Inside-Outside Algorithm for Macro Grammars

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Abstract

We propose an inside-outside algorithm for stochastic macro grammars. Our approach is based on types, which has been inspired by type-based approaches to reasoning about functional programs and higher-order grammars. By considering type derivations instead of ordinary word derivation sequences, we can naturally extend the standard inside-outside algorithm for stochastic context-free grammars to obtain the algorithm for stochastic macro grammars. We have implemented the algorithm and confirmed its effectiveness through an application to the learning of macro grammars.

Keywords: macro grammars, stochastic grammars, inside-outside algorithm, types

1. Introduction

The inside-outside algorithm (Baker, 1979) is a popular algorithm for learning stochastic context-free grammars (CFGs), and it has been used in various applications (Jelinek, 1985; Dodd, 1988). There are also many extensions so that the algorithm can handle various grammars, such as stochastic lexicalized tree-adjoining grammars (Schabes, 1992), projective and non-projective dependency grammars (Eisner, 1996; Koo et al., 2007), and multiple context-free grammars (MCFGs) (Kato et al., 2006).

In this paper, we extend the inside-outside algorithm for (stochastic, OI) macro grammars (Fischer, 1968), where each non-terminal may take parameters. Macro grammars (MGs) can generate non-context free languages, including non-semilinear languages, like $\{ww \mid w \in \{a, b\}^+\}$, $\{a^n b^n c^n \mid n > 0\}$ and $\{a^{2^n} \mid n \ge 0\}$. The class of languages generated by MGs coincides with the class of indexed languages and also with the level-2 language in Damm's OI-hierarchy of higher-order languages (Damm, 1982) (where level-0 and level-1 languages are regular and context-free languages respectively). Stochastic MGs would be useful for more faithfully representing stochastic language models than less expressive grammars like CFGs.

Extending the inside-outside algorithm for MGs is non-trivial. In CFGs, non-terminals in sequences derived from the initial symbol are rewritten in an arbitrarily order and they derive strings independently. This makes derivation modes like left-most derivation and right-most derivations indifferent and allows us to define *derivation trees*, based on which the inside-outside algorithm can be constructed. It is the case for TAGs and MCFGs as well. However, the situation is quite different when considering MG derivations, where a

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non-terminal may copy other non-terminals and those copies may derive different terms. Thus, it is tricky to come up with the right notion of derivation trees for designing an inside-outside algorithm.

Our key idea for extending the inside-outside algorithm is to use *intersection types*, which have been proved useful for reasoning about higher-order grammars (Kobayashi, 2013b; Kobayashi et al., 2013). By replacing the role of word derivations trees in the inside-outside algorithm for stochastic CFGs with that of *type derivation trees*, we can naturally obtain an inside-outside algorithm for MGs (and possibly also for arbitrary higher-order grammars (Damm, 1982; Kobele and Salvati, 2015), though it is left for future work).

We have implemented the algorithm and applied it to learn (non-stochastic) MGs. The learning of MGs proceeds as follows. Given a set of words, the goal is to find an MG that provides a good explanation of the words. To this end, we first fix a set of nonterminals and prepare a set of all the possible rules (in certain normal form), and run the inside-outside algorithm to maximize the probability that the words are generated. We then remove the rules whose probabilities are below a certain threshold. Finally, by removing the probabilities of the remaining rules, we obtain a non-stochastic MG. We have applied this procedure to several non-context free languages including non-semilinear ones and successfully obtained appropriate MGs.

Another potential application of our inside-outside algorithm is grammar-based data compression. Stochastic CFGs have been used for data compression, where a word is compressed as (the arithmetic coding of) its derivation sequence (Cameron, 1988; Tarhio, 2001; Naganuma et al., 2020). We expect that, by using stochastic MGs, we can achieve more compact coding of word data.

Related Work. As already mentioned, the inside-outside algorithm has been originally proposed for (stochastic) CFGs (Baker, 1979) and adapted later to other grammars (Schabes, 1992; Eisner, 1996; Koo et al., 2007; Kato et al., 2006). To our knowledge, the inside-outside algorithm for MGs is new. A distinguishing, novel feature of our inside-outside algorithm is the use of types, which allowed us to naturally extend the algorithm for CFGs. Type-based techniques have recently been used for higher-order grammars, albeit for different purposes such as higher-order model checking (Kobayashi, 2013b), pumping lemmas (Kobayashi, 2013a; Asada and Kobayashi, 2017), and data compression (Kobayashi et al., 2013).

Structure of the Paper. The rest of this paper is structured as follows. Section 2 gives the definition of stochastic macro grammars. Section 3 describes the inside-outside algorithm for stochastic macro grammars. Section 4 reports experiments, and Section 5 concludes the paper. The details omitted in this paper are found in an extended version of this paper (Kambe et al., 2021).

2. Stochastic Macro Grammars

In this section, we review the notion of macro grammars (Fischer, 1968) and define its stochastic extension.

Macro grammars are an extension of context-free grammars, where non-terminals may take parameters. For example, a macro grammar may contain a rule like $F \ x \to x \cdot x$, where

the non-terminal F takes a parameter x and \cdot denotes the word concatenation (we omit \cdot when there is no danger of confusion). Using the rule, F **a** and F **b** are rewritten to **aa** and **bb**.

Definition 1 (Macro grammars) A macro grammar (MG, for short) is a quadruple $\mathcal{G} = (\mathcal{A}, \mathcal{N}, \mathcal{R}, S)$ where:

(i) \mathcal{A} is a finite set of symbols called terminals; we use meta-variables a, b, c, \ldots for terminals;

(ii) \mathcal{N} is a map from a finite set of symbols called non-terminals to the set of nonnegative integers; $\mathcal{N}(F)$, called the arity of F, represents how many parameters F takes; we use meta-variables F, G, S, \ldots for non-terminals;

(iii) \mathcal{R} is a finite set of rewriting rules of the form $Fx_1 \dots x_{\mathcal{N}(F)} \to t$ where F is a nonterminal, $x_1, \dots, x_{\mathcal{N}(F)}$ are distinct variables, and t ranges over the set of terms defined by the following BNF:

$$t ::= x_i \mid a \mid t_1 \cdot t_2 \mid G t_1 \cdots t_{\mathcal{N}(G)}$$

We give higher precedence to concatenations (\cdot) than to applications, so that $F x \cdot x$ means $F(x \cdot x)$ instead of $(F x) \cdot x$. We sometimes insert parentheses explicitly to avoid confusion. By using the notation of λ -calculus, we sometimes write $F \to \lambda x_1, \ldots, x_k$. If for the rule $F x_1 \cdots x_k \to t$, and use meta-variables α, β, \cdots for the part $\lambda x_1, \ldots, x_k$. If thus, the rule is written $F \to \alpha$;

