

Minimal Macro-Based Rewritings of Formal Languages: Theory and Applications in Ontology Engineering (and Beyond)

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Abstract

In this paper, we introduce the problem of rewriting finite formal languages using syntactic macros such that the rewriting is minimal in size. We present polynomial-time algorithms to solve variants of this problem and show their correctness. To demonstrate the practical relevance of the proposed problems and the feasibility and effectiveness of our algorithms in practice, we apply these to biomedical ontologies authored in OWL. We find that such rewritings can significantly reduce the size of ontologies by capturing repeated expressions with macros. In addition to offering valuable assistance in enhancing ontology quality and comprehension, the presented approach introduces a systematic way of analysing and evaluating features of rewriting systems (including syntactic macros, templates, or other forms of rewriting rules) in terms of their influence on computational problems.

Introduction

KISS and DRY, standing for “Keep It Simple, Stupid” and “Don’t Repeat Yourself”, are key principles in software development. These principles prove advantageous in other contexts involving formal languages, including knowledge bases, formal specifications, and logical theories.

Despite the value of simplification and reduction of repetition, there is no universally applicable mechanism assisting with the associated refactoring of formal languages. Challenges arise from the need to preserve application-specific properties and the difficulty of specifying desirable and undesirable refactorings. In other words, there is a fine line between succinct simplicity and obscure terseness.

This paper proposes a formal framework for refactoring formal languages through automated conversions into smaller rewritings. The focus is on identifying rewriting mechanisms applicable in diverse situations and analysing their properties. One simple but effective refactoring strategy is the introduction of *names* for more complex recurring structures. Preserving syntactic structure is often important, motivating our exploration of rewriting mechanisms based on *syntactic macros*.

Consider the following example language consisting of formulas in propositional logic $\mathcal{L} = \{a \wedge b, (a \wedge b) \vee c, ((a \wedge b) \vee c) \wedge d\}$. A macro $m \mapsto a \wedge b$ can be used to “macrofy” \mathcal{L}

into $\mathcal{L}_m = \{m, m \vee c, (m \vee c) \wedge d\}$. Note that the expression $m \vee c$ occurs twice in the macrofied language \mathcal{L}_m . So, the question arises whether a rewriting mechanism allows for *nested* macro definitions, e.g., $m' \mapsto m \vee c$, or not.

Deciding what features to include in a rewriting mechanism, e.g., allowing for nesting or not, is not straightforward. To evaluate a feature’s impact, we propose to analyse its influence on computational problems *formulated w.r.t. rewriting mechanisms*. For instance, consider the above example and the problem of computing size-minimal rewritings. If the complexity of computing minimal rewriting with un-nested macros is lower than that of minimal rewriting with nested macros, then this effect of the feature “nesting” can inform its inclusion for practical purposes.

In this paper, we investigate a rewriting mechanism based on syntactic macros allowing for nesting. We show conditions under which the problem of finding size-minimal rewritings can be solved in polynomial time. We implement this rewriting mechanism and apply it to find size-minimal rewritings of large biomedical ontologies of practical relevance. The attained size reductions are comparable to, if not better than those of existing approaches, while also showcasing superior performance in terms of processing time.

Preliminaries

We define the technical terms used in the following sections. In particular, we introduce terms over a mixture of ranked, unranked, and mixed symbols, which will then enable us to apply our framework to the Web Ontology Language (OWL) which uses all three kinds of symbols.

Definition 1 (Alphabet, Terms, Language). A ranked alphabet \mathcal{F} is a finite set of symbols together with a function $\text{Ar} : \mathcal{F} \rightarrow \mathbb{N}$ that associates symbols with their arity. Symbols $f \in \mathcal{F}$ with $\text{Ar}(f) = 0$ are called constants and symbols with $\text{Ar}(f) = 1$ are called unary. An unranked alphabet \mathcal{U} is a set of symbols. A mixed alphabet $\mathcal{X} \subseteq \mathcal{F}$ is a subset of the ranked alphabet. An alphabet $\Sigma = \mathcal{F} \cup \mathcal{U}$ is a set of ranked or unranked symbols.

The set of terms $T(\Sigma)$ over an alphabet $\Sigma = \mathcal{F} \cup \mathcal{U}$ is inductively defined as follows:

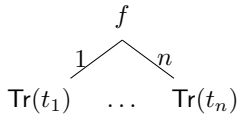
- $f \in T(\Sigma)$ if $f \in \mathcal{F}$ and $\text{Ar}(f) = 0$,
- $f(t_1, \dots, t_n) \in T(\Sigma)$ if $f \in \mathcal{F}$, $n \geq 1$, and $\text{Ar}(f) = n$,
- $f(t_1, \dots, t_n) \in T(\Sigma)$ if $f \in \mathcal{U}$ and $n \geq 1$, and

• $f(t_1, \dots, t_n) \in T(\Sigma)$ if $f \in \mathcal{X}$, $n \geq 1$, and $\text{Ar}(f) \leq n$, where $t_1, \dots, t_n \in T(\Sigma)$. A language \mathcal{L} over Σ is a set of terms $\mathcal{L} \subseteq T(\Sigma)$.

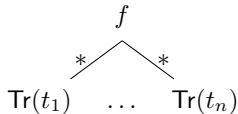
To define what it means for two terms to be identical, we introduce the notion of a term tree.

Definition 2 (Term Tree). Let Σ be an alphabet and $\Sigma = O \cup U \cup P$ a partition of Σ , where O , U , and P denote disjoint sets of ordered, unordered, and partially ordered symbols, respectively. Symbols $f \in P$ are associated with a function $\text{Or}: P \rightarrow \mathbb{N}$. The term tree $\text{Tr}(t)$ of a term $t \in T(\Sigma)$ is an unordered tree inductively defined as follows: if

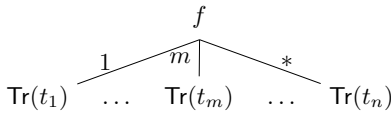
- t is a constant, then $\text{Tr}(t)$ is a node labelled with t ,
- $t = f(t_1, \dots, t_n)$ and $f \in \Sigma$ is ordered, then $\text{Tr}(t) =$



- $t = f(t_1, \dots, t_n)$ and $f \in \Sigma$ is unordered, then $\text{Tr}(t) =$



- $t = f(t_1, \dots, t_m, \dots, t_n)$ and $f \in \Sigma$ is partially ordered with $\text{Or}(f) = m$, then $\text{Tr}(t) =$



The notion of *term equality* then corresponds to the notion of graph isomorphism between term trees that preserves both node and edge labels. Similarly, the notion of a *subterm* relation is based on graph isomorphisms between restrictions of their corresponding term trees.

