Structured Generative Models of Natural Source Code

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Abstract

We study the problem of building generative models of natural source code (NSC); that is, source code written and understood by humans. Our primary contribution is to describe a family of generative models for NSC that have three key properties: First, they incorporate both sequential and hierarchical structure. Second, we learn a distributed representation of source code elements. Finally, they integrate closely with a compiler, which allows leveraging compiler logic and abstractions when building structure into the model. We also develop an extension that includes more complex structure, refining how the model generates identifier tokens based on what variables are currently in scope. Our models can be learned efficiently, and we show empirically that including appropriate structure greatly improves the models, measured by the probability of generating test programs.

1 Introduction

Source code is ubiquitous, and a great deal of human effort goes into developing it. An important goal is to develop tools that make the development of source code easier, faster, and less error-prone, and to develop tools that are able to better understand pre-existing source code. To date, this problem has been studied in communities other than machine learning, and indeed, many problems in this area are not well-suited to machine learning. Yet, source code is some of the most widely available data with many public online repositories. In recent years, massive open online courses (MOOCs) have also begun to collect source code in the form of homework assignments from tens of thousands of students (Huang et al., 2013). At the same time, the software engineering community has recently observed that it is useful to think of source code as natural—written by and meant to be understood by humans (Hindle et al., 2012). As a consequence, natural source code (NSC) has a great deal of statistical regularity beyond just the constraints imposed by the programming language.

The combination of these two observations—the availability of data, and the presence of statistical structure—opens up the possibility that machine learning tools could become useful in various tasks related to source code. From a machine learning perspective, constraints imposed by a language specification are some of the primary challenges. Yet, existing tools already capture this structure very well; for example, Microsoft’s IntelliSense MSDN (2013) makes code completion suggestions that are aware of a great deal of context, such as which variables are currently in scope. By viewing source code as data in a structured prediction problem one can combine a data-driven machine learning approach with the body of knowledge in programming languages and compilers research.

Existing tasks could be done in a more principled data-driven manner. For example, current auto-complete suggestions rely primarily on heuristics developed by an Integrated Development Environment (IDE) designer. With machine learning methods, we might be able to offer much improved completion suggestions by leveraging the massive amount of source code available in public repositories. Indeed, Hindle et al. (2012) have shown that even simple $n$-gram models are useful for
Figure 1: Samples of `for` loops generated by models in this work. Our model captures hierarchical structure and other patterns of variable usage and local scoping rules. Whitespace edited to improve readability.

improving code completion tools. Other tasks where machine learning might be applicable include automatic bug fixing, and defining code complexity metrics [Allamanis and Sutton 2013]. We can learn improved priors over programs for use in the recently re-popularized problem of programming by example [Halbert 1984; Gulwani 2011]. Finally, one might hope to solve new source code-related tasks that would not otherwise be possible, such as automatic translation between programming languages, automatic code summarization, and learning representations of source code for the purposes of visualization or discriminative learning.

One route toward these goals is to solve specific tasks related to source code. Indeed, there has been some recent work in this direction, particularly related to mining and suggesting API usage patterns [Bruch et al. 2009; Nguyen et al. 2012; Wang et al. 2013]. An alternative, which we pursue here, is to develop a generative model of source code, with the view that many of the above tasks become different forms of query on the same learned model (e.g., code completion is conditional sampling; bug fixing is model-based denoising; complexity metrics are probabilities of code snippets under the model [Allamanis and Sutton 2013]; representations may be derived from latent variables [Hinton and Salakhutdinov 2006] or from Fisher vectors [Jaakkola and Haussler 1998]). Hindle et al. (2012) and Allamanis and Sutton (2013) have taken this approach but with simple \( n \)-gram models. Our hope is that by building better generative models, we can make progress simultaneously towards several of the above-mentioned tasks, and that we can better isolate and tackle the core challenges that arise when applying machine learning methods to source code.

In this work we develop a family of generative models expressive enough to capture many of the important aspects of NSC: sequential and hierarchical structure, code-specific constraints, and naturalness. Our models combine natural language processing models of trees, distributed representations of source code elements like in neural probabilistic language models [Bengio et al. 2006], and compiler-like reasoning to enforce code-specific constraints. We show how to efficiently learn these models from a corpus of source code, and we show empirically that they far outperform the standard NLP models that have previously been applied to source code. Fig. 1[c] shows samples generated by models of NSC that we learn in this paper. Our full model (Fig. 1[c]) captures far more structure, both natural and structural, than existing models that have been applied to source code.

2 C#, Roslyn, Abstract Syntax Trees

While this work applies to any common imperative programming language like C/C++/Java, we focus specifically on C#. This decision is based on (a) the fact that large quantities of data are
readily available online, and (b) the recently released Roslyn C# compiler (MSDN, 2011) exposes APIs that allow easy access to a rich set of internal compiler data structures and processing results.