(iv) $S \in dom(\mathcal{N})$ is the start symbol, which satisfies $\mathcal{N}(S) = 0$;

For an MG $\mathcal{G} = (\mathcal{A}, \mathcal{N}, \mathcal{R}, S)$, the (outermost, leftmost¹) rewriting relation $t \Rightarrow_{\mathcal{G}, r} t'$ (where $r \in \mathcal{R}$) is inductively defined by:

- $F t_1 \cdots t_k \Rightarrow_{\mathcal{G}, F \to \lambda x_1, \dots, x_k, t} [t_1/x_1, \dots, t_k/x_k] t \text{ if } F \to \lambda x_1, \dots, x_k, t.$
- $t_1 \cdot t_2 \Rightarrow_{\mathcal{G},r} t'_1 \cdot t_2$ if $t_1 \Rightarrow_{\mathcal{G},r} t'_1$.
- $t_1 \cdot t_2 \Rightarrow_{\mathcal{G},r} t_1 \cdot t'_2$ if $t_2 \Rightarrow_{\mathcal{G},r} t'_2$ and t_1 contains no non-terminals.

Here, $[t_1/x_1, \ldots, t_k/x_k]t$ denotes the term obtained from t by simultaneously replacing each occurrence of x_i with t_i . We omit the subscripts \mathcal{G} and/or r when they are clear from the context or unimportant. We write $\Rightarrow_{\mathcal{G},r_1\cdots r_k}^*$ for the relational composition $\Rightarrow_{\mathcal{G},r_1}\cdots\Rightarrow_{\mathcal{G},r_k}$ (where k may be 0, in which case $\Rightarrow_{\mathcal{G},r_1\cdots r_k}^*$ is the identity relation on terms). Note that, given a term t and a sequence of rules $r_1, \ldots, r_k \in \mathcal{R}$, there exists at most one term t' such that $t \Rightarrow_{\mathcal{G},r_1\cdots r_k}^*$ t'.

The language generated by \mathcal{G} , written $\mathcal{L}(\mathcal{G})$, is defined as $\{w \in \mathcal{A}^* \mid S \Rightarrow^*_{\mathcal{G}} w\}$.

Remark 2 Fischer (1968) actually introduced two kinds of macro grammars: OI and IO. The MGs defined above are OI macro grammars. For the sake of simplicity, we excluded out the empty word ϵ from the set of terms. This is not a fundamental restriction, because any MG G with ϵ can be transformed to another MG G' without ϵ such that $\mathcal{L}(\mathcal{G}) \setminus \epsilon = \mathcal{L}(\mathcal{G}')$ (see, e.g., Asada and Kobayashi, 2016).

Below we often write \tilde{x} for a sequence of variables $x_1 \cdots x_k$.

^{1.} We need to fix the rewriting strategy to properly count the probability of a word being generated. We could alternatively choose the rightmost derivation.

Example 1 Consider the MG $\mathcal{G}_{2^n} = (\mathcal{A}, \mathcal{N}, \mathcal{R}, S)$ where $\mathcal{A} = \{a\}, \mathcal{N} = \{S \mapsto 0, F \mapsto 1\}$, and \mathcal{R} consists of:

$$S \rightarrow a \mid F a$$
 $F x \rightarrow x \cdot x \mid F(x \cdot x)$

(Here, we use the convention of writing multiple rules $F \tilde{x} \to t_1, \ldots, F \tilde{x} \to t_\ell$ that share the same left-hand side as $F \tilde{x} \to t_1 | \cdots | t_\ell$.) The word $a^4 = aaaa$ can be generated as follows.

$$S \Rightarrow_{S \to F \mathbf{a}} F \mathbf{a} \Rightarrow_{F x \to F(x \cdot x)} F(\mathbf{a} \cdot \mathbf{a}) \Rightarrow_{F x \to x \cdot x} \mathbf{a} \mathbf{a} \mathbf{a} \mathbf{a}.$$

The language $\mathcal{L}(\mathcal{G}_{2^n})$ is $\{a^{2^n} \mid n \geq 0\}$.

Definition 3 (Stochastic macro grammars) A stochastic macro grammar (SMG, for short) is a quintuple $\mathcal{G} = (\mathcal{A}, \mathcal{N}, \mathcal{R}, S, \phi)$, where $(\mathcal{A}, \mathcal{N}, \mathcal{R}, S)$ is an MG, and $\phi : \mathcal{R} \to (0, 1]$ assigns a non-zero probability to each rule. We require that $\sum_{F \to \alpha \in \mathcal{R}} \phi(F \to \alpha) = 1$ holds for each non-terminal $F \in dom(\mathcal{N})$.

The rewriting relation $\Rightarrow_{\mathcal{G},r}$ for $\mathcal{G} = (\mathcal{A}, \mathcal{N}, \mathcal{R}, S, \phi)$ is the one for the underlying MG $(\mathcal{A}, \mathcal{N}, \mathcal{R}, S)$.

The probability of a rewriting sequence $t \Rightarrow_{\mathcal{G},r_1\cdots r_k}^* t'$, written $\operatorname{Prob}(t \Rightarrow_{\mathcal{G},r_1\cdots r_k}^* t')$, is defined as $\prod_{i=1}^k \phi(r_i)$. For terms t and t', the probability that t' is obtained from t, written $\operatorname{Prob}(t \Rightarrow_{\mathcal{G}}^* t')$, is defined as the sum of the probabilities of all the rewriting sequences from t to t', i.e., $\sum_{r_1\cdots r_k\in\mathcal{R}^*,t\Rightarrow_{\mathcal{G},r_1\cdots r_k}^* t'} \operatorname{Prob}(t \Rightarrow_{\mathcal{G},r_1\cdots r_k}^* t')$. For a word $W \in \mathcal{A}^*$, we write $\operatorname{Prob}_{\mathcal{G}}(W)$ for $\operatorname{Prob}(S \Rightarrow_{\mathcal{G}}^* W)$. We write $\mathcal{L}(\mathcal{G})$ for the set $\{W \in \mathcal{A}^* \mid \operatorname{Prob}_{\mathcal{G}}(W) > 0\}$.

