] with [Marcelo Arenas](#), [Pablo Barceló](#), and [Leopoldo Bertossi](#) (Conference version at [AAAI'21](#))

## SHAP-score for explainable AI

Let  $X$  be a set of features,  $e$  an entity (that has a value  $e(x)$  for every feature  $x \in X$ ),  $M$  a model (that assigns a value to each entity),  $\mathcal{D}$  a probability distribution over the set of entities, and  $x$  a feature.



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The **SHAP score**  $\text{SHAP}_{\mathcal{D}}(M, e, x)$  is the Shapley value of  $x$  in the following game function  $\mathcal{G}_e$ :

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In other words,

$$\text{SHAP}_{\mathcal{D}}(M, e, x) \stackrel{\text{def}}{=} \sum_{S \subseteq X \setminus \{x\}} \frac{|S|!(|X| - |S| - 1)!}{|X|!} (\mathcal{G}_e(S \cup \{x\}) - \mathcal{G}_e(S))$$

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→ We **generalize** this result to more powerful classes of models, from the field of **knowledge compilation**

# Knowledge compilation

**Knowledge compilation:** a field of AI that studies various formalisms to represent Boolean functions...

- examples: truth tables, Boolean formulas in DNF/CNF, Boolean circuits, binary decision diagrams (OBDDs), binary decision trees, etc.

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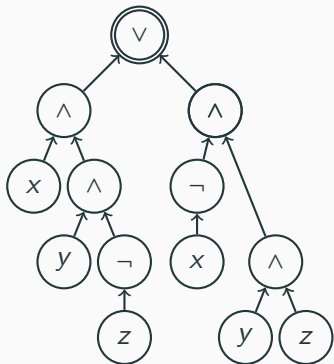
- examples: **satisfiability** in  $O(n)$  for truth tables or DNFs but NP-c for CNFs, **model counting** in  $O(n)$  for OBDDs but #P-hard for DNFs, etc.

**Deterministic and decomposable Boolean circuits:** the less restricted formalism of knowledge compilation that allows tractable model counting



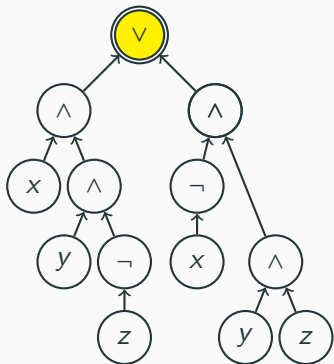
# Deterministic and decomposable Boolean circuits

(also called “**tractable Boolean circuits**”)



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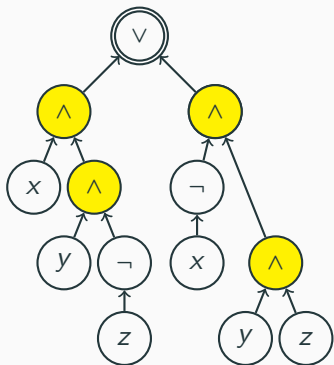
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- **Deterministic:** inputs of  $\vee$ -gates are mutually exclusive

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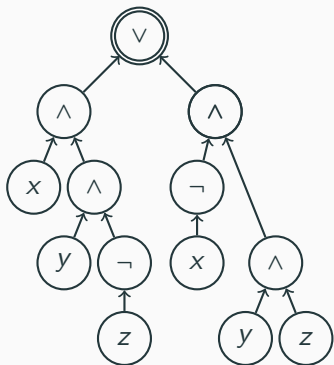
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- **Decomposable**: inputs of  $\wedge$ -gates are **independent** (no variable has a path to two different inputs of the same  $\wedge$ -gate)

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- **Decomposable**: inputs of  $\wedge$ -gates are **independent** (no variable has a path to two different inputs of the same  $\wedge$ -gate)

→ **model counting** or even **probability evaluation** can be solved in linear time

# Results

- Set  $X$  of **binary features**; so an entity  $e$  is a function from  $X$  to  $\{0, 1\}$
- A **deterministic and decomposable circuit**  $M$
- An **entity**  $e$  and a **feature**  $x \in X$
- We assume that the **distribution**  $\mathcal{D}$  is such that each feature  $y \in X$  has an **independent probability**  $p_y$  of being 1

# Results

- Set  $X$  of **binary features**; so an entity  $e$  is a function from  $X$  to  $\{0, 1\}$
- A **deterministic and decomposable circuit**  $M$
- An **entity**  $e$  and a **feature**  $x \in X$
- We assume that the **distribution**  $\mathcal{D}$  is such that each feature  $y \in X$  has an **independent probability**  $p_y$  of being 1

## Main result

Given as input  $M$ ,  $e$ ,  $x$  and  $p_y$  for every  $y \in X$ , we can compute the SHAP-score  $\text{SHAP}_{\mathcal{D}}(M, e, x)$  in time  $O(|M| \cdot |X|^2)$

## Proof sketch of main result (1/3)

Recall that  $\text{SHAP}_{\mathcal{D}}(M, e, x)$  is defined as

$$\sum_{S \subseteq X \setminus \{x\}} \frac{|S|!(|X| - |S| - 1)!}{|X|!} (\mathbb{E}_{e' \sim \mathcal{D}}[M(e') \mid e'(y) = e(y) \text{ for all } y \in S \cup \{x\}] - \mathbb{E}_{e' \sim \mathcal{D}}[M(e') \mid e'(y) = e(y) \text{ for all } y \in S])$$

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### Lemma

Computing SHAP-score can be reduced in polynomial time to the following problem.