Abstract syntax trees (ASTs) are the primary data structure used to reason about source code. The first task a compiler performs is to lex the code, which begins as a single string, into a sequence of tokens, \( \alpha_t \). Tokens are themselves strings that serve as the atomic syntactic elements of a programming language such as constants or variables. Given \( \alpha \), a compiler constructs an AST. The AST is a tree of nodes that represents the syntactic structure of code and that serves as an intermediate data structure used extensively by semantic analysis tools. The leaf nodes of the AST are the tokens, and internal nodes correspond to expressions, statements or other high level syntactic elements. From the AST, many crucial properties of the source code can be derived. For example, the tree structure is enough to determine which variables are in scope at any point in the program. See Fig. 2 for an example AST.

3 Log-bilinear Tree-Traversal Models

In this section, we describe Log-bilinear Tree-Traversal models (LTTs), which are a family of probabilistic models that produce ASTs. A key property of the model is that the tree is produced in a sequential fashion, according to some traversal order of the nodes in the tree. By generating the AST as a sequence we can exploit important knowledge, such as variable scoping and other context, at intermediate stages of the process.

More specifically, LTTs generate an AST with a depth-first recursive procedure. Starting at the root of the tree we sample the children and recurse from left to right. Along with this recursive hierarchical structure, there are also variables that evolve sequentially along the path of the tree traversal. After sampling, the source code can be read from the leaves of the tree, left to right. A detailed description of the generative procedure is given next.

3.1 Notation and Basic Generative Procedure

We begin with basic model notation. A node \( n \) can denote either a token such as “sum” or an internal node, such as Block or ForStatement. A children tuple \( C \) is a tuple of nodes. Sequential information is captured via traversal variables \( h_i \), that evolve sequentially in the depth-first traversal of the tree as it is being produced. We will distinguish throughout between deterministic and latent traversal variables. The former can be computed deterministically from the current partial tree (the set of nodes and tokens that have been instantiated at step \( i \)) that has been generated while the latter cannot. The relevance of this distinction will become clear in Sections 4 and 5. To refer to a collection of both deterministic and latent traversal variables, we will use the unqualified “traversal variables” term.
The basic generative procedure is defined by three distributions: (a) the prior over the root node and traversal variables, \( p(n, \mathbf{h}) \); (b) the distribution over children nodes conditioned on the parent node and \( \mathbf{h} \), denoted \( p(C \mid n, \mathbf{h}) \); and (c) the transition distribution for the \( \mathbf{h} \)s, denoted \( p(h_i \mid h_{i-1}) \). The generative procedure given in Algorithm 1 and illustrated in Fig. 3 produces a sequence of internal nodes \( (n_i)_{i=1}^N \), traversal variables \( (h_i)_{i=0}^N \), and the desired \( \alpha \).

LTT can be viewed as a Markov model equipped with a stack. As discussed in Section 4, this is a special case of a Probabilistic Pushdown Automata (PPDA) (Abney et al., 1999). We will now build upon this foundation by adding a log-bilinear parameterization and incorporating compiler logic. We note that while the depth-first traversal order is particularly well-suited for source code, other traversal orders are possible such as right-left or breadth-first. In order to compare to standard NLP models, we consider only depth-first order to ensure that tokens are produced in the same order that they are observed in the code.

Algorithm 1 Sampling from LTTs.

```markdown
initialize empty stack \( S \)
sample \( (n, h_0) \sim p(n, h_0) \)
push \( n \) onto \( S \)
\( (i, t) \leftarrow (1, 1) \)
while \( S \) is not empty do
  pop the top node \( n \) from \( S \)
  if \( n \) is an internal node then
    \( n_i \leftarrow n \)
    sample \( h_i \sim p(h_i \mid h_{i-1}) \)
    sample \( C_i \sim p(C_i \mid n_i, h_i) \)
    push \( n \) for \( n \in \text{REVERSED}(C_i) \) onto \( S \)
    \( i \leftarrow i + 1 \)
  else
    \( \alpha_i \leftarrow n \)
    \( t \leftarrow t + 1 \)
  end if
end while
```
3.2 Log-bilinear Parameterization

An important consideration is how to parameterize the distributions in the model, and in particular \( p(C \mid n, h) \). The general form that we use throughout is a log-bilinear form, where there is a real-valued vector representation of \((n_i, h_i)\) pairs, \( R_{con}(n_i, h_i) \), a real-valued vector representation for the children tuple, \( R_{ch}(C_i) \), and a bias term for the children, \( b_{ch}(C_i) \). These are combined via an inner product, which gives the negative energy of the children tuple

\[
-E(C_i; n_i, h_i) = R_{ch}(C_i)^T R_{con}(n_i, h_i) + b_{ch}(C_i)
\]

As is standard, this is then exponentiated and normalized to give the probability of sampling the children: \( p(C_i \mid n_i, h_i) \propto \exp \{-E(C_i; n_i, h_i)\} \). We take the support over which to normalize this distribution to be the set of children tuples observed as children of nodes of type \( n_i \) in the training set.