For an SMG $\mathcal{G} = (\mathcal{A}, \mathcal{N}, \mathcal{R}, S, \phi)$, we write $(\mathcal{G})^{\#}$ for the underlying MG $(\mathcal{A}, \mathcal{N}, \mathcal{R}, S)$. Note that $\mathcal{L}(\mathcal{G}) = \mathcal{L}((\mathcal{G})^{\#})$ holds.

Example 2 Consider the SMG $\mathcal{G}'_{2^n} = (\mathcal{A}, \mathcal{N}, \mathcal{R}, S, \phi)$ where $(\mathcal{A}, \mathcal{N}, \mathcal{R}, S)$ is as given in Example 1, and ϕ is given by:

$$\begin{split} \phi(S \to \mathbf{a}) &= 0.3, \qquad \phi(S \to F \, \mathbf{a}) = 0.7, \\ \phi(F \, x \to x \cdot x) &= 0.4, \quad \phi(F \, x \to F(x \cdot x)) = 0.6. \end{split}$$

Then, the probability for the derivation

$$S \Rightarrow_{S \to F a} F a \Rightarrow_{F x \to F(x \cdot x)} F(a \cdot a) \Rightarrow_{F x \to x \cdot x} aaaa$$

is $0.7 \times 0.6 \times 0.4 = 0.168$. Since this is the only derivation sequence for generating \mathbf{a}^4 , $Prob_{\mathcal{G}_{2n}'}(\mathbf{a}^4) = 0.168$.

In the rest of the paper, we impose a restriction to SMGs, so that for each word $W \in \mathcal{A}^*$, the set of rewriting sequences $S \Rightarrow_{\mathcal{G},r_1\cdots r_k}^* W$ is finite. For a term t, we write $||t||_0$ for the number of occurrences of symbols (terminals, non-terminals, and variables) in t, $||t||_1$ for the number of occurrences of symbols excluding non-terminals of non-zero arity. For example, if $\mathcal{N}(F) = 1$ and $\mathcal{N}(G) = 0$, then $||F(\mathbf{a} \cdot \mathbf{a} \cdot G)||_0 = 4$ while $||F(\mathbf{a} \cdot \mathbf{a} \cdot G)||_1 = 3$. We define the measure ||t|| of t by:

$$||t|| ::= (||t||_0, ||t||_1).$$

For example, $||F(x \cdot \mathbf{a})|| = (3, 2)$. We define the strict partial order < on ||t|| as the lexicographic order: (m, n) < (m', n') iff m < m' or $m = m' \land n < n'$.

Definition 4 (Expansive grammars) An SMG $\mathcal{G} = (\mathcal{A}, \mathcal{N}, \mathcal{R}, S, \phi)$ is expansive if (I) the start symbol S does not occur on the right-hand side of any rule and (II) for every rule $F x_1 \cdots x_k \to t \in \mathcal{R}$ such that $F \neq S$, (i) each variable x_i occurs at least once in t, and (ii) $||F x_1 \cdots x_k|| < ||t||$.

Note that the grammar \mathcal{G}'_{2^n} in Example 2 is expansive. The following property of expansive SMGs is important for our inside-outside algorithm. A proof is given in Kambe et al. (2021).

Lemma 5 Let $\mathcal{G} = (\mathcal{A}, \mathcal{N}, \mathcal{R}, S, \phi)$ be an expansive SMG. For every word $W \in \mathcal{A}^*$, the set of rewriting sequences $S \Rightarrow^*_{\mathcal{G}, r_1 \cdots r_k} W$ is finite.

Henceforth, we consider only expansive SMGs, and call them just SMGs.

Remark 6 Every context-free grammar in Chomsky normal form is expansive. To our knowledge, there is no such normal form for MGs. The definition of expansive grammars above is non-standard and ad hoc. We do not know whether every macro grammar can be transformed to an equivalent expansive grammar.

3. The Inside-Outside Algorithm for Macro Grammars

This section introduces our inside-outside algorithm for SMGs. Given an SMG \mathcal{G} and a finite set of words $\mathcal{W} = \{W_1, \ldots, W_Q\}$, the goal of the algorithm is to obtain a probability function ϕ that (locally) maximize $\prod_{q=1}^{Q} \operatorname{Prob}_{\mathcal{G}}(W_q)$ by iteratively updating ϕ .² At each iteration, the value of $\phi(A \to \alpha)$ is updated to $\frac{c(A \to \alpha)}{\sum_{A \to \beta} c(A \to \beta)}$, where $c(A \to \alpha)$ is the expected number of times the rule $A \to \alpha$ is used to derive the words in \mathcal{W} .

In the inside-outside algorithm for stochastic context-free grammars (SCFGs), $c(A \rightarrow \alpha)$ is obtained by considering the *inside probability inside*(A, i, j) and *outside probability outside*(A, i, j). For a word $W = a_1 \cdots a_n$, inside(A, i, j) (where $1 \le i \le j \le n$) denotes the probability that $a_i \cdots a_j$ is generated from A (or, the probability that the derivation tree for $a_i \cdots a_j$ whose root is A is obtained), and *outside*(A, i, j) denotes the probability that $a_1 \cdots a_n$ can be derived from the start symbol S: see Figure 1 (a) for an illustration.

In the case of SMG, the notion of a "derivation tree" is unclear, due to the existence of parameters. Our insight is that, by considering a "type derivation tree" corresponding to a derivation of a word, we can naturally define the *inside probability* and *outside probability*, and obtain an inside-outside algorithm based on those probabilities. For those who are familiar with type systems, Figure 1 (b) shows an illustration; it will be explained later. The reason why "types" come to play is that an SMG may be viewed as a (probabilistic) functional program; thus, a type system can be used to analyze the behavior of an SMG. In

^{2.} As in the case for stochastic context-free grammars, our inside-outside algorithm may be viewed as an instance of EM-algorithm (Dempster et al., 1977; Wu, 1983). Therefore, actually we can only guarantee that the value of $\prod_{q=1}^{Q} Prob_{\mathcal{G}}(W_q)$ increases monotonically at each iteration, and the algorithm converges to the value at a stationary point of $\prod_{q=1}^{Q} Prob_{\mathcal{G}}(W_q)$ (as a function of ϕ), not necessarily to a local maximum.

