

# Optimization Problems: Expressibility, Approximation Properties and Expected Asymptotic Growth of Optimal Solutions

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## Abstract

We extend the recent approach of Papadimitriou and Yannakakis that relates the approximation properties of optimization problems to their logical representation.

Our work builds on results by Kolaitis and Thakur who systematically studied the expressibility classes  $\text{MAX } \Sigma_n$  and  $\text{MAX } \Pi_n$  of maximization problems and showed that they form a short hierarchy of four levels. The two lowest levels,  $\text{MAX } \Sigma_0$  and  $\text{MAX } \Sigma_1$  coincide with the classes  $\text{MAX SNP}$  and  $\text{MAX NP}$  of Papadimitriou and Yannakakis; they contain only problems that are approximable in polynomial time up to a constant factor and thus provide a logical criterion for approximability. However, there are computationally very easy maximization problems, such as  $\text{MAXIMUM CONNECTED COMPONENT (MCC)}$  that fail to satisfy this criterion.

We modify these classes by allowing the formulae to contain predicates that are definable in least fixpoint logic. In addition, we maximize not only over relations but also over constants. We call the extended classes  $\text{MAX } \Sigma_i^{\text{FP}}$  and  $\text{MAX } \Pi_i^{\text{FP}}$ . The proof of Papadimitriou and Yannakakis can be extended to  $\text{MAX } \Sigma_1^{\text{FP}}$  to show that all problems in this class are approximable. Some problems, such as  $\text{MCC}$ , descend from the highest level in the original hierarchy to the lowest level  $\text{MAX } \Sigma_0^{\text{FP}}$  in the new hierarchy. Thus our extended class  $\text{MAX } \Sigma_1^{\text{FP}}$  provides a more powerful sufficient criterion for approximability than the original class  $\text{MAX } \Sigma_1$ .

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We separate the extended classes and prove that a number of important problems do not belong to  $\text{MAX } \Sigma_1^{\text{FP}}$ . These include  $\text{MAX CLIQUE}$ ,  $\text{MAX INDEPENDENT SET}$ ,  $\text{V-C DIMENSION}$  and  $\text{MAX COMMON INDUCED SUBGRAPH}$ .

To do this we introduce a new method that characterizes rates of growth of average optimal solution sizes. For instance, it is known that the expected size of a maximal clique in a random graph grows logarithmically with respect to the cardinality of the graph. We show that no problem in  $\text{MAX } \Sigma_1^{\text{FP}}$  can have this property, thus proving that  $\text{MAX CLIQUE}$  is not in  $\text{MAX } \Sigma_1^{\text{FP}}$ . This technique is related to *limit laws for various logics* and to the *probabilistic method* from combinatorics. We believe that this method may be of independent interest.

In contrast to the recent results on the non-approximability of many maximization problems, among them  $\text{MAX CLIQUE}$ , our results do not depend on any unproved hypothesis from complexity theory, such as  $\text{P} \neq \text{NP}$ .

# 1 Introduction

Although the notion of NP-completeness was defined in terms of *decision problems*, the prime motivation for its study and development was the apparent intractability of a large family of combinatorial *optimization problems*. NP-completeness of a decision problem rules out the possibility finding an optimal solution of the corresponding optimization problem in polynomial time unless  $P = NP$ . It does not exclude, however, the possibility that there are efficient algorithms which produce *approximate* solutions. In fact, for many optimization problems with NP-complete decision problems, there are simple and efficient algorithms that produce solutions differing from optimal solutions by at most a constant factor. For some problems, there even exist so-called *polynomial-time approximation schemes* (PTAS), which produce approximate solutions to any desired degree of accuracy. For other problems, notably the Traveling Salesperson Problem, there do not exist efficient approximations unless  $P = NP$  (see [10]). Until now the “structural” reasons for the different approximation properties of NP optimization problems have not been sufficiently understood.

Papadimitriou and Yannakakis [21] provided a new perspective by relating the approximation properties of optimization problems to their logical representation. Exploiting Fagin’s characterization of NP by existential second order logic [9], they defined two classes of optimization problems, MAX SNP and MAX NP, and showed that all problems in these classes are approximable in polynomial time up to a constant factor. They also identified a host of problems that are complete for MAX SNP with respect to so-called *L-reductions*, which preserve polynomial-time approximation schemes. Very recently, the classes MAX SNP and MAX NP have received a lot of attention due to results by Arora et al. [2] showing that problems which are hard for MAX SNP cannot have a PTAS, unless  $P = NP$ .

We present the syntactic criterion of Papadimitriou and Yannakakis in the more general form and notation provided by Kolaitis and Thakur [15].

**Definition 1.1** Recall that  $\Sigma_n$  (respectively  $\Pi_n$ ) are prefix classes in first order logic, consisting of formulae in prefix normal form with  $n$  alternating blocks of quantifiers beginning with  $\exists$  (respectively  $\forall$ ). The classes MAX  $\Sigma_n$  (respectively MAX  $\Pi_n$ ) consist of maximization problems  $Q$  whose input instances are finite structures  $A$  of a fixed signature  $\sigma$ , such that the cost of an optimal solution of  $Q$  on input  $A$  is definable by an expression

$$opt_Q(A) = \max_{\bar{S}} |\{\bar{x} : A \models \psi(\bar{x}, \bar{S})\}|$$

where  $\psi(\bar{x}, \bar{S})$  is a  $\Sigma_n$ -formula (respectively a  $\Pi_n$ -formula) and where  $\bar{S}$  are predicate variables not contained in  $\sigma$ .

## Examples.

1. MAX CUT (MC) is the problem of decomposing the vertex set of a given graph  $G$  into two subsets such that the number of edges between them is maximal. It is in MAX  $\Sigma_0$ :

$$opt_{MC}(G) = \max_U |\{(x, y) : G \models Exy \wedge (Ux \leftrightarrow \neg Uy)\}|.$$

2. MAX SAT is the problem of finding an assignment that satisfies the maximal number of clauses in a given propositional formula in CNF. Such a formula can be represented by

a structure  $F = (U; P, N)$  with universe  $U$  consisting of the clauses and the variables, and with binary predicates  $P$  and  $N$  where  $Pxy$  and  $Nxy$  say that variable  $y$  occurs positively, respectively negatively in clause  $x$ .  $\text{MAX SAT}$  is in  $\text{MAX } \Sigma_1$  with the defining expression

$$\text{opt}_Q(F) = \max_S |\{x : F \models (\exists y)((Sy \wedge Pxy) \vee (\neg Sy \wedge Nxy))\}|.$$

Kolaitis and Thakur proved that  $\text{MAX SAT} \notin \text{MAX } \Sigma_0$ .

3.  $\text{MAX CLIQUE}$  is the problem of finding a clique of maximal size in a graph. The size of such a clique in  $G$  is usually denoted by  $\omega(G)$ .  $\text{MAX CLIQUE}$  is in  $\text{MAX } \Pi_1$  because

$$\omega(G) = \max_C |\{x : G \models Cx \wedge (\forall y)(\forall z)(Cy \wedge Cz) \rightarrow (y = z \vee Eyz)\}|$$

It follows by simple monotonicity arguments [20] that  $\text{MAX CLIQUE}$  is not in  $\text{MAX } \Sigma_1$ . Note that by very recent results in [2], there exists an  $\varepsilon > 0$  such that the  $\text{MAX CLIQUE}$  problem cannot be approximated in polynomial-time within a factor of  $n^\varepsilon$ .

The syntactic criteria for  $\text{MAX SNP}$  and  $\text{MAX NP}$  used by Papadimitriou and Yannakakis are those for  $\text{MAX } \Sigma_0$  (where  $\psi(\bar{x}, \bar{S})$  is quantifier-free) and for  $\text{MAX } \Sigma_1$  (where  $\psi(\bar{x}, \bar{S})$  is existential). However, two remarks about the definitions of these classes should be made. First, the definition of  $\text{MAX } \Sigma_n$  as given above is not really sufficient to establish that all problems in  $\text{MAX } \Sigma_1$  are approximable up to a constant factor, at least if approximability means — as usually understood — that we can actually find in polynomial time a nearly optimal solution. The criterion as given by Definition 1 only allows us to determine the *cost* of an optimal solution up to a constant factor. We will therefore propose a modified notion for the logical representation of an optimization problem which requires that the formula models (in some sense to be made precise later) *all feasible solutions* of the problem, and not just the cost of an optimal one.

Second, it should be noted that in most papers the definitions of the classes  $\text{MAX SNP}$  and  $\text{MAX NP}$  have been interpreted differently than what was originally intended in [21]. While most authors (see [11, 16, 19, 20]) understood  $\text{MAX SNP}$ , respectively  $\text{MAX NP}$  to be *precisely*  $\text{MAX } \Sigma_0$  and  $\text{MAX } \Sigma_1$ , Papadimitriou and Yannakakis actually had in mind their closures under the appropriate reductions (although they did not really make this clear; but see the remark in [22]). In particular, these extended versions of  $\text{MAX SNP}$  and  $\text{MAX NP}$  can also contain minimization problems. Kann [13] defines yet another, intermediate version of  $\text{MAX SNP}$ .

We think that these different classes all have their merits, but it is important not to confuse them. The “pure” syntactic classes are interesting because they provide a logical criterion for approximability, and provide an opportunity to prove results about optimization problems using tools from logic (or, more precisely, finite model theory). In logic we have lower bound techniques that have no counterpart in computational complexity theory. In many cases these techniques (e.g. monotonicity arguments, Ehrenfeucht-Fraïssé games and limit laws) show that a problem does not satisfy a certain syntactic criterion, and thus establish separation and hierarchy results among the syntactic classes (without referring to unproved hypotheses from complexity theory). On the other hand, the closure classes may

be appropriate if one is interested in pure complexity results. But closing syntactic classes under a class of reductions that are defined in terms of computational complexity, rather than logical definability, precludes the use of the logical techniques.

This paper is about syntactic classes. One of our goals was to find a more general syntactic criterion for approximability than the one provided by Papadimitriou and Yannakakis. This is achieved using other results from finite model theory than just Fagin's theorem, in particular the close connection between *fixpoint logic* and polynomial-time computability. To avoid confusion, we will use the names  $\text{MAX } \Sigma_0$  and  $\text{MAX } \Sigma_1$ , introduced by Kolaitis and Thakur, rather than  $\text{MAX SNP}$  and  $\text{MAX NP}$ .

Kolaitis and Thakur [15, 16] systematically investigated the logical expressibility of optimization problems. They proved that the class  $\text{MAX } \mathcal{PB}$ , consisting of all polynomially bounded maximization problems, coincides with  $\text{MAX } \Pi_2$  and that there is proper hierarchy of four levels.

**Theorem 1.2**  $\text{MAX } \Sigma_0 \subsetneq \text{MAX } \Sigma_1 \subsetneq \text{MAX } \Pi_1 \subsetneq \text{MAX } \Pi_2 = \text{MAX } \mathcal{PB}$ .

It is interesting that the classes  $\text{MAX } \Pi_2$  and  $\text{MAX } \Pi_1$  are separated by  $\text{MAXIMUM CONNECTED COMPONENT (MCC)}$ , the problem of finding a connected component of maximal cardinality in a graph. This optimization problem is clearly solvable in polynomial time.

**Remark.** Surprisingly, the situation for *minimization problems* is not dual to the one for maximization problems. There is a proper hierarchy of only two levels:

$$\text{MIN } \Sigma_0 = \text{MIN } \Sigma_1 \subsetneq \text{MIN } \Pi_1 = \text{MIN } \mathcal{PB}.$$

Moreover, even the lowest class  $\text{MIN } \Sigma_0$  contains non-approximable problems. However, Kolaitis and Thakur [16] did isolate a different class (called  $\text{MIN } \text{F}^+\Pi_1$ ) all whose problems are approximable. This class is a proper subclass of  $\text{MIN } \Sigma_0$ .