Definition 3 (Subterms / Subtrees). Let t, t' be two edge- and node-labelled, unordered trees. We say that t is a subtree of t' if there exists a node n in t' and a (node- and edge-label preserving) isomorphism from the subtree of t' rooted at n to t . In this case, we refer to n as a position of t in t' and use $t'|_n$ for the subtree of t' rooted in n .

Let $t, t' \in T(\Sigma)$ be two terms. We say that t is a subterm of t' , denoted $t \preceq t'$, if $T(t)$ is a subtree of $T(t')$. We say that t and t' are equal, denoted $t = t'$, if they are both subterms of each other.

In the following, we rarely need to distinguish between terms and their corresponding trees and use *tree* and *term* interchangeably; we will not mention the arity or orderedness of symbols unless the context requires this.

Definition 4 (Substitution). The substitution of a term $u \in T(\Sigma)$ for a term $t' \preceq t$ at position p , written $t[u]_p$, is the replacement of t' in t at position p with u .

We will evaluate the feasibility and effectiveness of the algorithms introduced later on OWL ontologies (Grau et al. 2008; Motik et al. 2008). If readers are not familiar with OWL, it suffices to say that OWL has all

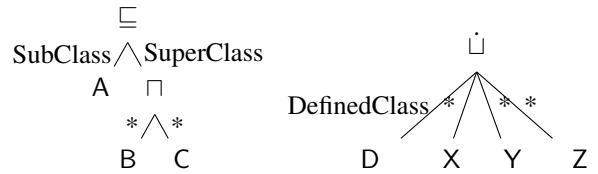


Figure 1: Example of term trees for OWL expressions.

kinds of symbols we consider here, i.e., ranked, unranked, mixed, as well as ordered, unordered, and partially ordered. Figure 1 shows two example term trees for the OWL expressions $\text{SubClassOf}(A, \text{ObjectIntersectionOf}(B, C))$ and $\text{DisjointUnion}(D, X, Y, Z)$ using Description Logic symbols \sqsubseteq , \sqcap , and \sqcup for the sake of readability. For instance, \sqsubseteq is a ranked and ordered symbol, whereas \sqcup is mixed with $\text{Ar}(\sqcup) = 3$ (because a class is defined as the disjoint union of two or more classes) and partially ordered with $\text{Or}(\sqcup) = 1$ (to mark the defined class). Also, we used descriptive names rather than numbers to indicate the order of terms.

Macros and Encodings

Macros for Formal Languages

A *macro* is understood as a rule that maps an input (in our case finite sets of terms, possibly using macros symbols) to an output (also terms). Such a mapping is usually used to expand a smaller input into a larger output.

Definition 5 (Macro Definition). Let M be a finite set of constant macro symbols disjoint from Σ . A set of macro definitions is a total function

$$\begin{aligned} \mathcal{M}: M &\rightarrow T(\Sigma \cup M) \setminus (\Sigma \cup M) \\ m &\mapsto t \end{aligned}$$

If $\mathcal{M}(m) = t$, we call $m \mapsto t$ a macro definition and m a macro for t .

The range of macro definitions is a set of non-constant terms. In the following, we omit the explicit exclusion of non-constant terms and simply write $\mathcal{M}: M \rightarrow T(\Sigma \cup M)$ to specify macro definitions for improved readability.

A macro's occurrence can be *expanded* to its associated output structure by replacing the macro symbol with the term it is defined to map to. Such an expansion may lead to the occurrence of other macros, giving rise to an iterative expansion process. The limit of this expansion process will be referred to as *the expansion* of a macro.

Definition 6 (Macro Expansion). Let $\mathcal{M}: M \rightarrow T(\Sigma \cup M)$ be a set of macro definitions and $t \in T(\Sigma \cup M)$ a term. The 1-step expansion $\mathcal{M}(t)$ of t w.r.t. \mathcal{M} is the term t' obtained by replacing all occurrences of any macro $m \in M$ in t with its expansion $\mathcal{M}(m)$. The n -step expansion of t w.r.t. \mathcal{M} is $\mathcal{M}^n(t) = \underbrace{\mathcal{M}(\dots \mathcal{M}(t))}_{n \text{ times}}$. The expansion of a macro, written

$\mathcal{M}^*(t)$, is the least fixed-point of \mathcal{M} applied to t .

The fixed-point $\mathcal{M}^*(m)$ of a macro m does not necessarily exist. Consider the macro definition $m \mapsto \text{succ}(m)$.

While the n -step expansion of m is well-defined for any $n \in \mathbb{N}$, the expansion $\mathcal{M}^*(m)$ does not exist.

The inverse of macro expansion is macro *instantiation*, i.e., replacing a term with a macro symbol that can be expanded to the term.

Definition 7 (Macro Instantiation). *Let $\mathcal{L} \subseteq T(\Sigma \cup M)$ be a language and $\mathcal{M}: M \rightarrow T(\Sigma \cup M)$ a set of macro definitions. A macro $m \in M$ can be instantiated in \mathcal{L} if there exists an n s.t. $\mathcal{M}^n(m)$ occurs in \mathcal{L} , i.e., there is a $t \in \mathcal{L}$ and a position p with $t|_p = \mathcal{M}^n(m)$. In this case, we also say m can be instantiated in t . We refer to the act of replacing $t|_p$ with m as instantiating m in t at position p . The term m occurring at position p in $t|m|_p$ is an instantiation of m .*

Since we are interested in macros for terms, we will restrict macro definitions so that the expansion of a macro is required to exist, for which we introduce some terminology.

