Gymnasium Bäumlihof

MATURAARBEIT

Theoretical Informatics: Formal languages and Descriptive Complexity

A study of the connection of first-order logic and context-sensitive languages

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Foreword

Some years ago, the Lego Mindstorms sparkled my interest in informatics and programming. By attending some courses at the Phænovum in Lörrach, I was able to learn how to program using Java, my first text-based programming language. At that time, I was planning to work at Boston Dynamics, as I loved being able to physically see what I had achieved. But then came the RoboCup robot [Rob97]. It was meant to be a rolling robot for playing football on a miniature playing field. After two years, we were still unable to follow the ball because the Corona pandemic prevented us from working on site together. Also, and to a greater extent, it didn't work because the hardware never did what it was meant to, and we passed interminable hours just trying to make it roll forward. As may have become apparent, I got tired of it and decided to move on to something which didn't include too much hardware and was more abstract.

So I decided to participate in the Swiss Olympiad in Informatics, which organizes national programming contests and selects various teams for international Olympiads. There, I got and still get quite a lot of interesting problems which I love to solve, found like-minded friends and was able to participate at some international competitions. Over the years, I began to notice that I enjoy solving tasks theoretically way more than implementing them. That is also something that got reflected in my competition scores, where I often came out knowing I solved a lot in theory, but failed to get the points. Some internships at informatics firms confirmed that actual programming is still too concrete for me.

Now let's get more abstract. Thanks to the "Schülerstudium", I attended a course on the mathematical background of computer science [HR22] and one on the theory of computer science [Rög23]. There, I learned more about Complexity Theory, computability, logic and the Chomsky Hierarchy. The way in which proofs could be made to hold for every problem with certain properties has fascinated me ever since. Further, logic is a tool which captures mathematical reasoning, and can thus be seen as a formalization of every "logical" thought we have. Also, I don't have to bother with implementation any more.

Using books, I began to inform myself more, and found out about the domain of Descriptive Complexity. This domain relates different kinds of logic to different classes of problems in computer science. So I knew I wanted to do my Matura project in this domain, but had difficulties finding an open question which seamed approachable. I asked multiple people if they had a more exact idea what I could do. In the end, a friend at the informatics Olympiad asked *ChatGPT*, which told me I could study the connection between the Chomsky Hierarchy and Descriptive Complexity. Refining this proposition a bit, I came up with (almost) the current question of relating logic and context-

sensitive languages. Then, I found out there exists a characterization using second-order logic, so I added "first-order logic" to the question.

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1. Introduction

In our daily lives, we are in contact with various kinds of algorithms at all times. Searching on Google, sending texts, asking questions to AI chatbots, searching for the fastest route with a navy; all of these consume resources in energy, storage space and time. According to a report from 2021, 3.7 % of global carbon emissions come from the IT domain, with an upward tendency. This is similar to that of the airline industry [Cli21]. At this scale, it is thus vitally important to understand and find out if the resource consumption can be reduced.

To find out how we can improve, we first need to understand how computers work, what we can compute, and why solving some problems is more difficult than solving others. The field of study that investigates this is called Complexity Theory. This is done by abstraction of computational models and of the problems themselves. It is then often possible to find classes of similar problems which allow for generalizations. However, it has proven to be very hard to find proofs of either optimality of algorithms or the separations of complexity classes. One of the emblematic open problems is the P versus NP question, of which we will speak more in appendix B.2.5. Nevertheless, some significant results concerning the complexity of problems on average in the real world and most importantly in cryptography have been made.

One of the subfields of Complexity Theory is Descriptive Complexity. It relates mathematical logic to different complexity classes. This allows us to get new insights into the underlying structure of problems of certain classes. The other main field present in this work, formal languages, is concerned with the abstraction of computational problems as sets, which is often helpful for proofs. This then allows us to define multiple formalisms which describe these sets. Our formal language class of focus, context-sensitive languages, is part of the "Chomsky Hierarchy" introduced by the famous linguist Noam Chomsky.

Towards the end of the 20th century, many equivalences were proven between fragments and extensions of various logics to complexity classes, including all classes in the Chomsky hierarchy. A great summary of all the results is found in Neil Immermans paper "Languages that capture complexity classes" [Imm87].

In this work, we will first introduce the relevant theory. After this, a personal study of connections between first-order logic and context-sensitive languages is presented.

Both chapter 2 and chapter 3 present the most important theory of formal languages and Descriptive Complexity, respectively. Additionally, in section 3.4 full proofs concerning equivalence of context-sensitive languages with logics and automata are presented. These proofs are written in a way trying to show the motivation behind certain crucial steps. Further, some details have been omitted for the sake of simplicity and length of this work. For the same purpose, many proofs, explanation, and examples for other languages in the Chomsky hierarchy were moved to appendix B.

1. INTRODUCTION

After this introduction to the material, we go on in chapter 4 with my personal studies about connections between first-order logic and context-sensitive language. In this process, different paths that I tried are presented and investigated. Towards the end of the chapter, the direct connection to context-sensitive languages fades and the objects of study becomes more related to Savitch's Theorem, which plays a great role in the theory of space-bounded computation. The most complicated proof is given in section 4.5 and concerns a simulation of alternating Turing machines using iterative logic. This divergence from the original working question was due to the hope that researching other, more loosely connected problems would help in the end for the core problem. Also, I tried to pursue ideas I had instead of trying paths where I did not make any progress.

Finally, in chapter 5 we reflect on what was accomplished in this work. A review about the working process is presented, and finally we discuss further possibilities of research.

For the relevant mathematical background, appendix A contains the basic definitions of Set Theory, first and second-order logic, and Turing machines.

A full collection of description, proofs, techniques, and context information about Descriptive Complexity and languages in the Chomsky Hierarchy is given in appendix B.

The entire work is written in English because all mathematical literature is in that language.

2. Formal languages

2.1 Definition

In informatics, we often get an input as a string of characters, and want to compute some function on it. In Complexity Theory, we mostly focus on decision problems where we only want to find out if some input fulfils some given property¹. To formalize this, there is the concept of formal languages. The following definitions are taken from the lecture Theory of Computer Science [Rög23]. For the mathematical background, refer to Appendix A.

Definition 2.1 (Alphabet). An alphabet Σ is a finite set of symbols

Definition 2.2 (Word). A word over some alphabet Σ is a finite sequence of symbols from Σ . We denote ε as the empty word, Σ^* as the set of all words over Σ , xy as the concatenation of x and y, x^n as the concatenation of x with itself n times, and |w| as the number of symbols in w.

Definition 2.3 (Formal language). A formal language is a set of words over some alphabet Σ , or equivalently a subset of Σ^*

For any computational decision problem, we can reformulate it as the problem of deciding if the input word is contained in the formal language consisting of all words which have the required property.

2.2 Chomsky Hierarchy

One of the multiple ways to categorize formal languages was invented by Avram Noam Chomsky, a modern linguist. It is based on the complexity of defining the language using formal grammars, which are a finite representation of formal languages (which can be infinite in the general case).

2.2.1 Grammars

A grammar can informally be seen as a set of rules telling us how to generate all words in a language.

Definition 2.4 (Grammar). A grammar is a 4-tuple $\langle V, \Sigma, R, S \rangle$ consisting of

- V The set of non-terminal symbols
- Σ The set of terminal symbols
- R A set of rules, formally over $(V \cup \Sigma)^*V(V \cup \Sigma)^* \times (V \cup \Sigma)^*$
- S The start symbol from the set V

¹This can be shown to be equivalent to computing functions

The non-terminal symbols in V are symbols that are not in Σ and exist for the purpose of steering the process of word generation. They do not appear in any of the final words generated by the grammar. Further, the rules dictate that there must be at least one non-terminal symbol on the left-hand side of any production rule. This is because $(V \cup \Sigma)^*V(V \cup \Sigma)^*$ means all words having one symbol in V enclosed by words in $(V \cup \Sigma)^*$, which are all words consisting of symbols in V and Σ . For better readability, we write rules in the form $a \to b$ instead of $\langle a, b \rangle$.

To generate the words, we have the concept of derivations.

Definition 2.5 (Derivation). First, we can define one derivation step.

We say u' can be derived from u if

- u is of the form xyz and u' is of the form xy'z for some words $x, y, y', z \in (V \cup \Sigma)^*$
- there exists a rule $y \to y'$ in R

We say that a word is in the *generated language* of a grammar if it consists only of symbols in Σ and can be derived in a finite number of steps from S.

Example 2.1. Consider the grammar $\langle \{S\}, \{a, b\}, R, S \rangle$ with

$$R = \left\{ S \to aSb, \quad S \to \varepsilon \right\}$$

The generated language for this grammar is $\{\varepsilon, ab, aabb, \dots\} = \{a^nb^n \mid n \in \mathbb{N}_0\}$

Now that we have a tool to describe some infinite languages using a finite description, we can further differentiate the complexity of a language by the minimum required complexity of the rules in any formal grammar describing that language. In the main section, we will only present the context-sensitive languages, as they are important for later chapters. In the context appendix explanations for regular languages (appendix B.1.1), context-free languages (appendix B.1.2) and recursive languages (appendix B.1.3) are provided.

2.2.2 Context-Sensitive Languages

The most important category of languages for this work can be defined by multiple equivalent restrictions on the grammars.

One restriction is that all rules have to be of the form $\alpha\beta\gamma \to \alpha\varphi\gamma$ with $\alpha, \gamma \in (\Sigma \cup V)^*$, $\beta \in V$ and $\varphi \in (\Sigma \cup V)^+$. This means that only the non-terminal is allowed to change. Additionally, if S is the start variable and never occurs on the right-hand side of any rule, we may include $S \to \varepsilon$.

Equivalently, we can require that for any rule $u \to v$ we have $|u| \le |v|$. This means that applying any rule will make the result longer. Again, we also allow the special rule $S \to \varepsilon$ if S does not occur on the right-hand side of any rule in R. These grammars are called noncontracting.

The last, most useful restriction for proofs is the Kuroda normal form [Pet22], where all rules have one of the following structures:

• $A \rightarrow BC$

- $AB \rightarrow CB$
- $A \rightarrow a$
- $S \to \varepsilon$ if S is the start symbol and does not occur on any right-hand side of a rule

where $A, B, C, S \in V$ and $a \in \Sigma$.

Example 2.2. Consider the grammar $\langle \{S, B\}, \{a, b, c\}, R, S \rangle$ with

$$R = \begin{cases} S \to abc, & S \to aSBc, \\ cB \to Bc, & bB \to bb \end{cases}$$

It generates the language $a^n b^n c^n$ for $n \in \mathbb{N}_1$ and is noncontracting.

The corresponding formalism for these languages is the linearly bounded nondeterministic Turing machine, which can only write on the tape cells that contained the input word in the beginning. This and an equivalent extension of second-order logic will be proven in section 3.4.1.

3. Descriptive Complexity

3.1 Aims

In mathematics, abstraction is one of the most important tools as it enables us to make general statements and prove them for all the concrete instantiations of a concept. Formal Logic takes this even further and makes it possible to abstract mathematical thought itself. In Computer science, we are often interested in the amount of resources needed to compute a certain function or solve a certain problem, speaking in terms of time and storage space. Different forms of logic have the power to describe different types of problems. By focusing on decision problems¹, we can say a corresponding logical characterization of a problem is a formula φ which is true if and only if a structure satisfies the required properties. By looking at the complexity of formulas which are needed to describe problems in terms of relations, operators, variables and other metrics, we can often find remarkably natural classes of logic corresponding to classes of problems.

Using these results, many insights into the underlying structure of real-world problems can be made which in turn can give us better ways to deal with them. Further, Descriptive Complexity has applications in database theory and computer aided verification and proofs.

3.2 Tools

As always, we first need to present some tools and techniques which will be used later in the proofs. Definition are again taken and modified from [Rög23] and [Imm99].

3.2.1 Complexity Theory

Complexity Theory is the study of the resources, measured mostly in time and space, needed to compute certain problems². Also, we do not really care about constants in the computation, and thus use a notation which omits these.

Definition 3.1 (Big-O notation). Let f, g be functions $f, g : \mathbb{N} \to \mathbb{R}_+$.

We say that $f \in \mathcal{O}(g)$ if there exists positive integers n_0, c such that for all $n \geq n_0$ we have

$$f(n) \le c \cdot g(n)$$

 $^{^{1}}$ Any problem can be reduced to boolean queries, for example by having a boolean querry meaning "the ith bit of an encoding of the answer is 1"

²The specific model of computation is not important as all give almost the same results. We will assume Turing machines

Complexity classes can then be defined as all the problems which have a Turing machine satisfying some bounds that can compute their solutions. Now we will define some common and important complexity classes.