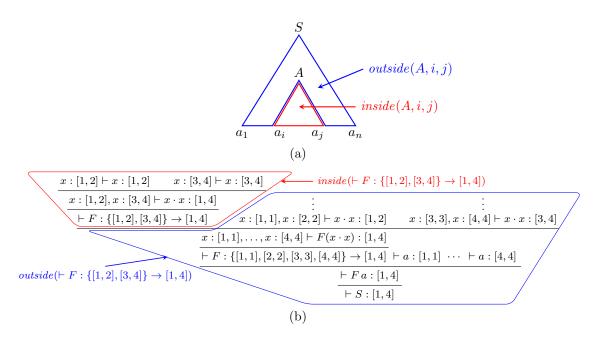


Figure 1: Inside and outside probabilities for SCFG (a) and SMG (b)

fact, types have recently been used for analyzing higher-order grammars (of which an MG can be considered a special case) (Kobayashi, 2013b; Kobayashi et al., 2013).

Remark 7 It would be possible to formalize an inside-outside algorithm without using the notion of types, but the resulting formalization would be more awkward. Also, we expect that the use of types allows us to extend the inside-outside algorithm for higher-order grammars of arbitrary orders, although it is left for future work.

We now define a type system. Below we fix an SMG $\mathcal{G} = (\mathcal{A}, \mathcal{N}, \mathcal{R}, S, \phi)$ and a word $W = a_1 \cdots a_n \in \mathcal{A}^*$. We write W[i, j] (where $1 \leq i \leq j \leq n$) for the subword $a_i \cdots a_j$.

The set of types, ranged over by τ , is defined by:

$$au ::= [i, j] \mid \sigma \to au \qquad \sigma ::= \{[i_1, j_1], \dots, [i_k, j_k]\}$$

Intuitively, [i, j] is the type of a term that may be used to generate W[i, j]. For example, if $W = a^4$, then as has types [1, 2], [2, 3], and [3, 4]. The type $\sigma \to \tau$ describes a function that takes an argument that has every type $\tau' \in \sigma$, and returns a value of type τ . For example, if there is a rule $F x \to x \cdot x$, F has type $\{[1,2],[3,4]\} \to [1,4]$. We require that a function of type $\sigma \to \tau$ must use the argument once for each $\tau' \in \sigma$. Thus, the function G with rule $G x \to \mathbf{a} \cdot \mathbf{a} \cdot \mathbf{a}$ has type $\{[3,4]\} \to [1,4]$, but not $\{[1,2],[3,4]\} \to [1,4]$ (because x is used to generate only W[3,4], not W[1,2]). A set of types of the form $\{[i_1, j_1], \ldots, [i_k, j_k]\}$ is so called an *intersection type* in the terminology of programming languages; we sometimes write $[i_1, j_1] \land \cdots \land [i_k, j_k]$ for it. We also just write [i, j] for $\{[i, j]\}$, and \top for \emptyset .

We restrict the shape of types as follows. We define $\tau^{\#}$ by:

$$[i, j]^{\#} = \{x \in \mathbf{Nat} \mid i \le x \le j\}$$
$$(\{[i_1, j_1], \dots, [i_k, j_k]\} \to \tau)^{\#} = \tau^{\#} \setminus ([i_1, j_1]^{\#} \cup \dots \cup [i_k, j_k]^{\#})$$

$$\frac{1}{x:[i,j] \vdash_W x:[i,j]} \qquad (\text{T-VAR}) \qquad \frac{W[i,i] = a}{\vdash_W a:[i,i]} \qquad (\text{T-TERM})$$

$$\Gamma_1 \vdash_W t_1:[i,j] \qquad \Gamma_2 \vdash_W t_2:[i+1,k]$$

$$\frac{\Gamma_1 \vdash_W t_1 : [i, j] \qquad \Gamma_2 \vdash_W t_2 : [j+1, k]}{\Gamma_1 \uplus \Gamma_2 \vdash_W t_1 \cdot t_2 : [i, k]}$$
(T-CONCAT)

$$\frac{\vdash_{W} F: \sigma_{1} \to \dots \to \sigma_{\mathcal{N}(F)} \to [i, j] \qquad \Gamma_{k,\tau} \vdash_{W} t_{k}: \tau \text{ for each } k \in \{1, \dots, \mathcal{N}(F)\}, \tau \in \sigma_{k}}{\biguplus_{k \in \{1, \dots, \mathcal{N}(F)\}, \tau \in \sigma_{k}} \Gamma_{k,\tau} \vdash_{W} F t_{1} \cdots t_{\mathcal{N}(F)}: [i, j]}$$
(T-APP)

$$\frac{F x_1 \cdots x_k \to t \in \mathcal{R} \qquad x_1 : \sigma_1, \dots, x_k : \sigma_k \vdash_W t : [i, j]}{\vdash_W F : \sigma_1 \to \dots \to \sigma_k \to [i, j]}$$
(T-RULE)

Figure 2: Typing rules

where **Nat** is the set of natural numbers. Intuitively, $\tau^{\#}$ denotes the set of positions generated by a term of type τ . We require: (i) in [i, j], it must be the case that $i \leq j$, and (ii) in $\{[i_1, j_1], \ldots, [i_k, j_k]\} \rightarrow [i, j], [i_{\ell}, j_{\ell}]^{\#} \cap [i_{\ell'}, j_{\ell'}]^{\#} = \emptyset$ for any $1 \leq \ell < \ell' \leq k$, and $(\bigcup_{\ell \in \{1, \ldots, k\}} [i_{\ell}, j_{\ell}]^{\#}) \subseteq [i, j]^{\#}$. Henceforth, we consider only types that satisfy the above restriction.

We consider a type judgment of the form $\Gamma \vdash_W t : \tau$, where Γ , called a type environment, is a set of bindings of the form x : [i, j]. Each binding x : [i, j] in a type environment means that x must be used as a value of type [i, j], i.e., may be used to generate W[i, j]. A type environment may contain more than one binding for each variable; for example, $\{x:[1,2], x:[3,4]\}$ means that x must be used for generating W[1,2], and also for generating W[3,4]. We sometimes write $x:\sigma$ to mean the type environment $\bigcup_{[i,j]\in\sigma} \{x:[i,j]\}$. The judgment $\Gamma \vdash_W t : \tau$ means that assuming that the variables in t are used according to Γ , t behaves as a value of type τ . For example, $\{x:[1,2], x:[3,4]\} \vdash_{\mathbf{a}^4} x \cdot x : [1,4]$ is a valid judgment. We often omit brackets and just write $x_1:[i_1,j_1], \ldots, x_k:[i_k,j_k]$ for $\{x_1:[i_1,j_1],\ldots,x_k:[i_k,j_k]\}$. When Γ is empty, we just write $\vdash_W t:\tau$ for $\emptyset \vdash_W t:\tau$. We usually fix W and omit the subscript W.