Definition 8 (Acyclic Macro Definitions). *For macros $m, m' \in M$, we say that m directly uses m' if m' occurs in $\mathcal{M}(m)$. Next, let uses be the transitive closure of directly uses. A set of macro definitions $\mathcal{M}: M \mapsto T(\Sigma \cup M)$ is acyclic if there are no ‘uses’ cycles in M , i.e., if there is no macro $m \in M$ that uses itself.*

Lemma 1. *Let $\mathcal{M}: M \mapsto T(\Sigma \cup M)$ be a set of macro definitions. Then:*

- (a) \mathcal{M} is acyclic iff $\mathcal{M}^*(t)$ exists for each $t \in T(\Sigma \cup M)$.
- (b) If $\mathcal{M}^*(t)$ exists, it is unique.
- (c) If $\mathcal{M}^*(t)$ exists then $\mathcal{M}^*(t) \in T(\Sigma)$.

So, acyclicity guarantees the existence of least fixed points for the expansion of macros. Lemma 1(a) is an immediate consequence of the close relationship between macro systems and finite, ground term rewriting systems (Baader and Nipkow 1998). Lemma 1(b) is due to \mathcal{M} being a function, and Lemma 1(c) is due to $\mathcal{M}^*(t)$ being a fixed-point and \mathcal{M} being total on M . In what follows, we restrict our attention to acyclic sets of macro definitions $\mathcal{M}: M \mapsto T(\Sigma \cup M)$.

Augmenting a language $\mathcal{L} \subseteq T(\Sigma)$ with a set of macro symbols M can be seen to define a new language $\mathcal{L}_M \subseteq T(\Sigma \cup M)$. If the expansion of all macros in \mathcal{L}_M w.r.t. some macro definitions $\mathcal{M}: M \rightarrow T(\Sigma \cup M)$ yields \mathcal{L} , then \mathcal{L}_M together with \mathcal{M} can be seen as an *encoding* of \mathcal{L} .

Definition 9 (Macro System, Macrofication, Language Encoding). *A macro system \mathfrak{M} is a tuple $(\mathcal{L}_M, \mathcal{M})$ where $\mathcal{L}_M \subseteq T(\Sigma \cup M)$ is a language and $\mathcal{M}: M \rightarrow T(\Sigma \cup M)$ a set of macro definitions. If $\mathcal{M}^*(\mathcal{L}_M) := \bigcup_{t \in \mathcal{L}_M} \mathcal{M}^*(t) = \mathcal{L}$,*

then \mathfrak{M} is an encoding of $\mathcal{L} \subseteq T(\Sigma)$. In this case, we will refer to \mathcal{L}_M as a macrofication of \mathcal{L} w.r.t. \mathcal{M} .

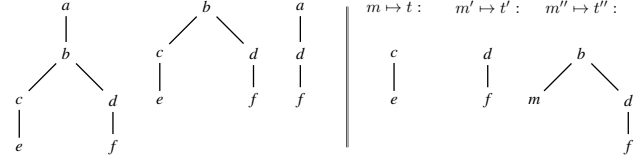
Example 1. *Consider the language $\mathcal{L} \subseteq T(\Sigma)$ over symbols $\Sigma = \{a, b, c, d, e, f\}$ which is given by the set of terms*

$$\mathcal{L} = \{a(b(c(e), d(f))), b(c(e), d(f)), a(d(f))\}.$$

Furthermore, consider the set of macro definitions

$$\mathcal{M} = \{m \mapsto c(e), m' \mapsto d(f), m'' \mapsto b(m, d(f))\}.$$

We can represent the terms in \mathcal{L} and in the macro definitions of \mathcal{M} as trees in the following way:



The 1-step expansion of m'' is the term $b(m, d(f))$ in which m is instantiated. Furthermore, the expansion (which in this case is the 2-step expansion) of m'' is $\mathcal{M}^(m'') = b(c(e), d(f))$. So, the macro system $\mathfrak{M} = (\mathcal{L}_M, \mathcal{M})$ with $\mathcal{L}_M = \{a(m''), m'', a(m'')\}$ encodes \mathcal{L} , i.e., $\mathcal{M}^*(\mathcal{L}_M) = \mathcal{L}$.*

Computational Problems

In the context of this work, we are interested in language encodings that are minimal in size. Before we can define the computational problem of finding size-minimal macro systems, we define the notion of their *size*.

Definition 10 (Size of Terms, Languages, Macros Definitions, Macro Systems). *Let \mathcal{L} be a finite language, $t \in \mathcal{L}$ a term, $d = m \mapsto t$ a macro definition, \mathcal{M} a set of macro definitions, and $\mathfrak{M} = (\mathcal{L}_M, \mathcal{M})$ a macro system. Then their size is defined as follows:*

- $size(t)$ is the number of nodes in t 's term tree,
- $size(\mathcal{L}) := \sum_{t \in \mathcal{L}} size(t)$,
- $size(d) := 1 + size(t)$,
- $size(\mathcal{M}) := \sum_{d \in \mathcal{M}} size(d)$,
- $size(\mathfrak{M}) := size(\mathcal{L}_M) + size(\mathcal{M})$.

We can now define minimal encodings w.r.t. their size.

Definition 11 (Size-Minimal Encodings). *Let $\mathfrak{M} = (\mathcal{L}_M, \mathcal{M})$ be an encoding of a language \mathcal{L} . Then \mathfrak{M} is called size-minimal encoding of \mathcal{L} w.r.t. \mathcal{M} if there is no encoding $\mathfrak{M}' = (\mathcal{L}'_M, \mathcal{M})$ of \mathcal{L} with $size(\mathfrak{M}') < size(\mathfrak{M})$.*

To avoid considering macro systems that can be trivially compressed, i.e., are not size-minimal, we will focus on sets of macro definitions that do not have duplicate macros.

Definition 12 (Reduced Sets of Macro Definitions). *A set of macro definitions is reduced if \mathcal{M}^* is injective, i.e., there are no $m, m' \in M$ with $m \neq m'$ and $\mathcal{M}^*(m) = \mathcal{M}^*(m')$.*

In what follows, we assume that all sets of macro definitions are reduced. Similarly, we will focus on encodings in which no macro can be instantiated anymore. In other words, all macros are *exhaustively* instantiated.