Definition 3.2 (DTIME[$\mathcal{O}(t)$]). We say that a decision problem is in DTIME[$\mathcal{O}(t)$] if there exists a deterministic Turing machine that takes a maximum of f(n) steps on any input of size n and $f \in \mathcal{O}(t)$.

Definition 3.3 (P). We say that a decision problem is in P if there exists a polynomial q such that the problem is in DTIME[$\mathcal{O}(q)$]

Definition 3.4 (DSPACE[$\mathcal{O}(t)$]). We say that a decision problem is in DSPACE[$\mathcal{O}(t)$] if there exists a deterministic Turing machine that visits a maximum of f(n) tape cells on any input of size n and $f \in \mathcal{O}(t)$.

Definition 3.5 (PSPACE). We say that a decision problem is in PSPACE if there exists a polynomial q such that the problem is in DSPACE[$\mathcal{O}(q)$]

We can go do the same for nondeterministic Turing machines, and get the corresponding complexity classes NTIME, NP, NSPACE, NPSPACE. There, we always take the maximum of tape cells and steps over any computation branch.

The complexity class P has a special meaning for computer scientists as these are the problems which are deemed "feasible" on modern computers.

3.2.2 Ehrenfeucht-Fraïssé Games

Ehrenfeucht-Fraïssé games are combinatorial games which are equivalent to first-order formulas and their extensions. Using these games, it is often possible to show inexpressibility results for certain problems in some logic \mathcal{L} .

As a motivation, we can look at what it means for a formula to hold on some structure. Assume the formula has the form $\forall x \varphi(x)$. Then this can be seen as some opponent choosing some element $a \in |\mathcal{A}|$ and us now needing to show that $\varphi(a)$ holds. The case where the formula has the form $\exists x \psi(x)$ can be treated similarly, but we can choose the element ourselves.

Now for the formal definition

Definition 3.6 (Ehrenfeucht-Fraïssé Game). The k-pebble Ehrenfeucht-Fraïssé Game \mathcal{G}_k is played by two players: the Spoiler and the Duplicator on a pair of structures \mathcal{A} and \mathcal{B} using k pairs of pebbles. In each move, the spoiler places one of the remaining pebbles on an element of one of the two structures. Then, the duplicator tries to match the move on the other structure by placing the corresponding pebble on an element. We say that the duplicator wins the k-pebble Ehrenfeucht-Fraïssé Game on \mathcal{A}, \mathcal{B} if after the k rounds, the map $i : |\mathcal{A}| \to |\mathcal{B}|$ defined as for all elements of $|\mathcal{A}|$ with a pebble and the constants as the element in $|\mathcal{B}|$ with the corresponding pebble or constant forms a partial isomorphism. A partial isomorphism is an isomorphism formed for some subset of the universe, with all relations restricted to that subset.

In this context, the spoiler wants to show that \mathcal{A} and \mathcal{B} are different, whereas the duplicator wants to show their equivalence.

As this is a zero-sum game of full information, one of the two players must have a winning strategy. It can be proven that if the duplicator has a winning strategy for the k-pebble Ehrenfeucht-Fraïssé on \mathcal{A} and \mathcal{B} if and only if \mathcal{A} and \mathcal{B} agree on all formulas with less or equal to k nested quantifiers. We can use these facts to prove inexpressibility of some problems in first-order logic by exhibiting two structures \mathcal{A}_k and \mathcal{B}_k for each k with one satisfying the problem constraints and the other not and a winning strategy for the duplicator on these two structures. This methodology can be extended to other logics by adding new moves or restrictions to the game.

3.3 Important Results

3.3.1 NSPACE[$\mathcal{O}(s(n))$] \subseteq DSPACE[$\mathcal{O}(s(n)^2)$]

This result is part of Savitch's Theorem, which introduces alternating Turing machines in an intermediate step. These Turing machines are a generalization of nondeterministic Turing machines, which can be seen as machine taking the "or" of all its computation paths.

Definition 3.7 (Alternating Turing Machine). An alternating Turing machine is a Turing machine with two types of states: the existential and universal gates. Now, the acceptance conditions change compared to a nondeterministic Turing machine and depends on the state we are currently in. If we are in an existential state, we accept if and only if at least one of the computations leading on from this configuration is accepting. If we are in a universal state, we accept if and only all the computations leading on from this configuration are accepting.

These ATMs are now capable of also taking the "and" of the child states and maintain the ability to take the "or" of its children.

We define ATIME[$\mathcal{O}(t)$] and ASPACE[$\mathcal{O}(t)$] analogously to NTIME[$\mathcal{O}(t)$] and NSPACE[$\mathcal{O}(t)$]. Now we can proceed to the (quite technical) proof of Savitch's Theorem as presented in [Imm99].

Theorem 3.1 (Savitch's Theorem). For all space constructible functions $t \ge \log n$ we have

$$NSPACE[\mathcal{O}(t)] \subseteq ATIME[\mathcal{O}(t^2)] \subseteq DSPACE[\mathcal{O}(t^2)]$$

Proof. We start with the first inclusion, NSPACE[$\mathcal{O}(t)$] \subseteq ATIME[$\mathcal{O}(t^2)$]. We now need to show that any NSPACE[$\mathcal{O}(t)$] Turing machine can be simulated by a ATIME[$\mathcal{O}(t^2)$] alternating Turing machine. Let N be a NSPACE[$\mathcal{O}(t)$] Turing machine. Without loss of generality, we assume that N clears its tape after accepting and goes back to the first cell.

Now consider G_w , the computation graph of N on input w. We now see that N accepts w if and only if there is a path from the start configuration s to the accepting configuration t. We now present a routine P(d, x, y) which asserts that there is a path of length at most 2^d from vertex x to y. Inductively, we can define P as follows:

$$P(d, x, y) = (\exists z)(P(d - 1, x, z) \land P(d - 1, z, y))$$

This formula asserts that there exists a middle vertex z for which there is a 2^{d-1} path from x to z and from z to y. Using an alternating Turing machine, we can evaluate the formula using an existential state to find the middle vertex z, and then a universal state covering both shorter paths.

Now for the runtime analysis, we see that we need $\mathcal{O}(t(n))$ time to write down the middle vertex z, as a configuration includes the tape, which has length $\mathcal{O}(t(n))$. Further, we then need to evaluate some P(d-1,z,y). By induction, we find that we need $\mathcal{O}(d\cdot t(n))$ time to compute P(d,x,y). By the fact that there are only $2^{\mathcal{O}(t(n))}$ possible configurations, we get that the initial d is also in $\mathcal{O}(t(n))$, and thus our total runtime is $\mathcal{O}(t(n)\cdot t(n)) = \mathcal{O}(t(n)^2)$.

For the second inclusion, we need to simulate a ATIME[$\mathcal{O}(s(n))$] machine A using a DSPACE[$\mathcal{O}(s(n))$] machine (here, we substituted s(n) for $t(n)^2$). Again, we consider the computation graph of A on input w. This graph has depth $\mathcal{O}(s(n))$ and size $2^{\mathcal{O}(s(n))}$.

We can systematically search this computation graph to get our answer. This is done by keeping a string of choices $c_1c_2...c_r$ of length $\mathcal{O}(s(n))$ made until this point. Note that this uniquely determines which state we are in.

Now, we can find the answer recursively. If we are in a halt state, we report this back to the previous state. In an existential state, we simulate its children, and if we get a positive result from one of them, we also return a positive result. In a universal state, we simulate its children, and if we get a positive result from all of them, we return a positive result.

In total, we use only $\mathcal{O}(s(n))$ space, to simulate A.

Thus, the second part of the theorem follows and by transitivity of \subseteq we have NSPACE[$\mathcal{O}(t(n))$] \subseteq DSPACE[$\mathcal{O}(t(n)^2)$].

We do not know if the containment is strict or not for any of the inclusions of the theorem. From this theorem, we also get the following interesting corollary.

Corollary 3.1.1. We have PSPACE = NPSPACE.

Proof.

$$\begin{split} \text{NPSPACE} &= \bigcup_{k \in \mathbb{N}}^{\infty} \text{NTIME}[\mathcal{O}(n^k)] \\ &\subseteq \bigcup_{k \in \mathbb{N}}^{\infty} \text{DTIME}[\mathcal{O}(n^{2k})] \\ &= \bigcup_{k \in \mathbb{N}}^{\infty} \text{DTIME}[\mathcal{O}(n^k)] \\ &= \text{PSPACE} \\ &\subseteq \bigcup_{k \in \mathbb{N}}^{\infty} \text{NTIME}[\mathcal{O}(n^k)] \\ &= \text{NPSPACE} \end{split}$$

3.3.2 Space Hierarchy Theorem

The Space Hierarchy Theorem states that for both nondeterministic and deterministic space, we have problems that can be solved using t(n) space, but not with any tighter space bound. Formally, we have

$$DSPACE[o(t)] \subsetneq DSPACE[\mathcal{O}(t)]$$

where o(t) is the set of functions f such that $f \in \mathcal{O}(t)$ but $t \notin \mathcal{O}(f)$, that is all functions that grow more slowly than t. This holds for all space constructible $t \ge \log n$. The same holds for NSPACE.

We will present a proof for deterministic space.

Proof. The proof uses a diagonalization argument by presenting some machine D that takes a Turing machine M and an input size in unary as input and does the opposite of M if it halts. We want to show that for all M which run in space $f(n) \in o(t(n))$, we have an input on which D and M do not agree. This would show that the language computed by D is not in DSPACE[o(t)], and thus the strict containment.

On input $\langle M, 1^k \rangle$ our machine D marks of $t(|\langle M, 1^k \rangle|)$ tape cells, which are the cells that are allowed for the computation. Further we also maintain a counter with size $|M| \cdot 2^{t(|\langle M, 1^k \rangle|)}$, which is the maximum amount of different configurations a Turing machine can pass before looping on a binary tape of size $t(|\langle M, 1^k \rangle|)$. Then, we simulate M on input $\langle M, 1^k \rangle$. If we transcend any bound, we reject. For all M in DSPACE[o(t)], there is a k such that $f(n) \leq t(n)$ by definition. On this input, the simulation finishes, and we can invert the output.

This directly gives us an input for which M and D differ, and thus proves our claim. Furthermore, D runs in DSPACE[$\mathcal{O}(t)$] as by construction we assured that we do not run infinitely and that we stay within the space bound.

3.4 Results concerning the Chomsky Hierarchy

Now that we have seen most of the required theory, we can start to apply it to the main theme of this work, the Chomsky Hierarchy. For this section, we define the vocabulary on strings to be $\sigma = \langle \{0, \ldots, n-1\}, Q_a, Q_b, \ldots, Q_z, \leq, 0, 1, \max \rangle$. The universe consists of the numbers from 0 to n-1, we have a unary predicate for each character in Σ , a total ordering on the universe, and the constants 0, 1 and $\max = n-1$. Again, only the results for context-sensitive languages are discussed in this section. Further results can be found in the context appendix under appendix B.2.

3.4.1 Context-Sensitive Languages

This is the language class that interests us most, as it has be studied less extensively then other language classes. Nevertheless, there are some known formalisms. One of them is the linear bounded nondeterministic Turing machine. The two directions of the proof were presented separately in [Kur64] and [Lan63].

Theorem 3.2. The class of context-sensitive languages is exactly the class of languages accepted by a linear bounded nondeterministic Turing machine.

Proof. For the direction from grammar to Turing machine, we only need to show that our Turing machine can simulate a derivation backwards. We know that every context-sensitive language has a noncontracting grammar G. Using this fact, we can construct a nondeterministic Turing machine N which scans the current tape and whenever it recognizes a pattern of the right-hand side of a production rule in G, it decides whether it replaces it or not by the left-hand side of the rule. If some computation branch of N ends up with only the start symbol of G on the tape, we accept. Essentially, N simulates a derivation of W from the start symbol backwards. Because we try all possibilities by nondeterminism, we know that if N does not accept W, there is no derivation ending in W from the start symbol of G. As we assumed G is noncontracting, replacing the right-hand side of a rule with the left-hand side never makes the word longer, and thus we only need O(|W|) space.

The other direction works by explicitly defining a grammar which simulates any linear bounded automaton backwards. Without loss of generality, we include an end marker #.