**New expressibility classes of optimization problems.** In this paper we extend the classes  $\text{MAX } \Sigma_i$  and  $\text{MAX } \Pi_i$  in several ways. Most importantly we allow the formulae to contain relations definable in least fixpoint logic. In addition, we maximize not only over relations but also over constants. We call the extended classes  $\text{MAX } \Sigma_i^{\text{FP}}$  and  $\text{MAX } \Pi_i^{\text{FP}}$ . The proof of Papadimitriou and Yannakakis can be extended to  $\text{MAX } \Sigma_1^{\text{FP}}$  to show that all problems in this class are approximable. Some problems, such as MCC, descend from the highest level  $\text{MAX } \Pi_2$  in the original hierarchy to the lowest level  $\text{MAX } \Sigma_0^{\text{FP}}$  in the new hierarchy. *Thus our extended class  $\text{MAX } \Sigma_1^{\text{FP}}$  provides a more powerful sufficient criterion for approximability than the original class  $\text{MAX } \Sigma_1$  of [21].* However, we also prove that even  $\text{MAX } \Sigma_1^{\text{FP}}$  does not contain all approximable problems; in fact, it does not even contain all polynomial time optimization problems. We discuss the question of how far the class  $\text{MAX } \Sigma_1$  can be extended while preserving approximability. For instance we show that we cannot allow fixpoint definitions (even existential fixpoint definitions) to contain relation variables over which we maximize.

**Separation of the extended classes by the probabilistic method.** We separate also the extended classes; e.g. we prove that

$$\text{MAX } \Sigma_0^{\text{FP}} \subsetneq \text{MAX } \Sigma_1^{\text{FP}} \subsetneq \text{MAX } \Pi_1^{\text{FP}} \subsetneq \text{MAX } \Pi_2^{\text{FP}} = \text{MAX } \mathcal{PB}.$$

Also, we prove that a number of important problems do not belong to  $\text{MAX } \Sigma_1^{\text{FP}}$ . These include  $\text{MAX CLIQUE}$ ,  $\text{MAX INDEPENDENT SET}$ ,  $\text{V-C DIMENSION}$  and  $\text{MAX COMMON INDUCED SUBGRAPH}$ .

To do this we have to use more sophisticated methods than the techniques of [20, 15] which break down in the presence of fixpoint definitions. We use two alternative methods.

The first method, introduced in the present paper, characterizes rates of growth of average optimal solution sizes. For instance, it is known [4] that the expected size of a maximal clique in a random graph of cardinality  $n$  grows asymptotically like  $2 \log n$ . We show that no problem in  $\text{MAX } \Sigma_1^{\text{FP}}$  can have this property, thus proving that  $\text{MAX CLIQUE}$  is not in  $\text{MAX } \Sigma_1^{\text{FP}}$ . This technique is related to *limit laws for various logics* [8, 17, 18] and to the *probabilistic method* from combinatorics [1]. We believe that this method may be of independent interest.

The second method uses special classes of structures where fixpoint logic has no more expressive power than quantifier-free formulae. On such classes we can apply monotonicity arguments that break down on arbitrary finite structures. With this technique we give an alternative proof that  $\text{MAX CLIQUE}$  is not in  $\text{MAX } \Sigma_1^{\text{FP}}$ . We also show that  $\text{MAX MATCHING}$  is not expressible by existential sentences with fixpoint definitions.

## 2 Preliminaries

**Definition 2.1** An NP *optimization problem* is a quadruple  $Q = (I_Q, \mathcal{F}_Q, f_Q, \text{opt})$  such that

- $I_Q$  is the set of *input instances* for  $Q$ .
- $\mathcal{F}_Q(I)$  is the set of *feasible solutions* for input  $I$ . Here, “feasible” means that the size of the elements  $S \in \mathcal{F}_Q(I)$  is polynomially bounded in the size of  $I$  and that the set  $\{(I, S) : S \in \mathcal{F}_Q(I)\}$  is recognizable in polynomial time.
- $f_Q : \{(I, S) : S \in \mathcal{F}_Q(I)\} \rightarrow \mathbb{N}$  is a polynomial-time computable function, called the *cost function*.
- $\text{opt} \in \{\max, \min\}$ .

For every NP optimization problem  $Q$ , the following decision problem is in NP: given an instance  $I$  of  $Q$  and a natural number  $k$ , is there a solution  $S \in \mathcal{F}_Q(I)$  such that  $f_Q(I, S) \geq k$  when  $\text{opt} = \max$ , (or  $f_Q(I, S) \leq k$ , when  $\text{opt} = \min$ ).

Let  $\text{opt}_Q(I) := \text{opt}_{S \in \mathcal{F}_Q(I)} f_Q(I, S)$ . An NP optimization problem is said to be *polynomially bounded* if there exists a polynomial  $p$  such that  $\text{opt}_Q(I) \leq p(|I|)$  for all instances  $I$ . We denote by  $\text{MAX } \mathcal{PB}$  ( $\text{MIN } \mathcal{PB}$ ) the set of all polynomially bounded maximization (minimization) problems.

**Approximation.** The *performance ratio* of a feasible solution  $S$  for an instance  $I$  of  $Q$  is defined as  $R(I, S) := \text{opt}_Q(I) / f_Q(I, S)$  if  $Q$  is a maximization problem and as  $R(I, S) := f_Q(I, S) / \text{opt}_Q(I)$  if  $Q$  is a minimization problem.

**Definition 2.2** We say that an NP optimization problem  $Q$  is *approximable up to a constant factor* if there exists a constant  $c > 0$  and a polynomial-time algorithm  $\Pi$  which produces, for every instance  $I$  of  $Q$ , a feasible solution  $\Pi(I)$  with performance ratio  $R(I, \Pi(I)) \leq c$ . APX is the class of all NP optimization problems that are approximable up to a constant factor.

A weaker notion of approximability that is sometimes used requires only that the *cost* of an optimal solution can be approximated; for instance, in the case of MAX CLIQUE it would only be required that the algorithm approximates the clique number  $\omega(G)$ , not that it actually finds a nearly optimal clique.

**Logical representation of optimization problems.** Let  $Q$  be an optimization problem whose input instances are finite structures of fixed vocabulary  $\sigma$ . The definition of the classes MAX  $\Sigma_n$  and MAX  $\Pi_n$  as given by Kolaitis and Thakur requires only that there is an appropriate logical definition of  $opt_Q(A)$ , the cost of an optimal solution. However, optimization problems can be modelled by logical formulae in a much closer way.

**Definition 2.3** A formula  $\psi(\bar{x}, \bar{S})$  of vocabulary  $\sigma \cup \{S_1, \dots, S_r\}$  represents  $Q$  if and only if the following holds.

- (i) For every instance  $A$  and every feasible solution  $S_0 \in \mathcal{F}_Q(A)$ , there exists an expansion  $B = (A, S_1, \dots, S_r)$  of  $A$  such that

$$f_Q(A, S_0) = |\{\bar{x} : B \models \psi(\bar{x}, \bar{S})\}|.$$

- (ii) Conversely, every expansion  $B = (A, S_1, \dots, S_r)$ , for which the set  $L = \{\bar{x} : B \models \psi(\bar{x}, \bar{S})\}$  is non-empty defines a feasible solution  $S_0$  for  $A$  with  $f_Q(A, S_0) = |L|$ ; moreover, this solution can be computed in polynomial time from  $B$ .

In particular, the cost of an optimal solution for  $A$  is  $opt_Q(A) = \max_{\bar{S}} |\{\bar{x} : A \models \psi(\bar{x}, \bar{S})\}|$ .

In all examples that we consider, the feasible solution defined by  $(A, S_1, \dots, S_r)$  will either be one of the  $S_i$  or the set  $\{\bar{x} : A \models \psi(\bar{x}, \bar{S})\}$  itself. Lautemann [19] has independently considered this more detailed logical representation of optimization problems. A more constructive alternative to Definition 1 might then be the following.

**Definition 2.4** MAX  $\Sigma_n$  is the class of all maximization problems that can be represented by  $\Sigma_n$ -formulae. The classes MAX  $\Pi_n$ , MIN  $\Sigma_n$  and MIN  $\Pi_n$  are defined analogously.

Clearly this definition is more restrictive than the one used by Kolaitis and Thakur. We think that it is justified by the following observations. First, the more restrictive definition is necessary to establish the result of Papadimitriou and Yannakakis that MAX  $\Sigma_1 \subseteq$  APX. Second, on all natural examples in the literature, the two definitions make no difference. Third, the results of Kolaitis and Thakur, in particular the fact that

$$\text{MAX } \Sigma_0 \subsetneq \text{MAX } \Sigma_1 \subsetneq \text{MAX } \Pi_1 \subsetneq \text{MAX } \Pi_2 = \text{MAX } \mathcal{PB}$$

remain true with the more restrictive definition. (However, the proof that MAX  $\Pi_2 =$  MAX  $\mathcal{PB}$  needs some modification.)

All results presented in this paper are true for both possible choices of logical representation of optimization problems. However, if the more liberal one (modelling only the cost of the optimal solution) is chosen, then the more liberal definition of approximability must also be adopted.

**Fixpoint logic.** It is well-known that the expressive power of first-order logic is limited by the lack of a mechanism for unbounded iteration or recursion. The most notable example of a query that is not first-order expressible is the transitive closure (TC) of a relation. This has motivated the study of more powerful languages that add recursion in one way or another to first-order logic. The most prominent of these are the various forms of *fixpoint logics*.

Let  $\sigma$  be a signature,  $P$  an  $r$ -ary predicate not in  $\sigma$  and  $\psi(\bar{x})$  be a formula of the signature  $\sigma \cup \{P\}$  with only positive occurrences of  $P$  and with free variables  $\bar{x} = x_1, \dots, x_r$ . Then  $\psi$  defines for every finite  $\sigma$ -structure  $A$  with universe  $|A|$  an operator  $\psi^A$  on the class of  $r$ -ary relations over  $|A|$  by

$$\psi^A : P \mapsto \{\bar{a} : (A, P) \models \psi(\bar{a})\}.$$

Since  $P$  occurs only positively in  $\psi$ , this operator is monotone, i.e.  $Q \subseteq P$  implies that  $\psi^A(Q) \subseteq \psi^A(P)$ . Therefore this operator has a *least fixed point* which may be constructed inductively beginning with the empty relation. Set  $\Psi^0 := \emptyset$  and  $\Psi^{j+1} := \psi^A(\Psi^j)$ . At some stage  $i$ , this process reaches a stable predicate  $\Psi^i = \Psi^{i+1}$ , which is the *least fixed point* of  $\psi$  on  $A$ , and denoted by  $\Psi^\infty$ . Since  $\Psi^i \subseteq \Psi^{i+1}$ , the least fixed point is reached in a polynomial number of iterations, with respect to the cardinality of  $A$ .

The fixed point logic (FO + LFP) is defined by adding to the syntax of first order logic the *least fixed point formation rule*: if  $\psi(\bar{x})$  is a formula of the signature  $\sigma \cup \{P\}$  with the properties stated above and  $\bar{u}$  is an  $r$ -tuple of terms, then

$$[\text{LFP}_{P, \bar{x}} \psi](\bar{u})$$

is a formula of vocabulary  $\sigma$  (to be interpreted as  $\Psi^\infty(\bar{u})$ ).