Definition 13 (Exhaustiveness of Encodings). *Let $\mathfrak{M} = (\mathcal{L}_M, \mathcal{M})$ be an encoding of a language \mathcal{L} . Then \mathfrak{M} is called*

- macrofication-exhaustive if no macro in \mathcal{M} can be instantiated in \mathcal{L}_M ,
- expansion-exhaustive if no macro in \mathcal{M} can be instantiated in the expansion of another macro in \mathcal{M} ,
- exhaustive if it is macrofication- and expansion-exhaustive,

The problem of finding a minimal encoding of a language can be formulated w.r.t. a given set of macro definitions, an equivalence class of macro definitions, or any set of macro definitions. We provide definitions for each of these cases.

First, we formulate the problem of finding a minimal encoding for a given language w.r.t. given macro definitions.

Problem 1. Given a finite language $\mathcal{L} \subseteq T(\Sigma)$ and \mathcal{M} a set of macro definitions, determine a size-minimal encoding of \mathcal{L} w.r.t. \mathcal{M} .

In Example 1, $\mathfrak{M} = (\mathcal{L}_M, \mathcal{M})$ with $\mathcal{L}_M = \{a(m''), m'', a(m')\}$ is a size-minimal encoding of \mathcal{L} with $size((\mathcal{L}_M, \mathcal{M})) = size(\mathcal{L}_M) + size(\mathcal{M}) = 5 + 11 = 16$. It is not hard to see, however, that \mathfrak{M} can be further compressed by instantiating m' in $\mathcal{M}(m'')$ without changing the expansion of m'' , i.e., without really changing \mathcal{M} . Hence next, we first define an equivalence of sets of macro definitions to capture this notion of "not really changing" and then use it to define a more general computational problem.

Definition 14 (Equivalence of Macro Definitions). Two sets of macro definitions $\mathcal{M}: M \rightarrow T(\Sigma \cup M)$ and $\mathcal{M}': M' \rightarrow T(\Sigma \cup M')$ are equivalent w.r.t. macro expansion if there exists a bijection $\mathcal{R}: M \leftrightarrow M'$ s.t. $\mathcal{M}^*(m) = \mathcal{M}'^*(\mathcal{R}(m))$ for all $m \in M$.

Problem 2 (Size-Minimal Encoding w.r.t. equivalent macro definitions). Given a finite language $\mathcal{L} \subseteq T(\Sigma)$ and \mathcal{M} a set of macro definitions, determine a size-minimal encoding $\mathfrak{M}' = (\mathcal{L}_{M'}, \mathcal{M}')$ of \mathcal{L} w.r.t. macro definitions equivalent to \mathcal{M} . That is, \mathcal{M}' is equivalent to \mathcal{M} and there does not exist an encoding $\mathfrak{M}'' = (\mathcal{L}_{M''}, \mathcal{M}'')$ of \mathcal{L} where \mathcal{M}'' is also equivalent to \mathcal{M} and $size(\mathfrak{M}'') < size(\mathfrak{M}')$.

Continuing with Example 1, $\mathfrak{M}' = (\mathcal{L}_{M'}, \mathcal{M}')$ with $\mathcal{L}_{M'} = \{a(m''), m'', a(m')\}$ and $\mathcal{M}' = \{m \mapsto c(e), m' \mapsto d(f), m'' \mapsto b(m, m')\}$ is a size-minimal encoding of \mathcal{L} w.r.t. macro definitions equivalent to \mathcal{M} : in addition to our observations regarding the minimality of \mathcal{L}_M above, we note that $size(\mathcal{M}') = size(\mathcal{L}_{M'}) + size(\mathcal{M}') = 5 + 10 = 15 < size(\mathcal{M}) = 16$, that \mathcal{M}' and \mathcal{M} are equivalent w.r.t. macro expansions, and that there is no equivalent set of macro definitions smaller than \mathcal{M}' .

Lastly, we formulate the general version of the problem by looking for a minimal encoding of an input language w.r.t. any possible set of macro definitions (following Definition 5). Here we are looking for the size-minimal encoding of an input language considering both the size of the encoded language and the size of the macro definitions.

Problem 3 (Size-Minimal Encoding via macro systems). Given a finite language $\mathcal{L} \subseteq T(\Sigma)$, determine a size-minimal encoding $\mathfrak{M} = (\mathcal{L}_M, \mathcal{M})$ of \mathcal{L} . That is, there exists no encoding \mathfrak{M}' of \mathcal{L} with $size(\mathfrak{M}') < size(\mathfrak{M})$.

Continuing with Example 1, the macrofication $\mathcal{L}_{M''} = \{a(m''), m'', a(d(f))\}$ together with the macro definitions $\mathcal{M}'' = \{m'' \mapsto b(c(e), d(f))\}$ is a size-minimal encoding of \mathcal{L} via macros systems. The size of the encoding is $size((\mathcal{L}_{M''}, \mathcal{M}'')) = size(\mathcal{L}_{M''}) + size(\mathcal{M}'') = 6 + 6 = 12$. Please note that \mathcal{M}'' contains no macro capturing the repeated occurrence of the "small" term $d(f)$ since it does not pay off as it only occurs once outside $\mathcal{M}''(m)$ and, for size minimality, we also consider the size of macro definitions.

Properties of Macros and Encodings

In the following, we restrict our attention to finite languages \mathcal{L} and reduced, finite macro definitions \mathcal{M} .

When trying to compute a minimal macrofication for an input language w.r.t. given set of macro definitions, the instantiation of one macro can affect the instantiate-ability of another macro: instantiating $m' \mapsto d(f)$ in the first term $a(b(c(e), d(f))) \in \mathcal{L}$ in Example 1 results in $t' = a(b(c(e), m'))$, in which m'' can no longer be instantiated. That is, m' and m'' depend on one another: since the instantiation of a macro ultimately corresponds to the replacement of its fixed-point expansion, we consider two macros to be mutually dependent if an exhaustive encoding w.r.t. their fixed-point expansions is not uniquely determined.