Let $N = \langle Q, \Sigma, \Gamma, \delta, q_0, q_{accept}, q_{reject} \rangle$ be a NSPACE[$\mathcal{O}(n)$] Turing machine. Then, we construct a grammar $G = \langle V, \Sigma, P, S \rangle$ with $V = \bigcup_{q_i \in Q} \bigcup_{a_j \in \Gamma} \{b_{q_i, a_j}\} \cup \{S, L, R, \#\} \cup \bigcup_{a_w \in \Gamma \setminus \Sigma} \{a_w\}$. The $b_{q, a}$ represent a position on the tape including the actual state and the actual character, in addition we also have the start state, the end marker and some utility non-terminals.

We now add the following rules to P:

- For each $a_i \in \Gamma$, we add a rule $S \to Lb_{q_{accept},a_i}R$ to P. These rules mean that we are in a final accept state. To extend the final tape, we add again for each $a_i \in \Gamma$ the rules $L \to La_i$, $L \to \#$, $R \to a_i R$ and $R \to \#$ to our rule set. These rules allow derivations from S to an end tape of the form $\#a_{i_1} \dots b_{q_{accept},a_{i_j}} \dots a_{i_k}\#$.
- For each rule $\langle a_k, q_l, L \rangle \in \delta(q_i, a_j)$, we add rule $b_{a_w,q_l}a_k \to a_w b_{a_j,q_i}$ for every $a_w \in \Gamma$. Similarly, for each rule $\langle a_k, q_l, R \rangle \in \delta(q_i, a_j)$, we add rule $a_k b_{a_w,q_l} \to b_{a_j,q_i} a_w$ for every $a_w \in \Gamma$. We can clearly see that these rules simulate the nondeterministic Turing machine backwards.
- For the start, we include $\#b_{a_i,q_0} \to \#a_i$ for all $a_i \in \Sigma$ This rule allows us to say that we are at the start of our computation and "remove" the read-write head to get our initial input word.

As for any word in G we can follow back the derivation to an accepting state, we have that both N and G define the same language.

Thus, we are done and have proven the equivalence of context-sensitive languages and linear bounded automata. \Box

Now that we showed this equivalence, we will show that the context-sensitive languages are equivalent to the languages definable in MSO(TC), where we supplement monadic second-order logic with a transitive closure operator.

For this, we first define the transitive closure of a formula.

Definition 3.8 (Transitive closure). Let $\phi\begin{pmatrix} k & k \\ a, b \end{pmatrix}$ be a formula with 2k free variables. We can see this formula as an edge relation over the graph with vertices c. Then, the transitive closure of the

formula $\left(TC_{\substack{k\\a,b}}^{k}\phi\begin{pmatrix}k\\a,b\end{pmatrix}\right)\begin{pmatrix}k\\u,v\end{pmatrix}$ is true if and only if there is a path in the $\stackrel{k}{c}$ graph from $\stackrel{k}{u}$ to $\stackrel{k}{v}$ using edges from ϕ . Equivalently, we can also define it to be the minimal relation such that if R(x,y) and R(y,z), then R(x,z).

Theorem 3.3. A language L is context-sensitive if and only if it can be described by a formula in MSO(TC).

Proof. We use theorem 3.2 and show the equivalence of MSO(TC) and $NSPACE[\mathcal{O}(n)]$ Turing machines. Then the theorem will follow immediately.

First, we show that any formula in MSO(TC) can be evaluated by NSPACE[$\mathcal{O}(n)$] Turing machine. The first step is to notice that any relation of MSO can be represented on the tape in $\mathcal{O}(n)$ space. So, for any sub-formula of the form $\left(TC_{k}^{k}\phi\left(\stackrel{k}{a},\stackrel{k}{b}\right)\right)\binom{k}{u},\stackrel{k}{v}$, we write down $\stackrel{k}{u}$ and guess the next vertex. Then, we can check if the transition is valid by evaluating phi. We can repeat this process until we reach $\stackrel{k}{v}$. Because Immerman showed that NSPACE is closed under complementation in [Imm88], we know that there is also a NSPACE[$\mathcal{O}(n)$] Turing machine that computes any formula of the form $\neg \left(TC_{k}^{k}\phi\left(\stackrel{k}{a},\stackrel{k}{b}\right)\right)\binom{k}{u},\stackrel{k}{v}$. The other parts of the formula can be evaluated easily in linear space as we just need to write down relations when quantifying and otherwise remember in which part of the constant-size formula we are at this moment.

For the other direction, consider a NSPACE[$\mathcal{O}(n)$] Machine N. As in the previous proof with the grammars, we enrich our logic with new symbols b_{a_i,q_i} for all pairs of states and symbols, which means that we add a relation Q_b for all such b to our vocabulary.

Now consider a tuple $\overline{X} = \langle Q_{b_1}, \dots, Q_{b_r} \rangle$. This tuple completely represents an instantaneous configuration of the tape and the machine. We can now write a formula $\varphi(\overline{X}, \overline{Y})$ which means that a transition from state \overline{X} to \overline{Y} is possible in N. This can be done by a big disjunction over all rules of N. As a transition a new character b_i is only determined by the actual character and the two characters left and right of it³, we can write all transitions of N in the form $\langle b_k, b_l, b_m \rangle \to \langle b_i, b_j, b_w \rangle$. If P is the set of all transitions, we have

$$\begin{split} \varphi(\overline{X},\overline{Y}) &\equiv \exists i \left(\forall j \left(|i-j| > 1 \to \bigwedge_{b_i} \left(Y_{Q_{b_i}}(j) \leftrightarrow X_{Q_{b_i}}(j) \right) \right) \land \\ \bigvee_{\langle b_k,b_l,b_m \rangle \to \langle b_u,b_v,b_w \rangle \in P} \left(X_{Q_{b_k}}(i-1) \land X_{Q_{b_l}}(i) \land X_{Q_{b_m}}(i+1) \land Y_{Q_{b_u}}(i-1) \land Y_{Q_{b_v}}(i) \land Y_{Q_{b_w}}(i+1) \right) \right) \end{split}$$

The first line asserts that apart from the indices where the head is and thus where we change something, the tape stays unchanged. The second line tells us that there exists a rule in P such that the characters in \overline{Y} at positions i-1, i, i+1 follow from the previous characters in \overline{X} .

Now, we can take the transitive closure over φ , starting with the input relations, and ending at an accepting position. Without loss of generality we can assume that N clears its tape after accepting,

³we include end markers for this to work without modification for the ends of the tape

so the end position is unique. Now, our formula of the transitive closure over φ holds if and only if there is an accepting path in N starting at the input word w.

This concludes the equivalence of MSO(TC) and context-sensitive languages. $\hfill\Box$

An interesting normal form for MSO(TC) can be derived from the proof.

Corollary 3.3.1. Every formula in MSO(TC) can be written in the form

$$\left(TC_{\overline{X},\overline{Y}}\varphi(\overline{X},\overline{Y})\right)\left(\overline{U},\overline{V}\right)$$

Proof. We have given an explicit way to convert any formula into a Turing machine and back in theorem 3.3. By construction this always gives us a formula of the required form. \Box

4. Personal Contribution

In this chapter, multiple tries at searches for new first-order logics and other related concepts are presented. The range of success as well as the range of the concrete themes are broad. I did not find a fundamentally new result about the characterization of context-sensitive languages using first-order logic, but managed to prove that various approaches could not work. Further, I also lowered some upper bounds for simulating alternating Turing machines using iterative logic. Using a restricted form of iterative logic, I could lower the bounds for an iterative simulation of a nondeterministic Turing Machine.

4.1 Direct Transformation

Similar to Immerman in [Imm99], we will use extended variables to model second-order variables in first-order logic. This will then directly give us a characterization of NSPACE[s(n)] without requiring any new insights, as we can just use the same technique as for second-order logic.

Definition 4.1 (Extended Variable). The logic FO-VAR[1, s(n)] has two types of variables. One are the normal domain variables, which we will denote by lowercase characters, ranging from 0 to n-1. Further, a formula can also include extended variables, which we will denote by uppercase characters, ranging from 0 to $2^{s(n)\log(n)}-1$, and thus having $s(n)\log(n)$ bits. The extended variables can not appear as an input to any predicate variables and can only be used in quantification and as an argument to the BIT relation. Thus, we can query if a specific bit in the binary representation is on. For extended variables with more than n bits, we can extend BIT to accept a tuple of domain variables encoding the position. This makes polynomial extended variables possible.

The extended variables in FO-VAR[1, s(n)] have exactly the same capabilities as second-order variables in second-order logic, as we can query it at a position, but can not do anything else. As we want to capture NSPACE[s(n)], we will now prove that SO(TC, arity k) = FO-VAR[1, $n^k/\log(n)$](TC).

Proof. We show by induction on the structures that every formula has a very similar equivalent For both, we show by induction that we can write an equivalent formula using the other logic.

Any atomic formula of SO(TC, arity k) which does not include any second-order variable is trivially writable in FO-VAR[1, $n^k/\log(n)$](TC). An atom of the form $Y(\overline{x})$ can be written as BIT(Y', \overline{x}) for Y' being an extended variable. We then understand this as Y being true with the variables \overline{x} exactly when BIT(Y', \overline{x}) is true. This always works as we have relations of at most arity k, and thus \overline{x} will never represent any higher number.

Using this, we then can induct. Conjunction, disjunction and negation do not change anything. When we quantify over a second-order variable, we can directly exchange this with quantifying over an extended variable, as by induction the subformulas without the quantification is equivalent and plugging in the new second-order / extended variable will not change this. Taking a transitive closure can also be done by replacing all second-order variables with extended variables.

By induction, we then have that all formulas in either of the logics has an equivalent formula in the other logic. \Box

Using this equivalence and the proof in section 3.4.1, we get that FO-VAR[1, $n^k/\log(n)$](TC) describes exactly the context-sensitive languages, and thus have our first characterization in first-order logic.

4.2 Analogues to Proof for DSPACE

For DSPACE[s(n)], there are multiple other characterizations in logic without using the transitive closure operator.

To understand the following, we first need to define the logic FO[t(n)], which formalizes iterative definitions, and then VAR[k] which restricts the number of variable but allows for unbounded FO iterations.

Definition 4.2 (FO[t(n)]). Let Q_1, \ldots, Q_n be a series of quantifiers, s_1, \ldots, s_n variables and M_1, \ldots, M_n be quantifier-free formulas. Then a quantifier block is $QB = (Q_1s_1.M_n) \ldots (Q_ns_n.M_n)$. Here, for a universal quantifier $(\forall s.M)\varphi \equiv \forall s(M \to \varphi)$. Also, for an existential quantifier $(\exists s.M)\varphi \equiv \exists s(M \land \varphi)$. Both of these effectively mean that we restrict the quantifiers to range only over the elements that satisfy M. Then, a formula of FO[t(n)] is of the form

$$([QB]^{t(n)}M_0)(\overline{c}/\overline{s})$$

where M_0 is a quantifier-free formula, $\bar{c} = c_1, \ldots, c_n$ is a tuple of constants and $\bar{s} = s_1, \ldots, s_n$ are the variables occurring in the quantifier block. Also, (\bar{c}/\bar{s}) means that in the beginning, we set $s_1 := c_n, \ldots, s_n := c_n$ and $[QB]^{t(n)}$ means QB literally repeated t(n) times. The truth values of these formulas for a specific structure are defined by iterating the quantifier block $t(|\mathcal{A}|)$ times.

So now we have a formalism for iterative procedures.

If we restrict the number of variables such that all s_i need to be in $\{x_1, \ldots, x_k\}$, apart from some boolean variables (variables which can only be 0 or 1), we get FO-VAR[t(n), k]. Additionally, we define

$$VAR[k] = \bigcup_{c=1}^{\infty} FO-VAR[2^{cn^k}, k]$$

This is the same as saying that we have unbounded iterations, as after at most 2^{cn^k} the truth values of the formula will loop. The c depends on the number of boolean variables included.

Now, we are ready to look at DSPACE. For DSPACE, we then have

$$DSPACE[n^k] = VAR[k+1]$$

A proof of this can be found in [Imm99]. In the main part of the proof, a construction is made to simulate a DSPACE Turing machine using VAR[k+1]. There, the relation $C_t(\overline{x}, \overline{b})$ is inductively defined to mean that at time t, the character on the tape at position \overline{x} is the one coded by \overline{b} , where \overline{b} is a tuple of boolean variables. Because the Turing machine we are contemplating is deterministic, this character is uniquely determined. Further, it only depends on the previous characters at positions $\overline{x}-1, \overline{x}$ and $\overline{x}+1$, as we include the head position and state in the characters. So this makes it possible for every position to go back in time and find out if we get to an ending state after n^k steps.