**Example.** Here is a fixpoint formula that defines the transitive closure of the binary predicate  $E$ :

$$\text{TC}(u, v) \equiv [\text{LFP}_{T, x, y} (x = y) \vee (\exists z)(Exz \wedge Tzy)](u, v).$$

On the class of all finite structures, (FO + LFP) has strictly more expressive power than first-order logic — it can express the transitive closure — but is strictly weaker than PTIME-computability. However, Immerman [12] and Vardi [23] proved that on *ordered structures* the situation is different. There (FO + LFP) characterizes precisely the queries that are computable in polynomial time. On the other hand, on very simple classes of structures, such as structures with empty signatures (i.e. sets), (FO + LFP) collapses to first-order logic.

### 3 Optimization problems definable by fixpoint logic

The fact that the problem MAXIMUM CONNECTED COMPONENT (MCC) appears only in the highest level MAX  $\Pi_2$  of the expressibility hierarchy suggests that we do not yet have



the “right” definitions. After all, MCC is computationally a very simple problem, and it appears high in the expressibility hierarchy just because first-order logic cannot express the transitive closure.

It is possible that there will always remain a certain “mismatch” between computational complexity and logical expressibility. But this mismatch is certainly not as big as the difference between first-order logic and PTIME. If we base our definitions on fixpoint logic (or other logical systems that allow recursion) rather than first-order logic, we obtain a closer relationship between logical and computational complexity.

**Definition 3.1** Let  $Q$  be a maximization problem whose instances are finite structures over a fixed vocabulary  $\sigma$ . We say that  $Q$  belongs to the class  $\text{MAX } \Sigma_i^{\text{FP}}$  if there exists a  $\Sigma_i$ -formula  $\psi(\bar{x}, \bar{c}, \bar{S}, \bar{P})$  of vocabulary  $\sigma \cup \{\bar{S}, \bar{c}\}$  (where  $\bar{S}$  and  $\bar{c}$  are tuples of predicate symbols and constants that do not occur in  $\sigma$ ) such that

- $\bar{P} = P_1, \dots, P_r$  are global predicates on  $\sigma$ -structures that are definable in fixpoint logic.
- the formula  $\psi(\bar{x}, \bar{c}, \bar{S}, \bar{P})$  represents  $Q$  (in the sense of Definition 2, with the obvious modifications). In particular,  $\text{opt}_Q(A) = \max_{\bar{S}, \bar{c}} |\{\bar{x} : A \models \psi(\bar{x}, \bar{c}, \bar{S}, \bar{P})\}|$ .

The classes  $\text{MAX } \Pi_i^{\text{FP}}$ ,  $\text{MIN } \Sigma_i^{\text{FP}}$  and  $\text{MIN } \Pi_i^{\text{FP}}$  are defined in an analogous way.

We insist that the fixpoint-predicates must not depend on the relations  $\bar{S}$  over which we maximize; we therefore call them *predefined fixpoint predicates*. (We will discuss this condition as well as the adequacy of our definitions and possible alternatives below).

The results of Kolaitis and Thakur [15] translate to these extended classes and prove

**Proposition 3.2** (i)  $\text{MAX } \Sigma_0^{\text{FP}} \subseteq \text{MAX } \Sigma_1^{\text{FP}} \subseteq \text{MAX } \Sigma_2^{\text{FP}} = \text{MAX } \Pi_1^{\text{FP}} \subseteq \text{MAX } \Pi_2^{\text{FP}} = \text{MAX } \mathcal{PB}$ .

(ii)  $\text{MIN } \Sigma_0^{\text{FP}} = \text{MIN } \Sigma_1^{\text{FP}} \subseteq \text{MIN } \Sigma_2^{\text{FP}} = \text{MIN } \Pi_1^{\text{FP}} = \text{MIN } \mathcal{PB}$ .

In this paper we will concentrate mainly on maximization problems. The increased expressive power provided by the fixpoint predicates has the effect that some problems occur in lower levels in the new hierarchy than they did in the original one.

**Example.** The problem MAXIMUM CONNECTED COMPONENT belongs to  $\text{MAX } \Sigma_0^{\text{FP}}$ . Its optimum on a graph  $G = (V, E)$  is definable by

$$\text{opt}_{\text{MCC}}(G) = \max_c |\{x : G \models [\text{TC } E](c, x)\}|.$$

Thus MCC descends from the highest level ( $\text{MAX } \Pi_2$ ) of the original hierarchy to the lowest level ( $\text{MAX } \Sigma_0^{\text{FP}}$ ) of the new hierarchy. This is interesting because, as we will see in a moment, also the extended class  $\text{MAX } \Sigma_1^{\text{FP}}$  (and therefore  $\text{MAX } \Sigma_0^{\text{FP}}$ , too) contains only problems in APX. Thus our approach provides a more powerful syntactic criterion for approximability than the original class  $\text{MAX } \Sigma_1$ . However, we will show that  $\text{MAX } \Sigma_1^{\text{FP}}$  does not capture all polynomial-time solvable maximization problems. Let us consider to what extent our definitions are adequate and discuss some alternatives.

**Maximization over constants.** Does maximization over constants really give more power? We prove that it does up to the level  $\text{MAX } \Sigma_1^{\text{FP}}$ , but that for  $\text{MAX } \Pi_1^{\text{FP}}$  and  $\text{MAX } \Pi_2^{\text{FP}}$ , we can do without it.

First of all, maximization over constants avoids trivialities. For instance, Kann [13] observed that the proof showing that  $\text{MAX CLIQUE}$  is not in  $\text{MAX } \Sigma_1$  applies even to graphs whose degree bounded by a constant  $d$ , although the problem becomes trivially solvable in polynomial time. With constants the optimum for  $\text{MAX CLIQUE}(d)$  can be defined (even without fixpoint predicates) by

$$\max_{c_0, \dots, c_d} |\{x : G \models \bigvee_i x = c_i \wedge \bigwedge_{i < j} (E c_i c_j \vee c_i = c_j)\}|.$$

Thus,  $\text{MAX CLIQUE}(d) \in \text{MAX } \Sigma_0^{\text{FP}} - \text{MAX } \Sigma_1$ . But even in the presence of fixpoint predicates, constants make a difference, as the following proposition shows.

**Proposition 3.3** *MAX CONNECTED COMPONENT is not expressible in  $\text{MAX } \Sigma_1^{\text{FP}}$  without maximization over constants.*

**PROOF.** Let  $G_n$  be the graph with  $n$  vertices and no edges. Obviously,  $\text{opt}_{\text{MCC}}(G_n) = 1$  for all  $n$ . Moreover, for every fixpoint-definable predicate  $P$ , there exists a natural number  $n_0$  such that  $P$  is in fact  $\Sigma_0$ -definable on  $\{G_n : n > n_0\}$ . Therefore, if MCC is expressible in  $\text{MAX } \Sigma_1^{\text{FP}}$  without constants, then there is an existential formula  $\psi(\bar{x}, \bar{S})$  (without fixpoint predicates), such that for all  $n > n_0$

$$\text{opt}_{\text{MCC}}(G_n) = \max_{\bar{S}} |\{\bar{x} : G_n \models \psi(\bar{x}, \bar{S})\}| = 1.$$

Choose a tuple  $\bar{u} \in G_n$  and predicates  $\bar{S}$  such that  $G_n \models \psi(\bar{u}, \bar{S})$ . Note that  $G_{2n}$  consists of two disjoint copies of  $G_n$ ; let  $\bar{S}^*$  be the union of the two copies of  $\bar{S}$ . Existential sentences are preserved by extensions, so there exist at least two tuples  $\bar{u}$ , satisfying  $G_{2n} \models \psi(\bar{u}, \bar{S}^*)$ . This contradicts the fact that  $\text{opt}_{\text{MCC}}(G_n) = 1$ .  $\blacksquare$

Another simple problem that requires maximization over constants is the *maximal degree*  $\Delta(G)$  of a graph, defined by

$$\Delta(G) = \max_c |\{x : G \models Ecx\}|.$$

Similar monotonicity arguments as above show that  $\Delta(G)$  is not definable in  $\text{MAX } \Sigma_1^{\text{FP}}$  without maximization over constants.

**Proposition 3.4** *Every problem in  $\text{MAX } \Pi_1^{\text{FP}}$  or  $\text{MAX } \Pi_2^{\text{FP}}$  can be expressed without maximization over constants.*

**PROOF.** Constants can be replaced by monadic predicates at the expense of a  $\Sigma_2$ -subformula. An expression

$$\text{opt}_Q(A) = \max_{\bar{c}, \bar{S}} |\{\bar{x} : A \models \psi(\bar{x}, \bar{c}, \bar{S})\}|$$

can be translated into

$$\text{opt}_Q(A) = \max_{\bar{C}, \bar{S}} |\{\bar{x} : A \models (\exists \bar{u})(\forall \bar{v}) \bigwedge_i (C_i v_i \leftrightarrow v_i = u_i) \wedge \psi(\bar{x}, \bar{u}, \bar{S})\}|.$$

The proof of Kolaitis and Thakur [15] that  $\text{MAX } \Sigma_2 = \text{MAX } \Pi_1$  and  $\text{MAX } \Sigma_3 = \text{MAX } \Pi_2$  applies also to this case and allows us to eliminate the leading existential quantifiers. ■

**Fixpoint definitions over the new predicates.** To strengthen our classes we could modify the definition of  $\text{MAX } \Sigma_i^{\text{FP}}$  so that the fixpoint predicates might depend also on the predicates  $\bar{S}$  over which we maximize. In fact, one could propose classes of all maximization problems  $Q$  such that

$$\text{opt}_Q(A) = \max_{\bar{S}} |\{\bar{x} : A \models \psi(\bar{x}, \bar{S})\}|$$

where  $\psi(\bar{x}, \bar{S})$  is a formula of (FO + LFP), possibly with restrictions on the quantifier structure. If we stipulate that  $\psi(\bar{x}, \bar{S})$  has the form  $[\text{LFP}_{R, \bar{z}} \varphi](\bar{u})$  with  $\varphi$  quantifier-free then we will remain inside  $\text{MAX } \Sigma_0$  because fixpoints over quantifier-free formulae are again  $\Sigma_0$ -definable. The next stronger possible class, motivated by the existential nature of the class  $\text{MAX } \Sigma_1$  is the class  $\text{MAX EFP}$  defined as above with the condition that  $\psi(\bar{x}, \bar{S}) \equiv [\text{LFP}_{R, \bar{z}} \varphi](\bar{u})$  where  $\varphi$  is existential. In particular  $\psi(\bar{x}, \bar{S})$  is a formula in *existential fixpoint logic* [3] or, equivalently, a query in  $\text{Datalog}(\neg)$ , i.e.  $\text{Datalog}$  with negations over the EDB-predicates [14]. However, this class is already too expressive.

**Proposition 3.5** *If  $P \neq NP$ , then  $\text{MAX EFP}$  contains non-approximable problems.*

**PROOF.** We consider the following variant of circuit satisfiability. A circuit is described by a finite structure  $C = (V, E, I, \text{out})$  where  $(V, E)$  is a directed acyclic graph,  $I \subseteq V$  is the set of sources (vertices with no incoming edges) describing the input nodes, every node in  $V - I$  has fan-in two, and  $\text{out}$  is a sink (no outgoing edges). Every non-input node is considered as a NAND-gate and  $\text{out}$  is the output node. Every subset  $S \subseteq I$  defines an assignment to the input nodes, and therefore a value  $f_C(S) \in \{0, 1\}$ , the value computed by  $C$  for input  $S$ .

Now the circuit-satisfiability problem is

$$\text{CIRCUIT-SAT} := \{C : (\exists S \subseteq I) f_C(S) = 1\}.$$

Since a Boolean formula is a special case of a circuit, it is clear that  $\text{CIRCUIT-SAT}$  generalizes  $\text{SAT}$  and is therefore NP-complete.