Variants of our models will define these vector representations \( R \) in different ways. Throughout we rely on the notion of an \( R \) matrix that can be indexed into with hashable objects to look up \( D \) dimensional real-valued vectors. \( R_x \) denotes the hash\((x)\)th row of the \( R \) matrix\(^1\). Similarly \( b_x \) looks up a real number. In the simple variant, each unique \( C \) sequence receives the unique representation \( R_{ch}(C_i) = R_{C_i} \) and \( b_{ch}(C_i) = b_{C_i} \). The representations for \((n, h)\) pairs are defined compositionally, as a sum of components. If we view \( h_i \) as a sequence of hashable variables, then \( h_{ij} \) represents the \( j \)th variable. For example, if we wanted two distinct binary traversal variables \( h_{i1} \) and \( h_{i2} \), then we can represent them as (key, value) tuples. We can write the representation as follows:

\[
R_{con}(n_i, h_i) = W^c_{10} R_{n_i} + \sum_{j=1}^{H} W^c_{j} R_{h_{ij}}
\]

(1)

The \( W^c \)'s are matrices that modulate the contribution of a variable in a position-dependent way. For computational efficiency we take \( W^c \)'s to be diagonal. In extensions to the basic models we also let the representation for children tuples be compositionally defined. The log-bilinear parameterization has the desirable property that the number of parameters grows linearly in the dimension of \( h \), so we can afford to have high dimensional traversal variables without worrying about exponentially bad data fragmentation.

4 Extended LTT Models

In this section we expand LTTs to leverage the full power that the framework admits. The extensions allow (a) traversal variables to depend arbitrarily on the history so long as their values can be determined with certainty based on the partial tree that exists up to the point where the variables are determined with certainty; (b) annotating nodes with richer types, as in lexicalized probabilistic context free grammars (Charniak [1997]); and (c) letting \( R_{ch} \) be compositionally defined, which becomes powerful when combined with deterministic reasoning about variable scoping.

4.1 Deterministic Traversal Variables

When introducing LTTs we restricted the traversal variables \( h_i \) to satisfy the first-order Markov property, but there is nothing restricting us from conditioning on any part of the tree that has already been produced. The only complication comes at inference time, if the variables are unobserved. However, if these variables are deterministic traversal variables and the unique value that has support can be computed efficiently, then as will be explained in Section 5 they can be as complicated as we like. That is, we can define the evolution of traversal variables by \( p(h_i \mid h_{0:i-1}, n_{1:i}, \alpha_{1:i}) \).

Examples where this is useful include variables representing any function of the path from the root of the AST to the current node or any autoregressive connections to the last \( n \) tokens or internal nodes. We consider variable scoping, a more elaborate deterministic relationship, in more detail in Section 4.3.

4.2 Annotating Nodes

Some features may not be deterministically computable from the current partial tree, but may help when predicting children nodes. Consider knowing that a BinaryExpression will evaluate to

\(^1\)In reality there are no collisions and we assign indices from 1 to the number of unique objects.
an object of type int. A whole class of such useful knowledge can be encoded by annotating nodes with extra information. This is accomplished by letting nodes take values in the cross-product space of the node type space and the annotation space. For example, when adding type annotations we might have nodes take value \((\text{BinaryExpression}, \text{int})\). This approach can cause certain problems. First, the range of parent nodes increases exponentially as we add annotations. Second, since the annotations are uncertain, there are more choices of node values at each step of the generative procedure, and this incurs a cost in log probabilities when evaluating a model. For example, we found that simply annotating expression nodes with type information led to worse log probabilities of generating held out data: while the cost of generating tokens decreased because the model had access to type information, the increased cost of generating type annotations along with nodetypes outweighed the improvement.

4.3 Identifier Token Scoping

In preliminary experiments, we found that children of \(\text{IdentifierToken}\) nodes are the source of greatest uncertainty when generating a program. \(\text{IdentifierToken}\) nodes are very common (e.g., variable and method names) and are parents of all tokens that are not language keywords (e.g., IntKeyword or EqualsToken) or constants (e.g., StringLiteral). Given that our goal in this work is to find models that have highest probability of generating held out programs, it is important to look for ways of improving parts of the model related to \(\text{IdentifierToken}\) nodes.

One of the most powerful features in predicting \(\text{IdentifierToken}\) at any given point is what variables have previously been declared and are currently in scope. Other useful cues include how recently the variable was declared, what the type the variable is, and how recently the variable has been assigned. We show how to incorporate such knowledge into LTTs.

Formally, our representation of scope is as a set of variable feature vectors. Each feature vector contains a string identifier corresponding to the variable along with other features of the variable, like those described above. A variable is “in scope” if there is a feature vector in the scope set that has a string identifier that is the same as the variable’s identifier.

When sampling an identifier token, there is a two step procedure. First, decide whether this identifier token will be sampled from the current scope. This is accomplished by annotating (as in Section 4.2) each \(\text{IdentifierToken}\) internal node with a binary variable that has the states \(\text{global}\) or \(\text{local}\). If \(\text{local}\), proceed to use the local scope model defined next. If \(\text{global}\), sample from a global identifier token model that gives support to all identifier tokens. Note that we consider the \(\text{global}\) option a necessary smoothing device, although ideally we would have a scope model complete enough to have all possible identifier tokens.

