

CBMM Memo No. 149

September 27, 2024

On the Power of Decision Trees in Auto-Regressive Language Modeling

Yulu Gan¹, Tomer Galanti², Tomaso Poggio¹, Eran Malach³

1: Center for Brains, Minds, and Machines, MIT, Cambridge, MA, USA

2: Texas A&M University

3: Kempner Institute, Harvard University

Abstract

Originally proposed for handling time series data, Auto-regressive Decision Trees (ARDTs) have not yet been explored for language modeling. This paper delves into both the theoretical and practical applications of ARDTs in this new context. We theoretically demonstrate that ARDTs can compute complex functions, such as simulating automata, Turing machines, and sparse circuits, by leveraging "chain-of-thought" computations. Our analysis provides bounds on the size, depth, and computational efficiency of ARDTs, highlighting their surprising computational power. Empirically, we train ARDTs on simple language generation tasks, showing that they can learn to generate coherent and grammatically correct text on par with a smaller Transformer model. Additionally, we show that ARDTs can be used on top of transformer representations to solve complex reasoning tasks. This research reveals the unique computational abilities of ARDTs, aiming to broaden the architectural diversity in language model development.



This material is based upon work supported by the Center for Brains, Minds and Machines (CBMM), funded by NSF STC award CCF-1231216.

On the Power of Decision Trees in Auto-Regressive Language Modeling

Yulu Gan

Massachusetts Institute of Technology
yulu_gan@mit.edu

Tomer Galanti

Texas A&M University
galanti@tamu.edu

Tomaso Poggio

Massachusetts Institute of Technology
tp@csail.mit.edu

Eran Malach

Harvard University
eran.malach@gmail.com

Abstract

1 Originally proposed for handling time series data, Auto-regressive Decision Trees
2 (ARDTs) have not yet been explored for language modeling. This paper explores
3 both the theoretical and practical applications of ARDTs in this new context. We
4 theoretically demonstrate that ARDTs can compute complex functions, such as
5 simulating automata, Turing machines, and sparse circuits, by leveraging “chain-
6 of-thought” computations. Our analysis provides bounds on the size, depth, and
7 computational efficiency of ARDTs, highlighting their surprising computational
8 power. Empirically, we train ARDTs on simple language generation tasks, showing
9 that they can learn to generate coherent and grammatically correct text on par
10 with a smaller Transformer model. Additionally, we show that ARDTs can be
11 used on top of transformer representations to solve complex reasoning tasks. This
12 research reveals the unique computational abilities of ARDTs, aiming to broaden
13 the architectural diversity in language model development.

14

1 Introduction

15 In recent years, Large Language Models (LLMs) have achieved outstanding results in tasks such as
16 natural language understanding, coding, and mathematical reasoning. LLMs predominantly utilize the
17 Transformer architecture Vaswani et al. (2023), establishing it as the standard in this field. However,
18 recent initiatives (Gu & Dao, 2023; Sun et al., 2023; Ma et al., 2023; De et al., 2024) have begun to
19 challenge the dominance of Transformers. These alternatives, while not yet matching Transformer
20 performance, offer advantages in terms of inference time efficiency. Moreover, some works are
21 revisiting traditional non-neural network models for language modeling, such as classical symbolic
22 models (Wong et al., 2023). These developments indicate a shift towards diverse, efficient, and
23 interpretable language modeling methodologies.

24 Tree-based models, particularly favored for handling tabular data (Grinsztajn et al., 2022), continue
25 to hold significant importance. While tree-based methods are mostly used for classification and
26 regression tasks, Auto-regressive Decision Trees (ARDTs) (Meek et al., 2002) have been studied for
27 time-series prediction, offering a simpler and more interpretable alternative to complex nonlinear
28 approaches. Although the ARDT approach was not originally designed for language tasks, it has
29 demonstrated considerable promise in various time-series datasets, outperforming traditional auto-
30 regressive models while maintaining ease of interpretation. Motivated by these results, our study
31 seeks to explore the potential of ARDTs for language prediction tasks, assessing whether they could
32 serve as a viable, interpretable alternative to complex, resource-intensive language models.

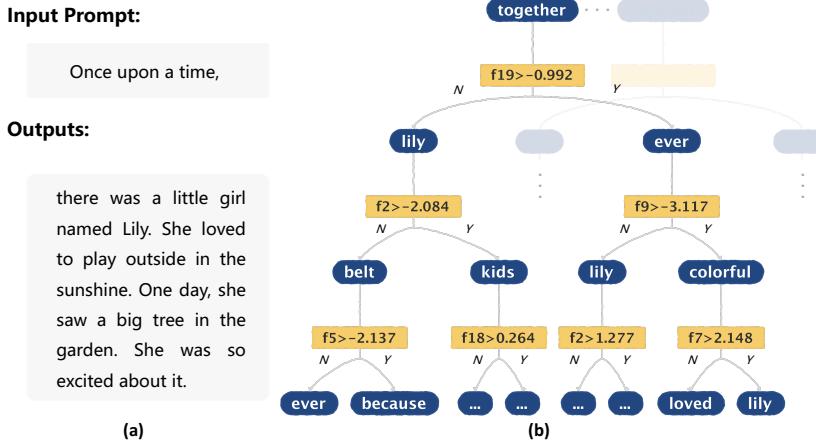


Figure 1: (a) An example of story continuation generated by our Auto-Regressive Decision Trees. We use decision trees and, remarkably, attain results comparable to Transformer-based models in terms of linguistic fluency. (b) The decision process of the decision trees. We visualize part of the tree ensemble, and can observe which word is most relevant for the splitting rule at each node.

33 To understand the power of ARDTs, we first conduct theoretical studies demonstrating that ARDTs,
 34 using decision trees as next-token predictors, can compute more complex functions than traditional
 35 decision trees. We explore the classes of functions ARDTs can compute, showing their ability to
 36 simulate functions computed by automata, Turing machines, or sparse circuits through intermediate
 37 “chain-of-thought” computations. We provide bounds on the size, depth, and run-time (measured
 38 by the number of intermediate tokens) required for ARDTs to simulate these function classes. Our
 39 findings highlight the surprising computational capabilities of ARDTs, underscoring their potential
 40 as a powerful and interpretable alternative for language prediction tasks requiring complex function
 41 computations.

42 Our experimental results further demonstrate the practical utility of ARDTs in language generation
 43 tasks. Utilizing standard auto-regressive inference methods, these models generate output sequences
 44 token-by-token, appending each new token to the input of the subsequent iteration. When trained on
 45 the TinyStories dataset Eldan & Li (2023), ARDTs produce coherent and grammatically accurate text
 46 (see in Fig 1). Notably, decision tree ensembles with approximately 0.3 million parameters outperform
 47 a Transformer model with around 1 million parameters on the same TinyStories dataset, highlighting
 48 their efficiency despite a smaller size. We discuss our approach to training interpretable decision
 49 trees, which enhances the transparency of the decision-making process in language generation.
 50 Furthermore, we assess the ability of tree-based models to execute various logical reasoning tasks.
 51 Notably, tree ensembles built on top of transformer embeddings and trained on specific downstream
 52 tasks perform comparably to larger general models like InstructGPT Ouyang et al. (2022) and
 53 PaLM-540B Chowdhery et al. (2022), under the conditions of these particular tasks.

54 Our contribution can be summarized as follows:

- 55 • We extend the application of ARDTs to language prediction tasks, adopting a novel approach
 56 that capitalizes on their inherent simplicity and interpretability. This aims to broaden the
 57 architectural diversity in language model development.
- 58 • Through theoretical analysis, we demonstrate that ARDTs can compute a broader array
 59 of complex functions than previously recognized, including the simulation of automata,
 60 Turing machines, and sparse circuits. These theoretical findings deepen our understanding
 61 of ARDTs’ computational capabilities.
- 62 • Our experimental results offer empirical evidence that ARDTs are capable of generating
 63 coherent and grammatically correct text, perform well compared to more complex models
 64 like small Transformers, and demonstrate solid reasoning abilities.