On the other hand, we can construct a formula  $\psi(S)$  in existential fixpoint logic such that

$$C \models \psi(S) \iff f_C(S) = 1.$$

We can assume that we have two distinct constants 0 and 1 available. Then

$$\psi(S) \equiv [\text{LFP}_{B, x, i} \varphi(S, B, x, i)](\text{out}, 1)$$

where  $\varphi(S, B, x, i)$  is the disjunction of the subformulae

$$\begin{aligned}Ix \wedge Sx \wedge i &= 1 \\Ix \wedge \neg Sx \wedge i &= 0 \\i &= 1 \wedge (\exists y)(Eyx \wedge By0) \\i &= 0 \wedge (\exists y)(\exists z)(Eyx \wedge Ezx \wedge By1 \wedge Bz1)\end{aligned}$$

Note that  $\varphi(S, B, x, i)$  inductively defines the predicate  $Bxi$  saying that the value computed by  $C$  at node  $x$  is  $i$ .

We now can define a problem  $Q \in \text{MAX EFP}$  by

$$\text{opt}_Q(C) = \max_S |\{x : C \models \psi(S)\}|.$$

Note that  $x$  does not occur freely in  $\psi$ , so  $\text{opt}_Q(C) = |V|$  if  $C \in \text{CIRCUIT-SAT}$  and  $\text{opt}_Q(C) = 0$  otherwise. Therefore, if  $Q$  were approximable up to any constant  $\varepsilon > 0$ , then the corresponding approximation algorithm would solve the **CIRCUIT-SAT** problem, and it would follow that  $P = NP$ .  $\blacksquare$

**Maximization over total orderings.** Papadimitriou and Yannakakis [21] proposed another direction for generalization: to maximize over total orderings. A natural problem expressible in this way is **MAX SUBDAG**: given a digraph  $G$ , find an acyclic subgraph of  $G$  with maximal number of edges. The expression defining the optimum for this problem is

$$\text{opt}_Q(G) = \max_{\prec} |\{(x, y) : G \models Exy \wedge x < y\}|.$$

This suggests the following definition.

**Definition 3.6** For every class  $M$ , as defined in Definitions 2 or 3, let  $M(<)$  defined in the same way as  $M$ , except that some of relations over which we optimize are binary predicates  $<_1, <_2, \dots$ , which do not run over all binary predicates, but only over total orderings of the given structure. We write the defining expression of an optimization problem in  $M(<)$  on an input structure  $A$  as

$$\text{opt}_Q(A) = \text{opt}_{\prec, \bar{S}, \bar{c}} |\{\bar{x} : A \models \psi(\bar{x}, \bar{c}, \prec, \bar{S}, \bar{P})\}|.$$

As remarked in [21] this feature does not destroy approximability:  $\text{MAX } \Sigma_1^{\text{FP}} \subseteq \text{APX}$ . (We prove a more general fact below.)

Note that for classes  $\text{MAX } \Pi_1$  and above, maximization over orderings does not increase the expressive power, because total orderings are axiomatizable by  $\Pi_1$ -formulae. Thus  $\text{MAX } \Pi_1(<) = \text{MAX } \Pi_1$  and  $\text{MAX } \Pi_1^{\text{FP}}(<) = \text{MAX } \Pi_1^{\text{FP}}$ , etc.

**Maximization over general classes of relations.** How far can we generalize the idea of the previous paragraph? Instead of just maximizing over orderings, we could maximize over any specified class of predicates. Let  $\bar{C} = C_1, \dots, C_q$  where each  $C_i$  is a class of relations of some fixed arity  $r_i$ . We now maximize over tuples  $\bar{S} = S_1, \dots, S_q$  of relations, subject to

the condition that  $S_i \in \mathcal{C}_i$ . The expression defining the cost of an optimal solution then has the form

$$\text{opt}_Q(A) = \text{opt}_{\bar{S} \in \bar{\mathcal{C}}, \bar{c}} |\{\bar{x} : A \models \psi(\bar{x}, \bar{c}, \bar{S}, \bar{P})\}|.$$

For any class  $M$  of Definitions 2 or 3, and any  $\bar{\mathcal{C}}$ , this defines a new class  $M(\bar{\mathcal{C}})$ . The classes  $M(<)$  are special cases.

In view of our goal to find a good criterion for approximability, we ask what condition  $\bar{\mathcal{C}}$  must satisfy so that problems in  $\text{MAX } \Sigma_1^{\text{FP}}(\bar{\mathcal{C}})$  be approximable. We give such a condition here, and prove a general form of the Theorem of Papadimitriou and Yannakakis.

**Definition 3.7** For every  $n \in \mathbb{N}$ , let  $\mathcal{C}(n)$  be a class of relations of fixed arity  $r$  over  $n$  and let  $\mathcal{C} = \bigcup_n \mathcal{C}(n)$ . We say that  $\mathcal{C}$  is *well-behaved* if for every  $k \in \mathbb{N}$  there exists a number  $\varepsilon(k) > 0$  such that for all  $n$  and for any set of conditions  $\alpha_1, \dots, \alpha_k$  of the form  $S(\bar{u})$  or  $\neg(S\bar{u})$ , (where  $\bar{u}$  are  $r$ -tuples over  $n$ ) the probability that  $\alpha_1 \wedge \dots \wedge \alpha_k$  is satisfied by a randomly chosen relation  $S \in \mathcal{C}(n)$ , is computable in polynomial time, and is either 0 or at least  $\varepsilon(k)$ .

**Examples.**

- The class of all  $r$ -ary relations is well-behaved with  $\varepsilon(k) = 2^{-k}$ .
- If we fix, in a consistent manner, an ordering on  $k$  pairs of elements then there are at least  $n!/(2k)!$  ways to extend this to a total ordering. Thus, the class of all total orderings is also well-behaved with  $\varepsilon(k) = ((2k)!)^{-1}$ .
- The class of unary functions, represented by binary relations, is not well-behaved. If we fix one value  $f(u) = v$ , then the probability that a function on  $n$  satisfies this condition is  $1/n$ .
- The class  $\mathcal{E} = \bigcup \mathcal{E}(n)$  of equivalence relations is not well-behaved. An equivalence relation on  $n$  satisfies a condition  $u \sim v$  with probability  $|\mathcal{E}(n-1)|/|\mathcal{E}(n)|$ . The asymptotic estimate for  $|\mathcal{E}(n)|$  (called the  $n$ -th Bell number) developed in [7] proves that his quotient tends to 0 as  $n$  goes to infinity.

A tuple  $\bar{\mathcal{C}}$  of well-behaved classes is again well-behaved, in the sense that the probability that any  $k$  atomic formulae  $S_i(\bar{u})$  or  $\neg S_i(\bar{u})$  are satisfied has the properties required by Definition 3.

**Theorem 3.8** *If  $\bar{\mathcal{C}}$  is well-behaved then every maximization problem in  $\text{MAX } \Sigma_1^{\text{FP}}(\bar{\mathcal{C}})$  is approximable up to a constant factor.*

PROOF. Let  $Q$  be a maximization problem, such that for all input structures  $A \in I_Q$

$$\text{opt}_Q(A) = \max_{\bar{S} \in \bar{\mathcal{C}}, \bar{c}} |\{\bar{x} : A \models (\exists \bar{y})\psi(\bar{x}, \bar{y}, \bar{c}, \bar{S}, \bar{P})\}|$$

where  $\psi$  is a quantifier-free formula with predefined fixpoint predicates  $\bar{P}$ . Fix an input structure  $A$  of cardinality  $n$ . The fixpoint predicates can be evaluated in polynomial time, so we may assume that they are part of the input, and not worry about them anymore.

Moreover, there are only polynomially many possible tuples  $\bar{c}$ , so we can compute the optimum for each of them separately; thus we can assume that the value of  $\bar{c}$  is fixed. To enhance readability we drop  $\bar{P}$  and  $\bar{c}$  and write  $\psi(\bar{x}, \bar{y}, \bar{S})$  in the sequel.

We consider the class  $\bar{\mathcal{C}}(n)$  as a probability space  $\Omega$  with uniform distribution. Define the random variable  $X^A$  on  $\Omega$  by

$$X^A(\bar{S}) = |\{\bar{u} : A \models (\exists \bar{y})\psi(\bar{u}, \bar{y}, \bar{S})\}|.$$

Obviously  $\text{opt}_Q(A) = \max(X^A) \geq E(X^A)$  where  $E(X^A)$  is the expected value of  $X^A$ . Note that  $X^A$  can be written as the sum of the indicator random variables

$$X_{\bar{u}}^A(\bar{S}) = \begin{cases} 1 & \text{if } A \models (\exists \bar{y})\psi(\bar{u}, \bar{y}, \bar{S}) \\ 0 & \text{otherwise} \end{cases}$$

By linearity of expectation  $E(X^A) = \sum_{\bar{u}} E(X_{\bar{u}}^A)$ . In this sum we can discard those  $X_{\bar{u}}^A$  which are identically 0, so let

$$B^A := \{\bar{u} : X_{\bar{u}}^A \neq 0\} = \{\bar{u} : A \models (\exists \bar{y})\psi(\bar{u}, \bar{y}, \bar{S}) \text{ for some } \bar{S} \in \bar{\mathcal{C}}(n)\}$$

Now

$$E(X^A) = \sum_{\bar{u} \in B^A} E(X_{\bar{u}}^A) \leq |B^A|.$$

Fix  $\bar{u} \in B^A$ . There exist predicates  $\bar{S}^* \in \Omega$  and a tuple  $\bar{v}$  such that  $A \models \psi(\bar{u}, \bar{v}, \bar{S}^*)$ . This formula depends only a fixed number  $\alpha_1, \dots, \alpha_k$  of  $\bar{S}$ -atoms, and every tuple  $\bar{S} \in \Omega$  respecting the values of  $\alpha_1, \dots, \alpha_k$  on  $\bar{S}^*$  will also satisfy  $\psi(\bar{u}, \bar{v}, \bar{S})$ . Since  $\bar{\mathcal{C}}$  is well-behaved, the probability that a randomly chosen  $\bar{S}$  has this property is at least  $\varepsilon(k)$ . Thus,  $E(X_{\bar{u}}^A) \geq \varepsilon(k)$  for every  $\bar{u} \in B^A$ . This implies

$$|B^A| \geq \max(X^A) \geq E(X^A) \geq \varepsilon(k)|B^A|$$

and, in particular,  $E(X^A) \geq \varepsilon(k) \text{opt}_Q(A)$ .

It remains to prove that an assignment  $\bar{S}^* \in \Omega$  with  $X^A(\bar{S}^*) \geq E(X^A)$  can be found in polynomial time. Enumerate all atoms  $S_i(\bar{u})$  as  $\alpha_1, \dots, \alpha_m$ . Clearly  $m$  is a polynomial in  $n$ . We determine truth-values for  $\alpha_1, \dots, \alpha_m$  as follows.