Definition 15 (Macro Dependency). Let $\mathcal{M}: M \rightarrow T(\Sigma \cup M)$ be a set of macro definitions. Two macros m and m' are independent if a macrofication-exhaustive encoding of any finite language $\mathcal{L} \subseteq T(\Sigma)$ w.r.t. $\{m \mapsto \mathcal{M}^*(m), m' \mapsto \mathcal{M}^*(m')\}$ is uniquely determined. Otherwise, the two macros are mutually dependent on one another.

Determining the dependency relationship between two macros can be reduced to the subterm relationship between their fixed-point expansions, in which case we say that one macro contains the other. If we focus on reduced sets of macro definitions, the "=" case is immaterial and so ignored.

Definition 16 (Macro Containment). Let $\mathcal{M}: M \rightarrow T(\Sigma \cup M)$ be a set of macro definitions with $m, m' \in M$ and $m \neq m'$. Then m contains m' , if $\mathcal{M}^*(m') \preceq \mathcal{M}^*(m)$. By abuse of notation, we will write $m \preceq m'$ if m is contained in m' .

Lemma 2 (Macro Dependency is Macro Containment). Let $\mathcal{M}: M \rightarrow T(\Sigma \cup M)$ be a set of macro definitions. Two macros $m, m' \in M$ are dependent iff $m \preceq m'$ or $m' \preceq m$.

Proof. Consider two macros $m, m' \in M$ with $\mathcal{M}^*(m) = t$ and $\mathcal{M}^*(m') = t'$.

"If" direction: assume w.l.o.g. that $m \preceq m'$ and set $\mathcal{M}_\downarrow = \{m \mapsto t, m' \mapsto t'\}$. Consider $\mathcal{L} = \{t'\}$ and a position p in t' s.t. $t'|_p = t$. So, $(\{m'\}, \mathcal{M}_\downarrow)$ and $(t'[m]_p, \mathcal{M}_\downarrow)$ are different macrofication-exhaustive encodings of \mathcal{L} since $m' \neq t'[m]_p$.

"Only if" direction: We show the contrapositive. Assume that neither $m \preceq m'$ nor $m' \preceq m$, i.e., there exists no position p in t such that $t|_p = t'$ and no position p in t' such that $t'|_p = t$. Hence, instantiating one of them in a term cannot affect the instantiate-ability of the other, and thus m and m' are not dependent. \square

Lemma 3. Let $\mathfrak{M} = (\mathcal{L}_M, \mathcal{M})$ be an encoding of a language \mathcal{L} . Then if \mathfrak{M} is a size-minimal encoding of \mathcal{L} w.r.t. \mathcal{M} , then it is macrofication-exhaustive;

Proof. This follows immediately from the definitions of size and "can be instantiated", and from the fact that $size(\mathcal{M}^n(m)) \geq 2$ for all $n \geq 1$. \square

Algorithms for Encodings

Polynomial Time Algorithm for Solving Problem 1

We start with an algorithm that constructs a size-minimal encoding w.r.t. a given set of macro definitions in polynomial time (i.e., solves Problem 1), which will lay the foundation for solving Computational Problem 2 and ultimately

Computational Problem 3. An extended version of this paper offers more detailed proofs, concrete algorithms, implementation details, additional examples, and a more elaborate discussion of results (Kindermann et al. 2023).

The following lemma shows that, for two dependant macros, the containing one should be instantiated with priority to get a size-minimal encoding. Note that contained macros might still be instantiated in a size-minimal encoding if they appear outside of the containing one.

Lemma 4 (Instantiation Precedence for Dependent Macros). *Let $\mathfrak{M} = (\mathcal{L}_M, \mathcal{M})$ be a macro system with $\mathcal{M}: M \rightarrow T(\Sigma \cup M)$ that encodes a language $\mathcal{L} \subseteq T(\Sigma)$. If there exist two macros $m, m' \in M$ with $m \prec m'$ s.t.*

- (a) *m is instantiated instead of m' in \mathcal{L}_M , or*
- (b) *m is instantiated instead of m' in some macro definition $m_d \mapsto t \in \mathcal{M}$,*

then there exists a macro system \mathfrak{M}' that encodes \mathcal{L} with $size(\mathfrak{M}') < size(\mathfrak{M})$.

Proof. Set $\mathcal{M}^*(m) = t$ and $\mathcal{M}^*(m') = t'$. By definition, $m \prec m'$ implies $t \prec t'$, i.e., t occurs in t' at some position p . Assume (a). Then, there exists a term $u \in \mathcal{L}_M$ s.t. $t'[m]_p$ occurs at position q in u . Since $\mathcal{M}^*(t'[m]_p) = \mathcal{M}^*(m')$ and $t'[m]_p$ is not a constant term, we have $size(t'[m]_p) > size(m')$. So, we can construct \mathcal{L}'_M by replacing u in \mathcal{L}_M with $u[m']_q$ and construct $\mathfrak{M}' = (\mathcal{L}'_M, \mathcal{M})$ with $size(\mathfrak{M}') < size(\mathfrak{M})$ as required. The same argument can be made for (b) and \mathcal{M} , if u is the expansion of a macro rather than a term in \mathcal{L}_M . \square

The next result shows that, from a set of pairwise independent macros, *all* should be instantiated and exhaustively.