65 **2 Related Work**

66 **Decision Trees.** Tree based models have been widely used for solving different classification and
67 regression tasks in machine learning (Navada et al., 2011). The ID3 algorithm was introduced by
68 Quinlan (1986), and has been widely used for decision tree learning, along with the CART (Breiman
69 et al., 1984; Lewis, 2000) algorithm. Decision tree ensembles, such as random forests (Breiman,
70 2001) and gradient boosted trees (Friedman, 2002), are also very popular. Despite continuous
71 advancements in deep learning, decision tree ensembles still outperform neural network based models
72 on tabular datasets (Shwartz-Ziv & Armon, 2022). Different from traditional decision trees, we use
73 auto-regressive decision trees to perform language prediction tasks more efficiently.

74 **Learning Theory for Decision Trees.** There are a few theoretical works studying the power of
75 decision trees in solving machine learning problems. The work of Brutzkus et al. (2020) shows that
76 the ID3 algorithm can learn sparse functions in some setting. Kearns & Mansour (1996) show that
77 decision trees are equivalent to boosting methods for amplifying the performance of weak learners
78 on the distribution. Other works focus on other aspects of decision tree learnability (Rivest, 1987;
79 Blum, 1992; Ehrenfeucht & Haussler, 1989; Bshouty & Burroughs, 2003). We note that from the
80 approximation point of view, decision trees can be regarded as splines with free knots. For instance,
81 piecewise constant hierarchical splines functions, similar to neural networks with threshold activation
82 can also be seen as decision trees. Note that ReLU networks can be viewed as piecewise hierarchical
83 linear splines (Anselmi et al., 2015; Yarotsky, 2016), and so decision trees can represent ReLU
84 networks (see Aytekin (2022)), though possibly with an exponential number of parameters. We note
85 that none of the works mentioned above studies the theory of auto-regressive decision trees, which is
86 a novel contribution of our paper.

87 **Decision Trees for Language.** Despite gaining popularity in several fields of machine learning, tree
88 based models are not widely used for language generation. Past works have utilized auto-regressive
89 decision trees for time-series analysis (Meek et al., 2002), or use trees for basic language modeling
90 (Potamianos & Jelinek, 1998). Decision trees were also used in parsing (Magerman, 1995; Heeman,
91 1999; Nallapati & Allan, 2002), modeling syntax (Filimonov, 2011) and language identification
92 (Hakkinen & Tian, 2001).

93 **3 Theory**

94 To explore the capabilities of ARDTs, we initially undertake theoretical studies demonstrating that
95 using decision trees as next-token predictors enables ARDTs to process significantly more complex
96 functions than “standard” decision trees. Firstly, we define the theoretical setting of our analysis
97 in Section 3.1. We then examine the various classes of functions that an ARDT can compute, as
98 discussed in Sections 3.2, 3.3, and 3.4. Here, the computation involves the ARDT receiving an
99 input sequence, such as a question, generating a series of intermediate tokens that describe the
100 thought process, and finally producing the output token. Specifically, we demonstrate that functions
101 computed by Automata, Turing machines, or sparse circuits can be emulated by an ARDT using
102 these intermediate “chain-of-thought” computations. Additionally, we provide bounds on the size,
103 depth, and runtime (measured by the number of intermediate tokens) required for ARDTs to simulate
104 these classes of interest. Our findings affirm that ARDTs, by leveraging decision trees for next-token
105 prediction, can handle far more complex functions than “standard” decision trees.

106 **Comment 1.** *The results in this section are representation results. That is, we study which functions
107 can, in theory, be represented by auto-regressive decision trees. We do not provide any formal results
108 on whether such functions can be learned from data. The question of how decision trees can be
109 trained to produce “chain-of-thought” responses to input questions is beyond the scope of this work.*

110 **3.1 Setting**

111 We adapt the standard definition of a decision tree, as described by Quinlan (1986), to include
112 modifications that allow for the processing of vector sequences of arbitrary lengths. Firstly, we
113 establish a vocabulary \mathbb{D} , which serves as our token dictionary. Next, we define an input embedding
114 $\Psi : \mathbb{D} \rightarrow \mathbb{R}^d$. For any sequence of tokens $s \in \mathbb{D}^n$, $\Psi(s) \in \mathbb{R}^{n \times d}$ represents the embedding applied
115 individually to each token. The space comprising sequences of d -dimensional vectors is denoted by

116 $\mathcal{X} = \mathbb{R}^{* \times d}$. Subsequently, we define a decision tree \mathcal{T} that receives an input $\mathbf{x} \in \mathcal{X}$ and outputs a
 117 token $y \in \mathbb{D}$.

118 In our experiments, detailed in Section 4, we apply a weighted-average operator to the word vectors of
 119 the sequence, where the average vectors are used as an input to the decision trees. For the theoretical
 120 analysis we study a different approach for using decision trees over vector sequences, where instead
 121 of averaging word vectors we ‘‘concatenate’’ them. That is, the decision tree is applied to the L
 122 most recent words, in a ‘‘sliding window’’ fashion. We note that experimentally we observed that
 123 both the ‘‘sliding-window’’ and the weighted-average approach produced similar results, and use the
 124 weighted-average technique in our experiments for computational reasons.

125 We start by defining a decision tree \mathcal{T} that gets inputs of a fixed length L , namely $\mathcal{T} : \mathbb{R}^{L \times d} \rightarrow \mathbb{D}$.
 126 We refer to the value L as the *context length* of \mathcal{T} , and this value will correspond to the maximal
 127 length of a sequence that affects the computation of the tree. In this case, we treat the input $\mathbf{x} \in \mathbb{R}^{L \times d}$
 128 as a vector, and let \mathcal{T} be a standard decision tree operating on vectors of size $L \cdot d$. Namely, \mathcal{T} is
 129 defined by a binary tree, where each node corresponds to an input feature $x_{i,j}$ and some threshold
 130 $\tau \in \mathbb{R}$. Each leaf corresponds to some output token $y \in \mathbb{D}$. The output of the tree \mathcal{T} is computed
 131 by starting at the root, and for each internal node with feature $x_{i,j}$ and threshold τ , moving to the
 132 right node if $x_{i,j} \geq \tau$ and otherwise moving to the left node. When reaching a leaf, we output the
 133 value $y \in \mathbb{D}$ corresponding to the leaf. The *size* of the tree \mathcal{T} is the number of leaves in the tree, and
 134 its *depth* is the maximum length of a path from root to leaf. Note that the runtime of computing the
 135 output of \mathcal{T} corresponds to the *depth* of the tree.

136 Now, given some tree over length- L inputs $\mathcal{T} : \mathbb{R}^{L \times d} \rightarrow \mathbb{D}$, we apply \mathcal{T} to an input of arbitrary
 137 length $\mathbf{x} \in \mathcal{X}$ using the following simple rule: if \mathbf{x} has length shorter than L , we pad it to length L
 138 by prepending the input, adding additional padding ($\langle \text{PAD} \rangle$) tokens at the beginning; if \mathbf{x} is longer
 139 than L , we apply \mathcal{T} only to the last L tokens in \mathbf{x} . This induces a decision tree with arbitrary length
 140 inputs $\mathcal{T} : \mathcal{X} \rightarrow \mathbb{D}$.

141 Finally, we use the tree \mathcal{T} as a next-token predictor function, applied over some input using auto-
 142 regressive computation. That is, we define a sequence-to-sequence predictor $\mathcal{T}^{\text{AR}} : \mathbb{D}^* \rightarrow \mathbb{D}^*$
 143 induced from the tree \mathcal{T} as follows: for every input $\mathbf{s} \in \mathbb{D}^n$, recursively define $s_{n+1} =$
 144 $\mathcal{T}(\Psi(s_1, \dots, s_{n+1}))$, and let $\mathcal{T}^{\text{AR}}(s_1, \dots, s_n) = (s_{n+1}, s_{n+2}, \dots)$. We call \mathcal{T}^{AR} an *auto-regressive*
 145 *decision tree* (ARDT).