Suppose values for  $\alpha_1, \dots, \alpha_i$  are already computed, and let  $\beta_i$  be the conjunction of those  $\alpha_j$  and  $\neg\alpha_j$  (for  $j \leq i$ ) that have been set to TRUE. Now we define  $\alpha_{i+1}$  to be TRUE if

$$E(X^A | (\beta_i \wedge \alpha_{i+1})) \geq E(X^A | (\beta_i \wedge \neg\alpha_{i+1}))$$

and FALSE otherwise. Note that these conditional expectations can be computed in polynomial time, by the same arguments as in the first part of this proof and because  $\bar{\mathcal{C}}$  is well-behaved. At the end,  $\beta_m$  determines relations  $\bar{S}^*$ , so  $E(X^A | \beta_m) = X^A(\bar{S}^*)$ . Note that

$$\begin{aligned} E(X^A | \beta_i) &= P(\alpha_{i+1} | \beta_i) E(X^A | (\beta_i \wedge \alpha_{i+1})) + P(\neg\alpha_{i+1} | \beta_i) E(X^A | (\beta_i \wedge \neg\alpha_{i+1})) \\ &\leq E(X^A | \beta_{i+1}) \end{aligned}$$

where  $P(\alpha_{i+1} | \beta_i)$  is the conditional probability that  $\alpha_{i+1}$  holds, given that  $\beta_i$  is TRUE. In particular

$$E(X^A) = E(X^A | \beta_0) \leq E(X^A | \beta_m) = X^A(\bar{S}^*).$$

This technique for “derandomizing” a probabilistic argument is well known. Alon and Spencer [1] call it *the method of conditional expectations*. ■

## 4 Probabilistic methods

Let  $Q$  be an optimization problem whose input instances are finite structures over a fixed vocabulary  $\sigma$ . We now consider the behaviour of  $\text{opt}_Q(A)$  on a *randomly chosen*  $\sigma$ -structures  $A$ . Fix  $n$  and let  $\Omega$  be the probability space of all  $\sigma$ -structures over universe  $n$ , with uniform distribution; then  $\text{opt}_Q$  is a random variable on  $\Omega$  whose expected value is denoted by  $E(\text{opt}_Q)$ .

We will establish a probabilistic (necessary) criterion for membership in  $\text{MAX } \Sigma_1^{\text{FP}}$ . In fact it holds for any class  $\text{MAX } \Sigma_1^{\text{FP}}(\bar{C})$  provided that  $\bar{C}$  is  $\Sigma_2$ -axiomatizable. In particular, our criterion applies to  $\text{MAX } \Sigma_1^{\text{FP}}(<)$ , since linear orderings are in fact  $\Pi_1$ -axiomatizable.

**Theorem 4.1 (Probabilistic criterion for  $\text{MAX } \Sigma_1^{\text{FP}}$ )** *Let  $Q$  be a problem in  $\text{MAX } \Sigma_1^{\text{FP}}(\bar{C})$  where  $\bar{C}$  is  $\Sigma_2$ -axiomatizable. Then there exists a polynomial  $p(n)$  and a constant  $\varepsilon > 0$  such that*

$$p(n) \geq E(\text{opt}_Q) \geq \varepsilon p(n)$$

or  $E(\text{opt}_Q)$  decreases to 0 exponentially fast as  $n$  goes to infinity.

Before we prove Theorem 4.1, we assemble some results from the theory of asymptotic probabilities that we need. As usual, we denote by  $\mu_n(\psi)$  the probability that the sentence  $\psi$  is true in a random structure with universe  $n$ .

**Fact 4.2** *For every formula  $\varphi(\bar{x})$  in fixpoint logic, there exists a quantifier-free first-order formula  $\alpha(\bar{x})$  and a constant  $c > 0$  such that*

$$\mu_n((\forall \bar{x})[\varphi(\bar{x}) \leftrightarrow \alpha(\bar{x})]) > 1 - c^n$$

for large enough  $n$ .

In fact this result is true even for stronger logics than fixpoint logic, e.g. the infinitary logic  $L_{\infty\omega}^\omega$ . It is essentially Theorem 3.13 in [18]. The second fact that we need is a generalization of the 0-1 law for strict  $\Sigma_1^1$ -sentences, due to Kolaitis and Vardi [17]. Strict  $\Sigma_1^1$ -formulae have the form  $(\exists \bar{S})(\exists \bar{y})(\forall \bar{z})\varphi$  where  $\varphi$  is quantifier-free. A dyadic rational is a rational number whose denominator is a power of two.

**Fact 4.3** *Let  $\psi(\bar{x})$  be a strict  $\Sigma_1^1$ -formula with free variables  $\bar{x} = x_1, \dots, x_k$ . For every  $k$ -tuple  $\bar{u} \in \mathbb{N}^k$ , there exists a dyadic rational  $p_{\bar{u}}$ , such that  $\mu_n(\psi(\bar{u}))$  tends to  $p_{\bar{u}}$  exponentially fast. Moreover,  $p_{\bar{u}}$  only depends on the equality type of  $u_1, \dots, u_k$  (not on  $\bar{u}$  itself).*

Finally we will need a Lemma about binomial distributions  $b(n, k, p) := \binom{n}{k} p^k q^{n-k}$  where  $0 \leq p \leq 1$  and  $q = 1 - p$ .

**Lemma 4.4** *If  $\varepsilon > 0$  and  $k \geq (1 + \varepsilon)pn$ , then  $b(n, k, p)$  tends to 0 exponentially fast as  $n$  goes to infinity.*

For a proof, see [4, p. 10] or [1, Appendix A].

PROOF OF THEOREM 4.1. Let  $Q \in \text{MAX } \Sigma_1^{\text{FP}}(\bar{\mathcal{C}})$ . We first assume that  $\text{opt}_Q$  can be expressed without maximization over constants, i.e. that there exists a  $\Sigma_1$ -formula  $\psi(\bar{x}, \bar{S})$  (with predefined fixpoint predicates) such that

$$\text{opt}_Q(A) = \max_{\bar{S} \in \bar{\mathcal{C}}} |\{\bar{x} : A \models \psi(\bar{x}, \bar{S})\}|.$$

The proof of Theorem 3.8 shows that for some constant  $\varepsilon > 0$ ,  $|B^A| \geq \text{opt}_Q(A) \geq \varepsilon |B^A|$  where

$$B^A = \{\bar{u} : A \models (\exists \bar{S} \in \bar{\mathcal{C}}) \psi(\bar{u}, \bar{S})\}.$$

On  $\Omega$ , we define the random variable  $X(A) := |B^A|$ . It follows that  $E(X) \geq E(\text{opt}_Q) \geq \varepsilon E(X)$ . It suffices to prove that  $E(X)$  converges to a polynomial  $F(n)$ . We write  $X$  as the sum of the indicator random variables

$$X_{\bar{u}}(A) := \begin{cases} 1 & \text{if } \bar{u} \in B^A \\ 0 & \text{otherwise} \end{cases}$$

By linearity of expectation,  $E(X) = \sum_{\bar{u}} E(X_{\bar{u}})$ . Let  $\alpha(\bar{S})$  be a  $\Sigma_2$ -axiom for  $\bar{\mathcal{C}}$ . Then  $E(X_{\bar{u}})$  is the probability that the formula

$$\eta(\bar{u}) \equiv (\exists \bar{S})(\alpha(\bar{S}) \wedge \psi(\bar{u}, \bar{S}))$$

holds on a random structure with universe  $n$ . Fact 4.2 tells us that except on an exponentially decreasing fraction of structures, the predefined fixpoint predicates are definable by quantifier-free formulae. If we substitute them into  $\eta(\bar{u})$ , then we obtain a strict  $\Sigma_1^1$ -formula  $\varphi(\bar{u})$  such that, for some constant  $c > 0$ ,

$$|E(X_{\bar{u}}) - \mu_n(\varphi(\bar{u}))| < c^n.$$

Now, by Fact 4.3, the probability  $\mu_n(\varphi(\bar{u}))$  converges exponentially fast to a dyadic rational  $p_{\bar{u}}$  which only depends on the equality type of  $\bar{u}$ . If  $k$  is fixed then the number of equality types of  $k$ -tuples is also fixed; moreover, the number of  $k$ -tuples of equality type  $e$  over  $n$  is a polynomial  $f_e(n)$ . Let  $p_e$  be the asymptotic probability of  $\varphi(\bar{u})$  for tuples of equality type  $e$ . It follows that  $E(X)$  converges exponentially fast to the polynomial

$$F(n) = \sum_e p_e f_e(n).$$

With maximization over constants, the situation becomes more complicated. We now have

$$\text{opt}_Q(A) = \max_{\bar{c}, \bar{S}} |\{\bar{x} : A \models \psi(\bar{x}, \bar{c}, \bar{S})\}|.$$

To establish Theorem 3.8 we fixed for every input structure  $A$  an optimal tuple  $\bar{c}$  which then was considered as part of the input. Since  $\bar{c}$  depends on  $A$  this no longer works when  $A$  is a random input. Therefore, let

$$B^A(\bar{c}) := \{\bar{x} : A \models (\exists \bar{S} \in \bar{\mathcal{C}}) \psi(\bar{x}, \bar{c}, \bar{S})\}.$$

On every input structure  $A$  we then have

$$\max_{\bar{c}} |B^A(\bar{c})| \geq \text{opt}_Q(A) \geq \varepsilon \max_{\bar{c}} |B^A(\bar{c})|$$



for a fixed constant  $\varepsilon > 0$ . Let  $X := \max_{\bar{c}} |B^A(\bar{c})|$ ; it suffices to prove that there exists a polynomial  $F(n)$  such that  $E(X) \sim F(n)$ .

As above, we find a strict  $\Sigma_1^1$ -formula  $\varphi(\bar{c}, \bar{u})$  such that, for any fixed  $(\bar{c}, \bar{u})$ , the expectation that  $\bar{u} \in B^A(\bar{c})$  is exponentially close to the asymptotic probability of  $\varphi(\bar{c}, \bar{u})$ . Again, the asymptotic probability of  $\varphi(\bar{c}, \bar{u})$  is a dyadic rational that depends only on the equality type of  $(\bar{c}, \bar{u})$ .

Let  $D$  be the set of equality types of  $\bar{c}$  in  $n$ ; clearly, the size of  $D$  is bounded (independently of  $n$ ) and the cardinality of every  $d \in D$  is a polynomial  $f_d(n)$ . Each equality type  $e$  of tuples  $(\bar{c}, \bar{u})$  is an extension of an equality type  $d \in D$ ; we write  $d \prec e$  when this occurs. If  $\bar{c} \in d \prec e$ , let  $U_e(\bar{c}) = \{\bar{u} : (\bar{c}, \bar{u}) \in e\}$ . The cardinality of  $U_e(\bar{c})$  is described by a polynomial  $g_e(n)$  (which depends only on  $e$ ). We denote the asymptotic probability of  $\varphi(\bar{c}, \bar{u})$  (for  $(\bar{c}, \bar{u}) \in e$ ) by  $p_e$ . If  $\bar{c} \in d$  is fixed, then the arguments in the first part of this proof show that  $E(|B^A(\bar{c})|) = \sum_{d \prec e} E(|B^A(\bar{c}) \cap U_e(\bar{c})|)$  converges exponentially fast to  $G_d(n) := \sum_{d \prec e} p_e g_e(n)$  which is a polynomial. Eventually one of the  $G_d(n)$  will dominate all the other ones, so asymptotically  $F(n) := \max_{d \in D} G_d(n)$  is a polynomial. This implies that

$$E(X) = E(\max_{\bar{c}} |B^A(\bar{c})|) \geq \max_{\bar{c}} E(|B^A(\bar{c})|) \sim \max_{d \in D} \sum_{d \prec e} p_e g_e(n) = F(n).$$

It remains to prove that asymptotically  $E(X)/F(n) < 1 + \varepsilon$  for every  $\varepsilon > 0$ . We first prove a Lemma.