The scope set can be updated deterministically as we traverse the AST by recognizing patterns that correspond to when variables should be added or removed from the scope. We implemented this logic for three cases: parameters of a method, locally declared variables, and class fields that have been defined prior in the class definition. We do not include class fields defined after the current point in the code, and variables and methods available in included namespaces. Note that it is this incompleteness that necessitates the \(\text{global}\) option described above, but these three cases are very common and cover many interesting cases.

All that remains is to define how to draw a child of a \((\text{IdentifierToken}, \text{local})\) parent node. Given the scope set which contains variable feature vectors \(\{v_u\}\), the probability of selecting token \(\alpha\) is proportional to \(p(\alpha | n_i, h_i) \propto \exp\{-E(\alpha; n_i, h_i)\}\), where we normalize only over the variables currently in scope, and where the representation of the possible children is defined compositionally. Specifically, we let \(R_{ch}(\alpha)\) and \(b_{ch}(\alpha)\) be defined as follows:

\[
R_{ch}(\alpha) = \sum_{u=1}^{V} W^{ch}_{v_{iu}} R_{v_{iu}} \quad b_{ch}(\alpha) = \sum_{u=1}^{V} b_{v_{iu}}.
\]

For example, if a variable in scope has feature vector \((\text{identifier}=\text{``i''}, \text{type}=int, \text{how recently declared}=3, \text{how recently assigned}=0)\), then its corresponding \(R_{ch}\) would be a context matrix-modulated sum of representations for \((\text{identifier}=\text{``i''}, \text{type}=int, \text{how recently declared}=3)\), and \(\text{how}\)
5 Inference and Learning in LTTs

In this section we show how to train and evaluate LTTs by showing how to compute the log probability of a token sequence and the gradient of the log probability with respect to model parameters.

**Only Deterministic Traversal Variables.** In the first case, we assume that any traversal variables \( h_i \) that appear in the model can be computed deterministically from the current partial tree. In this case, for each program \( \alpha_m \), we use the compiler to compute the full AST corresponding to \( \alpha_m \), then we use the AST to deterministically compute the only valid setting of the traversal variables. At this point, all variables in the model can be treated as observed. Since LTTs are directed models, this means that the total log probability is a sum of log probabilities at each production, and learning decomposes into independent problems at each production. Thus, we can simply stack all productions into a single training set and follow standard gradient-based procedures for training log-bilinear models. More details will be described in Section 7 but generally we follow Mnih and Teh (2012).

**Latent Traversal Variables.** In the second case, we allow latent traversal variables that need to be summed over in order to compute the probability of a token sequence. In this case, the traversal variables couple the learning across different productions from the same tree. For simplicity and to allow efficient exact inference, we consider only the case in which latent traversal variables are discrete (although this restriction could easily be lifted if one was willing to use approximate inference). In this case, we can formulate an EM algorithm for the learning where an exact E step can be implemented using the forward-backward algorithm.

More formally, under the above assumptions the probability of \( \alpha \) takes the following form:

\[
\sum_{h_{0:N}} p(n_1, h_0) \prod_{i=1}^N p(C_i | n_i, h_i) p(h_i | h_{i-1}) \times p(h_i^d | h_{0:i-1}, n_{1:i}, \alpha_{1:i})
\]

(3)

where we use the notation \( h_i \) to mean a latent traversal variable and \( h_i^d \) to mean a set of deterministic traversal variables, and where \( h \) represents the union of \( \{h_i^l\} \) and \( h_i^d \). Firstly, the \( p(h_i^d | \cdot) \) terms drop off because as above we can use the compiler to compute the AST from \( \alpha \) then use the AST to deterministically fill in the only legal values for the \( h_i^d \) variables, which makes these terms always equal to 1. It then becomes clear that the sum can be computed using the forward-backward algorithm.

For learning, we follow the standard EM formulation and lower bound the data log probability with a free energy of the following form (which for brevity drops the prior and entropy terms):

\[
\sum_{i=2}^N \sum_{h_i^l, h_{i-1}^l} Q_i, i-1(h_i^l, h_{i-1}^l) \log P(h_i^l | h_{i-1}^l) \\
+ \sum_{i=1}^N \sum_{h_i^l} Q_i(h_i^l) \log p(C_i | n_i, h_i)
\]

(4)

In the E step, the \( Q \)'s are updated optimally given the current parameters using the forward backward algorithm. In the M step, given \( Q \)'s, the learning decomposes across productions. We represent the transition probabilities using a simple tabular representation and use stochastic gradient updates. For the emission terms, it is again straightforward to use standard log-bilinear model training. The only difference from the previous case is that there are now \( K \) training examples for each \( i \), one for each possible value of \( h_i^l \), which are weighted by their corresponding \( Q_i(h_i^l) \). A simple way of handling this so that log-bilinear training methods can be used unmodified is to sample \( h_i^l \) values from the corresponding \( Q_i(\cdot) \) distribution, then to add unweighted examples to the training set with \( h_i^l \) values being given their sampled value. This can then be seen as a stochastic incremental M step.
Method | Train | Valid | Test
--- | --- | --- | ---
2-gram | -4.28 | -4.98 | -5.13
3-gram | -2.94 | -5.05 | -5.25
4-gram | -2.70 | -6.05 | -6.31
5-gram | -2.68 | -7.22 | -7.45
PCFG | -3.67 | -4.04 | -4.23
LTT-∅ | -3.67 | -4.04 | -4.24
LBL 10-gram | -3.19 | -4.62 | -4.87

Figure 4: Baseline model log probabilities per token.