The typing rules for deriving valid type judgments are given in Figure 2. In the figure, $\exists \exists denotes the disjoint union: \Gamma_1 \exists \Gamma_2$ is defined to be $\Gamma_1 \cup \Gamma_2$ only if $\Gamma_1 \cap \Gamma_2 = \emptyset$.

Figure 1 (b) shows a type derivation tree for $\vdash_W S : [1,4]$ for the SMG in Example 2 and $W = \mathbf{a}^4$. The type derivation tree corresponds to the derivation sequence $S \Rightarrow_{S \to F \mathbf{a}} F \mathbf{a} \Rightarrow_{F x \to F(x \cdot x)} F(\mathbf{a} \cdot \mathbf{a}) \Rightarrow_{F x \to x \cdot x} \mathbf{a} \mathbf{a} \mathbf{a} \mathbf{a}$. The judgment $\vdash F : \{[1,2],[3,4]\} \to [1,4]$ in the type derivation tree corresponds to the second use of F (in $F(\mathbf{a} \cdot \mathbf{a})$) and represents that the argument $\mathbf{a} \cdot \mathbf{a}$ is used for generating the subwords W[1,2] and W[3,4]. This is not a coincidence. Every type derivation tree for $\vdash_W S : [1,|W|]$ corresponds to a derivation sequence for W, and vice versa. Thus, we can calculate the probability $Prob_{\mathcal{G}}(W)$ by summing up the probabilities of type derivation trees, instead of considering derivation sequences, as discussed below. We write T for a type derivation tree, and $\mathbf{DT}(\Gamma \vdash t : \tau)$ for the set of type derivation trees whose conclusion is $\Gamma \vdash t : \tau$.³ We write $occ(T, F \to \alpha)$ for the number of times the rule $F \to \alpha$ is used in (applications of the rule T-RULE) T. The probability Prob(T) of a type derivation tree T is defined by:

$$Prob(T) = \prod_{F \to \alpha \in \mathcal{R}} \phi(F \to \alpha)^{occ(T, F \to \alpha)}$$

For a type judgment $\Gamma \vdash_W t : \tau$, its inside probability $inside(\Gamma \vdash_W t : \tau)$ is defined by:

$$inside(\Gamma \vdash_W t : \tau) = \sum_{T \in \mathbf{DT}(\Gamma \vdash_W t : \tau)} Prob(T)$$

Thus, the inside probability $inside(\Gamma \vdash_W t : \tau)$ is analogous to the inside probability for SCFG, where derivation trees have been replaced by type derivation trees. The theorem below guarantees that our inside probability correctly models the probability that a word is generated. A proof is given in Kambe et al. (2021).

Theorem 8 Let $\mathcal{G} = (\mathcal{A}, \mathcal{N}, \mathcal{R}, S, \phi)$ be an SMG and $W \in \mathcal{A}^*$. Then $Prob_{\mathcal{G}}(W) = inside(\vdash_W S : [1, |W|])$.

For a type environment Γ , we write $\Gamma \downarrow_{[i,j]}$ for the restricted type environment $\{x : [i',j'] \in \Gamma \mid i \leq i' \leq j' \leq j\}$; $\Gamma \downarrow_{[i,j]}$ is undefined if there exists $x : [i',j'] \in \Gamma$ such that $[i,j]^{\#} \cap [i',j']^{\#} \neq \emptyset$ but $[i',j']^{\#} \not\subseteq [i,j]^{\#}$. We write \mathbf{Ty}_W for the set of (valid) types, where all the indexes *i* occurring in them must satisfy $1 \leq i \leq |W|$ (so that they are valid indexes for *W*). As in the case for SCFG, the inside probability $inside(\Gamma \vdash t : \tau)$ can be inductively calculated as follows.

^{3.} We view type derivation trees as *unordered* trees, where the order of children of each node is irrelevant. For example, $\frac{T_1 \quad T_2}{\Gamma \vdash t : \tau}$ and $\frac{T_2 \quad T_1}{\Gamma \vdash t : \tau}$ are considered the same trees.

Here, $inside(\Gamma \vdash_W t : \tau) = 0$ if it does not match any of the above definitions (e.g., $inside(x : [1,2] \vdash_W x : [1,3]) = 0$). Each equation for $inside(\Gamma \vdash_W t : \tau)$ sums up the probabilities of all the possible derivations for $\Gamma \vdash_W t : \tau$. In the fourth clause, we assume k > 0; the case where t is an arity-0 non-terminal is covered by the last clause. The correctness of this calculation is discussed in Kambe et al. (2021).

Remark 9 A careful reader may notice that the above algorithm for calculating inside ($\Gamma \vdash t:\tau$) is circular: in the definition of inside ($\vdash_W F:\sigma_1 \rightarrow \cdots \rightarrow \sigma_k \rightarrow [i, j]$), F may occur in t, so that inside ($\vdash_W F:\sigma_1 \rightarrow \cdots \rightarrow \sigma_k \rightarrow [i, j]$) may show up again in the calculation of inside $(x_1:\sigma_1,\ldots,x_k:\sigma_k\vdash_W t:[i, j])$. This is actually not a problem. Thanks to the restriction to expansive grammars (recall Definition 4), we can actually prove that in any type derivation tree T, each type judgment may occur at most once. Thus, when recursively calculating inside ($\Gamma \vdash_W t:\tau$), we can consider that inside ($\Gamma \vdash_W t:\tau$) = 0 when it is encountered again. Without the restriction to expansive grammars, we would need to compute the least fixpoint of the equations above, which is computationally more expensive.