**Lemma 4.5** *Let  $d \in D$  and  $d \prec e$ . Then, for every  $\varepsilon > 0$ , the probability that there exists a tuple  $\bar{c} \in D$  such that*

$$|B^A(\bar{c}) \cap U_e(\bar{c})| \geq (1 + \varepsilon)p_e g_e(n)$$

*tends to 0 exponentially fast.*

**PROOF.** Fix  $k = k(n)$  and define the random variable  $Y(A)$  to be the number of tuples  $\bar{c} \in d$  such that  $B^A(\bar{c}) \cap U_e(\bar{c})$  has cardinality  $k$ . We can write  $Y$  as the sum of the indicator random variables

$$Y_{\bar{c}, U}(A) = \begin{cases} 1 & \text{if } U = B^A(\bar{c}) \cap U_e(\bar{c}) \\ 0 & \text{otherwise} \end{cases}$$

where  $\bar{c}$  has equality type  $d$  and  $U$  is a subset of  $U_e(\bar{c})$  of cardinality  $k$ . Let  $m := g_e(n)$ ,  $p := p_e$  and  $q := 1 - p$ . Markov's inequality and linearity of expectation give

$$P(Y \geq 1) \leq E(Y) = \sum_{\bar{c}, U} E(Y_{\bar{c}, U}) = f_d(n) \binom{m}{k} p^k q^{m-k} = f_d(n) b(m, k, p).$$

By Lemma 4.4, if  $k \geq (1 + \varepsilon)pm = (1 + \varepsilon)p_e g_e(n)$  then  $b(m, k, p)$  converges to 0 exponentially fast. Thus the same holds for the probability that there exists a tuple  $\bar{c}$  for which  $|B^A(\bar{c}) \cap U_e(\bar{c})|$  exceeds  $(1 + \varepsilon)p_e g_e(n)$ .  $\blacksquare$

Suppose that  $E(X) \geq (1 + \varepsilon)F(n)$ . Then there is a constant  $\varepsilon > 0$  such that there exists with non-negligible probability at least one tuple  $\bar{c}$  (of equality type, say,  $d$ ) with  $|B^A(\bar{c})| \geq (1 + \varepsilon)G_d(n)$ . But then there must exist an extension  $e$  of  $d$  such that with non-negligible probability there is a  $\bar{c}$  with  $|B^A(\bar{c}) \cap U_e(\bar{c})| \geq (1 + \varepsilon)p_e g_e(n)$ .

The Lemma just proved shows that this is not the case. This proves the theorem.  $\blacksquare$

**Applications.** As usual in graph theory, let  $\omega(G)$ ,  $\alpha(G)$  and  $\chi(G)$  denote the size of a maximum clique, the size of a maximum independent set and the chromatic number of a graph  $G$ . We use the following results from the theory of random graphs (see [1, 4]).

**Fact 4.6** (i)  $E(\omega) = E(\alpha) \sim 2 \log n$ ,

(ii)  $E(\chi) \sim n/(2 \log n)$ .

Together with our probabilistic criterion, this implies that MAX CLIQUE and MAX INDEPENDENT SET are not in MAX  $\Sigma_1^{\text{FP}}(<)$ .

There are other important maximization problems  $Q$  for which  $E(\text{opt}_Q)$  does not grow like  $\Theta(p(n))$  for any polynomial  $p(n)$ , and which therefore are not in MAX  $\Sigma_1^{\text{FP}}(<)$ . Examples include the following.

**V-C DIMENSION.** Given a collection  $S_1, \dots, S_m$  of subsets of a finite set  $M$ , find a set  $T \subseteq M$  of maximal cardinality which is shattered by  $S_1, \dots, S_m$  (this means that every subset of  $T$  occurs as  $T \cap S_i$  for some  $i$ ). The cardinality of  $T$  is called the *Vapnik-Chervonenkis dimension* of  $S_1, \dots, S_m$ ; it plays an important rôle e.g. in learning theory. We can represent a collection  $S_1, \dots, S_m$  of subsets of  $n$  by a binary predicate  $S$  over  $\max(n, m)$  such that  $S_i = \{j : (i, j) \in S\}$ .

**MAX COMMON INDUCED SUBGRAPH (MCIS).** Given two graphs  $G$  and  $H$ , find a graph of maximal cardinality which is an induced subgraph of both  $G$  and  $H$ .

**MAX CLIQUE MINOR (MCM).** Given a graph  $G$ , find a clique of maximal size which is a minor (i.e. a contraction of a subgraph) of  $G$ . The size of such a clique is called the *contraction clique number* of  $G$ , abbreviated  $\text{ccl}(G)$ . It is known [5] that for all almost all graphs,  $\text{ccl}(G) \sim n(\log n)^{-1/2}$ .

**LONGEST CHORDLESS PATH (LCP).** Given a graph  $G$ , find a set  $V$  of nodes, as large as possible, such that  $G|_V$  is a simple path.

Note that to apply the probabilistic criterion to these (and other) problems, it is not necessary to determine  $E(\text{opt}_Q)$  explicitly. Theorem 4.1 implies the following proposition.

**Proposition 4.7** *Let  $Q$  be a maximization problem. If, over the probability space  $\Omega$  of all  $\sigma$ -structures with universe  $n$ ,*

$$1 \leq E(\text{opt}_Q) = o(n)$$

*then  $Q \notin \text{MAX } \Sigma_1^{\text{FP}}(<)$ .*

In fact, if we can show that for all  $\varepsilon > 0$ , the probability that  $\text{opt}_Q(A) \geq \varepsilon|A|$  tends to 0 exponentially fast then  $E(\text{opt}_Q) = o(n)$  follows because  $\text{opt}_Q$  is polynomially bounded.

There is a large class of graph problems, for which this can be established by the following method. For any property  $P$  of graphs, let  $c_n(P)$  be the number of graphs with vertex set  $n$  that satisfy  $P$ . Let MAX INDUCED SUBGRAPH WITH PROPERTY  $P$  (MIS( $P$ )) be the problem of maximizing the cardinality of a set of nodes  $V$  in a given graph  $G$ , such that the induced subgraph  $G|_V$  has property  $P$ . The problems MAX CLIQUE, MAX INDEPENDENT SET, LONGEST CHORDLESS PATH are special cases of MIS( $P$ ); another example is MAX INDUCED  $k$ -COLOURABLE SUBGRAPH.

**Theorem 4.8** *If  $0 \leq \log c_n(P) \leq n^2/2 - n^{1+\delta}$  for some  $\delta > 0$ , then  $\text{MIS}(P) \notin \text{MAX } \Sigma_1^{\text{FP}}(<)$ .*

**PROOF.** For  $r = r(n)$ , let  $Y_r(G)$  be the random variable whose value is the number of induced subgraphs in  $G$  of cardinality  $r$  with property  $P$ . Clearly  $\text{opt}_{\text{MIS}(P)}(G) = \max\{r : Y_r(G) > 0\}$ . By linearity of expectation

$$E(Y_r) = \binom{n}{r} c_r(P) 2^{-\binom{r}{2}}.$$

Stirling's formula implies that  $\binom{n}{r} = 2^{O(r)}$  for  $n = O(r)$ . It follows that

$$P(Y_r \geq 1) \leq E(Y_r) = 2^{O(r) + \log c_r(P) - \binom{r}{2}} \leq 2^{-r^{1+\delta} + O(r)}$$

which tends to 0 exponentially fast as  $n$ , and hence  $r$ , goes to infinity. Hence,  $1 \leq E(\text{opt}_{\text{MIS}(P)}) = o(n)$  and by Proposition 4.7 it follows that  $\text{MIS}(P) \notin \text{MAX } \Sigma_1^{\text{FP}}(<)$ . ■

The arguments that show that  $\text{MCIS}$  and  $\text{V-C-DIMENSION}$  are not in  $\text{MAX } \Sigma_1^{\text{FP}}(<)$  are very similar.

We also obtain results for minimization problems.

**Theorem 4.9** *MIN COLOURING is not in  $\text{MIN } \Sigma_1^{\text{FP}}$ .*

**PROOF.** Recall that  $\text{MIN } \Sigma_1^{\text{FP}} = \text{MIN } \Sigma_0^{\text{FP}}$ . Suppose that the chromatic number could be defined by

$$\chi(G) = \min_{\bar{S}, \bar{c}} |\{\bar{x} : G \models \psi(\bar{x}, \bar{c}, \bar{S})\}|$$

where  $\psi$  is quantifier-free (possibly with predefined fixpoint predicates) and  $\bar{x} = x_1, \dots, x_k$ . It follows that  $\chi(G)$  can be defined as

$$\chi(G) = n^k - \max_{\bar{S}, \bar{c}} |\{\bar{x} : G \models \neg\psi(\bar{x}, \bar{c}, \bar{S})\}| = n^k - \text{opt}_Q(G)$$

with a maximization problem  $Q \in \text{MAX } \Sigma_0^{\text{FP}}$ . But this implies that  $E(\chi) = n^k - \Theta(p(n))$  for some polynomial  $p$ , which is not the case, since  $E(\chi) \sim n/(2 \log n)$ . ■

There also is a probabilistic criterion for membership in  $\text{MAX } \Pi_1^{\text{FP}}$ , which will allow us to separate  $\text{MAX } \Pi_2^{\text{FP}}$  from  $\text{MAX } \Pi_1^{\text{FP}}$ .

**Theorem 4.10 (Probabilistic criterion for  $\text{MAX } \Pi_1^{\text{FP}}$ )** *For every problem  $Q \in \text{MAX } \Pi_1^{\text{FP}}$  and every natural number  $k \in \mathbb{N}$ , the property that  $\text{opt}_Q(A) > k$  satisfies a 0-1 law.*

**PROOF.** We again use the fact that except on an exponentially decreasing fraction of structures, fixpoint predicates are definable by quantifier-free formulae. Thus, the optimum for  $Q \in \text{MAX } \Pi_1^{\text{FP}}$ , is defined on almost all structures by an expression

$$\text{opt}_Q(A) = \max_{\bar{S}, \bar{c}} |\{\bar{x} : A \models \psi(\bar{x}, \bar{c}, \bar{S})\}|$$

where  $\psi(\bar{x}, \bar{c}, \bar{S})$  is a  $\Pi_1$ -formula.

Then, the property that  $\text{opt}_Q(A) > k$  is expressed by the strict  $\Sigma_1^1$ -formula

$$(\exists \bar{S})(\exists \bar{c})(\exists \bar{x}_0) \cdots (\exists \bar{x}_k) \bigwedge_{0 \leq i < j \leq k} (\bar{x}_i \neq \bar{x}_j) \wedge \bigwedge_{0 \leq i \leq k} \psi(\bar{x}_i, \bar{c}, \bar{S}).$$

The theorem now follows from the 0-1 law for strict  $\Sigma_1^1$ -formulae. ■

We did not find natural optimization problems that do not satisfy this criterion. However, we can cook up artificial ones such as **MAXIMUM CONNECTED COMPONENT WITH PERFECT MATCHING (MCCPM)** which, given a graph, asks for a maximum connected component that admits a perfect matching. Note that MCCPM is solvable in polynomial time.

**Proposition 4.11**  $\text{MCCPM} \notin \text{MAX } \Pi_1^{\text{FP}}$ .

**PROOF.** With probability tending to 1, a random graph is connected. Obviously, a graph of odd cardinality cannot have a perfect matching, but almost all graphs of even cardinality admit a perfect matching. Thus,  $\text{opt}_{\text{MCCPM}}(G)$  tends to 0 on graphs with odd cardinality, and to  $|G|$  on graphs of even cardinality. ■

**Corollary 4.12**  $\text{MAX } \Pi_1^{\text{FP}} \subsetneq \text{MAX } \Pi_2^{\text{FP}} = \text{MAX } \mathcal{PB}$ .

## 5 Monotonicity properties

The simple monotonicity properties that were used in [20, 15] to separate expressibility classes of optimization problems do not survive in the presence of fixpoint definitions. Nevertheless we can make use of them to prove inexpressibility results for  $\text{MAX } \Sigma_1^{\text{FP}}$  and  $\text{MIN } \Sigma_1^{\text{FP}}$  by looking at classes of structures where fixpoint logic collapses to  $\Sigma_0$ -formulae. Although such classes cannot contain very interesting structures, they somewhat surprisingly suffice to show that prominent problems such as **MAX CLIQUE**, **MAX MATCHING** and **MIN COLOURING** are not in  $\text{MAX } \Sigma_1^{\text{FP}}$  and  $\text{MIN } \Sigma_1^{\text{FP}}$  respectively.