If we want to extend this to nondeterministic Turing machines using $C_t(\overline{x}, \overline{b}) \equiv$ the character at position \overline{x} can be \overline{b} at time t, we run into problems. As we don't have the guarantee that the computation is deterministic, we can not say any more that we depend on the $C_{t-1}(\overline{x}, \overline{b})$ only. Doing this would mean that impossible states could be reached, and thus we would have false positives. One way to fix this is by remembering the nondeterministic choices we made in the previous steps. In the worst case, this would take $\mathcal{O}(2^{cn^k})$ additional bits. But we already know by Savitch's Theorem (section 3.3.1) and the equivalence for DSPACE that we only need $n \cdot (k+2)$ bits to represent a NSPACE[n^k] computation.

More generally, any proof which would show that NSPACE[n^k] can be expressed in VAR[r(n)], where VAR[r(n)] is the generalization of VAR[k] which means that a total of $r(n) + \mathcal{O}(1)$ bits are allowed, with $n \cdot (k+1) \le r(n) < n \cdot (k+2)$ would be an improvement on Savitch's Theorem. That is because the proof for DSPACE[n^k] can easily be extended to more general polynomial functions, Immerman did this in [IBB99]. Actually, this is a two-way relationship: if Savitch's Theorem can be improved, we can describe NSPACE with less than k+2 variables and unbounded iterations.

4.3 Mixing iterations and transitive closure

One question that came up during the process of finding a logic which is smaller than

$$FO-VAR[s(n), s(n)/\log(n)]$$

but still captures NSPACE[s(n)]. This led to the idea of mixing up iterative procedures with the transitive closure operator. I will now show that this approach will not help much and any restriction done this way would be mean that there exists a restriction using only iterative procedures that also contains NSPACE[s(n)].

The first is surrounding a formula in FO-VAR[$t(n), r(n)/\log(n)$] with a TC operator using variables of size r(n). For this to contain NSPACE[s(n)], we need for any formula of the form $(\text{TC}_{a,b}\varphi)(c,d)$ that there exists a quantifier block, a formula ϕ and some constants \overline{e}, f, g such that

$$\left(\mathrm{TC}_{a,b}\left([QB]^{t(n)}\phi(\overline{e}/\overline{s})\right)\right)(f,g) \equiv (\mathrm{TC}_{a,b}\varphi)(c,d)$$

We know that we can simulate any TC formula with variables of size r(n) using r(n) iterations of a quantifier block. Thus, we can rewrite the formula as

$$\left(\mathrm{TC}_{a,b}\left([QB]^{t(n)}\phi(\overline{e}/\overline{s})\right)\right)(f,g) \equiv [QB_1]^{r(n)}[QB_2]^{t(n)}\phi(\overline{e}/\overline{s},c/a,d/b)$$

The two quantifier blocks can then be merged into one by additionally maintaining a counter variable of size $\log(r(n))$ so that the quantifier block acts as the first one would during the first r(n) round and then acts like the other one.

The other case where we write the TC formula after the quantifier block is similar, then we have

$$([QB]^{t(n)} (TC_{a,b}\phi) (f,g)) (\overline{e}/\overline{s}) \equiv (TC_{a,b}\varphi)(c,d)$$

For $c \cdot r(n) > \log(t(n))$ with some fixed c, we can do the same counting trick. As a $t(n) > 2^{cr(n)}$ does not add any expressive power, we can assume that this is true.

Thus, in both cases, we have a formula in FO-VAR $[r(n) + t(n), r(n)/\log(n)]$. Now, there are multiple cases

- $r(n) \le t(n)$ Then, FO-VAR $[r(n) + t(n), r(n)/\log(n)] = \text{FO-VAR}[t(n), r(n)/\log(n)]$. This is only interesting in the case where r(n) < s(n)
- r(n) > t(n) Then, FO-VAR $[r(n) + t(n), r(n)/\log(n)] = \text{FO-VAR}[r(n), r(n)/\log(n)]$. This is again only interesting when r(n) < s(n).

We thus get that anything interesting in this case happens only when we have less variable bits than s(n). Using Savitch's Theorem once more, we also get that $r(n) > \sqrt{n}$. Another interesting result is that Savitch's Theorem can be improved for some possible results as

$$FO-VAR[t(n), r(n)/\log(n)] \subset DSPACE[t(n)r(n)]$$

which would be smaller than $s(n)^2$ in some of these cases. The same method also means that $t(n)r(n) \ge s(n)$ because of Savitch's Theorem and the Space Hierarchy Theorem (section 3.3.2). As this is an open problem since 50 years, this seems to be a very difficult endeavour.

4.4 Restricting universal quantification

One further approach that I attempted was restricting universal quantification in the FO-VAR formulas, which I called FO \exists -VAR. In FO \exists -VAR, universal quantification is only allowed over boolean variables. We will denote the boolean variables by b_j . Further, the requirement of the M_i to be quantifier-free is dropped. This step was motivated by the fact that nondeterministic Turing machines in essence capture existential quantification.

A similar idea to the one in Savitch's Theorem, guessing the middle of the path and checking both shorter sides. A formula in FO \exists -VAR[$s(n), s(n)/\log(n)$] which is equivalent to a formula in

FO-VAR[1,
$$s(n)/\log(n)$$
] of the form $\left(TC_{\overline{X},\overline{Y}}\varphi\right)(\overline{C},\overline{D})$ is

$$QB \equiv (\forall b_1.M_1)(\exists \overline{Z})(\forall b_2)(\exists \overline{A}, \overline{B}.M_2)(\exists \overline{X}, \overline{Y}.M_3)$$

$$M_1 \equiv \neg(\forall \overline{z}(\operatorname{BIT}(\overline{X}, \overline{z}) \leftrightarrow \operatorname{BIT}(\overline{Y}, \overline{z})) \lor \varphi(\overline{X}, \overline{Y}))$$

$$M_2 \equiv (b_2 \land \forall \overline{z}(\operatorname{BIT}(\overline{X}, \overline{z}) \leftrightarrow \operatorname{BIT}(\overline{A}, \overline{z})) \land \forall \overline{z}(\operatorname{BIT}(\overline{B}, \overline{z}) \leftrightarrow \operatorname{BIT}(\overline{Z}, \overline{z}))) \lor (\neg b_2 \land \forall \overline{z}(\operatorname{BIT}(\overline{Z}, \overline{z}) \leftrightarrow \operatorname{BIT}(\overline{A}, \overline{z})) \land \forall \overline{z}(\operatorname{BIT}(\overline{B}, \overline{z}) \leftrightarrow \operatorname{BIT}(\overline{Y}, \overline{z})))$$

$$M_3 \equiv \forall \overline{z}(\operatorname{BIT}(\overline{X}, \overline{z}) \leftrightarrow \operatorname{BIT}(\overline{A}, \overline{z})) \land \forall \overline{z}(\operatorname{BIT}(\overline{B}, \overline{z}) \leftrightarrow \operatorname{BIT}(\overline{Y}, \overline{z}))$$

and finally

$$[QB]^{cs(n)}(false)(\overline{C}/\overline{X},\overline{D}/\overline{Y})$$

for some c. This formula needs some explanation. We let M_1 be the breaking condition, being false whenever either \overline{X} and \overline{Y} are the same or connected directly. So in QB, the first quantification means that we break with true whenever we have a connection, as when this happens, we quantify over the empty set, which is defined as true. After this, a middle configuration \overline{Z} is guessed, and both sides b_2 are checked. In M_2 , we then check that \overline{A} and \overline{B} are the new endpoints which are defined by b_2 and $\overline{X}, \overline{Z}, \overline{Y}$. After this, we copy \overline{A} to \overline{X} and \overline{B} to \overline{Y} in M_3 . When iterating this we guess a path from \overline{C} to \overline{D} , checking every connection between adjacent states.

More generally, for any function $r(n) \leq 2^{cs(n)}$, we can define a formula in

$$FO\forall, \exists \text{-VAR}[s(n)/\log(r(n)), \log(r(n)), s(n)r(n)/\log(n)]$$

Here, we define FO \forall , \exists -VAR[t(n), f(n), s(n)] to contain all formulas which have t(n) iterations, extended variables of f(n) bits which can be universally quantified and $s(n)\log(n)$ bit extended variables which can be used in existential quantification. These formulas are very similar to the one defined for FO \exists -VAR from above. The only difference lies in the splitting. Instead of splitting paths into two parts, we split them into r(n) parts. Thus, for a path of length $2^{cs(n)}$, we need

$$\log_{r(n)} \left(2^{cs(n)} \right) = \frac{\log \left(2^{cs(n)} \right)}{\log(r(n))} = cs(n) / \log(r(n))$$

iterations. As for simulating this formula with a Turing machine, the product of the number of iterations and the size of the extended variables is important, we do not gain any tighter results from this.

4.5 Alternating bounds

In the proof of Savitch's Theorem, we use alternating Turing machines as an intermediate step for proving that NSPACE[s(n)] is a subset of DSPACE[s(n)2]. We can also add another intermediate step using FO-VAR[$s(n), s(n)/\log(n)$] with the method shown in section 4.4. It is also quite easy to simulate any formula in FO-VAR[$t(n), s(n)/\log(n)$] with an alternating Turing machine in ATSR[t(n)s(n), s(n), t(n)], where in this new class ATSR, we specify time, space and reversals. With

reversals, we mean the number of times we switch from universal states to existential states and back. We do this by writing the current values of all variables during the iterated quantifier part and evaluating the quantifier-free FO formulas, which can be done efficiently.

We will now investigate two ways of simulating an ATSR[t(n), s(n), r(n)] Turing machine using FO-VAR.

The first one is a straightforward simulation of each step of the computation. For this, we encode the whole state of the Turing machines in a tuple of s(n) bit extended variables, and always guess the next step. Also, we assume without loss of generality that a predicate $existential(\overline{X})$ exists and that there exists exactly one accepting state, denoted by \overline{E} .

$$QB \equiv (\forall b.M_1)(\exists \overline{A}.\varphi(\overline{X}, \overline{A}))(\forall \overline{B}.M_2)(\exists \overline{X}.\forall \overline{z}(\mathrm{BIT}(\overline{X}, \overline{z}) \leftrightarrow \mathrm{BIT}(\overline{B}, \overline{z})))$$

$$M_1 \equiv \neg \forall \overline{z}(\mathrm{BIT}(\overline{X}, \overline{z}) \leftrightarrow \mathrm{BIT}(\overline{E}, \overline{z}))$$

$$M_2 \equiv (existential(\overline{X}) \rightarrow \forall \overline{z}(\mathrm{BIT}(\overline{A}, \overline{z}) \leftrightarrow \mathrm{BIT}(\overline{B}, \overline{z}))) \land \varphi(\overline{X}, \overline{B})$$

with

$$([QB]^{t(n)}(false))(\overline{S}/\overline{X})$$

This gives us a formula in FO-VAR[t(n), $s(n)/\log(n)$] which simulates the procedures of an alternating Turing machine. To simplify it, some M_i are not quantifier-free. These can be moved out in an equivalent way, but make the formula less readable. The inner formulas work as follows: The formula QB starts of with checking if we already achieved our goal and the actual configuration is the accepting configuration using M_1 . Next, if we are not done yet, we first existentially guess the next configuration, restricting this quantification to only those configurations which are directly connected to the actual one. In M_2 we either retain this existentially guessed next state if we are in an existential state (thus effectively doing nothing) or ignore the existentially quantified state and just quantify universally over all states which are connected to the current one. The last thing we do is copying \overline{B} to \overline{X} , preparing it to be the new start of the path.

By combining the above techniques for switching between universal and existential quantification with the path-halving method from Savitch's Theorem, we get an even stronger result.