The outside probability $outside(\Gamma \vdash_W t : \tau)$, which intuitively expresses the probability that $\vdash_W S : [1, |W|]$ is derived from $\Gamma \vdash_W t : \tau$, can also be calculated analogously to the case of SCFG. Let **Terms**_{\mathcal{G}} be the set of terms that occur in the rewriting rules of \mathcal{G} . Then $outside(\Gamma \vdash_W t : \tau)$ is given by:

$$\begin{aligned} & outside(\vdash_{W} S:[1,|W|]) = 1, \\ & outside(\Gamma \vdash_{W} t:[i,j]) = \\ & \left(\sum_{t:t'\in\mathbf{Terms}g,j+1\leq k,\Gamma'\downarrow_{[i,j]}=\Gamma} \\ & outside(\Gamma' \vdash_{W} t\cdot t':[i,k]) \times inside(\Gamma'\downarrow_{[j+1,k]} \vdash_{W} t':[j+1,k])\right) \\ & + \left(\sum_{t':t\in\mathbf{Terms}g,k\leq i-1,\Gamma'\downarrow_{[i,j]}=\Gamma} \\ & outside(\Gamma' \vdash_{W} t'\cdot t:[k,j]) \times inside(\Gamma'\downarrow_{[k,i-1]} \vdash_{W} t':[k,i-1])\right) \\ & + \left(\sum_{F\tilde{x} \to t\in\mathcal{R},\Gamma=\{x_{1}:\sigma_{1},\ldots,x_{k}:\sigma_{k}\}} \phi(F\tilde{x} \to t) \times outside(\vdash_{W} F:\sigma_{1} \to \cdots \to \sigma_{k} \to [i,j])\right) \\ & + \left(\sum_{Ft_{1}\cdots t_{k}\in\mathbf{Terms}g,t=t_{\ell},\Gamma'\downarrow_{[i,j]}=\Gamma,\sigma_{1} \to \cdots \to \sigma_{\ell} \uplus \{[i,j]\} \to \cdots \to \sigma_{k} \to [i',j']\in\mathbf{Ty}_{W} \\ & outside(\Gamma' \vdash_{W} Ft_{1} \cdots t_{k}:[i',j']) \\ & \times inside(\vdash_{W} F:\sigma_{1} \to \cdots \to \sigma_{\ell} \uplus \{[i,j]\} \to \cdots \to \sigma_{k} \to [i',j']) \\ & \times \prod_{1\leq m\leq k,[i'',j'']\in\sigma_{m}} inside(\Gamma'\downarrow_{[i'',j'']} \vdash_{W} t_{m}:[i'',j''])\right), \qquad (\text{if } t\neq S) \end{aligned}$$

Although the equations above may look complicated, they can systematically be obtained from the intuition on outside probabilities. Unlike inside probabilities, the case where t is an arity-0 non-terminal is covered by the second clause since such t as a premise does not appear in T-RULE except when t = S.

Now we are ready to describe our inside-outside algorithm, which takes a set of words $\mathcal{W} = \{W_1, \ldots, W_Q\}$ and an SMG $\mathcal{G} = (\mathcal{A}, \mathcal{N}, \mathcal{R}, S, \phi)$ as inputs, and output an SMG $\mathcal{G}' = (\mathcal{A}, \mathcal{N}, \mathcal{R}, S, \phi')$. The overall algorithm is shown in Algorithm 1.

In Step 1, $c(F \to \alpha)$ denotes the expected number of times the rule $F \to \alpha$ is used for deriving W_1, \ldots, W_Q . It is calculated by:

$$c(F \to \alpha) = \sum_{q=1}^{Q} \frac{\phi(F \to \alpha)}{Prob_{\mathcal{G}}(W_q)} \sum_{\sigma_1 \to \dots \to \sigma_k \to [i,j] \in \mathbf{Ty}_{W_q}} (1)$$

$$outside(\vdash_{W_q} F : \sigma_1 \to \dots \to \sigma_k \to [i,j]) \times inside(x_1 : \sigma_1, \dots, x_k : \sigma_k \vdash_{W_q} t : [i,j]).$$

In Step 2, $\phi(F \to \alpha)$ is re-estimated by:

$$\phi'(F \to \alpha) = \frac{c(F \to \alpha)}{\sum_{F \to \beta \in \mathcal{R}} c(F \to \beta)}.$$
(2)

The probability function ϕ is repeatedly updated until the change in $\prod_{q=1}^{Q} \operatorname{Prob}_{\mathcal{G}}(W_q)$ is less than the given threshold ϵ .

Algorithm 1: The Inside-Outside Algorithm

Given an SMG $\mathcal{G} = (\mathcal{A}, \mathcal{N}, \mathcal{R}, S, \phi)$, a set of words $\mathcal{W} = \{W_1, \ldots, W_Q\}$, and a threshold ϵ

- 1. For each $F \to \alpha \in \mathcal{R}$, calculate $c(F \to \alpha)$ by equation 1
- 2. For each $F \to \alpha \in \mathcal{R}$, calculate $\phi'(F \to \alpha)$ by equation 2

3.
$$\mathcal{G}' \leftarrow (\mathcal{A}, \mathcal{N}, \mathcal{R}, S, \phi')$$

4. If
$$\frac{\prod_{q=1}^{Q} Prob_{\mathcal{G}'}(W_q)}{\prod_{q=1}^{Q} Prob_{\mathcal{G}}(W_q)} < 1 + \epsilon$$
, then output \mathcal{G}' ; otherwise let $\mathcal{G} \leftarrow \mathcal{G}'$ and go back to step 1

Like the inside-outside algorithm for SCFG (Lafferty, 2000), our algorithm for SMG can be viewed as an instance of EM algorithm, hence satisfies the following property.

Theorem 10 (correctness of the inside-outside algorithm) In Algorithm 1, the value of $\prod_{q=1}^{Q} \operatorname{Prob}_{\mathcal{G}}(W_q)$ increases monotonically at each iteration.

See Kambe et al. (2021) for a proof.

Remark 11 If the arity of every non-terminal is 0 and all the rules in \mathcal{R} are in Chomsky normal form, then our algorithm coincides with the standard inside-outside algorithm for SCFG. See Kambe et al. (2021) for more details.

As for the complexity of the algorithm, the worst-case complexity for computing the inside probabilities for a word W is exponential in |W|, unfortunately. This is because in general we need to consider a type of the form $\sigma_1 \to \cdots \to \sigma_k \to [i, j]$ for each non-terminal of arity k, and each σ_i is a *set* of intervals of the form [i', j']. Even under the well-formed condition, there are as many as $k^{O(|W|)}$ possible types, hence also $k^{O(|W|)}$ possible type judgements to be considered when computing the inside and outside probabilities. This problem is similar to that of the extremely high complexity of higher-order model checking

(and related problems on higher-order grammars) (Ong, 2006; Kobayashi and Ong, 2011). In practice, however, we expect that we can often avoid the exponential blow-up by considering only relevant types, as in practical algorithms for higher-order model checking (Kobayashi, 2013b; Broadbent and Kobayashi, 2013; Ramsay et al., 2014).