As usual, we identify  $n$  with the set  $\{0, \dots, n-1\}$  and denote the group of all permutations on  $n$  by  $S_n$ .

**Definition 5.1** For all natural numbers  $n, m$ , we define the graphs  $K_{n;m} = (n \times m, E_{n,m})$  where  $E_{n,m} = \{((x, y)(x', y')) : x \neq x'\}$ .  $K_{n;m}$  is the complete  $n$ -partite graph where each partition class contains exactly  $m$  vertices.

Let  $\sigma \in S_n$  and  $\pi_1, \dots, \pi_m \in S_m$ . Then the bijection  $(i, j) \mapsto (\sigma i, \pi_i j)$  on  $n \times m$  is an automorphism of  $K_{n;m}$ , and every automorphism of  $K_{n;m}$  can be described in this way.

**Definition 5.2** For  $k$ -tuples  $\bar{u}, \bar{v}$  in  $K_{n;m}$  we write  $\bar{u} \equiv_k \bar{v}$  if there is an automorphism  $f$  of  $K_{n;m}$  with  $f u_i = v_i$  for  $i = 1, \dots, k$ . The equivalence classes with respect to  $\equiv_k$  are called  $\equiv_k$ -types.

The following lemma is easy to prove.

**Lemma 5.3** *There exists a function  $f : \mathbb{N} \rightarrow \mathbb{N}$  such that the number of  $\equiv_k$ -types in  $K_{n;m}$  is bounded by  $f(k)$  (independently of  $n$  and  $m$ ). Furthermore every  $\equiv_k$ -type is uniformly definable by a quantifier-free formula. This means that there exist quantifier-free formulae  $e_1(\bar{x}), \dots, e_{f(k)}(\bar{x})$  such that every  $\equiv_k$ -type in any  $K_{n;m}$  is defined by precisely one formula  $e_i(\bar{x})$ .*

Note that for small  $n, m$ , some of the  $\equiv_k$ -types may not occur in  $K_{n;m}$ . However, for every  $k$ , there exists a  $n_0$  such that for  $n, m > n_0$ , the number of  $\equiv_k$ -types in  $K_{n;m}$  is precisely  $f(k)$ .

**Proposition 5.4** *For any formula  $\varphi(\bar{x}) \in L_{\infty\omega}^\omega$  there exists a  $\Sigma_0$ -formula  $\alpha(\bar{x})$  and a number  $n_0$  such that for all  $n, m > n_0$*

$$K_{n;m} \models (\forall \bar{x})(\varphi(\bar{x}) \leftrightarrow \alpha(\bar{x})).$$

PROOF. Take  $n, m$  large enough such that every  $\equiv_k$ -type  $e_i$  is realized by some  $k$ -tuple  $\bar{u}_i$  in  $K_{n;m}$ . Let  $I(\varphi) = \{i \leq f(k) : K_{n;m} \models \varphi(\bar{u}_i)\}$  and set

$$\alpha(\bar{x}) \equiv \bigvee_{i \in I(\varphi)} e_i(\bar{x}).$$

■

The following result gives us a useful monotonicity criterion to prove inexpressibility results even for  $\text{MAX } \Sigma_1^{\text{FP}}(<)$  and  $\text{MIN } \Sigma_1^{\text{FP}}(<)$ :

**Theorem 5.5** *Let  $Q$  be an optimization problem on graphs in either  $\text{MAX } \Sigma_1^{\text{FP}}(<)$  or  $\text{MIN } \Sigma_1^{\text{FP}}(<)$ . Then either  $\text{opt}_Q(K_{n;m}) = O(1)$  or there exists a constant  $n_0$  such that  $\text{opt}_Q(K_{n;m}) < \text{opt}_Q(K_{n;m+1})$  for all  $n, m > n_0$ .*

PROOF. By proposition 5.4 there exists for every optimization problem  $Q$  in  $\text{MAX } \Sigma_1^{\text{FP}}(<)$  or  $\text{MIN } \Sigma_1^{\text{FP}}(<)$  an existential first-order formula  $\psi(\bar{x}, \bar{c}, \bar{<}, \bar{S})$  (without fixpoint predicates) such that

$$\text{opt}_Q(K_{n;m}) = \text{opt}_{\bar{S}, \bar{<}, \bar{c}} |\{\bar{x} : K_{n;m} \models \psi(\bar{x}, \bar{c}, \bar{<}, \bar{S})\}|$$

for all large enough  $n, m$ .

Suppose that  $\text{opt}_Q(K_{n;m}) \neq O(1)$ . For any large enough  $n, m$ , fix predicates  $\bar{S}$ , orderings  $\bar{<}$  and constants  $\bar{c} = c_1, \dots, c_r$  in  $K_{n;m}$  such that the set

$$L_m(\bar{S}, \bar{<}, \bar{c}) := \{\bar{u} : K_{n;m} \models \psi(\bar{u}, \bar{c}, \bar{<}, \bar{S})\}$$

realizes an optimal solution, i.e.  $\text{opt}_Q(K_{n;m}) = |L_m(\bar{S}, \bar{<}, \bar{c})|$ .

Since  $\text{opt}_Q(K_{n;m})$  is unbounded, we can choose a tuple  $\bar{u} = (u_1, \dots, u_k) \in L_m(\bar{S}, \bar{<}, \bar{c})$  such that at least one of the  $u_i$  is different from all constants  $c_1, \dots, c_r$ . Fix  $u_i = (x_i, y_i)$ .

First, consider the case where  $Q$  is a *maximization problem*. Let  $\pi : K_{n;m+1} \rightarrow K_{n;m}$  be the projection with  $\pi(x, m) = (x, u_i)$  and  $\pi(x, y) = (x, y)$  for all  $y < m$ , and extend it to tuples in the obvious way. We extend  $\bar{S}$  to predicates  $\bar{S}^*$  over  $K_{n;m+1}$  by defining  $\bar{S}^*(\bar{z}) = \bar{S}(\pi\bar{z})$ . We also extend any ordering  $<$  on  $K_{n;m}$  to an ordering  $<^*$  on  $K_{n;m+1}$  by

letting  $(x, m)$  be the immediate successor of  $(x, y_i)$ . Let  $\bar{v}$  be the tuple obtained from  $\bar{u}$  by replacing (every occurrence of)  $u_i$  by  $m$ . Since  $\psi$  is an existential formula, it follows that  $L_m(\bar{S}, \bar{<}, \bar{c}) \cup \{\bar{v}\} \subseteq L_{m+1}(\bar{S}^*, \bar{<}^*, \bar{c})$ . Thus  $\text{opt}_Q(K_{n;m}) < \text{opt}_Q(K_{n;m+1})$ .

Now let  $Q$  be a *minimization problem*. We show that  $\text{opt}_Q(K_{n;m-1}) < |L_m(\bar{S}, \bar{<}, \bar{c})|$ .

First, since every permutation  $\pi$  of  $m$  gives an automorphism  $(\text{id} \times \pi)$  of  $K_{n;m}$ , we can assume without loss of generality, that  $c_1, \dots, c_r \in K_{n;m-1}$ .

Let  $\bar{S}^*$  and  $\bar{<}^*$  be the restrictions of  $\bar{S}$  and  $\bar{<}$  to  $K_{n;m-1}$ . Since  $\psi$  is existential, it follows that  $L_{m-1}(\bar{S}^*, \bar{<}^*, \bar{c}) \subseteq L_m(\bar{S}, \bar{<}, \bar{c})$ . If the inclusion is strict, then we are done.

Suppose  $L_{m-1}(\bar{S}^*, \bar{<}^*, \bar{c}) = L_m(\bar{S}, \bar{<}, \bar{c})$ . Take a tuple  $\bar{u} \in L_m(\bar{S}, \bar{<}, \bar{c})$  containing the element  $u_i$  which is different from all constants  $c_1, \dots, c_r$ , and let  $\sigma$  be the automorphism of  $K_{n;m}$  that switches  $u_i = (x_i, y_i)$  with  $(x_i, m-1)$ . Define  $\bar{T}(\bar{z}) = \bar{S}(\sigma\bar{z})$  and define new orderings  $\bar{<}$  by  $z \prec_i z'$  iff  $\sigma z <_i \sigma z'$ . It follows that for all  $\bar{x}$

$$\bar{x} \in L_m(\bar{T}, \bar{<}, \bar{c}) \iff \sigma\bar{x} \in L_m(\bar{S}, \bar{<}, \bar{c}) = L_{m-1}(\bar{S}^*, \bar{<}^*, \bar{c}).$$

Thus  $|L_m(\bar{T}, \bar{<}, \bar{c})| = \text{opt}_Q(K_{n;m})$ . Again, let  $\bar{T}^*$  and  $\bar{<}^*$  be the restrictions of  $\bar{T}$  and  $\bar{<}$  to  $K_{n;m-1}$ . Then  $L_{m-1}(\bar{T}^*, \bar{<}^*, \bar{c}) \subseteq L_m(\bar{T}, \bar{<}, \bar{c})$ . But  $\sigma u_i$  is in  $K_{n;m} - K_{n;m-1}$  so

$$\sigma\bar{u} \in L_m(\bar{T}, \bar{<}, \bar{c}) - L_{m-1}(\bar{T}^*, \bar{<}^*, \bar{c}).$$

This implies that  $\text{opt}_Q(K_{n;m-1}) < \text{opt}_Q(K_{n;m})$ . ■

**Theorem 5.6** (i) MAX CLIQUE is not in MAX  $\Sigma_1^{\text{FP}}(<)$ .

(ii) MIN COLOURING is not in MIN  $\Sigma_1^{\text{FP}}(<)$ .

PROOF. As usual, let  $\omega(G)$  and  $\chi(G)$  denote the size of a maximum clique and the chromatic number of  $G$ . Obviously,  $\omega(K_{n;m}) = \chi(K_{n;m}) = n$  is independent of  $m$ . The claim now follows from Theorem 5.5. ■

A very similar criterion applies to the structures  $K_n^d = (n, R^d)$  with the  $d$ -ary predicate  $R^d = \{(a_1, \dots, a_d) : a_i \neq a_j \text{ for all } i \neq j\}$ .

**Theorem 5.7** Let  $Q$  be an optimization problem on  $d$ -ary relations in either MAX  $\Sigma_1^{\text{FP}}(<)$  or MIN  $\Sigma_1^{\text{FP}}(<)$ . Then either  $\text{opt}_Q(K_n^d) = O(1)$  or there exists a constant  $n_0$  such that  $\text{opt}_Q(K_n^d) < \text{opt}_Q(K_{n+1}^d)$  for all  $n > n_0$ .

The proof is very similar to the proof of Theorem 5.5. As applications, we present the problems to find a maximum matching in a graph and to find a maximum (disjoint) covering in a  $d$ -dimensional predicate.

MAX MATCHING(MM) is the problem of finding a set of independent edges of maximal size in a given graph. It is well-known that this is solvable in polynomial-time. A *covering* of a  $d$ -dimensional predicate  $R$  is a subset  $M \subseteq R$  of mutually disjoint  $d$ -tuples (i.e. if  $\bar{u} \in M$  and  $\bar{v} \in M$  then  $u_i \neq v_j$  for all  $i, j \leq d$ ). MAX  $d$ -COVER ( $MdC$ ) is the problem of finding a maximum covering of a given  $d$ -dimensional predicate. Note that MAX 2-COVER is MAX MATCHING. For all  $d$ , MAX  $d$ -COVER is in APX. Panconesi and Ranjan [20] proved that MAX  $d$ -COVER is not in MAX  $\Sigma_1$ . We extend this to the following result.