Lemma 5 (Instantiation of Independent Macros). *Let \mathcal{L} be a language and $\mathcal{M}: M \rightarrow T(\Sigma \cup M)$ a (reduced) set of macro definitions s.t. any two macros in M are independent. Furthermore, let $\mathfrak{M} = (\mathcal{L}_M, \mathcal{M})$ be an encoding of \mathcal{L} s.t. for all $t \in \mathcal{L}$ and all positions p with $t|_p = \mathcal{M}^*(m)$, we have $t[m]_p \in \mathcal{L}_M$. Then there is no encoding \mathfrak{M}' of \mathcal{L} w.r.t. \mathcal{M} s.t. $size(\mathfrak{M}') < size(\mathfrak{M})$.*

Proof. Assume that such a smaller $\mathfrak{M}' = (\mathcal{L}'_M, \mathcal{M})$ exists. Then there exists a macro $m \in M$ that is instantiated in some term $t \in \mathcal{L}$ at position p in \mathcal{L}'_M but not in \mathcal{L}_M . Since there is no $m' \in M$ s.t. m and m' are dependent, there is no macro that instantiates a subterm of $t|_p$ in \mathcal{L}_M . This means that $t|_p$ occurs in \mathcal{L}_M . However, this is a contradiction to our assumptions about \mathcal{L}_M since $\mathcal{M}^*(m) = t|_p$. \square

Theorem 1. *A size-minimal encoding of a finite language $\mathcal{L} \subseteq T(\Sigma)$ w.r.t. a finite set of (reduced) macro definitions $\mathcal{M}: M \rightarrow T(\Sigma \cup M)$ exists, is unique, and can be constructed in polynomial time w.r.t. the size of \mathcal{L} and \mathcal{M} .*

Proof. The existence of a minimal encoding is trivial. Since both \mathcal{L} and \mathcal{M} are finite, all possible encodings can be enumerated and compared w.r.t. their size.

Next, we sketch out a simple algorithm to compute a minimal encoding of \mathcal{L} w.r.t. \mathcal{M} and show that each step preserves uniqueness and is polynomial:

- 1.(a) compute $\mathcal{M}^*(m)$ for each $m \in M$
- (b) determine all dependencies between macros in \mathcal{M} , and
- (c) compute the associate Hasse-Diagram of macro dependencies \prec .

This can be constructed by a naive algorithm in $O(|\mathcal{M}|^2 * \mu^2)$ steps, where μ is the maximum $size(\mathcal{M}^*(m))$ of $m \in M$ since subtree isomorphism of labelled, un-ordered trees can be decided in quadratic time (Valiente 2002). We can further reduce this to $O(|\mathcal{M}|^2 * \tau^2)$ steps, where τ is the maximum $size(t)$ of $t \in \mathcal{L}$ since any macro with extension larger than τ can never be instantiated and thus be ignored.

2. Starting from the top, traverse the Hasse-Diagram of macro dependencies in a breadth-first manner (starting with maximally containing macros) and exhaustively instantiate all macros m on each level in \mathcal{L} , i.e., compute $\mathcal{L}_{S \cup \{m\}} := \{t' \mid t' \text{ is obtained by replacing all occurrences of } \mathcal{M}^*(m) \text{ in } t \in \mathcal{L}_S \text{ with } m\}$ starting from $\mathcal{L}_\emptyset = \mathcal{L}$.

Since the macros on each level are independent (due to \mathcal{M} being reduced) and since we exhaustively instantiate a macro before we possibly instantiate macros it contains, the resulting macro system $\mathfrak{M} = (\mathcal{L}_M, \mathcal{M}_M)$ is unique and size-minimal; see Lemmas 5 and 4.

Each of these $|\mathcal{M}|$ steps for macros m can be carried out in $|\mathcal{L}| * \tau^2$: we need to test all terms in \mathcal{L} whether they contain $\mathcal{M}^*(m)$ which can be assumed to have size $\leq \tau$.

Thus, the worst-case runtime of the algorithm described above is $O(|\mathcal{M}|^2 * \tau^2 + |\mathcal{M}| * |\mathcal{L}| * \tau^2)$. \square

Generalising this to non-reduced macro systems is straightforward and we only lose uniqueness.

Polynomial Time Algorithm for Solving Problem 2

Theorem 2. *A size-minimal encoding of a finite language $\mathcal{L} \subseteq T(\Sigma)$ w.r.t. the class of equivalent macro definitions of a finite set of (reduced) macro definitions $\mathcal{M}: M \rightarrow T(\Sigma \cup M)$ exists, is unique up to macro renaming, and can be constructed in polynomial time w.r.t. the size of \mathcal{L} and \mathcal{M} .*

Proof. Define the language \mathcal{L}' to be the union of terms in \mathcal{L} and in \mathcal{M} , i.e., $\mathcal{L}' = \mathcal{L} \cup \{\mathcal{M}^*(t) \mid m \mapsto t \in \mathcal{M}\}$. Then the size of \mathcal{L}' is bounded by $2 * size(\mathcal{L}) * size(t_{max})$, where t_{max} is the largest term in \mathcal{L} . So, a size-minimal encoding of \mathcal{L}' with respect to \mathcal{M} is unique and can be computed in polynomial time according to Theorem 1. Let $\mathfrak{M}' = (\mathcal{L}'_M, \mathcal{M})$ be such an encoding. Then the terms $t' \in \mathcal{L}'_M$ that correspond to terms of macro definitions have been compressed to be size minimal. Let $t'_m \in \mathcal{L}'_M$ be the term that corresponds to the expansion of m , i.e., $\mathcal{M}^*(m) = \mathcal{M}^*(t'_m)$, and let $\mathcal{L}_{M'}$ be the set of remaining terms in \mathcal{L}'_M . Then $\mathcal{M}' = \{m \mapsto t'_m \mid m \in M\}$ is equivalent to \mathcal{M} and $\mathfrak{M} = (\mathcal{L}_{M'}, \mathcal{M}')$ is a size-minimal encoding w.r.t. macro definitions equivalent to \mathcal{M} . Note that as a consequence of Theorem 1, the encoding \mathfrak{M} is unique up to permutations over the macro symbols M .

It is straightforward to extend the algorithm described in the proof of Theorem 1 to also maximally compress

\mathcal{M} : in Step 2, in addition to computing $\mathcal{L}_{S \cup \{m\}}$ for each $m \in M$, also compute $\mathcal{M}_{S \cup \{m\}} := \{m'' \mapsto t' \mid t' \text{ is obtained by replacing all occurrences of } \mathcal{M}^*(m) \text{ in } t \text{ with } m, \text{ for any } m'' \mapsto t \in \mathcal{M}_S\}$, with $\mathcal{M}_\emptyset = \mathcal{M}$. \square

Note that in the previous result, uniqueness only holds up to renaming of macros, because equivalence of macro definitions allows this. As previously remarked for Problem 1, uniqueness (up to renaming) stems from the reducedness of the macro definitions. We may allow macro definitions to be non-reduced but must then choose which of two equivalent macro definitions to instantiate at any applicable position.