4. Experiments

We have implemented the inside-outside algorithm for SMGs, and applied it to learning of MGs. Given a set of words $\mathcal{W} = \{W_1, \ldots, W_Q\}$, the goal is to obtain an SMG $\mathcal{G} = (\mathcal{A}, \mathcal{N}, \mathcal{R}, S, \phi)$ such that the probability $\prod_{q=1}^{Q} Prob_{\mathcal{G}}(W_q)$ is high. To this end, we apply the following procedure.

- 1. Fix \mathcal{N} , the set of non-terminals and their arities.
- 2. Let \mathcal{R} be the set of all the possible rewriting rules (modulo certain constraints on the shape of rules, to ensure that the number of rules is finite; see below for details).
- 3. Randomly assign the initial probability to each rule.
- 4. Run the inside-outside algorithm (Algorithm 1, with the threshold $\epsilon = 10^{-5}$).
- 5. Remove the rules whose probabilities are 10^2 times smaller than the average of the probabilities of rules of the same non-terminal, and output the resulting grammar.

Since the inside-outside algorithm is not guaranteed to converge to the global maximum, we ran the steps 3-5 above ten times, and output the grammar with the largest value of $\prod_{q=1}^{Q} Prob_{\mathcal{G}}(W_q)$.

As the benchmark set, we picked the languages $L_{\mathbf{a}^{2^n}} = \{\mathbf{a}^{2^n} \mid n \ge 0\}, L_{ww} = \{ww \mid w \in \{\mathbf{a}, \mathbf{b}\}^+\}, L_{waw} = \{waw \mid w \in \{\mathbf{a}, \mathbf{b}\}^+\}, and L_{www} = \{www \mid w \in \{\mathbf{a}, \mathbf{b}\}^+\}, and for each language, we set <math>\mathcal{W}$ to the subset of the language consisting of words of length up to 9. For example, \mathcal{W} was set to $\{\mathbf{a}, \mathbf{aa}, \mathbf{a}^4, \mathbf{a}^8\}$ for $L_{\mathbf{a}^{2^n}}$. We fixed \mathcal{N} to $\{S \mapsto 0, F \mapsto 1\}$.

To ensure that the number of rewriting rules is finite, we restricted the right-hand side of each rule to one of the following forms for certain constants c_1 and c_2 :

- (i) the concatenation $t_1 \cdot \ldots \cdot t_k$ of terms t_1, \ldots, t_k , where $k \leq c_1$, and at most one of t_1, \ldots, t_k may be an application $F u_1 \ldots u_\ell$ (with u_1, \ldots, u_ℓ are variables or terminals); all the other t_i 's must be variables or terminals.
- (ii) $F t_1 \ldots t_k$, where the number of symbols occurring in the term is less than or equal to c_2 .

In the experiments, c_1 was set to 2 for $L_{a^{2^n}}$, and 3 for the other languages. We set $c_2 = 3$ for all the languages. For example, for $L_{a^{2^n}}$, possible right-hand sides that match (i) are:

$$x$$
, a, $x \cdot x$, $x \cdot a$, $a \cdot x$, $a \cdot a$, $x \cdot F x$, $a \cdot F x$, $x \cdot F a$, ...,

and those that match (ii) are:

$$Fx, Fa, F(x \cdot x), F(a \cdot x), F(x \cdot a), \dots$$

These are ad hoc restrictions introduced to avoid an explosion of the number of rewriting rules; our algorithm itself works without these restrictions (as long as the number of rules is finite).

Table 1 shows the results of our experiments. The column "ideal grammars" shows (the rewriting rules of) a simple (expansive) MG for each language. The column "learned grammars" shows the grammar obtained by our procedure (with the probability of each rule being omitted). The P column gives the value of $\prod_{W \in \mathcal{W}} Prob_{\mathcal{G}}(W)$ for the learned grammar. The column "time" gives the total running time of ten runs, measured in seconds.

As seen in the table, our procedure returned correct grammars for all the five languages, although the learned grammars are a little more complex than ideal ones. Out of the ten runs of Steps 3–5 of the procedure, the grammars shown in the table were obtained seven times for L_{ww} , and ten times for other languages. Interestingly, we found that for all the five languages, the learned grammars have larger values of $\prod_{W \in \mathcal{W}} \operatorname{Prob}_{\mathcal{G}}(W)$ than the ideal grammars (with optimal probability assignment). For example, for the language $L_{\mathbf{a}^{2^n}}$, the value of $\prod_{W \in \mathcal{W}} \operatorname{Prob}_{\mathcal{G}}(W)$ for the ideal grammar is 1.6×10^{-3} , which is smaller than that of the learned grammar. Thus, the learned grammar may actually be preferable to the "ideal" grammar for the purpose of data compression based on stochastic grammars (Naganuma et al., 2020).