**INPUT:** binary features  $X$ , entity  $e$ , deterministic and decomposable circuit  $M$ , integer  $k$ .

**OUTPUT:**  $\sum_{\substack{S \subseteq X \\ |S|=k}} \mathbb{E}_{e' \sim \mathcal{D}}[M(e') \mid e'(y) = e(y) \text{ for all } y \in S]$



## Proof sketch of main result (2/3)

Goal: compute  $\sum_{\substack{S \subseteq X \\ |S|=k}} \mathbb{E}_{e' \sim \mathcal{D}} [M(e') \mid e'(y) = e(y) \text{ for all } y \in S]$ .

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**Goal:** compute  $\sum_{\substack{S \subseteq X \\ |S|=k}} \mathbb{E}_{e' \sim \mathcal{D}} [M(e') \mid e'(y) = e(y) \text{ for all } y \in S]$ .

- **Step 1:** **smooth** the circuit. A Boolean circuit is *smooth* if for every  $\vee$ -gate  $g$ , every input gate of  $g$  sees the same set of variables. We can smooth  $M$  in  $O(|M| \cdot |X|^2)$

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- **Step 2:** for every gate  $g$  of the circuit and  $\ell \in \{0, \dots, |\text{var}(g)|\}$ , define the value

$$\alpha_g^\ell \stackrel{\text{def}}{=} \sum_{\substack{S \subseteq \text{var}(g) \\ |S|=\ell}} \mathbb{E}_{e' \sim \mathcal{D}} [M_g(e') \mid e'(y) = e(y) \text{ for all } y \in S]$$

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and **compute the values  $\alpha_g^\ell$  by bottom-up induction** on the circuit

## Proof sketch of main result (3/3)

Compute  $\alpha_g^\ell \stackrel{\text{def}}{=} \sum_{\substack{S \subseteq \text{var}(g) \\ |S|=\ell}} \mathbb{E}_{e' \sim \mathcal{D}} [g(e') \mid e'(y) = e(y) \text{ for all } y \in S]$

for every gate  $g$  and integer  $\ell \in \{0, \dots, |\text{var}(g)|\}$

- $g$  is a **variable gate** with variable  $y$ . Then  $\alpha_g^0 = p_y$  and  $\alpha_g^1 = e(y)$
- $g$  is an **OR gate** with inputs  $g_1, g_2$ . Then  $\alpha_g^\ell = \alpha_{g_1}^\ell + \alpha_{g_2}^\ell$
- $g$  is an **AND gate** with inputs  $g_1, g_2$ .

$$\text{Then } \alpha_g^\ell = \sum_{\substack{\ell_1 \in \{0, \dots, |\text{var}(g_1)|\} \\ \ell_2 \in \{0, \dots, |\text{var}(g_2)|\} \\ \ell_1 + \ell_2 = \ell}} \alpha_{g_1}^{\ell_1} \cdot \alpha_{g_2}^{\ell_2}$$

- $g$  is a  $\neg$ -gate with input  $g_1$ . Then  $\alpha_g^\ell = \binom{|\text{var}(g)|}{\ell} - \alpha_{g_1}^\ell$

→ We can compute all the values  $\alpha_g^\ell$  in time  $O(|M| \cdot |X|^2)$

# Reduction from computing expectations

Computing expectations problem for a class  $\mathcal{C}$ : Given as input a model  $M \in \mathcal{C}$  and independent probability values on the features, what is the expected value of  $M$ ?

## Reduction (folklore)

For any class  $\mathcal{C}$  of models and under the uniform distribution, computing expectations for  $\mathcal{C}$  reduces to the problem of computing SHAP-scores for  $\mathcal{C}$

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- (One application of the **efficiency axiom**. Notice the **difference with Shapley( $q$ )** (open problem))
- ⇒ Computing SHAP-score is  $\#P$ -hard for CNF or DNF formulas, for instance
  - When a problem is hard, try to **approximate it**
  - We will use the notion of **Fully Polynomial-time Randomized Approximation Scheme (FPRAS)**.



Let  $\Sigma$  be a finite alphabet and  $f : \Sigma^* \rightarrow \mathbb{R}$  be a problem. Then  $f$  is said to have an FPRAS if there is a randomized algorithm  $\mathcal{A} : \Sigma^* \times (0, 1) \rightarrow \mathbb{N}$  and a polynomial  $p(u, v)$  such that, given  $x \in \Sigma^*$  and  $\epsilon \in (0, 1)$ , algorithm  $\mathcal{A}$  runs in time  $p(|x|, 1/\epsilon)$  and satisfies the following condition:

$$\Pr(|f(x) - \mathcal{A}(x, \epsilon)| \leq \epsilon f(x)) \geq \frac{3}{4}.$$

- **Example:** model counting for DNF formulas has a FPRAS [KLM89]

# No FPRAS for DNFs

## Lemma

Computing the SHAP-score for models given as **monotone DNF formulas** has no FPRAS unless  $NP=RP$

This is in contrast to model counting (computing expectations) for DNFs which has a FPRAS!

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## Lemma

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This is in contrast to model counting (computing expectations) for DNFs which has a FPRAS!

- (We did not identify a class of models for which computing the SHAP-score is intractable but where it can be approximated)

Thanks for your attention!



Marcelo Arenas, Pablo Barceló, Leopoldo E. Bertossi, and Mikaël Monet.

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