6 Related Work

The LTTS described here are closely related to several existing models. Firstly, a Hidden Markov Model (HMM) can be recovered by having all children tuples contain a token and a Next node, or just a token (which will terminate the sequence), and having a single discrete latent traversal variable. If the traversal variable has only one state and the children distributions all have finite support, then an LTT becomes equivalent to a Probabilistic Context Free Grammar (PCFG). PCFGs and their variants are components of state-of-the-art parsers of English [McClosky et al., 2006], and many variants have been explored. For example, Charniak (1997) and Klein and Manning (2003) consider annotating internal nodes, and Matsuzaki et al. (2005) has explored latent annotations. Aside from the question of the order of the traversals, Tree Traversal models are essentially special cases of Probabilistic Pushdown Automata (PPDA) (for definition and weak equivalence to PCFGs, see Abney et al. (1999)). Log-bilinear parameterizations have been applied widely in language modeling, for n-gram models [Saul and Pereira, 1997; Mnih and Hinton, 2007; Mnih and Teh, 2012] and PCFG models [Charniak, 2000; Klein and Manning, 2002; Titov and Henderson, 2007; Henderson and Titov, 2010]. To be clear, our claim is not that general Tree Traversal models or the log-bilinear parameterizations are novel; however, we believe that the full LTT construction, including the tree traversal structure, log-bilinear parameterization, and incorporation of deterministic logic to be novel and of general interest.

The problem of modeling source code is relatively understudied in machine learning. We previously mentioned Hindle et al. (2012) and Allamanis and Sutton (2013), which tackle the same task as us but with simple NLP models. There is also quite a bit of work on mining frequent API usage patterns for use in suggesting method calls on a variable and program point currently under consideration. These approaches use some amount of basic machine learning, typically following the approach of defining a similarity measure between code contexts, then re-ranking candidate method calls based on frequency [Bruch et al., 2009; Nguyen et al., 2012; Wang et al., 2013]. The other related work that we are aware of is Liang et al. (2010), which uses a sophisticated non-parametric model to encode the prior that programs should factorize repeated computation, but there is no learning from existing source code, and the prior is only applicable to a functional programming language with quite simple syntax rules. Our approach builds a sophisticated and learned model and supports the full language specification of a widely used imperative programming language.

7 Experimental Analysis

In this section we describe experiments that we ran in order to better understand how the models proposed in this work perform in practice. In all experiments, we used a dataset that we collected from TopCoder.com. There are 2261 C# programs which make up 140k lines of code and 2.4M parent nodes in the collective abstract syntax trees. These programs are solutions to programming competitions, and there is some overlap in programmers and in problems across the programs. We created training splits based on the user identity, so the set of users in the test set are disjoint from those in the training or validation sets (but the training and validation sets share users). The overall split proportions are 20% test, 10% validation, and 70% train. The evaluation measure that we use throughout is the log probability under the model of generating the full program. All logs are base 2. To make this number more easily interpretable, we divide by the number of tokens in each program, and report the average log probability per token.
| Method       | Train | Valid | Test  |
|--------------|-------|-------|-------|
| LTT-∅        | -3.67 | -4.04 | -4.24 |
| LTT-Seq      | -2.54 | -3.25 | -3.46 |
| LTT-Hi       | -2.28 | -3.30 | -3.53 |
| LTT-HiSeq    | **-2.10** | **-3.06** | **-3.28** |

Figure 5: Log probabilities of LTT models augmented with deterministically determinable latent variables.

| Method        | Train | Valid | Test  |
|---------------|-------|-------|-------|
| LTT-∅         | -3.67 | -4.04 | -4.24 |
| LTT-latent    | **-3.23** | **-3.70** | **-3.91** |
| LBL HMM       | -9.61 | -9.97 | -10.10 |

Figure 6: Log probabilities of LTT-latent models augmented with latent variables and learned with EM.

| Method                   | Train | Valid | Test  |
|--------------------------|-------|-------|-------|
| LTT-HiSeq (50)           | -2.10 | -3.06 | -3.28 |
| LTT-HiSeq-Scope (2)      | -2.28 | -2.65 | -2.78 |
| LTT-HiSeq-Scope (10)     | -1.83 | -2.29 | -2.44 |
| LTT-HiSeq-Scope (50)     | -1.54 | -2.18 | -2.33 |
| LTT-HiSeq-Scope (200)    | **-1.48** | **-2.16** | **-2.31** |
| LTT-HiSeq-Scope (500)    | -1.51 | **-2.16** | -2.32 |

Figure 7: Log probabilities of LTT models with deterministic traversal variables and scope model. Number in parenthesis is the dimension of the representation vectors.