146 In the rest of this section, we will analyze the capacity of ARDTs to simulate some function classes.
 147 Following Malach (2023), we give the following definition:

Definition 2. For some class \mathcal{F} of functions $f : \mathbb{D}^n \rightarrow \mathbb{D}$, we say \mathcal{F} can be simulated by
 auto-regressive decision-trees in length complexity T , if for every $f \in \mathcal{F}$ there exists \mathcal{T}^{AR}
 s.t. for all $\mathbf{s} \in \mathbb{D}^n$, we have $\mathcal{T}_T^{\text{AR}}(\mathbf{s}) = f(\mathbf{s})$ (where $\mathcal{T}_T^{\text{AR}}$ indicates the output of \mathcal{T}^{AR} at
 iteration T).

148
 149 In other words, we say that the tree \mathcal{T}^{AR} can compute the function f , if given some input sequence
 150 \mathbf{s} , it generates T tokens followed by the correct output $f(\mathbf{s})$. That is, we allow the tree to use T
 151 intermediate tokens as ‘‘chain-of-thought’’ before outputting the correct answer.

152 3.2 Simulating Automata

153 An automaton \mathcal{A} is defined over an alphabet Σ , using a set of states Q , an initial state $q_0 \in Q$ and a
 154 transition function $\delta : Q \times \Sigma \rightarrow Q$. We always assume that $|\Sigma| \geq 2$ and $|Q| \geq 2$. The automaton \mathcal{A}
 155 gets an input string $\mathbf{x} \in \Sigma^*$, and computes an output state $\mathcal{A}(\mathbf{x}) \in Q$ by starting at state q_0 and at
 156 each iteration i transitioning to the next state based on the i -th token x_i , namely $q_i = \delta(q_{i-1}, x_i)$.
 157 The automaton then returns the state reached at the final iteration.

158 Let $\mathcal{F}_n^{\text{Aut}}$ is the class of all functions computed by automata over strings of length n . Namely,
 159 $\mathcal{F}_n^{\text{Aut}}$ is the class of functions $f : \Sigma^n \rightarrow Q$ s.t. for all $f \in \mathcal{F}_n^{\text{Aut}}$ there exists an automaton \mathcal{A} s.t.
 160 $\mathcal{A}(\mathbf{x}) = f(\mathbf{x})$ for all $\mathbf{x} \in \Sigma^n$.

161 The class of functions computed by Automata has been well-studied from the early days computer
 162 science theory (Hopcroft et al., 2001), and has various important connections to language problems.
 163 This class of functions is also interesting in the context of reasoning tasks for language modeling. For

164 example, the *Web-of-Lies* and *Navigate* problems in the Big-Bench Hard dataset (Srivastava et al.,
 165 2023) can be solved by finite state Automata.

166 We show that ARDTs can simulate Automata:

Theorem 3. Let $\mathbb{D} = \Sigma \cup Q \cup \{\langle \text{PAD} \rangle\}$. Then, $\mathcal{F}_n^{\text{Aut}}$ can be simulated by ARDTs of size $O(|\mathbb{D}|^2)$, depth $O(\log |\mathbb{D}|)$ and context length $L \geq n$, in length complexity $O(n)$.

167
 168 Note that ARDTs simulate Automata very efficiently: the total run-time of the ARDT guaranteed by
 169 Theorem 3 is $O(n \log |\mathbb{D}|)$, which corresponds to the time it takes to read all the input bits. In this
 170 sense, no algorithm can simulate Automata significantly faster than ARDT.

171 In the proof, we construct an ARDT that, at every iteration i , outputs the state of the Automaton at
 172 step i (denoted q_i). The state at step $i + 1$ is only a function of the i -th state, given by the most recent
 173 token generated by the model; and the i -th input, which is always given by looking back $n + 1$ tokens.
 174 Therefore, a simple tree, applied as a *sliding-window* over the input, can compute the transition matrix
 175 to find the next state. The full proof is given in Appendix A.

176 Next, we show that the above result implies a *separation* between ARDTs and standard decision trees.
 177 Specifically, we show that if we use a decision-tree over the input to directly predict the final output
 178 of the Automata, without outputting intermediate states, then the size of the decision tree must be
 179 exponential in the length of the input:

Theorem 4. There exists some $f \in \mathcal{F}_n^{\text{Aut}}$ s.t. any decision tree that computes f has size
 $\geq \Omega(2^n)$.

180
 181 This shows that the fact that ARDTs can perform intermediate computations auto-regressively (e.g.,
 182 perform *chain-of-thought*) significantly improves their efficiency¹. To prove the result, we show that
 183 computing the *parity* of a sequence of bits (i.e., whether the number of bits is even or odd) requires a
 184 tree of exponential size, but can be easily computed by a simple 2-state Automaton.

185 *Proof of Theorem 4.* Consider the binary alphabet $\Sigma = \{0, 1\}$ and the state set $Q = \{\text{even}, \text{odd}\}$,
 186 with $|\Sigma| = 2$ and $|Q| = 2$. We define a function $f : \Sigma^n \rightarrow Q$ as follows:

$$f(\mathbf{x}) = \begin{cases} \text{even} & \text{if } \sum x_i \bmod 2 = 0, \\ \text{odd} & \text{otherwise.} \end{cases}$$

187 The function f describes the parity of the sum of bits in \mathbf{x} and can be efficiently computed by an
 188 automaton that toggles between states even and odd upon encountering a 1.

189 Suppose a decision tree \mathcal{T} computes f . We claim that the size of \mathcal{T} must be at least 2^n . Assume for
 190 contradiction that \mathcal{T} has fewer than 2^n leaves. Since \mathcal{T} is a decision tree, we assume that all its leaves
 191 are reachable by some input $\mathbf{x} \in \{0, 1\}^n$.

192 Consider a leaf l of \mathcal{T} reached by some input \mathbf{x} , at a depth less than n . This implies that there exists
 193 at least one bit index $j \in [n]$ such that no decision node in \mathcal{T} queries x_j on the path to l . Define
 194 $\mathbf{x}' \in \{0, 1\}^n$ by flipping x_j in \mathbf{x} , while keeping all other bits unchanged:

$$x'_i = \begin{cases} x_i & \text{if } i \neq j, \\ \neg x_j & \text{if } i = j. \end{cases}$$

195 Since \mathbf{x}' alters \mathbf{x} only at the unqueried index j , it follows the same path in \mathcal{T} and reaches the same leaf
 196 l . Therefore, $\mathcal{T}(\mathbf{x}) = \mathcal{T}(\mathbf{x}')$. However, the definition of f guarantees $f(\mathbf{x}) \neq f(\mathbf{x}')$ as their parities
 197 are different, leading to a contradiction. Thus \mathcal{T} cannot compute f with fewer than 2^n leaves. \square

¹This is an example of how compositional sparsity can defeat the curse of dimensionality (Poggio, 2022). A function may not be approximated by a decision tree without an exponential number of parameters but may be represented efficiently by composing intermediate sparse functions, as ARDTs do.

198 **3.3 Simulating Turing Machines**

199 A Turing machine \mathcal{M} is defined over an alphabet Σ , using a space set Q , initial state $q_0 \in Q$ and
200 transition function $\delta : Q \times \Sigma \rightarrow Q \times \Sigma \times \{\langle \text{LEFT} \rangle, \langle \text{RIGHT} \rangle\}$. The Turing machine has a tape,
201 where each cell contains a symbol from Σ . The *head* of the Turing machine is initialized at the
202 leftmost cell on the tape in state $q_0 \in Q$. At each iteration of the machine, it reads the symbol $s \in \Sigma$
203 and given the head state $q \in Q$ uses $\delta(q, s)$ to determine the new state of the head, the symbol to
204 write under the head, and whether to move the head left or right on the tape.

205 In our setting, we consider Turing machines with fixed memory M , i.e. Turing machines with access
206 to a tape with M cells. In particular, this means that the Turing machine \mathcal{M} operate on inputs with
207 $< M$ tokens. At the initial step, the input is written on the tape. If the input size is shorter than M ,
208 we add empty tokens $\{\emptyset\} \in \Sigma$ after the input sequence. We consider Turing machines with fixed
209 runtime T , namely we let the machine run for T iterations and then halt it. The output of the machine
210 is the rightmost symbol on the tape after T iterations. So, we define $\mathcal{M} : \Sigma^M \rightarrow \Sigma$ to be the function
211 computed by the machine after T steps. We denote by $\mathcal{F}_{M,T}^{\text{Turing}}$ the class of functions computed by
212 Turing machines with memory of size M and runtime T .