Polynomial Time Algorithm for Solving Problem 3

Recall that the minimal encoding of a language with equivalent macro definitions is unique (up to renaming) by Theorem 2. For the set of reduced macro definitions \mathcal{M} and language \mathcal{L} , we denote the minimal encoding without renaming macro symbols by $\mathfrak{M}_{min}^{\mathcal{L}, \mathcal{M}}$. In Problem 3, we are thus interested in determining a set of macro definitions $\mathcal{M}_{opt} \in \text{argmin}_{\mathcal{M}} \text{size}(\mathfrak{M}_{min}^{\mathcal{L}, \mathcal{M}})$ for a given language \mathcal{L} .

To determine which macro definitions to include in such a minimal encoding, it will be elementary to consider *occurrences* and *sizes* of subterms in encodings.

Definition 17 (Occurrences & Dominance of terms). *Consider an encoding $\mathfrak{M} = (\mathcal{L}_M, \mathcal{M})$ of $\mathcal{L} \subseteq T(\Sigma)$. The number of occurrences of a term $t \in T(\Sigma \cup M)$ in \mathfrak{M} is defined as follows: $occ_{\mathfrak{M}}(t) :=$*

$$\sum_{t' \in \mathcal{L}_M} |\{p \mid t'|_p = t\}| + \sum_{m' \in M} |\{p \mid \mathcal{M}(m')|_p = t\}|.$$

We write $occ_{\mathcal{L}}(t)$ as a short form of $occ_{(\mathcal{L}, \emptyset)}(t)$, and say a term t is dominated by a term t' in \mathcal{L} if $t \preceq t'$ and $occ_{\mathcal{L}}(t) = occ_{\mathcal{L}}(t')$. In this case, we also say t' dominates t .

The first key observation is that, if t is dominated by t' in \mathcal{L} , then t only occurs within t' in \mathcal{L} and also only occurs exactly once in t' . It is not hard to show that \mathcal{M}_{opt} contains no macro definition $m \mapsto t$ where $\mathcal{M}_{opt}^*(t)$ is dominated by a term $t' \neq \mathcal{M}_{opt}^*(t)$ in \mathcal{L} : otherwise the encoding could be further compressed by removing $m \mapsto t$ and adding $m \mapsto t'$.

Another key observation is that \mathcal{M}_{opt} only contains macro definitions $m \mapsto t$ where $occ_{\mathcal{L}}(\mathcal{M}_{opt}^*(t)) \geq 2$, because introducing macros for terms that occur once increases the size of the encoding by 1.

These two observations allow us to characterise the set of macro definitions for a minimal encoding of a language.

Theorem 3. *For a finite language $\mathcal{L} \subseteq T(\Sigma)$ where Σ does not include unary symbols, a size-minimal encoding of \mathcal{L} is given by $\mathfrak{M}_{min}^{\mathcal{L}, \mathcal{M}}$ w.r.t. macro definitions*

$$\mathcal{M} := \{m_t \mapsto t \mid t \text{ subterm in } \mathcal{L} \text{ with } occ_{\mathcal{L}}(t) \geq 2 \text{ and } \nexists \text{ subterm } t' \text{ in } \mathcal{L} \text{ dominating } t \text{ in } \mathcal{L}\}$$

and can be constructed in time polynomial in $\text{size}(\mathcal{L})$.

Proof (Sketch). As noted above, a size-minimal encoding does not include any macro definition s.t. its expansion is a dominated term or a term only occurring once. However,

macro definitions for other (non-constant) terms, occurring at least twice and of size of at least three, cannot increase but can decrease the size of (exhaustive) encodings. Since Σ doesn't contain unary symbols, any non-constant term t in any language encoding will be of size of at least three. Namely its root symbol plus at least two arguments. We can use these arguments recursively to justify the introduction and exhaustive instantiation of all macro definitions in \mathcal{M} . \square

The algorithm sketched in the proofs of Theorems 1 and 2 can be easily extended to one for Problem 3 by constructing \mathcal{M} prior to the 1st step: considering all nodes n in all term trees $t \in \mathcal{L}$, determine how often $t|_n$ occurs in \mathcal{L} and, if this is more than once, whether t_n is dominated, i.e., contained by other subterms with equal number of occurrences.

Empirical Evaluation

We investigate whether the 3 algorithms presented in Section can be implemented to efficiently and effectively rewrite large OWL ontologies of practical relevance.

Implementation: We implement the three algorithms described above for OWL ontologies in Java (17 LTS) using the OWL API (5.1.15) and JGraphT (1.5) to handle ontologies and trees, respectively. All experiments were run on an Apple M2 Max processing unit with 96GB of RAM under the operating system macOS Ventura (13.5). All source code is available at <https://github.com/ckindermann/AAAI2024>.

Corpus: We use 5 large ontologies that were originally selected for the evaluation of a related approach, cf. (Nikitina and Koopmann 2017). The latest version of each ontology was downloaded from BioPortal¹ on August 8, 2023. In the case of SNOMED the most recent release of February 2023 was used. The size of each ontology is shown in the third column of Table 1, where S stands for SNOMED, G for Galen, C for Genomic CDS, F for FYPO, and N for NCIT.

Setup: An axiom of the form *EquivalentClasses*(N, C) can be seen as macro definition of the form $N \mapsto C$ if N is a named class and C is a complex class expression. To apply our approach, however, we require macro definitions to be functions and acyclic (see Definition 8). For an ontology \mathcal{O} , let $\mathcal{M}_{\mathcal{O}} \subseteq \mathcal{O}$ denote the set of macro definitions obtained from \mathcal{O} 's *EquivalentClasses*(N, C) axioms without axioms that (a) are involved in cycles or (b) in which N occurs more than once in this set of axioms. Note that we do not reduce $\mathcal{M}_{\mathcal{O}}$ because we are interested in the impact of *macro instantiation* on the size of an encoding of an ontology rather than the impact of *removing redundant* definitions.