On a high level, the plan is to do the following:

- 1. From the actual starting vertex, find all reachable vertices using only vertices which have the same type as the starting vertex.
 - (a) For existential states, we can use the normal technique of halving paths naively
 - (b) For universal states, we need to quantify for all ending vertices and then consider two cases
 - i. We claim that there is no path using only universal states going to this vertex. Then, we need to show that for each middle vertex, one of the two new paths still does not exist.
 - ii. We claim that a path exists. In this case, we can try to find a path normally.
- 2. Repeat with all the reached vertices

Before presenting the formula, we can first think of how much iterations we need to do. Because of the halving trick, we use $\log(a)$ iterations for a path of length a with only one quantifier type. To get an upper bound on the total number of iterations, we can use Jensen's inequality ([Mar19], p.28). We then get

$$\frac{\sum_{j=0}^{r(n)} \log(a_j)}{r(n)} \le \log\left(\frac{\sum_{j=0}^{r(n)} a_j}{r(n)}\right) = \log\left(\frac{t(n)}{r(n)}\right)$$

because of the condition that $\sum_{j=0}^{r(n)} a_j = t(n)$. Multiplying this with r(n), we get that a path can require a maximum of $r(n) \log \left(\frac{t(n)}{r(n)}\right)$ iterations. Thus, the formula is in FO-VAR $[r(n) \log \left(t(n)/r(n)\right), s(n)/\log (n)]$

The formula is then as follows:

$$QB \equiv (\forall b_0.M_1)(\exists b_0.N_1)(\exists b_1.M_2)(\exists Z_e.M_3)(\forall Z.N_2)$$

$$(\exists b_{2e})(\forall b_2.N_3)(\exists A, B.M_4)(\forall S, E.M_5)(\exists A, B.M_6)(\exists I, X.M_7)(\exists b_0.N_4)(\exists b_{path}.N_5)$$

$$M_1 \equiv b_{path} \rightarrow \neg (I = Y \land (S = E \lor \varphi(S, E)))$$

$$N_1 \equiv \neg b_{path} \rightarrow \neg (S = E \lor \varphi(S, E))$$

$$M_2 \equiv \neg b_1 \leftrightarrow (S = E \lor \varphi(S, E))$$

$$M_3 \equiv existential(Z_e) \leftrightarrow existential(X)$$

$$N_2 \equiv (b_{path} \rightarrow Z = Z_e) \land (existential(Z) \leftrightarrow existential(X))$$

$$N_3 \equiv \neg b_{path} \rightarrow b_2 = b_{2e}$$

$$M_4 \equiv (b_1 \land ((\neg b_2 \land A = S \land B = Z) \lor (b_2 \land A = Z \land B = E))) \lor (\neg b_1 \land A = I \land (B = Y \lor (existential(B) \leftrightarrow \neg existential(I))))$$

$$M_5 \equiv S = A \land (((b_1 \lor existential(S)) \land E = B) \lor (\neg (b_1 \lor existential(S)) \land (E = Y \lor (existential(E) \leftrightarrow \neg existential(S)))))$$

$$M_6 \equiv (\neg b_1 \land S = A \land E = B) \lor (b_1 \land X = A \land I = B)$$

$$M_7 \equiv X = A \land I = B$$

$$N_4 \equiv b_0 = b_{path}$$

$$N_5 \equiv (b_1 \land b_{path} = b_0) \lor (\neg b_1 \land (existential(X) \rightarrow b_{path}))$$

and $([QB]^{r(n)\log(t(n)/r(n))}(\neg b_{path}))$ $(true/b_{path}, AS/S, AS/X, AS/I, AS/S, AS/E, AE/Y)$ being the final formula. First, we will look at the meaning of the variables:

Y: the accepting configuration

X: the actual starting configuration from which we started the search

I: the vertex for which we are checking that a connection from X exists

S: the start of the path we are checking right now

E: the end of the path we are checking right now

 Z, Z_e : the guessed middle configuration of a path from S to E

 A, B, b_0 : variables used for copying or as dummies

 b_{path} : whether we are trying to show that there is a path or that there is no path from S to E

 b_1 : remember whether S and E are connected

 b_2, b_{2e} : which half of the $S \to Z \to E$ path should be checked

As this formula is quite intricate, it is proposed to read it in four goes.

- 1. First, we look at the formula in the easiest case: We are still trying to find a path from X to I using S and E, which are not connected. In this case, we have b_{path} and b_1 as true. Then, QB works like this: First, in M_1 , we check that we are not done, which we aren't as S and E are not connected. As b_{path} is true, N_1 does not affect anything. In M_2 , b_1 is set to true. Then we guess a middle configuration between S and E which has the same type as X in M_3 . N_2 just copies Z_e into Z. Next, we choose a side of the path. As b_{path} is true, this is done universally, because N_3 ignores the choice that was made with b_{2e} . In this case, M_4 copies the relevant new starting and ending points to A and B. Because b_1 is true, we then copy A and B to S and E in M_5 . When combining M_6 and M_7 , we just retain X and I to make them stay the same using A and B. The same happens with b_{path} using N_4 , N_5 and b_0 . So in the end, we get a new configuration with a guessed middle configuration replacing either the former ending or starting point. If no path exists, this will continue until the formula $\neg b_{path}$ marks this branch as false.
- 2. The second option we look at is when we do not want a path to exist. In that case, we have ¬b_{path}. Because of this, M₁ does not have any effect. In N₁, we check that we did not find any connection after all, and if we did find one, this logical branch will be false because of the existential quantification. If we get N₁ is true, we get on to M₂, which will establish b₁. The formula N₂ completely ignores M₃, which thus has no effect. N₂ itself then universally quantifies over all middle vertices Z which could lie on a path between S and E. The next two quantifiers have the effect of quantifying existentially which half of S → Z → E is not connected. This half must exist as otherwise a path from S to E exists, which we want to be false in this case. Because we again have b₁ as true, M₄ will copy the relevant part of the path to A and B. These are then copied back to S and E in M₅. M₆, M₇, N₄ and N₅ do the same as in the connection case, which was resetting S, E, X and I to the same value. If effectively no path exists, we will continue doing this until we hit ¬b_{path}. At this point, the branch will then be true, as effectively, no path exists from X to I by making these choices.
- 3. The third possibility we need to consider is that we are presently trying to do a path from X to I and that we succeed in finding a connection between S and E. In this case, we have b_{path} and $\neg b_1$. In this case, we look at what happens when the current component, and thus X, is universal. In M_1 , if I = Y, we are done, as we reached the accepting configuration. Otherwise, we can again ignore N_1 , and M_2 will set b_1 to false. We can ignore the quantification for Z and b_2 as they will not be used in this iteration of the formula. In M_4 , A and B are guessed such that A is the new starting vertex, which was the ending vertex before, and B is either the ending vertex or a vertex of the other type. Then, M_5 copies A to S, marking it as the starting vertex. Further, because we changed quantification type, we have that a valid S must now be

existential. Thus, we also copy B too E directly. After that, we copy back S to A and E to B in M_6 , for them to set X and I accordingly. The last change happens in N_5 , where we set b_{path} to be true. Thus, the state is set for a new block of existential states.

4. The last option is similar to the third one, with the difference that the actual state X is existential. In this case, we have b_{path} and $\neg b_1$. In M_1 , if I = Y, we are done, as we reached the accepting configuration. Otherwise, we can again ignore N_1 , and M_2 will set b_1 to false. We can ignore the quantification for Z and b_2 as they will not be used in this iteration of the formula. In M_4 , A and B are guessed such that A is the new starting vertex, which was the ending vertex before, and B, which will be ignored later, is either the ending vertex or a vertex of the other type. Then, M_5 copies A to S, marking it as the starting vertex. Further, because we changed quantification type, we have that a valid S must now be existential. Thus, we quantify universally over all vertices which are either the ending vertex or have the other type. After that, we copy back S to A and E to B in M_6 , for them to set X and E accordingly. The last change happens in N_5 , where we quantify existentially over both possibilities we set for that new ending vertex, having a path, or not. Thus, the state is set for a new block of universal states.

The complete formula sets the starting conditions to be such that we are trying to find a path with $b_{path} = true$, and that all of X, S, E and I are set to the staring configuration AS. The ending Y is set to the desired ending AE. This starting configuration will trigger either case three or four and make the first cycle possible.

These results allow for enclosing the ATSR class quite with only a logarithmic overhead between two FO-VAR classes.

FO-VAR $[a(n), s(n)/\log n] \subseteq ATSR[a(n)s(n), s(n), a(n)] \subseteq FO-VAR[a(n)\log(s(n)), s(n)/\log n]$

5. Conclusion and Direction

5.1 Conclusion

In this work, we investigated multiple logics in relation to Savitch's Theorem. This has led us to have a better notion of how all these logics are related to $\mathrm{NSPACE}[s(n)]$ and thus also to linear-bounded automata and context-sensitive languages.

In the beginning, we introduced the theory of formal languages and the Chomsky Hierarchy. Afterward, the main tools of Descriptive Complexity, including Complexity Theory and Ehrenfeucht-Fraïssé Games where presented. Savitch's Theorem is the next proof included in this work which is then present throughout the work. Then, the equivalence between context-sensitive languages and linear bounded automata is shown, giving a framework for what comes next.

Personally, I investigated multiple ideas I got during the time I read the theory.

The first one was a direct transformation of the results of connections between second-order transitive closure logic and nondeterministic space Turing machines to first-order logic. This approach does not contain any new insights, but is a good showcase of the close correlation between first- and second-order logic.

After this, I wanted to explicitly prove that some methods could not work. This branch of the work started with the investigation of the proof that DSPACE is equivalent to VAR[k+1]. There, I showed that naively applying this method gives wrong results, and that a natural extension by remembering decisions is suboptimal. A full proof was impossible to make as it is unclear how to generalize this direction of work. The difficulty of this problem is again illustrated by Savitch's Theorem, which has not been improved for a long time and thus makes it seem unlikely that a simulation of NSPACE machines with subquadratic DSPACE machines is possible.

The next method I tried was mixing transitive closure logic with iterative logic. This turned out to be not very powerful, as any interesting result in one of the mixed logics would imply one in pure iterative logic. Nevertheless, some upper and lower bounds were shown using Savitch's Theorem and the Space Hierarchy Theorem.

In an attempt to make FO-VAR less powerful, I then considered restricting universal quantification. A new formula made this possible, but also for this restriction, I was unable to find a way to simulate it using the transitive closure. The generalization of this idea by adding more bits to the extended variables and decreasing the iteration count gives an interesting space-time tradeoff, but does not solve the inherent problem of simulating this formula by NSPACE machines.

The most complicated result I was able to get does not really have any connection to contextsensitive languages at all. It concerns the simulation of alternating Turing machines using FO-VAR. There a quite tight containment could be found which bounds some alternating Turing machine class from above and below by a factor of only $\log(s(n))$. This result involved the combination of different techniques used in the results described above. This result could lead onto a path to describe alternating space-time classes exactly using logic.

5.1.1 Working process

Generally, this work was a great learning opportunity for me. I was able to see how scientific research is done and could immerse myself in a domain that interests me. I knew that I could not plan with any significant results, and indeed I worked on a lot of different branches, but most of the time hit a dead end.

In the beginning of the working process, I spend a lot of time reading multiple books about Descriptive Complexity and logic. Then, I researched more papers on the topic and tried to understand lower and upper bounds that were described there. This took a bit more time than expected, but I still was able to start investigating myself early enough. As this is my first scientific research work, I did not know exactly how to approach it, so I wrote to Dr. Královi from the ETH Zürich. His tips game me good conditions to start. During the months that followed, I tried multiple directions and read a lot of papers concerning new things I wanted to prove. Quite soon, Ms. Sprunger and I discussed that starting to write the theoretical part of the project would be good so that I would not have too much stress in the end. I did this during the summer break, experiencing some difficulties in the simplification of the proofs enough while still maintaining there correctness. Afterward, I continued doing research. Two months before handing in, the International Olympiad in Informatics took place. My time plan did not account for this very well, so I had to work quite a lot in the last two weeks to write down what I had done.

Overall, I think that there are three main points which could be improved:

- First, I often feel that my proofs are not explained in a way that is clear and concise. This makes it difficult for the reader to follow the arguments and understand the underlying thought process.
- Another point is the methods of research. I found it difficult to find any resources on this matter
 for the highly abstract field of mathematics. Further, I had no mentor on this project which
 could help me along the right way.
- The time management was suboptimal, as I spend a lot of time on branches that where clearly not working and thus did not have time to investigate everything I wanted. Also, I did not start writing down my own research until very late, which generated some stress in the end.

5.2 Directions

In the future, multiple topics could be investigated further to get an even deeper understanding on what happens in Savitch's Theorem.

In all proofs concerning equivalences between transitive closure logics and NSPACE[s(n)], we assumed that s(n) is at most polynomial. This is still a quite profound limitation, and no characterization

for superpolynomial bounds is known to me. Finding a generalization could lead to new insights that would help in the polynomial case, and in the end to the case where s(n) = n and we have exactly the context-sensitive languages.