213 **Comment 5.** *Turing machines are typically defined with infinite number of tape cells, and are
214 allowed to run arbitrarily long before halting. However, for every given input length, any computable
215 function always uses a fixed memory and run-time (which depend on the input length).*

216 We now show any Turing machine with fixed memory and run-time can be simulated by an ARDT:

Theorem 6. *Let $\mathbb{D} = \Sigma \cup Q \cup \{\langle \text{PAD} \rangle, \langle \text{SEP} \rangle\}$ ². Then, $\mathcal{F}_{M,T}^{\text{Turing}}$ can be simulated by ARDTs
of size $O(|\mathbb{D}|^4)$, depth $O(\log |\mathbb{D}|)$ and context length $L = M + 3$, with length complexity
 $O(MT)$.*

217 To prove the result, we show that an ARDT can compute the state of the Turing machine at each
218 iteration. Specifically, we encode the state of the machine as a sequence of tokens from \mathbb{D} , where we
219 put a token $q \in Q \subseteq \mathbb{D}$ indicating the state of the head before the token that the head reads. This
220 way, the transition between states is a function that only depends locally on the tokens surrounding
221 the position of the head, where all other (non-state) tokens can be copied as-is from one state to
222 the next. Similarly to the proof in the previous section, this operation can be realized by a small
223 *sliding-window* tree. The full proof is given in Appendix A.

225 **3.4 Simulating Sparse Circuits**

226 A circuit \mathcal{C} over some alphabet Σ is defined as a directed-acyclic-graph (DAG), with n input nodes
227 and one output node. Each internal (non-input) node with k incoming edges corresponds to some
228 function $g : \Sigma^k \rightarrow \Sigma$ computed by the node over its incoming inputs. For some input $x \in \Sigma^n$, the
229 output of the circuit \mathcal{C} is the value of the output node, when setting the input nodes of \mathcal{C} to x_1, \dots, x_n .
230 The size of the circuit \mathcal{C} is the number of nodes in the computational graph. We say that \mathcal{C} is k -sparse,
231 if the maximal in-degree of every node in the graph is k . Denote by $\mathcal{F}_{N,k}^{\text{Circuit}}$ the class of functions
232 computed by k -sparse circuits of size N .

233 We note that sparse circuits are an extension of sparse Boolean circuits, and so can represent Turing
234 machines with bounded memory (Arora & Barak, 2009). In this sense, this class is “equivalent” to the
235 class of functions computed by Turing machines. However, some functions may be more efficient to
236 compute using sparse circuits, and so it is interesting to understand how ARDTs can directly simulate
237 sparse circuits, as demonstrated in the following theorem:

Theorem 7. *Let $\mathbb{D} = \Sigma \cup \{\langle \text{PAD} \rangle\}$. Then, $\mathcal{F}_{N,k}^{\text{Circuit}}$ can be simulated by ARDTs of size
 $O(N|\mathbb{D}|^k \log |\mathbb{D}|)$ and context length $L \geq N$, in length complexity $O(N)$.*

238

²We introduce a new separator token $\langle \text{SEP} \rangle$, that is used during the generation of the ARDT, but is not part of the alphabet or state set of the Turing machine.

239 *Proof of Theorem 7.* Consider a k -sparse circuit \mathcal{C} with N total nodes, where $N - n$ are internal
 240 nodes. Let $g_1, \dots, g_{N-n} : \Sigma^k \rightarrow \Sigma$ be the functions computed at the internal nodes, ordered
 241 topologically so that each function depends only on the inputs or the results of preceding nodes. Let
 242 g_{N-n} denote the function computed by the output node.

243 Define $f_i : \Sigma^{n+i-1} \rightarrow \Sigma$ as the output of the i -th node in this ordering, considering all inputs and
 244 outputs from previous nodes. Each f_i is effectively a k -Junta. By Lemma 10, there exists a decision
 245 tree \mathcal{T}_i of size $O(|\mathbb{D}|^k)$ such that $\mathcal{T}_i(\Psi(\mathbf{x})) = f_i(\mathbf{x})$ for all $\mathbf{x} \in \Sigma^{n+i-1}$.

246 To accommodate inputs $\mathbf{x} \in \Sigma^N$, we modify each tree \mathcal{T}_i to ignore the first $N - n - i + 1$ inputs.
 247 This adaptation does not affect the size of the tree.

248 Let $\mathbf{z} = \Psi(\langle \text{PAD} \rangle) \in \{0, 1\}^d$. Construct a tree as follows: begin with the rightmost branch of the
 249 tree, using functions $h_{1,1}, \dots, h_{1,d}, \dots, h_{N-n,1}, \dots, h_{N-n,d}$. For each node $i \in [N - n]$ and each
 250 bit $j \in [d]$, define:

$$h_{i,j} = \begin{cases} 1\{\Psi(\mathbf{x})_{i,j} \geq 1\} & \text{if } z_j = 1, \\ 1\{\Psi(\mathbf{x})_{i,j} < 1\} & \text{if } z_j = 0. \end{cases}$$

251 Attach tree $\mathcal{T}_{N-n-i+1}$ at each left node (i, j) .

252 Observe that during the i -th iteration, the string begins with $N - n - i \langle \text{PAD} \rangle$ tokens, allowing \mathcal{T}_i
 253 to process the pertinent part of the input. After $N - n$ iterations, the constructed tree calculates the
 254 output token as specified by \mathcal{C} . \square

255 4 Experiments

256 In this section, we experimentally validate the capabilities of ARDTs as demonstrated in the previous
 257 section and prove their language modeling potential. In Section 4.2, we first train a model based
 258 on ARDTs and test its ability to continue stories on Tinystories Eldan & Li (2023), which involves
 259 extending narratives similar to a finite state automaton. ARDTs generate coherent text that builds on
 260 existing stories, also requiring the interpretation of complex contexts and emotions. This showcases
 261 the effectiveness of sparse circuits in managing significant yet limited inputs.

262 Additionally, in Section 4.3, we assess the model’s reasoning abilities on the Big-Bench-Hard Suzgun
 263 et al. (2022) dataset, where tasks often involve evaluating the truthfulness of propositions, effectively
 264 emulating a Turing machine as it processes inputs to determine a definitive outcome (true or false).

265 4.1 Setting

266 To align with the theory section, we designed our experiments to closely mirror the theoretical
 267 settings as closely as possible. We here provide a detailed description of our implementation of
 268 Auto-regressive Decision Trees (ARDTs) for next-token prediction tasks. Our objective is to utilize
 269 ARDTs as a language model that receives a sequence of input tokens x_1, \dots, x_n and predicts the
 270 subsequent token x_{n+1} . Initially, we employ a Word2Vec embedding Mikolov et al. (2013), denoted
 271 by Ψ , to convert the sequence tokens into word embeddings $\Psi(x_1), \dots, \Psi(x_n), \Psi(x_{n+1}) \in \mathbb{R}^{100}$.
 272 We then compute a weighted average of these embeddings with exponential decay, prioritizing the
 273 most recent tokens: $\bar{v} = \sum_{i=1}^n \alpha^{n-i+1} \Psi(x_i)$, where $\alpha \in (0, 1)$. Using XGBoost Chen & Guestrin
 274 (2016), we train an ensemble of decision trees, \mathcal{T} , which takes the input vector \bar{v} and predicts the
 275 embedding of the next token $\Psi(x_{n+1})$, aiming to minimize the mean squared error (MSE) loss. We
 276 train this model using sequences of varying lengths sampled from our dataset. During inference,
 277 the model generates text auto-regressively. At each step, it receives the current sequence \bar{v} , outputs
 278 the predicted embedding of the next token $\hat{u} = \mathcal{T}(\bar{v})$, and identifies the token whose embedding is
 279 closest to this prediction, i.e., $\hat{x} = \arg \min_x \|\Psi(x) - \hat{u}\|_2$. This token is then used as the next token
 280 in the sequence. The input vector is updated with the new token using $\bar{v} \leftarrow \alpha \bar{v} + \Psi(\hat{x})$, and the
 281 process repeats for the next iteration. Figure 2 illustrates the training and inference pipeline.