**Experimental Protocol.** For all of our experiments, we used a validation set to choose hyperparameter values. These include the strength of a smoothing parameter and the epoch at which to stop training (if applicable). We did a coarse grid search in each of these parameters and the numbers we report (for train, validation, and test) are all for the settings that optimized validation performance. For the gradient-based optimization, we used AdaGrad [Duchi et al., 2011] with stochastic mini-batches. Unless otherwise specified, the dimension of the latent representation vectors was set to 50. Occasionally the test set will have tokens or children tuples unobserved in the training set. In order to avoid assigning zero probability to the test set, we locally smoothed every children distribution with a default model that gives support to all children tuples. The numbers we report are for a mixture of our models with this default model. Details of this smoothed model, along with additional experimental details, appear in the Appendix. There is an additional question of how to represent novel identifiers in the scope model. We set the representations of all features in the variable feature vectors that were unobserved in the training set to the zero vector 0.

**Baselines and Basic Log-bilinear Models.** We begin by training generic language models to serve as baselines. The natural choices are n-gram models and PCFG-like models. In the n-gram models we use additive smoothing, with the strength of the smoothing hyperparameter chosen to optimize validation set performance. Similarly, there is a smoothing parameter in the PCFG-like models that is chosen to optimize validation set performance. We also explored the effect of the log-bilinear parameterization in two ways. First, we trained a PCFG model that was identical to the first PCFG model but with the parameterization defined using the standard log-bilinear parameterization. This is the most basic LTT model, with no traversal variables (LTT-∅). The result was nearly identical to the standard PCFG. Next, we trained a 10-gram model with a standard log-bilinear parameterization, which is equivalent to the models discussed in [Mnih and Teh, 2012]. This approach dominates the basic n-gram models, allowing longer contexts and generalizing better. Results appear in Fig. 4.

**Deterministic Traversal Variables.** Next, we took the LTT-∅ model and added deterministic traversal variables that include hierarchical and sequential information. The hierarchical information is how deep in the AST a node is, the kind of the node’s parent, and a sequence of 10 ancestor history variables, which store for the last 10 ancestors, the kind of the node and the index
| Method             | Total  | Token | Tree  |
|-------------------|--------|-------|-------|
| LTT-∅             | -4.23  | -2.78 | -1.45 |
| LTT-Seq           | -3.53  | -2.28 | -1.25 |
| LTT-Hi            | -3.46  | -2.18 | -1.28 |
| LTT-HiSeq         | -3.28  | -2.08 | -1.20 |
| LTT-HiSeq-Scope   | -2.33  | -1.10 | -1.23 |

Figure 8: Breakdowns of test log probabilities by whether the cost came from generating the tree structure or tokens. For all models $D = 50$.

of the child that would need to be recursed upon to reach the current point in the tree. The sequential information is the last 10 tokens that were generated.

In Fig. 5 we report results for three variants: hierarchy only (LTT-Hi), sequence only (LTT-Seq), and both (LTT-HiSeq). The hierarchy features alone perform better than the sequence features alone, but that their contributions are independent enough that the combination of the two provides a substantial gain over either of the individuals.

**Latent Traversal Variables.** We also explore adding latent traversal variables to the models, which means that we turn to using EM learning. In all cases, we used 32 discrete latent states. Here, results were more mixed. While the latent-augmented LTT (LTT-latent) outperforms the LTT-∅ model, the gains are smaller than achieved by adding the deterministic features. As a baseline, we also trained a log-bilinear-parameterized standard HMM, and found its performance to be far worse than other models. We also tried a variant where we added latent traversal variables to the LTT-HiSeq model from the previous section, but the training was too slow to be practical due to the cost of computing normalizing constants in the E step. See Fig. 6.

**Scope Model.** The final set of models that we trained incorporate the scope model from Section 4.3 (LTT-HiSeq-Scope). The features of variables that we use are the identifier string, the type, where the variable appears in a list sorted by when the variable was declared (also known as a de Bruijn index), and where the variable appears in a list sorted by when the variable was last assigned a value. Here, the additional structure provides a large additional improvement over the previous best model (LTT-HiSeq). See Fig. 7.

**Analysis.** To understand better where the improvements in the different models come from, and to understand where there is still room left for improvement in the models, we break down the log probabilities from the previous experiments based on the value of the parent node. The results appear in Fig. 8. In the first column is the total log probability number reported previously. In the next columns, the contribution is split into the cost incurred by generating tokens and trees respectively. We see, for example, that the full scope model pays a slightly higher cost to generate the tree structure than the Hi&Seq model, which is due to it having to properly choose whether IdentifierTokens are drawn from local or global scopes, but that it makes up for this by paying a much smaller cost when it comes to generating the actual tokens.