In the context of Savitch's Theorem, it is interesting to investigate the computation graphs of NSPACE and DSPACE machines. This has been discussed on the theoretical computer science stack exchange in [Bar10]. A motivation for this is that the number of nodes in both graphs are the same, only the number of edges vary.

Another direction that could be investigated is looking at normal forms. One that seems to have some potential is the Kuroda Normal Form described in [Kur64]. This approach could yield a semantic restriction similar to the one for context-free languages described in appendix B.2.3.

After showing that mixing TC and iterative procedures does not give any strong characterizations in section 4.3 and seeing that all interesting cases happen when the extended variables have less than s(n) bits, one direction that took up most of the time and yielded very little results came up. A very interesting result would have been to show that any iterative formula simulating a TC computation needs to have at least variables of the same size, as this would have shown that the path of investigating any logic which is a subset of these logics. To do this I read multiple papers concerning hierarchies over the transitive closure, Generalized quantifiers and alternating space-time. One of the most interesting of these is "A double arity hierarchy theorem for transitive closure logic" [GH96] which combines both and shows strict hierarchies on unordered graphs. The main problem with these approaches is that they can not be generalized to include string structures, which are inherently ordered. This makes it impossible to connect them to Turing machines which work with these structures. Some steps in this direction were made in the chapter about proving lower bounds in [Imm99].

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A. Mathematical Background

The definitions are taken from the lectures Discrete Mathematics in Computer Science [HR22] and Theory of Computer Science [Rög23], as well as from the book Descriptive Complexity [Imm99].

A.1 Set Theory

Set An unordered collection of distinct elements, written with curly braces {}

Tuple An ordered collection of elements, written with pointed braces $\langle \rangle$

Set operations There are multiple ways to form new sets from already existing sets:

Union denoted as \cup , an element is in $A \cup B$ if and only if it is in A or B

Intersection denoted as \cap , an element is in $A \cap B$ if and only if it is in A and B

Cartesian product denoted as \times , $A \times B$ is the set of 2-tuples $\langle a, b \rangle$ with an element a of A and an element b of B

Cartesian power A^k denotes the Cartesian product of A with itself repeated k times

Power set denoted as $\mathcal{P}(A)$, contains all subsets of A

A.2 First-Order Logic

We abbreviate first-order logic as FO.

Variable A variable is an element that can have a value from a set

Universe The set over which variables and constants can range

Relation A relation of arity k, $R(x_1, ..., x_k)$ can be either true or false for any k-tuple of variables. In this work we always consider an equality relation =, an ordering relation \leq , and BIT(x, y), which means that the y^{th} bit of x is 1 in binary notation, to be present

Vocabulary A tuple $\tau = \langle R_1^{a_1}, \dots, R_r^{a_r}, c_1, \dots, c_s \rangle$ of relations R_i with arity a_i and constants c_j^1

Structure A tuple $\mathcal{A} = \langle |\mathcal{A}|, R_1^{\mathcal{A}}, \dots, R_r^{\mathcal{A}}, c_1^{\mathcal{A}}, \dots, c_s^{\mathcal{A}} \rangle$ where $|\mathcal{A}|$ is the universe, the constants are assigned a value from $|\mathcal{A}|$, and each relation is assigned a truth value for each a_i -tuple in $|\mathcal{A}|^{a_i}$. The set of all structures for a given universe is denoted as STRUCT $[\tau]$

 $^{^{1}}$ We omit functions, which are included in most textbook definitions, as they can be simulated by a relation in our case

First-Order Formula A first-order formula is inductively defined as follows:

Atoms Any formula of the form $R(x_1, ..., x_k)$ for some relation of arity k is called an atomic formula

Conjunction If φ and ψ are formulas, $(\varphi \wedge \psi)$ is a formula

Disjunction If φ and ψ are formulas, $(\varphi \lor \psi)$ is a formula

Negation If φ is a formula, $\neg \varphi$ is a formula

Existential quantification If φ is a formula, $\exists x \varphi$ is a formula

Universal quantification If φ is a formula, $\forall x \varphi$ is a formula

Free variables A variable is called free if there is an occurrence of it in a formula which is not bound by a quantifier whose scope surrounds it

Semantics For any structure, we can assign a truth value to any formula over the corresponding vocabulary. If the formula contains free variables, these need to be assigned a value from the universe first. We say \mathcal{A} satisfies ϕ , denoted as $\mathcal{A} \models \phi$, if and only if ϕ is true under the interpretation of the constant and relations in \mathcal{A} . This truth value is inductively assigned to all formulas as follows:

Atoms For a formula ϕ of the form $R(x_1, \ldots, x_k)$, we have $\mathcal{A} \models \phi$ if and only if the interpretation of the relation $R^{\mathcal{A}}$ maps $\langle x_1, \ldots, x_k \rangle$ to true

Conjunction We have $\mathcal{A} \models (\varphi \land \psi)$ if and only if $\mathcal{A} \models \varphi$ and $\mathcal{A} \models \psi$

Disjunction We have $\mathcal{A} \models (\varphi \lor \psi)$ if and only if $\mathcal{A} \models \varphi$ or $\mathcal{A} \models \psi$

Negation We have $\mathcal{A} \models \neg \varphi$ if and only if $\mathcal{A} \not\models \varphi$

Existential quantification We have $\mathcal{A} \models \exists x \varphi$ if and only if there exists a $y \in |\mathcal{A}|$ such that $\mathcal{A} \models \varphi(y/x)$, where $\varphi(y/x)$ denotes φ with any occurrence of x replaced with the element y

Universal quantification We have $\mathcal{A} \models \forall x \varphi$ if and only if for all $y \in |\mathcal{A}|$ we have $\mathcal{A} \models \varphi(y/x)$

First-Order Queries A first-order query is a map from structures over one vocabulary σ to structures over another vocabulary τ . The mapping is done in such a way that first-order formulas define the universe, which is a subset of $|\mathcal{A}|^k$ for some k, the relation symbols, and all the constants. For a more formally thorough definition see [Imm99]

Isomorphism An isomorphism is a map $I: |\mathcal{A}| \to |\mathcal{B}|$ with \mathcal{A}, \mathcal{B} over the same vocabulary which satisfies the following properties:

- I is bijective
- for every available relation R_i of arity a_i and every a_i -tuple $\overline{e} = \langle e_1, \dots, e_{a_i} \rangle$ in $|\mathcal{A}|^{a_i}$, we have

$$R_i^{\mathcal{A}}(e_1,\cdot,e_{a_i}) \Leftrightarrow R_i^{\mathcal{B}}(I(e_1),\cdot,I(e_{a_i}))$$

• for every constant symbol c_j , we have $I(c_j^A) = c_j^B$

If such an I exists for two structures \mathcal{A} and \mathcal{B} , we write $\mathcal{A} \cong \mathcal{B}$

A.3 Second-Order Logic

In second-order logic, we extend the capabilities of first-order logic with the ability to quantify over relations. We thus also need to extend our definitions. We abbreviate second-order logic as SO.

- SO variables A relation that is not given in the vocabulary and can be substituted with a specific interpretation
- SO formula In addition to the inductive rules from the FO formulas, we can quantify over secondorder formulas
 - **SO Existential quantification** If φ is a formula, then $\exists V \varphi$ is a formula
 - **SO Universal quantification** If φ is a formula, then $\forall V \varphi$ is a formula
- SO Semantics Here we also need to extend the FO semantics
 - **SO Existential quantification** We have $\mathcal{A} \models \exists V \varphi$ if and only if there exists a relation U over $|\mathcal{A}|$ such that $\mathcal{A} \models \varphi(U/V)$, where $\varphi(U/V)$ denotes φ with any occurrence of V replaced with U
 - **SO Universal quantification** We have $\mathcal{A} \models \forall V \varphi$ if and only if for all relations U over $|\mathcal{A}|$ we have $\mathcal{A} \models \varphi(U/V)$

A.4 Turing Machines

Turing machines are the most common model of computation.

Informal definition A Turing machine is an automaton with a finite number of states and an infinite tape. Using a read/write head, which can read one symbol on the tape, modify one symbol on the tape and move left and right, a Turing Machine can compute functions

Formal definition Formally, a Turing machine is a 7-tuple $M = \langle Q, \Sigma, \Gamma, \delta, q_0, q_{accept}, q_{reject} \rangle$, where

- Q is the set of states
- Σ is the alphabet of the input word
- Γ is the set of symbols which can be written or read on the tape, which we call the tape alphabet
- δ is the transition function, with $\delta: \Gamma \times Q \to \Gamma \times Q \times \{L,R\}$. This means that when a Turing machine is in state n and reads a on the tape, δ tells us to which state we should transition, which symbol we should write and which direction we should move the read/write head
- q_0 the start state

 q_{accept} the accepting state

 q_{reject} the rejecting state

- Turing computation At the beginning, the Turing machine is in the start state, the input word is written on a consecutive part of the tape and the read/write head is on the first character of the input word. In the following steps, the machine state changes according to the transition function. If at some point the machine enters the accepting or the rejecting state, the computation halts, and the Turing machine is said to have accepted / rejected the input. It can happen that the machine continues indefinitely or loops. In that case, we also say that it has rejected its input. In this work, we will ignore the tape content after the computation and focus on decision problems.
- **Decidability** If a Turing machine halts on all inputs, we say that it decides a problem, as we can always be sure that the machine will accept or reject an input in finite time.
- Nondeterministic Turing machine We can extend the transition function δ to allow multiple transitions from a given state. Formally, we then have $\delta: \Gamma \times Q \to \mathcal{P}(\Gamma \times Q \times \{L,R\})$. If at some point there are multiple transitions that are possible from the current state, we can take any of them. If there exists any computational path which leads to an accepting state, the nondeterministic Turing machine accepts. This is not analogous to how real sequential computers work, but allows interesting results, and is as powerful as a normal deterministic Turing machine.
- **Space/Time-Constructible functions** A function f(n) is time constructible if there exists a Turing machine which on input 1^n writes f(n) in binary on its tape in time f(n). Space-constructible functions are defined analogously.
- Church-Turing Thesis The Church-Turing Thesis states that anything that can be done on a real-world computer can be done using a Turing machine.

B. Mathematical Context and further proofs

B.1 Formal languages

B.1.1 Regular Languages

The regular languages have the most restricted type of grammars. Formally, any regular language can be described by a grammar with rules in $V \times (\Sigma \cup \Sigma V \cup \varepsilon)$. This means that we only have exactly one non-terminal on the left-hand side and the right-hand side is either a terminal, the empty word or a terminal symbol followed by a non-terminal symbol.

Example B.1. Consider the grammar $\langle \{S, O\}, \{a\}, R, S \rangle$ with

$$R = \begin{cases} S \to aO, & S \to \varepsilon, \\ O \to aS \end{cases}$$

The generated language are exactly all words with even length.

The regular languages have been studied quite thoroughly and have multiple equivalent formalisms:

- The language is recognized by a Deterministic finite automaton, which process the input word one character at a time
- The language can be decided by a read-only Turing machine, that is a Turing machine that can not modify it's tape
- The language can be described by a regular expression

For a more in-depth analysis of regular languages and equivalent formalisms refer to appendix B.2.2 and [Str94].

B.1.2 Context-Free Languages

The context-free languages extend the regular languages by allowing arbitrary right-hand sides for the rules of the defining grammar. Formally, that gives us rules in $V \times (\Sigma \cup V)^*$. Most valid arithmetic expressions, logical formulas and formally correct code in programming languages are context-free, as we can see the non-terminal symbols as types which are then converted to specific expressions of that type.

Example B.2. Consider the grammar $\{\{\mathbf{Exp}, \mathbf{NumF}, \mathbf{Num}\}, \{0, 1, (,), -, +\}, R, \mathbf{Exp}\}$ with

$$R = \begin{cases} \mathbf{Exp} \rightarrow \mathbf{NumF}, & \mathbf{Exp} \rightarrow (\mathbf{Exp} + \mathbf{Exp}), \\ \mathbf{Exp} \rightarrow (\mathbf{Exp} - \mathbf{Exp}), & \mathbf{Exp} \rightarrow (-\mathbf{Exp}), \\ \mathbf{Num} \rightarrow 0\mathbf{Num}, & \mathbf{Num} \rightarrow 1\mathbf{Num}, \\ \mathbf{Num} \rightarrow \varepsilon, & \mathbf{NumF} \rightarrow 0, \\ \mathbf{NumF} \rightarrow 1\mathbf{Num} \end{cases}$$

This generates the language of all well-formed formulas using addition and subtraction over binary numbers. For clarity, **Exp** denotes an arbitrary expression, **NumF** any number without leading zeroes and **Num** any number (possibly empty or with leading zeroes).