282 **Comment 8.** *We note that the setting described above deviates from the theory setting. 1) While
 283 the theoretical analysis focuses on the representational power of a single auto-regressive decision
 284 tree, the experiments utilize ensembles of decision trees. Notably, tree ensembles are more expressive,
 285 which suggests that our positive findings should also extend to these ensembles. 2) For simplicity,
 286 our theoretical study examines trees that generate a single output token in each iteration, rather
 287 than producing a word vector, which is the approach used in the experiments. 3) The decision trees*

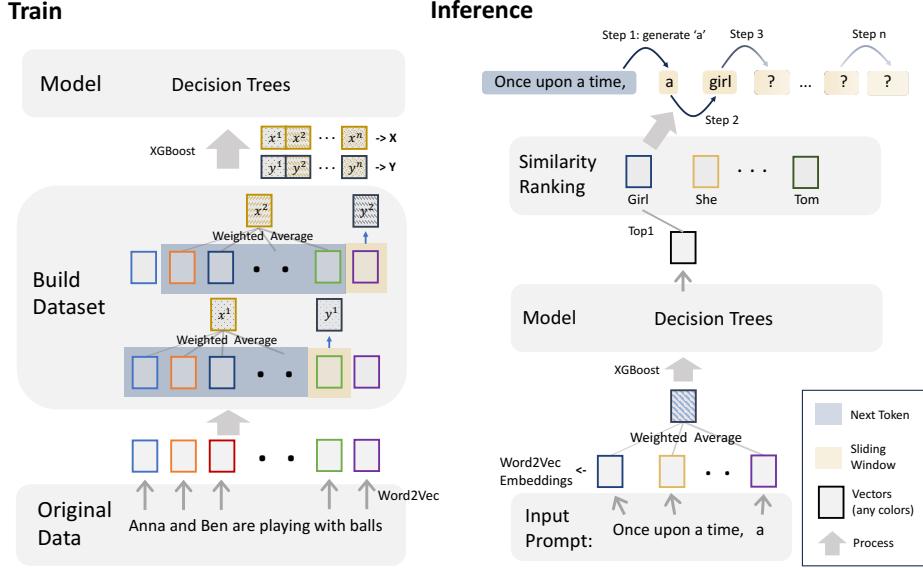


Figure 2: **The Pipeline of Our Method.** (a) **Training.** First, we employ a Word2Vec model to convert words into embeddings. Next, we utilize a sliding window approach to construct a dataset for training decision trees. Within this window, we performed a weighted average calculation, and the following token after the window was used as the label. (b) **Inference.** We use our trained Decision Trees for the purpose of next-token prediction.

288 *discussed theoretically operate on concatenated token vectors within a sliding window, in contrast to*
 289 *the use of vector averages in the experimental setting.*

290 4.2 The Ability to Generate Coherent Stories

291 We test ARDTs’ ability to generate stories with the *TinyStories* Eldan & Li (2023) dataset, which is a
 292 widely-used high-quality synthetic dataset of short stories that contain words that a 3 to 4-year-old
 293 child can understand, generated by GPT-3.5 and GPT-4. Details can be found in Appendix B.2.

294 For experiments conducted on TinyStories, we strictly follow Eldan & Li (2023) and employ the
 295 multidimensional score provided by GPT-4, as detailed in Appendix B.5.

296 For baselines to compare with ARDTs, we selected several Transformer-based models. These
 297 include two small Transformers trained on the TinyStories dataset (TinyStories-1M and TinyStories-
 298 33M Eldan & Li (2023)), as well as GPT-4 OpenAI et al. (2023), to illustrate the performance
 299 differences between non-neural network methods and the Transformer architecture.

300 For our evaluation, we provide the models with 100 story beginnings (refer to examples in Ap-
 301 pendix B.4), each consisting of fewer than 6 words, generated by GPT-4. We use these beginnings as
 302 inputs to the model, allowing the it to perform next token prediction, ultimately generating outputs of
 303 20 words. For the ground truth row in Table 1, we grade complete stories from the dataset.

304 As shown in Table 1, ARDTs achieved performance comparable to GPT-4 and TinyStories-33M
 305 on four metrics: grammar, creativity, consistency, and plot. Our model outperforms TinyStories-
 306 1M, a Transformer-based model with 1M parameters, despite being smaller in size. These results
 307 demonstrate that although tree-based models are generally considered inferior to large neural networks,
 308 surprisingly, they can compete with small Transformers when trained on the TinyStories dataset.

309 4.3 Evaluating ARDTs in Language Reasoning Tasks

310 We now explore the potential of using decision trees for logical reasoning tasks using the Big-Bench-
 311 Hard dataset. The Big-Bench-Hard dataset, detailed in Appendix B.2, contains 23 challenging
 312 reasoning tasks from the BIG-Bench benchmark. We selected four representative reasoning tasks for
 313 evaluation, with examples provided in Appendix B.2.

Table 1: Experiment Results on TinyStories: The results show that an auto-regressive tree can achieve better performance as the GPT-Neo architecture and exhibit competitive performance compared to both GPT-4 and TinyStories-33M.

	Model Architecture	Parameters*	Grammar†	Creativity†	Consistency†	Plot†
TinyStories-1M	GPT-Neo	1M	4.42	2.70	6.32	3.65
TinyStories-33M	GPT-Neo	33M	7.80	6.87	9.10	7.65
GPT-4	GPT-4	1800B	9.93	8.51	9.32	8.24
Ground Truth	/	/	8.21	6.32	7.87	7.56
ARDTs (Ours)	Decision Tree	0.3M	7.85	4.10	7.36	5.39

* For our decision trees, we report the total number of tree nodes in the ensemble as the parameter count.

† To minimize the impact of inconsistency on our results and enhance the robustness of our evaluation metrics, we calculated the average scores from ten assessments for each of the 100 stories. Each story was evaluated ten times using the same prompt provided to GPT-4.

314 Each task involves training a separate decision tree ensemble. These ensembles utilize a weighted
 315 average of input word embeddings, as described in Section 4.1, using the word embedding layer
 316 from a pre-trained GPT-2 model trained on WebText. Each model is trained with 200 examples
 317 and tested on 50 examples. We also experiment with decision trees trained on top of a pre-trained
 318 GPT-2 Transformer model, where the output vectors from GPT-2 serve as input features for the
 319 decision trees, combining GPT-2’s advanced language understanding with the analytical capabilities
 320 of decision trees.

321 For establishing baselines, we follow the methodology of Suzgun et al. (2022) and use accuracy as
 322 the metric. InstructGPT, Codex, and PaLM 540B are used as baselines.

323 As presented in Table 2, our model demonstrates substantial effectiveness in reasoning tasks, with
 324 performance comparable to state-of-the-art methods. For instance, we observe improvements of
 325 7.4% in Boolean Expression tasks, 2% in Navigate tasks, and 7.8% in Sports Understanding tasks.
 326 Moreover, we find that further enhancements are possible by integrating decision trees with the GPT-2
 327 Transformer, underscoring the significant impact of word embeddings on performance. However, this
 328 paper focuses on highlighting the potential of the ARDTs architecture, not word embeddings. Our
 329 results show that the ARDTs model has strong reasoning abilities.

Table 2: Experimental Results on BIG-Bench-Hard. Lin: Linear Embedding; GPT: GPT-2 Embedding. The results demonstrate that ARDTs possess good reasoning capabilities.