Expanding all macros exhaustively in $\mathcal{O} \setminus \mathcal{M}_{\mathcal{O}}$ yields the language $\mathcal{L} = \mathcal{M}_{\mathcal{O}}^*(\mathcal{O} \setminus \mathcal{M}_{\mathcal{O}})$ without macro symbols and without their definitions. By abuse of notation, $(\mathcal{L}, \mathcal{M}_{\mathcal{O}})$ can be seen as an encoding of \mathcal{O} and can be used as an input macro system for Problems 1 and 2. For Problem 3, we use \mathcal{O} as the input language but remove all axioms involving unary symbols, i.e., *ComplementOf*.²

¹See <https://bioportal.bioontology.org/>

²Which caused the removal of only one axiom in one ontology.

P	O	$size(\mathcal{O})$	$size(\mathcal{L}_M)$	$size(\mathcal{M})$	Prop. Red.	# Axioms	# Ch. Axioms	# \mathcal{M}
1	S	3 657 845	1 291 740	2 269 878	3%	227 909	9 199	132 588
2			1 291 740	2 269 878	3%	227 909	9 199	132 588
3			2 013 130	293 779	37%	360 497	188 066	54 883
1	G	198 568	104 752	90 435	2%	25 563	686	9 968
2			104 752	87 961	3%	25 563	1 152	9 968
3			151 442	16 496	15%	35 531	14 433	3 624
1	C	35 361	31 905	2 627	2%	3 992	177	330
2			31 905	2 528	3%	3 992	210	330
3			20 501	2 340	35%	4 322	585	439
1	F	289 643	138 740	90 886	21%	37 481	5 524	7 550
2			138 740	90 874	21%	37 481	5 525	7 550
3			144 021	64 298	28%	45 030	18 650	9 814
1	N	1 149 850	830 107	319 743	0%	237 060	0	19 069
2			830 107	319 743	0%	237 060	0	19 069
3			913 719	36 158	17%	256 129	60 752	9 019

Table 1: Statistics on Minimising Ontologies showing the size of the ontology \mathcal{O} , its macrofication \mathcal{L}_M , and its macro definitions \mathcal{M} (in the case of Problem 1 and 2, definitions are measured by the size of associated axioms), the proportional size reduction, Prop. Red. (measured by $(1 - (size(\mathcal{L}_M) + size(\mathcal{M})) / size(\mathcal{O})) * 100$), the number of axioms of the input language (# Axioms), the number of changed axioms (# Ch. Axioms), and the number of macro definitions (# \mathcal{M}).

Reduction Results: In Table 1, we list statistics for the size-minimal encoding for each pair of the 3 computational problems and 5 ontologies. We can see that size-minimal encodings w.r.t. Problem 3 lead to significantly larger size-reductions compared to Problem 1 and 2, suggesting that the introduction of *new macro symbols* can capture and reveal structural patterns in ontologies that cannot be encoded via existing named classes defined via *EquivalentClasses* axioms, i.e., macros in Problem 1 and 2.

A comparison with the size reduction of class expressions reported for a related approach, cf. (Nikitina and Koopmann 2017), reveals that encodings w.r.t. Problem 3 often yield comparable reductions while reducing larger proportions of class expressions.

Processing Time: We can compute each size-minimal encoding for each ontologies w.r.t. any of the three problems in less than a minute. This is a significant improvement over existing approaches, cf. (Nikitina and Koopmann 2017), where minimising 100 concepts in SNOMED was reported to take on average 3–10 minutes depending on concept size.

Related Work

The notion of a “macrofication”, i.e., the idea of refactoring source code by introducing macros in an automated manner, has already been proposed (Schuster, Disney, and Flanagan 2016). The motivation for reversing macro expansion, or what we call macro instantiation, is improved readability and maintenance. However, the objective of smaller rewritings is subjected to the condition of not altering program behaviour rather than aiming for size-minimality.

Automated rewriting mechanisms for OWL ontologies, designed to aide ontology comprehension and maintenance include techniques for removing redundancies based on entailment (Grimm and Wissmann 2011), removing redundancies based on templates (Skjæveland et al. 2018), reusing equivalent named classes (Kindermann and Skjæveland 2022), repairing unsatisfiable classes (Kalyanpur et al.

2006), and adding missing but desired as well as removing undesired relationships (Mougin 2015). While all of these approaches reduce an ontology’s size, none of the proposed techniques aim for size-minimality.

Existing rewriting approaches for OWL ontologies, aiming for some notion of size-minimality are based on entailment (Baader, Küsters, and Molitor 2000; Nikitina and Koopmann 2017). However, these approaches only work for non-expressive Description Logics, namely $\mathcal{AL}\mathcal{E}$ and \mathcal{EL} , and must be restricted further, e.g., to exclude the important OWL constructor *IntersectionOf* (Nikitina and Schewe 2013) or to require a notion of semantic acyclicity (Koopmann and Nikitina 2016) to mitigate unfavourable computational characteristics, limiting their application in practice.

Besides earlier versions of this work, cf. (Kindermann 2021), this is the first rewriting study that formalises both the arity and orderdness of symbols and is thus truly applicable to complex languages such as OWL.

Conclusions and Outlook

In this paper, we present a rewriting mechanism for finite formal languages based on (nested) syntactic macros. Using this mechanism, we demonstrate the feasibility and effectiveness of computing size-minimal rewritings for large ontologies of practical relevance in the biomedical domain.

The presented work can be extended in a variety of ways. The complexity of the general Problem 3, for languages over alphabets including unary symbols, remains an open question. Moreover, different features of macro systems can be investigated, e.g., *1-step macros* (no nesting), or *parameterised macros* of the form $m(x_1, x_2) \mapsto a(x_1, b(c, x_2))$, with variables that can be bound to input arguments.

Another interesting direction for future work are user studies to investigate the usefulness of size-minimal encodings in potential use-case scenarios. Such studies may shed light on what kind of interaction mechanisms are required for assisting with refactoring tasks in practice.

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