Those languages have less known formalisms, the Push-Down Automaton (again see [Rög23]) being the most common. For a characterization of the context-free languages using logic, see appendix B.2.3.

B.1.3 Recursive Languages

The recursive languages are the most general languages in the hierarchy, as they don't have any restrictions on the rules. It can be shown that this set of languages is equivalent to the languages recognizable by a Turing machine. By the Church-Turing thesis, this means that these are exactly the languages that can be computed by any of our computers and algorithms. Thus, we have a huge number of equivalent formalisms, including a RAM machine, while-programs and lambda calculus.

It is worth noting that there are languages which are not recursive. One of the most important example of these languages is the set of all (descriptions) of Turing machines which halt on every input, also known as the halting problem. For the characterization using logic, again refer to appendix B.2.4.

B.2 Descriptive Complexity

B.2.1 Reduction and Completeness

A reduction can informally be seen as a method of using a problem we already solved to solve a new problem by converting this new problem into an instance of the old problem. These reductions can be very useful to define complete problems for complexity classes, which in turn enables us to prove theorems for all problems of a specific complexity class.

Definition B.1 (first-order reduction). Let \mathcal{C} be a complexity class and A and B be two problems over vocabularies σ and τ . Now suppose that there is some first-order query $I: \mathrm{STRUC}[\sigma] \to \mathrm{STRUC}[\tau]$ for which we have the following property:

$$A \in A \Leftrightarrow I(A) \in B$$

Then I is a first-order reduction from A to B, denoted as $A \leq_{fo} B$.

First-order reductions can then be used to show that some problem is also a member in some complexity class, as in most complexity classes, we can compute the first-order query, and then we are

left with a problem that we already know is in the required class. The converse can also be shown: for some problem B which is not in some complexity class C, if we have $B \leq_{fo} A$, then A is also not in C, as otherwise B would also be in C, which is a contradiction.

Using the reductions, we can define completeness.

Definition B.2 (Completeness via first-order reductions for Complexity Class \mathcal{C}). We say some problem A is complete for \mathcal{C} via \leq_{fo} if and only if

- $A \in \mathcal{C}$
- for all $B \in \mathcal{C}$, we have $B \leq_{fo} A$

Informally, a complete problem captures the essence of the complexity class. Further, they have an application in some proofs of equivalences between complexity classes \mathcal{C} and logics \mathcal{L} . These proofs follow the following steps as in [Imm99]:

- 1. Show that $\mathcal{L} \subseteq \mathcal{C}$ by providing a way to convert any formula $\varphi \in \mathcal{L}$ into an algorithm in \mathcal{C} .
- 2. Find a complete problem T for \mathcal{C} via first-order reductions.
- 3. Show that \mathcal{L} is closed under first-order reductions, that is that any formula can be extended by first-order quantifiers and boolean connectives and stay in \mathcal{L} .
- 4. Find a formula for T in \mathcal{L} , which shows $T \in \mathcal{L}$.

The above steps work, as for any problem B in C, there is a first-order reduction I to T, and both \mathcal{L} and \mathcal{C} are complete via these reductions, so we also have $B \in \mathcal{L} = \mathcal{C}$.

B.2.2 Regular Languages

Here, we will show that the regular languages are captured exactly by second-order logic where we restrict ourselves to quantify only over predicates of arity one and do not include \leq . Further, we also are not allowed to use \leq , but have access to equality x=y and the successor relation x=y+1. We call this class SOM[+1].

First we need to present a formal definition of deterministic finite automata.

Definition B.3 (DFA). A deterministic finite automaton is a 5-tuple $M = \langle Q, \Sigma, \delta, q_0, F \rangle$ where

- Q is the set of states
- Σ is the alphabet
- δ is the transition function mapping a state and a symbol to the next state, so formally $\delta: Q \times \Sigma \to Q$.
- q_0 the start state

F a subset of Q which are the accepting states.

We say that a DFA D accepts a word $w \in \Sigma^*$ if when starting at the start state, if we go through w and always transition to the next state according to the actual symbol in w and the actual state, we end up in an accepting state.

In [Rög23] and [Str94] there is a proof of the following fact we will use in our proof for SOM[+1]:

Theorem B.1. For any alphabet Σ , there is a DFA recognizing language $L \subseteq \Sigma^*$ if and only if it is regular.

Now we can start to prove our main theorem for regular languages.

Theorem B.2. For any alphabet Σ , a language $L \subseteq \Sigma^*$ is expressible in SOM[+1] if and only if it is regular.

Proof. First we show that any regular language can be expressed in SOM[+1]. Let L be regular, end D_L be a DFA recognizing the language. We assume L does not contain the empty word, otherwise we can recognize the language $L \setminus \{\varepsilon\}$ and then add $\varphi \vee \forall x (x \neq x)$, which adds the empty string back.

Now let D_L have k states. We can existentially quantify unary relations X_1, \ldots, X_k to have the meaning that $X_i(y)$ is true if and only if D_L is in state i after y steps. Then, we need to make consistency checks. We present formulas for each of the consistency checks, and then can take the "and" of those to get our final formula $\exists X_1, \ldots, X_k (\varphi_1 \wedge \varphi_2 \wedge \varphi_3)$.

The start state is q_i We have

$$\varphi_1 := \bigwedge_{i=1}^k (i = j \leftrightarrow X_j(0))$$

We end in an accepting state Let T_i be the set of all characters which lead from q_i to an accepting state. Then we have

$$\varphi_2 := \bigwedge_{i=1}^k \left(X_i(\max) \to \bigvee_{a \in T_i} Q_a(\max) \right)$$

We move according to the transition function We have

$$\forall x \left(\forall y \left(y = x + 1 \to \left(\bigwedge_{i=1}^k \bigwedge_{a \in \Sigma} \left((X_i(x) \land Q_a(x)) \to X_{\delta(i,a)}(y) \right) \right. \right. \\ \left. \land \bigwedge_{i=1}^k \bigwedge_{a \in \Sigma} \left((X_i(y) \land Q_a(x)) \to \bigvee_{r=1}^k (X_r(x) \land \delta(r,a) = j) \right) \right) \right) \right)$$

By induction, we can show that always exactly one *i* satisfies $X_i(x)$ for any *x*. Thus, if the created formula is satisfied, we know that D_L accepts the word, and thus we have described *L* in SOM[+1].

For the other direction, we need to introduce two new concepts.

One of them is the nondeterministic finite automaton, which is analogous to the nondeterministic Turing machine as it can also have multiple transitions going from the same state. As with the nondeterministic Turing machine and the Turing machine, both the DFA and the NFA have the same expressive power.

The other concept is that of $(\mathcal{V}_1, \mathcal{V}_2)$ -structures. These structures are generalizations of our former vocabulary σ as they have characters in $A \times \mathcal{P}(\mathcal{V}_1) \times \mathcal{P}(\mathcal{V}_2)$. These structures are useful as we can make \mathcal{V}_1 to be the set of free first-order variables in a formula φ and \mathcal{V}_2 be the set of free second-order variables in the formula. If at a position i in our $(\mathcal{V}_1, \mathcal{V}_2)$ -structures we have x in the first-order component of its character, we see this as meaning that x = i. For the second-order variables in the third component, an X at position i means that X(i) holds.

Now, we can prove by induction that all formulas in SOM[+1] with free variables in \mathcal{V}_1 and \mathcal{V}_2 are regular. Sentences, the formulas without free variables are the special case where $\mathcal{V}_1, \mathcal{V}_2 = \emptyset$.

First, we need to check that the $(\mathcal{V}_1, \mathcal{V}_2)$ -structures are consistent, and no first-order variable x appears more than once. This can be done by a NFA which has one state for each subset of variables, and extends its subset while going over the string. If a variable appears twice, we enter a state that always loops and rejects.

Then, we see that the atomic formulas can be checked, as x = y, x = y + 1 and $Q_a(x)$ are easy to check, and checking X(x) is equivalent to looking if the occurrence of x has X in the third component. We always need to take the intersection with the NFA which checks if the structure is valid.

All boolean connectives are also valid, as regular languages are closed under complement, intersection and union as seen in [Rög23].

The most difficult case is a formula of the form $\exists x \varphi$ (as $\forall x \varphi \equiv \neg \exists x \neg \varphi$)). If $\exists x \varphi$ is over $(\mathcal{V}_1, \mathcal{V}_2)$ -structures, then φ is over $(\mathcal{V}_1 \cup \{x\}, \mathcal{V}_2)$ -structures. By induction, we know that φ defines a regular language and thus there is a NFA N which recognizes it. For the new automaton, we duplicate our states, with the meanings "used x" and "not used x". If we are in a state where x was used, we can not take any transition with x in the second set. If we are in a state where x was not used, we can take a transition with x in the second set and go to the corresponding state with x used or take a transition where x is not used and go to the corresponding state where x was not used.

The remaining case with second-order variables is treated analogously, without the restriction on the number of times the variable is used, so we do not need to duplicate our states.

By induction, we have thus showed the other direction, and we see that SOM[+1] and the regular languages are equivalent.

B.2.3 Context-Free Languages

For the context-free languages, we will show that they have an underlying structure that includes matchings.

A matching relation is a binary relation M on the universe $\{0, \ldots, n-1\}$ which has the following properties:

increasing If M(i, j), then i < j

uniqueness Any k in the universe appears at most once in the relation

non-crossing If we were to draw arcs for the matching, none of them would intersect. Formally, if M(i,j) and M(k,l), then either j < k or l < i

Visually, we can think of these relations as nested ranges over the universe.

With matchings, we can define $FO(\exists Match)$ as the first-order logic extended with existential quantification over matching relations.

Theorem B.3. For any alphabet Σ , a language $L \subseteq \Sigma^*$ is expressible in $FO(\exists Match)$ if and only if it is context-free.

For this, we first introduce a normal form for context-free grammars. The proof that every context-free grammar can be converted to this form can be found in [LST95].

Lemma B.4. Every context free language has a grammar which satisfies

- All rules are of one of the two forms
 - $-S \rightarrow \alpha \text{ with } \alpha \in \Sigma$
 - $-X \to \alpha u\beta \text{ with } \alpha, \beta \in \Sigma \text{ and } u \in (\Sigma \cup V)^*$
- For all production rules with a right-hand side that has at least one non-terminal we define its pattern. The pattern of rule $X \to v_0 X_1 v_2 X_2 \dots X_s v_s$ is defined to be $v_0 |v_1| \dots |v_s|$, where | is a new symbol not in Σ We require that for any two rules with the same pattern, they have the same left-hand side and thus the source non-terminal can be uniquely identified by the pattern.

For a specific arch $\langle i,j \rangle$ in a matching M on some word structure, we can also determine a pattern. For this, we go through all indices from i to j and add the character at the actual position. If we are at a starting point of some arch $\langle k,l \rangle$, instead of adding the actual character, we add | and continue at l+1.

Now, we can start with the proof of our theorem.

Proof. We want to find a formula such that for all arches $\langle i, j \rangle$ in M, the substring from i to j can be derived from the non-terminal for which we have a rule with the pattern of $\langle i, j \rangle$.

For this, we say that arch $\langle i,j \rangle$ corresponds to a production rule p if they have the same pattern. For any string u, we have a formula $\phi_u(i,j)$ which means that the substring from i to j is u. This formula is easy to write as we only need to check each character one by one using the successor relation. We can express correspondence to $p \equiv X \to v_0 X_1 v_2 X_2 \dots X_s v_s$ (including rules with terminal right-hand side) by the following formula:

$$\mathcal{X}_{p}(x,y) \equiv \exists x_{1}, y_{1}, \dots, x_{s}, y_{s} \left((x < x_{1} \land x_{1} < y_{1} \land y_{1} < x_{2} \land \dots \land y_{s} < y \right) \land$$

$$(\phi_{v_{0}}(x, x_{1} - 1) \land \phi_{v_{1}}(y_{1} + 1, x_{2} - 1) \land \dots \land \phi_{v_{s}}(y_{s} + 1, y)) \land$$

$$(M(x_{1}, y_{1}) \land \dots \land M(x_{s}, y_{s}) \land M(x, y)) \land$$

$$\forall k, l \left(M(k, l) \rightarrow \left((x \leq k \land l \leq y) \lor (x_{1} \leq k \land l \leq y_{1}) \lor \dots \lor (x_{s} \leq k \land l \leq y_{s}) \right) \right)$$

The first line means that the v_i are in the right order, the second that they do correspond, the third that there are arches between the v_i and the last that there are no other arches.