BIG-Bench Hard	Srivastava et al. (2023)					Ours		
	Random	SOTA	Human-Rater	InstructGPT	Codex	PaLM 540B	Lin	GPT
Boolean Expressions	50	68.5	79.4	90	88.4	83.2	72.0	85.3
Navigate	50	56	81.9	68	50.4	62.4	55.4	69.2
Web-of-Lies	50	59.6	81.3	51.6	51.6	51.2	53.2	71.1
Sports Understanding	50	68.1	70.8	71.6	72.8	80.4	72.3	83.9
All Tasks (avg)	50	63.1	78.4	70.3	65.8	69.3	63.2	77.4

330 5 Discussion

331 The findings in this paper demonstrate that tree-based models have potential in language generation.
 332 Although they do not yet match the performance of large language models, they possess certain
 333 advantages that make them valuable for studying the emergence of intelligence on a smaller scale.
 334 Decision trees are easier to interpret (see Appendix C for more on interpretability using ARDTs),
 335 simpler to understand and analyze mathematically, and fast to train. Moreover, unlike standard neural
 336 networks, the inference time for decision trees typically increases *logarithmically* with their size: a
 337 tree with depth d can have 2^d nodes but only requires traversing $O(d)$ nodes per input.

338 This paper serves as a preliminary exploration into using ARDTs for language modeling tasks.
 339 We aim to inspire further research that integrates tree-based models into current language model

340 pipelines, leveraging their unique strengths to enhance language generation capabilities. We believe
341 incorporating tree-structured models into hybrid models with Transformers could be a promising
342 direction for future research.

343 **5.1 Acknowledgement**

344 The first author would like to thank Shimian Li (Peking University) for helping to enhance the
345 appearance of Figures 1, 2, and 4.

346 **References**

347 Anselmi, F., Rosasco, L., Tan, C., and Poggio, T. Deep convolutional networks are hierarchical kernel
348 machines. *Center for Brains, Minds and Machines (CBMM) Memo No. 035*, 2015.

349 Arora, S. and Barak, B. *Computational complexity: a modern approach*. Cambridge University Press,
350 2009.

351 Aytekin, C. Neural networks are decision trees, 2022.

352 Bird, S., Klein, E., and Loper, E. *Natural language processing with Python: analyzing text with the
353 natural language toolkit*. "O'Reilly Media, Inc.", 2009.

354 Blum, A. Rank-r decision trees are a subclass of r-decision lists. *Information Processing Letters*, 42
355 (4):183–185, 1992.

356 Breiman, L. Random forests. *Machine learning*, 45:5–32, 2001.

357 Breiman, L., Friedman, J., Olshen, R., and Stone, C. *Classification and Regression Trees*. Wadsworth
358 Publishing, 1984.

359 Brutzkus, A., Daniely, A., and Malach, E. Id3 learns juntas for smoothed product distributions. In
360 *Conference on Learning Theory*, pp. 902–915. PMLR, 2020.

361 Bshouty, N. H. and Burroughs, L. On the proper learning of axis-parallel concepts. *The Journal of
362 Machine Learning Research*, 4:157–176, 2003.

363 Chen, T. and Guestrin, C. XGBoost: A scalable tree boosting system. In *Proceedings of the 22nd ACM
364 SIGKDD International Conference on Knowledge Discovery and Data Mining*, KDD '16, pp. 785–
365 794, New York, NY, USA, 2016. ACM. ISBN 978-1-4503-4232-2. doi: 10.1145/2939672.2939785.
366 URL <http://doi.acm.org/10.1145/2939672.2939785>.

367 Chowdhery, A., Narang, S., Devlin, J., Bosma, M., Mishra, G., Roberts, A., Barham, P., Chung, H. W.,
368 Sutton, C., Gehrmann, S., Schuh, P., Shi, K., Tsvyashchenko, S., Maynez, J., Rao, A., Barnes,
369 P., Tay, Y., Shazeer, N., Prabhakaran, V., Reif, E., Du, N., Hutchinson, B., Pope, R., Bradbury,
370 J., Austin, J., Isard, M., Gur-Ari, G., Yin, P., Duke, T., Levskaya, A., Ghemawat, S., Dev, S.,
371 Michalewski, H., Garcia, X., Misra, V., Robinson, K., Fedus, L., Zhou, D., Ippolito, D., Luan, D.,
372 Lim, H., Zoph, B., Spiridonov, A., Sepassi, R., Dohan, D., Agrawal, S., Omernick, M., Dai, A. M.,
373 Pillai, T. S., Pellan, M., Lewkowycz, A., Moreira, E., Child, R., Polozov, O., Lee, K., Zhou, Z.,
374 Wang, X., Saeta, B., Diaz, M., Firat, O., Catasta, M., Wei, J., Meier-Hellstern, K., Eck, D., Dean,
375 J., Petrov, S., and Fiedel, N. Palm: Scaling language modeling with pathways, 2022.

376 De, S., Smith, S. L., Fernando, A., Botev, A., Cristian-Muraru, G., Gu, A., Haroun, R., Berrada, L.,
377 Chen, Y., Srinivasan, S., Desjardins, G., Doucet, A., Budden, D., Teh, Y. W., Pascanu, R., Freitas,
378 N. D., and Gulcehre, C. Griffin: Mixing gated linear recurrences with local attention for efficient
379 language models, 2024.

380 Ehrenfeucht, A. and Haussler, D. Learning decision trees from random examples. *Information and
381 Computation*, 82(3):231–246, 1989.

382 Eldan, R. and Li, Y. Tinystories: How small can language models be and still speak coherent english?,
383 2023.

384 Filimonov, D. *Decision tree-based syntactic language modeling*. University of Maryland, College
 385 Park, 2011.

386 Friedman, J. H. Stochastic gradient boosting. *Computational statistics & data analysis*, 38(4):
 387 367–378, 2002.

388 Grinsztajn, L., Oyallon, E., and Varoquaux, G. Why do tree-based models still outperform deep
 389 learning on typical tabular data? *Advances in Neural Information Processing Systems*, 35:507–520,
 390 2022.

391 Gu, A. and Dao, T. Mamba: Linear-time sequence modeling with selective state spaces, 2023.

392 Hakkinen, J. and Tian, J. N-gram and decision tree based language identification for written words.
 393 In *IEEE Workshop on Automatic Speech Recognition and Understanding, 2001. ASRU'01.*, pp.
 394 335–338. IEEE, 2001.

395 Heeman, P. A. Pos tags and decision trees for language modeling. In *1999 Joint SIGDAT Conference
 396 on Empirical Methods in Natural Language Processing and Very Large Corpora*, 1999.

397 Hopcroft, J. E., Motwani, R., and Ullman, J. D. Introduction to automata theory, languages, and
 398 computation. *Acm Sigact News*, 32(1):60–65, 2001.

399 Kearns, M. and Mansour, Y. On the boosting ability of top-down decision tree learning algorithms. In
 400 *Proceedings of the twenty-eighth annual ACM symposium on Theory of computing*, pp. 459–468,
 401 1996.

402 Lewis, R. J. An introduction to classification and regression tree (cart) analysis. In *Annual meeting of
 403 the society for academic emergency medicine in San Francisco, California*, volume 14. Citeseer,
 404 2000.

405 Ma, X., Zhou, C., Kong, X., He, J., Gui, L., Neubig, G., May, J., and Zettlemoyer, L. Mega: Moving
 406 average equipped gated attention, 2023.

407 Magerman, D. M. Statistical decision-tree models for parsing. *arXiv preprint cmp-lg/9504030*, 1995.

408 Malach, E. Auto-regressive next-token predictors are universal learners. *arXiv preprint
 409 arXiv:2309.06979*, 2023.

410 Meek, C., Chickering, D. M., and Heckerman, D. Autoregressive tree models for time-series analysis.
 411 In *Proceedings of the 2002 SIAM International Conference on Data Mining*, pp. 229–244. SIAM,
 412 2002.

413 Mikolov, T., Chen, K., Corrado, G., and Dean, J. Efficient estimation of word representations in
 414 vector space, 2013.

415 Nallapati, R. and Allan, J. Capturing term dependencies using a sentence tree based language model.
 416 In *Proceedings of CIKM*, volume 2, pp. 383–390. Citeseer, 2002.