**Theorem 5.8** MAX MATCHING and MAX  $d$ -COVER are not in MAX  $\Sigma_1^{\text{FP}}(<)$ .

PROOF.  $\text{opt}_{\text{MDC}}(K_{dn}^d) = \text{opt}_{\text{MDC}}(K_{dn+1}^d) = n$ , so the claim follows from Theorem 5.7. ■

To complete the picture we prove that the problem MAX SAT separates MAX  $\Sigma_1$  from MAX  $\Sigma_0^{\text{FP}}$ .

**Theorem 5.9** MAX SAT  $\not\subseteq$  MAX  $\Sigma_0^{\text{FP}}$ .

PROOF. We consider propositional formulae depending on the variables  $X_0, \dots, X_{m-1}$ . Let  $p \subseteq m$ ; we say that a clause has type  $p$  if it has the form

$$\bigvee_{i \in p} X_i \vee \bigvee_{i \notin p} \neg X_i.$$

Let  $\mathcal{B}_{n,m}$  be the set of Boolean formulae  $F$  in CNF satisfying the following two conditions:

- every clause of  $F$  has type  $p$  for some  $p \subseteq m$ ;
- for every  $p \subseteq m$ ,  $F$  contains at least  $n$  clauses of type  $p$ .

Note that an assignment of truth values to the variables  $X_0, \dots, X_{m-1}$  is also described by a subset  $q \subseteq m$  and that the assignment  $q$  makes clauses of type  $p$  false if and only if  $p$  is the complement of  $q$ .

As described above, we encode formulae by finite structures over the vocabulary  $\sigma = \{C, P, N\}$  whose universe is the disjoint union of the set of clauses and the set of variables, where  $C$  identifies the set of clauses, and where  $Pxy$  and  $Nxy$  say that the variable  $y$  occurs positively (respectively negatively) in clause  $x$ . With respect to this encoding we have the following.

**Lemma 5.10** For every formula  $\varphi(\bar{x})$  in (FO + LFP) there exists a natural number  $n_0$  and a quantifier-free first-order formula  $\alpha(\bar{x})$  which is equivalent to  $\varphi(\bar{x})$  on  $\mathcal{B}_{n,m}$ , provided that  $n, m \geq n_0$ .

The proof is a straightforward application of Ehrenfeucht-Fraïssé games.

Towards a contradiction, we now suppose that MAX SAT (abbreviated MS) is in MAX  $\Sigma_0^{\text{FP}}$ , i.e.

$$\text{opt}_{\text{MS}}(F) = \max_{\bar{c}, \bar{S}} |\{\bar{x} : F \models \psi(\bar{x}, \bar{c}, \bar{S})\}|$$

where  $\psi$  is a  $\Sigma_0$ -formula, possibly containing fixpoint predicates, and where  $\bar{x} = x_1, \dots, x_r$ ,  $\bar{c} = c_1, \dots, c_s$  and  $\bar{S} = S_1, \dots, S_t$ . If we restrict attention to formulae  $F \in \mathcal{B}_{n,m}$  where  $n, m$  are sufficiently large compared to  $r, s$  and  $t$  then we can eliminate the fixpoint predicates and assume that  $\psi$  is a quantifier-free first-order formula.

If  $a$  is a clause in a formula  $F$ , we denote by  $F_a$  the formula obtained by removing clause  $a$ . Now, let  $G$  be a formula in  $\mathcal{B}_{n,m}$  which contains  $n$  clauses of type  $m$  and at least  $n+1$  clauses of every type  $p \subsetneq m$ . Note that the optimal assignments for  $G$  are all those which make at least one variable true. Furthermore, removing any clause  $a$  of type  $m$  from  $G$  does

not change the maximal number of satisfiable clauses, but removing  $j \leq 2$  clauses of any other type does reduce the number of satisfiable clauses by  $j$ . In particular

$$\text{opt}_{\text{MS}}(G_a) = \begin{cases} \text{opt}_{\text{MS}}(G) & \text{if } a \text{ has type } m \\ \text{opt}_{\text{MS}}(G) - 1 & \text{if } a \text{ has type } p \subsetneq m. \end{cases}$$

We now fix values for  $\bar{c}$  and  $\bar{S}$  on  $G$  such that  $\text{opt}_{\text{MS}}(G) = |L(\bar{c}, \bar{S})|$  where

$$L(\bar{c}, \bar{S}) = \{\bar{w} : G \models \psi(\bar{w}, \bar{c}, \bar{S})\}.$$

In the sequel, we call a clause in  $G$  *generic* if it is different from the constants  $c_1, \dots, c_r$ .

**Lemma 5.11** *Let  $a$  be any generic clause in  $G$ . If  $a$  has type  $m$  then no tuple  $\bar{w} \in L(\bar{c}, \bar{S})$  contains  $a$ . However, if  $a$  has type  $p \neq m$ , then there exists precisely one tuple  $\bar{w} \in L(\bar{c}, \bar{S})$  containing  $a$ ; this tuple does not contain any other generic clause.*

**PROOF.** First, suppose that  $a$  has type  $m$ , and let  $\bar{w}$  be a tuple in  $L(\bar{c}, \bar{S})$  containing  $a$ . We add a clause  $a'$  also of type  $m$  to  $G$  and obtain a new formula  $F$  with  $\text{opt}_{\text{MS}}(F) = \text{opt}_{\text{MS}}(G)$ . However, we can extend  $\bar{S}$  to predicates  $\bar{S}'$  over  $F$  in such a way that  $a'$  remains indistinguishable from  $a$ . The tuple  $\bar{w}'$ , obtained from  $\bar{w}$  by substituting  $a'$  for  $a$  is then contained in  $L(\bar{c}, \bar{S}')$ . Thus, it would follow that  $\text{opt}_{\text{MS}}(F) \geq \text{opt}_{\text{MS}}(G) + 1$  which is false. This proves the first part.

Now, let  $a$  have type  $p \neq m$ . Suppose that no tuple in  $L(\bar{c}, \bar{S})$  contains  $a$  and let  $\bar{S}''$  be the restriction of  $\bar{S}$  to  $G_a$ . Then  $L(\bar{c}, \bar{S}'')$  in  $G_a$  coincides with  $L(\bar{c}, \bar{S})$  on  $G$ , hence  $\text{opt}_{\text{MS}}(G_a) \geq \text{opt}_{\text{MS}}(G)$  which is false.

Now, suppose that there are two distinct tuples  $\bar{v}$  and  $\bar{w}$  in  $L(\bar{c}, \bar{S})$  that contain  $a$ . As above, we add a copy  $a'$  of  $a$  to  $G$  to obtain a new formula  $F$ , and extend  $\bar{S}$  to predicates  $\bar{S}'$  over  $F$ . Note that  $\text{opt}_{\text{MS}}(F) = \text{opt}_{\text{MS}}(G) + 1$ . But the tuples  $\bar{v}'$  and  $\bar{w}'$ , obtained from  $\bar{v}$  and  $\bar{w}$  by substituting  $a'$  for  $a$  are then contained in  $L(\bar{c}, \bar{S}')$ . Thus, it would follow that  $\text{opt}_{\text{MS}}(F) \geq \text{opt}_{\text{MS}}(G) + 2$ , which is false.

Finally we assume that some tuple  $\bar{w} \in L(\bar{c}, \bar{S})$  contains two generic clauses  $a, a'$ . Then they both must have type different from  $m$  and do not occur in any other tuple in  $L(\bar{c}, \bar{S})$ . Thus, if we remove both clauses  $a, a'$  from  $G$  we obtain a formula  $F$  with  $\text{opt}_{\text{MS}}(F) = \text{opt}_{\text{MS}}(G) - 2$ . However, by taking the restriction of  $\bar{S}$  to  $F$ , we would remove only the tuple  $\bar{w}$  from  $L(\bar{c}, \bar{S})$  and could conclude that  $\text{opt}_{\text{MS}}(F) \geq \text{opt}_{\text{MS}}(G) - 1$ , whence a contradiction. This proves the lemma.  $\blacksquare$

To prove the theorem, we now fix a type  $p \subseteq m$  with the following properties:

- (i) For all  $i \leq s$ , if  $c_i$  stands for a variable  $X_j$ , then  $j \in p$ , i.e.  $X_j$  occurs positively in clauses of type  $p$ .
- (ii)  $p$  is neither too large nor too small:  $|p|, |m - p| > r + s$ .

Choose a generic clause  $a$  of type  $p$ ; there exists precisely one tuple  $\bar{w} \in L(\bar{c}, \bar{S})$  containing  $a$ .

We distinguish two possibilities.



First, we assume that  $\bar{w}$  consists only of  $a$  and (possibly) of constants from  $c_1, \dots, c_s$ . In this case we add to  $G$  a clause of type  $m$  and obtain a formula  $G$  with  $\text{opt}_{\text{MS}}(F) = \text{opt}_{\text{MS}}(G)$ . For any tuple  $\bar{u}$ , let  $\bar{u}'$  be the tuple obtained by replacing occurrences of  $a$  by  $a'$ . We extend  $\bar{S}$  to predicates  $\bar{S}'$  over  $F$  in such a way that  $\bar{S}'(\bar{u}') = \bar{S}(\bar{u})$ . Then, despite the fact that  $a$  and  $a'$  have different types, the tuples  $\bar{w}$  and  $\bar{w}'$  are indistinguishable by quantifier-free formulae  $\psi(\bar{w}, \bar{c}, \bar{S})$  (here we use property (i)). It follows that  $\text{opt}_{\text{MS}}(F) = \text{opt}_{\text{MS}}(G) + 1$  which is false.

In the second case,  $\bar{w}$  contains some element  $v$  which is neither  $a$  nor a constant from  $c_1, \dots, c_s$ . By the Lemma, it can only be a variable, say  $X_j$ . We fix another variable, say  $X_k$  which is different from all constants  $c_1, \dots, c_s$ , does not occur in  $\bar{w}$ , and satisfies the condition that  $k \in p \leftrightarrow j \in p$  (by condition (ii), such a variable must exist).

We now add to  $G$  clauses  $b_1, \dots, b_q$  of type  $p$ , where  $q = \text{opt}_{\text{MS}}(G)$ , to obtain a formula  $F$ . Clearly  $\text{opt}_{\text{MS}}(F) = 2\text{opt}_{\text{MS}}(G)$ . On the other hand, for any tuple  $\bar{u}$  and  $k \leq q$ , let  $\bar{u}'_i$  be obtained by replacing occurrences of  $a$  by  $b_i$ ; moreover, let  $\bar{u}''_i$  be the tuple by replacing occurrences of  $X_j$  in  $\bar{u}'_i$  by  $X_k$ . Let  $\bar{S}'$  be any extension of  $\bar{S}$  to  $F$ , satisfying the condition that for all  $\bar{u}$  and all  $i \leq q$ ,  $\bar{S}'(\bar{u}'_i) = \bar{S}(\bar{u})$ . We modify  $\bar{S}'$  to a new predicates  $\bar{S}''$ . For any tuple  $\bar{v}$ , let  $\bar{v}^*$  be constructed by replacing occurrences of  $X_k$  by  $X_j$ ; then we set  $\bar{S}''(\bar{v}) = \bar{S}'(\bar{v}^*)$ .

It is easy to see that  $\bar{w}$  and all tuples  $\bar{w}'_i, \bar{w}''_i$  are contained in  $L(\bar{c}, \bar{S}'')$ . This implies that  $\text{opt}_{\text{MS}}(F) \geq 2\text{opt}_{\text{MS}}(G) + 1$  which is false. The theorem is proved.  $\blacksquare$

**Corollary 5.12**  $\text{MAX } \Sigma_0^{\text{FP}} \subsetneq \text{MAX } \Sigma_1^{\text{FP}} \subsetneq \text{MAX } \Pi_1^{\text{FP}} \subsetneq \text{MAX } \Pi_2^{\text{FP}} = \text{MAX } \mathcal{PB}$ .

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