Now, we want to be more general, and express the that the pattern of $\langle i, j \rangle$ corresponds to some production rule with left-hand side X. Let $\widetilde{\mathcal{X}}_X(x,y)$ be the disjunction of all \mathcal{X}_p with left-hand side

X. Because our normal form says that the pattern uniquely determines the left-hand side, for each arch which has arches underneath, we have a unique corresponding non-terminal.

Now, we want to have a formula which expresses not only correspondence for a production rule p, but also that the non-terminals are correct. For this, we supplement our formula \mathcal{X}_p with a new line, expressing that the non-terminals correspond.

$$\widetilde{\mathcal{X}}_{p}(x,y) \equiv \exists x_{1}, y_{1}, \dots, x_{s}, y_{s} \left((x < x_{1} \land x_{1} < y_{1} \land y_{1} < x_{2} \land \dots \land y_{s} < y \right) \land \\
\left(\phi_{v_{0}}(x, x_{1} - 1) \land \phi_{v_{1}}(y_{1} + 1, x_{2} - 1) \land \dots \land \phi_{v_{s}}(y_{s} + 1, y) \right) \land \\
\left(M(x_{1}, y_{1}) \land \dots \land M(x_{s}, y_{s}) \land M(x, y) \right) \land \\
\forall k, l \left(M(k, l) \rightarrow \left((x \le k \land l \le y) \lor (x_{1} \le k \land l \le y_{1}) \lor \dots \lor (x_{s} \le k \land l \le y_{s}) \right) \\
\left(\widetilde{\mathcal{X}}_{X_{1}}(x_{1}, y_{1}) \land \dots \land \widetilde{\mathcal{X}}_{X_{s}}(x_{s}, y_{s}) \right) \right)$$

Finally, with P being our set of rules, we have a formula that tells us a word can be derived from the start symbol:

$$\exists M \left(\widetilde{\mathcal{X}}_S(0, \max) \land \forall x, y \left(M(x, y) \to \bigvee_{p \in P} \widetilde{\mathcal{X}}_p(x, y) \right) \right)$$

Now, by construction, if and only if a word satisfies the formula, there is a derivation from S for the word, as each arch can be seen as a derivation step, which we check is valid with our formula. We used our assumption from the normal form to show that the $\tilde{\mathcal{X}}_p$ are only satisfied when the arches which are non-terminal do not belong to any other non-terminal symbol then the one in the rule. If two terminal rules coincide, we do not care as no further derivation is possible.

Now, we come to the other direction. This direction requires some new notation and lemmas. We will use the notion of tree languages.

Definition B.4 (Tree Language). In a tree language, we have a rooted tree, which has an order on its vertices in leftmost depth-first way¹. Each node has a label, and each label has an arity which corresponds to the out-degree of the node. A tree language is the set of all trees over a finite label set.

We define the leaf alphabet of a tree language to be the set of 0-ary labels. For any tree T in a tree language, we define the yield of T to be the leaf labels concatenated according to the order relation from left to right.

The vocabulary of a tree language \mathcal{T} is $\tau = \langle \{0, \dots, n-1\}, Q_a, Q_b, \dots, Q_z, \leq, 0, 1, \max, C^2 \rangle$ In addition to the relations for each label, there is a child relation C(i, j) which means "node i is a child of node j".

Now, we present two lemmas for recognizable tree languages and their relation to context-free languages.

Lemma B.5 ([MW67]). A language $L \subseteq \Sigma^*$ is context free if and only if there is a recognizable tree language T with leaf alphabet Σ for which a word is in L if and only if it is the yield of some tree in T.

¹The order which we find by doing a depth-first search on the tree, entering the leftmost node first

Lemma B.6 ([TW68]). A tree language T is recognizable if and only if there is a monadic second-order sentence that recognizes it.

We now present some relations that can be written in MSO on trees.

Lf(i) Node i is a leaf Lf(i) $\equiv \forall x \neq C(x, i)$

 $\mathbf{Lc}(i,j)$ Node i is the leftmost child of j $\mathbf{Lc}(i,j) \equiv C(i,j) \land \forall x (C(x,j) \rightarrow i < x)$

 $\mathbf{Rc}(i,j)$ Node i is the rightmost child of j $\mathbf{Rc}(i,j) \equiv C(i,j) \land \forall x (C(x,j) \to x < i)$

 $\mathbf{An}(i,j)$ Node i is an ancestor or j

$$\operatorname{An}(i,j) \equiv \exists U(U(i) \land U(j) \land \forall x(U(x) \rightarrow ((x \neq i \leftrightarrow \exists y(C(x,y) \land U(y))) \land (x \neq j \leftrightarrow \exists y(C(y,x) \land U(y))))))$$

 $\mathbf{Pt}(U,i,j)$ Node i is an ancestor or j, j is a leaf and U contains all nodes in the path from i to j.

$$Pt(U, i, j) \equiv U(i) \wedge U(j) \wedge Lf(j) \wedge \forall x (U(x) \rightarrow ((x \neq i \leftrightarrow \exists y (C(x, y) \wedge U(y))) \wedge (x \neq j \leftrightarrow \exists y (C(y, x) \wedge U(y)))))$$

Using these two lemmas, we can continue by presenting for any formula φ in FO(\exists Match) a formula ϕ in MSO over trees such that

$$w \models \varphi \Leftrightarrow \text{there exists a tree } T \text{ with yield } w \text{ such that } T \models \phi$$

For this, we present a class of trees which correspond to a word with a matching. For any word w with matching M, we can construct a tree over $\Sigma \cup \{\oplus^2, \odot^2\}$. We do this using an intermediate step. First, we construct a tree with wrong arity for nodes of type \oplus by assigning one node of type \oplus to each arch, with edges to every direct arch underneath it and every character directly underneath it. If we have multiple trees, we add a new \odot node on top with an edge to all roots of these trees. To fix the arity issue, we repeat the following procedure until there are no nodes with more than outdegree 2.

Take some node with outdegree greater than 2. Take the two leftmost children and add a ⊙ node with an edge to both, and an edge from the new node to the former parent. This procedure will eventually terminate as we always decrease the outdegree of some node by one and add a valid node.

We can see that this procedure can also be done backward if and only if for any node of type \oplus , the leaf on the leftmost and rightmost path of a node are distinct and no \oplus node occurs on the path between the two. We can express this property of a tree by the following formula.

$$\Upsilon \equiv \forall x (Q_{\oplus}(x) \to (\exists y, z, U_y, U_z (y \neq z \land \operatorname{Pt}(U_z, x, z) \land \operatorname{Pt}(U_y, x, y) \land \forall r (U_y(r) \to ((r = y \lor \exists w (U_y(w) \land \operatorname{Rc}(w, r))) \land (r = y \lor r = x \lor Q_{\odot}(r)))) \land \forall r (U_z(r) \to ((r = z \lor \exists w (U_z(w) \land \operatorname{Lc}(w, r))) \land (r = y \lor r = x \lor Q_{\odot}(r)))))))$$

Here, in the first line we assert that for every node with label \oplus , we have two distinct leaves y, z with paths U_y and U_z . The second and third line assert the same for x and y, that they are the rightmost / leftmost leaf and that no other \oplus type node lies on the path from them to x.

Now, we want to convert our formula φ over strings with a matching to a formula γ over trees. Then we can assert that the tree represents a string with matching and the yield satisfies φ using $\Upsilon \wedge \gamma$.

For this, we need to restrict any quantifiers in φ to the leaves by replacing $\exists x \phi$ with $\exists x Lf(x) \land \phi$ and $\forall x \phi$ with $\forall x Lf(x) \rightarrow \phi$. Further, we replace M(z,y) by

$$m(z,y) \equiv \exists x (Q_{\oplus}(x) \land (\exists U_y, U_z(y \neq z \land \operatorname{Pt}(U_z, x, z) \land \operatorname{Pt}(U_y, x, y) \land \forall r (U_y(r) \to ((r = y \lor \exists w (U_y(w) \land \operatorname{Rc}(w, r))) \land (r = y \lor r = x \lor Q_{\odot}(r)))) \land \forall r (U_z(r) \to ((r = z \lor \exists w (U_z(w) \land \operatorname{Lc}(w, r))) \land (r = y \lor r = x \lor Q_{\odot}(r)))))))$$

which is very similar to Υ .

This is already everything we need to do, and thus we can conclude that

$$w \models \varphi \Leftrightarrow \text{there exists a tree } T \text{ with yield } w \text{ such that } T \models \Upsilon \land \gamma$$

Thus, we have proved both directions and see that the context free languages are exactly captured by $FO(\exists Match)$

B.2.4 Recursive Languages

The most general case is interesting as it gives us a logical formalism for all problems which are computable at all.

The proof relies on Diophantine sets. Those sets are the sets that correspond to the tuples which have a solution for some Diophantine equation. A Diophantine equation is a polynomial equation P with a tuple \overline{x} of parameters and a tuple \overline{y} of variables. A tuple \overline{x} has a solution if there exists a tuple \overline{y} such that $P(\overline{x}, \overline{y}) = 0$. The famous MRDP Theorem states that the Diophantine sets are exactly the computable sets. At the same time, this shows that Hilbert's 10^{th} problem is unsolvable. A full proof of these facts can be found in [Mat96].

With this new characterization, there is a quite straightforward characterization of computable sets. The logic FO($\exists \mathbb{N}$) consists of all formulas $\phi(\overline{x}) \equiv \exists \overline{y}(\varphi(\overline{x}, \overline{y}))$ with φ having only bounded quantifiers (of the form $\exists x < y$ or $\forall x < y$), addition, multiplication, equality, and any constant natural number [Ent20]. The existential quantifiers at the beginning are allowed to range over all the natural numbers.

These formulas can define exactly the Diophantine sets, as the formulas we present are exactly those that mean "there is a tuple \overline{y} of natural numbers such that some polynomial is satisfied". Thus, they also define exactly all computable sets.

B.2.5 Open questions

The domain of Descriptive Complexity is full of open questions as the proofs of lower bounds seems to be very difficult in most cases. Further, even separation between complexity classes which seem to take an exponential amount of resources compared to another one in practice can not be shown to be different.

$\mathbf{P} \stackrel{?}{=} \mathbf{NP}$

The P vs. NP question is the most emblematic question in Descriptive Complexity Theory. In practice, for any NP-complete problem, only exponential worst-case algorithms are known. This leads to the widely believed conjuncture that $P \neq NP$. The problem is one of the seven Millennium Problems and a solution of equality or inequality is worth 1 Million US dollars.

The consequences of a solution stating that P = NP could have many practical advantages if it was constructive and had a low constant, as many important problems in research and logistics could be solved quickly. It would also mean the breakdown of most of modern cryptography, which relies on problem being intractable. On a conceptual level, it would mean that finding a proof to a problem is not harder than verifying its correctness, which would greatly impact the work of mathematicians. If a proof of the contrary would be known, this would focus the research more on the average case complexity of NP problems, but because of the continued lack of success on the question, this shift has already widely taken place.

$\mathbf{NSPACE}[\mathcal{O}(n)] \overset{?}{=} \mathbf{DSPACE}[\mathcal{O}(n)]$

This problem is known under the name first Linear bounded automaton problem since its proposal by Kuroda in [Kur64], and asks if nondeterminism adds power in the context of bounded space. This comes from the fact that a NSPACE[$\mathcal{O}(n)$] Turing machine can be seen as a Turing machine with a linear bound on its space usage. This theorem is of interest as we know that NSPACE[$\mathcal{O}(n)$] is equivalent to the context-sensitive languages by section 3.4.1.

Since the proposal, there were two advances. One is the proof that NSPACE is closed under complement. The contrary would have implied NSPACE[$\mathcal{O}(n)$] \neq DSPACE[$\mathcal{O}(n)$] as DSPACE is closed under complement. The second advance is Savitch's Theorem in section 3.3.1 which already gives a bound for simulating NSPACE using DSPACE machines. It is not known if this theorem is optimal, that is whether the blow-up by a power of 2 is optimal or if we can do better.

An equality would imply that the context-sensitive languages can be recognized by a deterministic linear bounded automaton, which could make recognizing words in context-sensitive languages easier and faster.

C. Independence declaration (German)

Ich, Yaël Arn, 4A

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