417 Navada, A., Ansari, A. N., Patil, S., and Sonkamble, B. A. Overview of use of decision tree algorithms
 418 in machine learning. In *2011 IEEE control and system graduate research colloquium*, pp. 37–42.
 419 IEEE, 2011.

420 OpenAI, :, Achiam, J., and Steven Adler, e. a. Gpt-4 technical report, 2023.

421 Ouyang, L., Wu, J., Jiang, X., Almeida, D., Wainwright, C. L., Mishkin, P., Zhang, C., Agarwal,
 422 S., Slama, K., Ray, A., Schulman, J., Hilton, J., Kelton, F., Miller, L., Simens, M., Askell, A.,
 423 Welinder, P., Christiano, P., Leike, J., and Lowe, R. Training language models to follow instructions
 424 with human feedback, 2022.

425 Poggio, T. Compositional sparsity: a framework for ml. *Center for Brains, Minds and Machines
 426 (CBMM) Memo No. 138*, 2022.

427 Potamianos, G. and Jelinek, F. A study of n-gram and decision tree letter language modeling methods.
 428 *Speech Communication*, 24(3):171–192, 1998.

429 Quinlan, J. R. Induction of decision trees. *Machine learning*, 1:81–106, 1986.

430 Rivest, R. L. Learning decision lists. *Machine learning*, 2:229–246, 1987.

431 Shwartz-Ziv, R. and Armon, A. Tabular data: Deep learning is not all you need. *Information Fusion*,
432 81:84–90, 2022.

433 Srivastava, A., Rastogi, A., and Abhishek Rao, e. a. Beyond the imitation game: Quantifying and
434 extrapolating the capabilities of language models, 2023.

435 Sun, Y., Dong, L., Huang, S., Ma, S., Xia, Y., Xue, J., Wang, J., and Wei, F. Retentive network: A
436 successor to transformer for large language models, 2023.

437 Suzgun, M., Scales, N., Schärli, N., Gehrmann, S., Tay, Y., Chung, H. W., Chowdhery, A., Le, Q. V.,
438 Chi, E. H., Zhou, D., and Wei, J. Challenging big-bench tasks and whether chain-of-thought can
439 solve them, 2022.

440 van der Maaten, L. Barnes-hut-sne, 2013.

441 Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., Kaiser, L., and
442 Polosukhin, I. Attention is all you need, 2023.

443 Wong, L., Grand, G., Lew, A. K., Goodman, N. D., Mansinghka, V. K., Andreas, J., and Tenenbaum,
444 J. B. From word models to world models: Translating from natural language to the probabilistic
445 language of thought, 2023.

446 Yarotsky, D. Error bounds for approximations with deep relu networks. *CoRR*, abs/1610.01145, 2016.
447 URL <http://arxiv.org/abs/1610.01145>.

448 **A Additional Proofs**

449 For any \mathbb{D} , let $d = \lceil \log(|\mathbb{D}|) \rceil + 1$ and let $\Psi : \mathbb{D} \rightarrow \{0, 1\}^d$ be a one-to-one mapping of tokens to
450 Boolean vectors, s.t. $\Psi_1(s) = 1$ for all $s \in \mathbb{D}$.

451 **Definition 9.** A function $f : \mathbb{D}^L \rightarrow \mathbb{D}$ is called *k*-Junta if there exists a set of separate indexes
452 $i_1, \dots, i_k \in [L]$ and function $g : \mathbb{D}^k \rightarrow \mathbb{D}$ s.t. $f(\mathbf{x}) = g(x_{i_1}, \dots, x_{i_k})$.

453 **Lemma 10.** For every *k*-Junta $f : \mathbb{D}^L \rightarrow \mathbb{D}$, there exists a tree \mathcal{T} of size $O(|\mathbb{D}|^k)$ and depth
454 $O(k \log |\mathbb{D}|)$ s.t. $\mathcal{T}(\Psi(\mathbf{x})) = f(\mathbf{x})$ for all $\mathbf{x} \in \mathbb{D}^L$.

455 *Proof.* Let \mathcal{T} the perfect binary tree of depth dk , where each level of the tree corresponds to a pair
456 $(j, l) \in [k] \times [d]$, and all the nodes at the level implement the condition $\Psi_l(x_{i_j}) \geq 1$. Observe that in
457 this construction, each leaf correspond to a specific choice of values for $\Psi(x_{i_1}), \dots, \Psi(x_{i_k})$, and we
458 can set its output to be $g(x_{i_1}, \dots, x_{i_k})$. \square

459 *Proof of Theorem 3.* Let \mathcal{A} be some automaton, defined by transition function $\delta : Q \times \Sigma \rightarrow Q$, and we
460 can arbitrarily extend it to $\delta : \mathbb{D}^2 \rightarrow \mathbb{D}$ s.t. $\delta(x, \langle \text{PAD} \rangle) = q_0$ for all $x \in \mathbb{D}$. Then, from Theorem 10
461 there exists some tree \mathcal{T} of size $O(|\mathbb{D}|^2)$ s.t. for all $\mathbf{x} \in \mathbb{D}^L$ it holds that $\mathcal{T}(\Psi(\mathbf{x})) = \delta(x_L, x_{L-n})$.

462 We prove by induction that for all $i \in [n]$ it holds that $\mathcal{T}_i^{\text{AR}}(\mathbf{x}) = q_i$, where q_i is the state of the
463 automaton \mathcal{A} at iteration i .

464 • Let $\mathbf{z} \in \mathbb{R}^{L,d}$ be the padded output of $\Psi(\mathbf{x})$, i.e. $\mathbf{z} =$
465 $[\Psi(\langle \text{PAD} \rangle), \dots, \Psi(\langle \text{PAD} \rangle), \Psi(x_1), \dots, \Psi(x_n)]$. Note that since $x_{L-n} = \langle \text{PAD} \rangle$
466 we have $\mathcal{T}_1^{\text{AR}}(\mathbf{x}) = \mathcal{T}(\mathbf{z}) = \delta(x_L, \langle \text{PAD} \rangle) = q_1$.

467 • Assume that $\mathcal{T}_{1:i-1}^{\text{AR}}(\mathbf{x}) = (q_1, \dots, q_{i-1})$. Therefore,

$$\begin{aligned} \mathcal{T}_i^{\text{AR}}(\mathbf{x}) &= \mathcal{T}(\Psi(\langle \text{PAD} \rangle, \dots, \langle \text{PAD} \rangle, x_1, \dots, x_n, q_1, \dots, q_{i-1})) \\ &= \delta(q_{i-1}, x_i) = q_i \end{aligned}$$

468 Therefore, the required follows. \square

469 *Proof of Theorem 6.* We encode the state of the Turing machine by a string $\mathbf{s} \in \mathbb{D}^{M+1}$ as follows:
470 if the head is in state $q \in Q$ and at position $i \in [M]$, and the memory is $m_1, \dots, m_M \in \Sigma$, we set
471 $\mathbf{s} = (m_1, \dots, m_{i-1}, q, m_i, \dots, m_M)$. That is, we add a token indicating the state of the head *before*
472 the cell where the head is located. Let $\delta : Q \times \Sigma \rightarrow Q \times \Sigma \times \{\langle \text{LEFT} \rangle, \langle \text{RIGHT} \rangle\}$ be the transition
473 function of the Turing machine. We define the following function $g : \mathbb{D}^4 \rightarrow \mathbb{D}^4$:

$$g(\mathbf{s}) = \begin{cases} x_2 & \text{if } x_1, x_2, x_3 \notin Q \\ q & \text{if } x_1 \in Q \text{ and } \delta(x_1, x_2) = (q, \alpha, \langle \text{RIGHT} \rangle) \\ \alpha & \text{if } x_1 \in Q \text{ and } \delta(x_1, x_2) = (q, \alpha, \langle \text{LEFT} \rangle) \\ \alpha & \text{if } x_2 \in Q \text{ and } \delta(x_2, x_3) = (q, \alpha, \langle \text{RIGHT} \rangle) \\ x_1 & \text{if } x_2 \in Q \text{ and } \delta(x_2, x_3) = (q, \alpha, \langle \text{LEFT} \rangle) \\ x_2 & \text{if } x_3 \in Q \text{ and } \delta(x_3, x_4) = (q, \alpha, \langle \text{RIGHT} \rangle) \\ q & \text{if } x_3 \in Q \text{ and } \delta(x_3, x_4) = (q, \alpha, \langle \text{LEFT} \rangle) \end{cases}$$