In the Appendix, we go further into the breakdowns for the best performing model, reporting the percentage of total cost that comes from the top parent kinds. IdentifierTokens from the global scope are the largest cost (30.1%), with IdentifierTokens covered by our local scope model (10.9%) and Blocks (10.6%) next. This suggests that there would be value in extending our scope model to include more IdentifierTokens and an improved model of Block sequences.

**Samples.** Finally, we qualitatively evaluate the different methods by drawing samples from the models. Samples of for loops appear in Fig. 1. To generate these samples, we ask (b) the PCFG and (c) the LTT-HiSeq-Scope model to generate a ForStatement. For (a) the LBL n-gram model, we simply insert a for token as the most recent token. We also initialize the traversal variables to reasonable values: e.g., for the LTT-HiSeq-Scope model, we initialize the local scope to include string[] words. We also provide samples of full source code files (CompilationUnit) from the LTT-HiSeq-Scope model in the appendix, and additional for loops. Notice the structure that the model is able to capture, particularly related to high level organization, and variable use and re-use. It also learns quite subtle things, like int variables often appear inside square brackets.
8 Discussion

Natural source code is a highly structured source of data that has been largely unexplored by the
machine learning community. In this paper we show how to build probabilistic models that capture
some of the structure that appears in NSC. One key to our approach is to leverage the great deal
of work that has gone into building compilers. The result is models that not only yield large im-
provements in quantitative measures over baselines, but also qualitatively produce far more realistic
samples.

There are many remaining modeling challenges. One question is how to encode the notion that
the point of source code is to do something. Relatedly, how do we represent and discover high
level structure related to trying to accomplish such tasks? There are also a number of specific sub-
problems that are ripe for further study. Our model of Block statements is naive, and we see that
it is a significant contributor to log probabilities. It would be interesting to apply more sophisticated
sequence models to children tuples of Blocks. Also, applying the compositional representation
used in our scope model to other children tuples would interesting. Similarly, it would be interesting
to extend our scope model to handle method calls. Another high level piece of structure that we only
briefly experimented with is type information. We believe there to be great potential in properly
handling typing rules, but we found that the simple approach of annotating nodes to actually hurt
our models.

More generally, this work’s focus was on generative modeling. An observation that has become
popular in machine learning lately is that learning good generative models can be valuable when the
goal is to extract features from the data. It would be interesting to explore how these models might
be used for this purpose in the case of NSC.

Our belief is that probabilistic modeling of source code provides a rich source of problems with the
potential to improve source code processing applications, and to stimulate new machine learning
research. We hope that this work will help drive both of these lines of work forward.

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Appendix

More Experimental Protocol Details

For all hyperparameters that were not validated over (such as minibatch size, scale of the random initializations, and learning rate), we chose a subsample of the training set and manually chose a setting that did best at optimizing the training log probabilities. For EM learning, we divided the data into databatches, which contained 10 full programs, ran forward-backward on the databatch, then created a set of minibatches on which to do an incremental M step using AdaGrad. All parameters were held fixed throughout the experiments, with the exception that we re-optimized the parameters for the learning that required EM, and we scaled the learning rate when the latent dimension changed. Our code used properly vectorized Python for the gradient updates and a C++ implementation of the forward-backward algorithm but was otherwise not particularly optimized. Run times (on a single core) ranged from a few hours to a couple days.

Smoothed Model

In order to avoid assigning zero probability to the test set, we assumed knowledge of the set of all possible tokens, as well as all possible internal node types – information available in the Roslyn API. Nonetheless, because we specify distributions over tuples of children nodes there are tuples in the test set that would be assigned zero probability under our models as described up to this point. To remedy this, we smooth every $p(C_i | h_i, n_i)$ by mixing it with a default distribution $p_{\text{def}}(C_i | h_i, n_i)$ over children that gives broad support.

$$p_\pi(C_i | h_i, n_i) = \pi p(C_i | h_i, n_i) + (1 - \pi) p_{\text{def}}(C_i | h_i, n_i)$$

For distributions whose children are all 1-tuples of tokens, the default model is an additively smoothed model of the empirical distribution of tokens in the train set. For other distributions we model the number of children in the tuple as a Poisson distribution, then model the identity of the children independently (smoothed additively).

This smoothing introduces trees other than the Roslyn AST with positive support. This opens up the possibility that there are multiple trees consistent with a given token sequence and we can no longer compute $\log p(\mathbf{\alpha})$ in the manner discussed in Section 5. Still we report the log-probability of the AST, which is now a lower bound on $\log p(\mathbf{\alpha})$.

| Parent Kind             | % Log prob | Count |
|-------------------------|------------|-------|
| (IdentifierToken, global) | 30.1        | 17518 |
| (IdentifierToken, local) | 10.9        | 27600 |
| Block                   | 10.6        | 3556  |
| NumericLiteralToken     | 4.3         | 8070  |
| Argument                | 3.6         | 10004 |
| PredefinedType          | 3.0         | 7890  |
| IfStatement             | 2.9         | 2204  |
| AssignExpression        | 2.4         | 2747  |
| ExpressionStatement     | 2.1         | 4141  |
| EqualsValueClause       | 2.0         | 3937  |
| StringLiteralToken      | 1.9         | 680   |
| AddExpression           | 1.9         | 1882  |
| ForStatement            | 1.6         | 1759  |