L	ideal grammar	learned grammar	P	time
$L_{\mathbf{a}^{2^n}}$	$ \begin{array}{c c} S \rightarrow \mathbf{a} \mid F \mathbf{a} \\ F x \rightarrow F (x \cdot x) \mid x \cdot x \end{array} $	$S \rightarrow \mathbf{a} \mid \mathbf{a} \cdot \mathbf{a} \mid F \mathbf{a} \mid F (\mathbf{a} \cdot \mathbf{a})$ $F x \rightarrow F (x \cdot x) \mid x \cdot x$	2.3×10^{-3}	1.1×10^4
L_{ww}	$\begin{array}{c} S \rightarrow F \mathbf{a} \mid F \mathbf{b} \\ F x \rightarrow F (x \cdot \mathbf{a}) \\ \mid F (x \cdot \mathbf{b}) \\ \mid x \cdot x \end{array}$	$ \begin{array}{c} S \rightarrow \mathbf{a} \cdot \mathbf{a} \mid \mathbf{b} \cdot \mathbf{b} \mid F \mathbf{a} \mid F \mathbf{b} \mid F (\mathbf{a} \cdot \mathbf{a}) \\ \mid F (\mathbf{a} \cdot \mathbf{b}) \mid F (\mathbf{b} \cdot \mathbf{a}) \mid F (\mathbf{b} \cdot \mathbf{b}) \\ F x \rightarrow F (x \cdot \mathbf{a}) \mid F (x \cdot \mathbf{b}) \\ \mid F (\mathbf{a} \cdot x) \mid F (\mathbf{b} \cdot x) \mid x \cdot x \end{array} $	2.0×10^{-53}	1.0×10^5
L_{waw}	$\begin{array}{c} S \rightarrow F \mathbf{a} \mid F \mathbf{b} \\ F x \rightarrow F (x \cdot \mathbf{a}) \\ \mid F (x \cdot \mathbf{b}) \\ \mid x \cdot \mathbf{a} \cdot x \end{array}$	$\begin{array}{c} S \rightarrow \mathbf{a} \cdot \mathbf{a} \cdot \mathbf{a} \mid \mathbf{b} \cdot \mathbf{a} \cdot \mathbf{b} \mid F \mathbf{a} \mid F \mathbf{b} \\ \mid F (\mathbf{a} \cdot \mathbf{a}) \mid F (\mathbf{a} \cdot \mathbf{b}) \\ \mid F (\mathbf{b} \cdot \mathbf{a}) \mid F (\mathbf{b} \cdot \mathbf{b}) \\ F x \rightarrow F (x \cdot \mathbf{a}) \mid F (x \cdot \mathbf{b}) \\ \mid F (\mathbf{a} \cdot x) \mid F (\mathbf{b} \cdot x) \mid x \cdot \mathbf{a} \cdot x \end{array}$	2.0×10^{-53}	$1.9 imes 10^5$
L_{aww}	$\begin{array}{c} S \rightarrow F \mathbf{a} \mid F \mathbf{b} \\ F x \rightarrow F (x \cdot \mathbf{a}) \\ \mid F (x \cdot \mathbf{b}) \\ \mid \mathbf{a} \cdot x \cdot x \end{array}$	$\begin{split} S & \rightarrow \mathbf{a} \cdot \mathbf{a} \cdot \mathbf{a} \mid \mathbf{a} \cdot \mathbf{b} \cdot \mathbf{b} \mid F \mathbf{a} \mid F \mathbf{b} \\ & \mid F \left(\mathbf{a} \cdot \mathbf{a} \right) \mid F \left(\mathbf{a} \cdot \mathbf{b} \right) \\ & \mid F \left(\mathbf{b} \cdot \mathbf{a} \right) \mid F \left(\mathbf{b} \cdot \mathbf{b} \right) \\ F x & \rightarrow F \left(x \cdot \mathbf{a} \right) \mid F \left(x \cdot \mathbf{b} \right) \\ & \mid F \left(\mathbf{a} \cdot x \right) \mid F \left(\mathbf{b} \cdot x \right) \mid \mathbf{a} \cdot x \cdot x \end{split}$	2.0×10^{-53}	$1.9 imes 10^5$
L _{www}	$\begin{array}{c} S \rightarrow F \mathbf{a} \mid F \mathbf{b} \\ F x \rightarrow F (x \cdot \mathbf{a}) \\ \mid F (x \cdot \mathbf{b}) \\ \mid x \cdot x \cdot x \end{array}$	$\begin{array}{c} S \rightarrow \mathbf{a} \cdot \mathbf{a} \cdot \mathbf{a} \mid \mathbf{b} \cdot \mathbf{b} \cdot \mathbf{b} \mid F \mathbf{a} \mid F \mathbf{b} \\ \mid F \left(\mathbf{a} \cdot \mathbf{a} \right) \mid F \left(\mathbf{a} \cdot \mathbf{b} \right) \\ \mid F \left(\mathbf{b} \cdot \mathbf{a} \right) \mid F \left(\mathbf{b} \cdot \mathbf{b} \right) \\ Fx \rightarrow F \left(x \cdot \mathbf{a} \right) \mid F \left(x \cdot \mathbf{b} \right) \\ \mid F \left(\mathbf{a} \cdot x \right) \mid F \left(\mathbf{b} \cdot x \right) \mid x \cdot x \cdot x \end{array}$	2.7×10^{-19}	1.4×10^5

Table 1: The experimental results

We report the result for the language $L_{ww} = \{ww \mid w \in \{a, b\}^+\}$ in more detail. Here are the probabilities of rewriting rules obtained for one of the successful runs:

$\phi(S \rightarrow \mathbf{a} \cdot \mathbf{a}) = 0.026,$	$\phi(S \rightarrow \mathbf{b} \cdot \mathbf{b}) = 0.032,$	$\phi(S \to F {\rm a}) = 0.018,$
$\phi(S \to F {\rm b}) = 0.0045,$	$\phi(S \to F(\mathbf{a} \cdot \mathbf{a})) = 0.23,$	$\phi(S \to F(\mathbf{a} \cdot \mathbf{b})) = 0.23,$
$\phi(S \to F(\mathbf{b} \cdot \mathbf{a})) = 0.23,$	$\phi(S \to F(\mathbf{b} \cdot \mathbf{b})) = 0.23,$	
$\phi(Fx \to F(x \cdot \mathbf{a})) = 0.17,$	$\phi(Fx \to F(x \cdot \mathbf{b})) = 0.17,$	$\phi(Fx \to F(\mathbf{a} \cdot x)) = 0.13,$
$\phi(Fx \to F(\mathbf{b} \cdot x)) = 0.13,$	$\phi(Fx \to x \cdot x) = 0.41.$	

5. Conclusions

We have developed an inside-outside algorithm for SMGs. The key idea was to consider type derivations (instead of word derivation sequences), which allowed us to naturally extend the inside-outside algorithm for stochastic CFGs. We have implemented the algorithm and applied it to the learning of MGs.

Future work includes an application of the algorithm to data compression based on stochastic grammars (Naganuma et al., 2020). The use of SMGs would allow us to compress data more compactly than stochastic CFGs. We also plan to extend the inside-outside algorithm for higher-order grammars (Damm, 1982; Kobele and Salvati, 2015) (where MGs correspond to order-2 OI grammars). We expect that our type-based approach can naturally be extended to deal with grammars of arbitrary order. In practice, the main bottleneck would be the explosion of the number of types to be considered. We plan to apply techniques for type-based higher-order model checking (Kobayashi, 2013b; Broadbent and Kobayashi, 2013) to cope with the problem.

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