Figure 9: Percent of log probability contributions coming from top parent kinds for LTT-HiSeqScope (50) model on test set.
for ( int i = 0 ; i < words . Length ; ++ i ) i = i . Replace ( "X" , i )

for ( int j = 0 ; j < words . X ; j ++ ) {
    if ( j [ j ] == - 1 ) continue;
    if ( words [ j ] != words [ j ] ) j += thisMincost ( 1 )
    else {
        j = ( j + 1 ) % 2
        words [ j + 1 ] += words [ 0 ]
    }
}

for ( int j = words ; j < words . Pair ; ++ j )
    for ( int i = 0 ; i < words . Length ; ++ i )
        isUpper ( i , i )

for ( int i = 0 ; i < words . Length ; ++ i )
    words [ i , i ] = words . Replace ( "*" , i * 3 )

for ( int j = 360 ; j < j ; )
    if ( ! words . ContainsKey ( j ) ) {
        if ( words . at + " " + j == j ) return ume ( j , j )
    else {
        j = 100
    }
}

for ( int c = 0 ; c < c ; ++ c )
    for ( int i = 0 ; i < c ; i ++ )
        if ( ! words [ i ] ) i = i

for ( int i = 0 ; i < words . Length ; i ++ )
    i . Parse ( i )

for ( int i = words ; i < 360 ; ++ i )
    words [ i ] = words [ i ]
    i = 4

Figure 10: More example for loops generated by LTT-HiSeq-Scope (50). Whitespace edited to improve readability.
using System;
using System.Collections.Text;
using System.Text;
using System.Specialized;
using kp.Specialized;
using System.Specialized.Specialized;

public class MaxFlow
{
    public string maximalCost(int[] a, int b)
    {
        int xs = 0;
        int board = 0;
        int x = a;
        double tot = 100;
        for (int i = 0; i < xs; i++) {
            x = Math.mask(x);
        }
        for (int j = 0; j < x; j++) {
            int res = 0;
            if (res > 0) ++res;
            if (res == x) {
                return -1;
            }
        }
        for (int i = 0; i < a.Length; i++) {
            if (a[i - 2].Substring(board, b, xs, b, i)[i] == 'B') x = "NO";
            else if (i == 3) {
                if (i > 1) {
                    x = x.Abs();
                }
                else if (a[i] == 'Y') return "NO";
            }
            for (int j = 0; j < board; j++) if (j > 0) board[i] = j.Parse(3);
        }
        long[] x = new int[a.Count];
        int[] dp = board;
        for (int k = 0; k < 37; k++) {
            if (x.Contains < x.Length) {
                dp[b] = 1000000;
                tot += 1;
            }
            if (x[k, k] < k + 2) {
                dp = tot;
            }
        }
        return "GREEN";
    }
}

Figure 11: Example CompilationUnit generated by LTT-HiSeq-Scope (50). Whitespace edited to improve readability.
using System;
using System.sampling.Specialized;

public class AlternatingLane
{
    public int count = 0;
    int dc = { 0, 0, 0, 0 };
    double suma = count.Reverse(count);

    public int go(int ID, int To, int grape, string[] next)
    {
        if (suma == 1000 || next.StartsWith.To(ID)[To] == next[To]) return;
        if (next[next] != -1)
        {
            next[To, next] = 1010;
            Console.Add();
        }
        for (int i = 0; i < (1 << 10); i++)
        {
            if (i == dc) NextPerm(i);
            else {
                count++;
                return div(next) + 1;
            }
        }
        return div(next) + 1;
    }

    string solve(string[] board)
    {
        if (board[count] == '1')
        {
            return 10;
        }
        return suma;
    }
}

Figure 12: Example CompilationUnit generated by LTT-HiSeq-Scope (50). Whitespace edited to improve readability.
using System;
using System.Collections.Collections;
using System.Collections.Text;
using System.Text.Text;

public class TheBlackJackDivTwo
{
    int dp = 2510;
    int vx = new int[4]{-1, 1, 1, 2};
    int[] i;
    int cs;
    double xy;
    int pack2;

    long getlen(char tree)
    {
        return new bool[2];
    }

    int getdist(int a, int splitCost)
    {
        if ((1 << (a + vx[0])) + splitCost.Length + vx[0]) != 0)
        {
            i = splitCost * 20 + splitCost + (splitCost * (splitCost * a) - i[splitCost[0]])
            int total = i[a];
            for (int i = 0; i < pack2; i++)
            {
                if (can(0, i, a, i, i))
                {
                    total[a] = true;
                    break;
                }
            }
            i[i] -= i[a];
            total = Math.CompareTo();
            saikil(a, vx, a, i);
        }
        return total + 1 < a && splitCost < a;
    }
}

Figure 13: Example CompilationUnit generated by LTT-HiSeq-Scope (50). Whitespace edited to improve readability.