Observe that the function $f : \mathbb{D}^{M+1} \rightarrow \mathbb{D}^{M+1}$ s.t. $f_i(\mathbf{s}) = g(s_{i-1}, s_i, s_{i+1}, s_{i+2})$ exactly defines the
transition between the encoded states of the Turing machine. Namely, if the state of the machine at
iteration i is \mathbf{s} , then the state at iteration $i+1$ is $f(\mathbf{s})$. We slightly modify g to handle the generation
of the first iteration, as follows:

$$\tilde{g}(\mathbf{s}) = \begin{cases} \langle \text{SEP} \rangle & x_1 = \langle \text{PAD} \rangle \text{ and } x_2 = \langle \text{PAD} \rangle \text{ and } x_3 = \langle \text{PAD} \rangle \\ q_0 & x_1 = \langle \text{PAD} \rangle \text{ and } x_2 = \langle \text{PAD} \rangle \text{ and } x_3 \neq \langle \text{PAD} \rangle \\ \langle \text{SEP} \rangle & x_2 = \langle \text{SEP} \rangle \\ g(\mathbf{s}) & \text{otherwise} \end{cases}$$

474 Now, from Lemma 10 there exists a tree \mathcal{T} of size $O(|\mathbb{D}|^4)$ s.t. $\mathcal{T}(\Psi(\mathbf{x})) = \tilde{g}(x_1, x_2, x_3, x_4)$.
 475 Let $s_1, \dots, s_T \in \mathbb{D}^{M+1}$ the encodings of the state of the Turing machine at iterations $1, \dots, T$. Let
 476 $\mathbf{x} \in \mathbb{D}^L$ be the encoding of the input, starting with $\langle \text{PAD} \rangle$ tokens, followed by one $\langle \text{BOS} \rangle$ token and
 477 the input string. Denote the output of the ARDT \mathcal{T}^{AR} after $T \cdot (M + 2)$ given the input \mathbf{x} , where we
 478 split the output into chunks of size $M + 2$ by:

$$\mathcal{T}^{\text{AR}}(\mathbf{x}) = (z_1, \dots, z_T) \in \mathbb{D}^{T \cdot (M+2)}, z_i \in \mathbb{D}^{M+2}$$

479 **Claim:** For all $i \in [T]$, it holds that $z_i = (\langle \text{SEP} \rangle, s_i)$.

480 **Prove:** We prove by induction on i .

481 • For $i = 1$, notice that the input begins with 3 $\langle \text{PAD} \rangle$ tokens, followed by the input tokens
 482 x_1, \dots, x_M , and therefore by definition of \tilde{g} we get $z_1 = (\langle \text{SEP} \rangle, q_0, x_1, \dots, x_M) =$
 483 $(\langle \text{SEP} \rangle, s_1)$.

• Assume the required holds for i . First, observe that

$$z_{i+1,1} = \mathcal{T}(\Psi(s_{i-1,M+1}, \langle \text{SEP} \rangle, s_{i,1}, \dots, s_{i,M+1})) = \langle \text{SEP} \rangle$$

484 Now, assume that $z_{i+1,1:j} = (\langle \text{SEP} \rangle, s_{i+1,1}, \dots, s_{i+1,j-1})$. Therefore

$$\begin{aligned} z_{i+1,j+1} &= \mathcal{T}(\Psi(s_{i,j-1}, s_{i,j}, s_{i,j+1}, \dots, s_{i,M+1}, \langle \text{SEP} \rangle, s_{i+1,1}, \dots, s_{i+1,j-1})) \\ &= g(s_{i,j-1}, s_{i,j}, s_{i,j+1}, s_{i,j+2}) = s_{i+1,j} \end{aligned}$$

485 and by induction we get $z_{i+1} = (\langle \text{SEP} \rangle, s_{i+1})$

486 Therefore, \mathcal{T} outputs the final token of iteration T after $T(M + 2)$ steps of auto-regression, which
 487 proves the theorem. \square

488 B Additional Implementation Details

489 B.1 Hardware & Computational Cost

490 Our experiments were conducted on a single NVIDIA A100 GPU. For the Tiny Stories experiments,
 491 the training process took approximately 1 hour, and it required about 1 second to generate 20 words
 492 during the inference phase.

493 B.2 Dataset Details

494 **Tiny Stories.** As shown in Tab. 3, the training and validation datasets of Tiny Stories contain
 495 147,273 and 21,990 stories, respectively. We use NLTK Bird et al. (2009) as the tokenizer to obtain
 496 420,351,665 and 4,329,963 tokens from the training dataset. In the training dataset and validation
 497 dataset, the number of words in the vocabulary is 27,455 and 11,273, respectively.

498 **BIG-Bench-Hard** is a dataset contains the selection of 23 difficult tasks from the BIG-Bench. These
 499 tasks are identified by their resistance to being outperformed by prior language model evaluations
 500 when compared to the average human evaluator. The BIG-Bench-Hard tasks often demand complex,
 501 multi-step reasoning, and the use of few-shot prompting without CoT, as previously utilized in
 502 BIG-Bench evaluations Srivastava et al. (2023), significantly underrepresents the true potential and
 503 performance of language models.

504 Four representative reasoning tasks we select for evaluate our ARDTs:

505 (1) *Boolean Expressions*. Example: not (True) and (True). Answer: False.

506 (2) *Navigate*. Example: If you follow these instructions, will you return to the starting point?
 507 Instructions: Turn left. Take 5 steps. Turn right. Answer: No.

508 (3) *Web-of-Lies*. Example: Delbert tells the truth. Delfina says Delbert lies. Antwan says Delfina tells
 509 the truth. Does Delfina tell the truth? Answer: No.

510 (4) *Sports Understanding*. Example: Is the following sentence plausible? "Elias Lindholm beat the
 511 buzzer." Answer: No.

Table 3: Basic Information about the Tinystories Dataset.

	Training dataset	Validation dataset
The number of stories	147,273	21,990
The number of tokens	420,351,665	4,329,963
The word count of each story.	54 - 5,498	63 - 4,254
Vocabulary	27455	11274

512 **B.3 Details about the Visualization of the Decision Trees**

513 To enable visualization that treats words as features, as shown in Algorithm 1, we map word
 514 embeddings into a lower-dimensional space. This process utilizes three primary inputs: word
 515 embeddings W in an $N \times 100$ matrix, where N represents the number of words and 100 the
 516 dimensionality of each embedding; cluster centers C in a 20×100 matrix, indicating 20 clusters
 517 within the 100-dimensional embedding space; and a mapping matrix M sized 100×20 , designed
 518 to reduce the embeddings' dimensionality to 20. The algorithm begins with an orthogonalization
 519 procedure, applying QR decomposition to the transpose of C (C^T) and returning the first 20 columns
 520 of Q^T , thereby establishing an orthogonal basis for the cluster space. It then projects the word
 521 embeddings W into this lower-dimensional space by multiplying them with the mapping matrix M .
 522 By iterating over each word embedding in W , the algorithm applies this projection and ultimately
 523 returns a set of transformed embeddings $\{E_1, \dots, E_N\}$, where each E_i provides a lower-dimensional
 524 representation of the corresponding word embedding. This approach allows us to treat each vector
 525 value as individual words, facilitating a more intuitive understanding of the data.

Algorithm 1 Map Word Embeddings to Lower Dimensional Space

```

input
  Word Embeddings  $W \subseteq \mathbb{R}^{N \times 100}$ 
  Cluster Centers  $C \subseteq \mathbb{R}^{20 \times 100}$ 
  Mapping Matrix  $M \subseteq \mathbb{R}^{100 \times 20}$ 
procedure ORTHOGONALIZE( $C$ )
   $Q, R \leftarrow$  QR Decomposition( $C^T$ )
  return  $Q[:, : 20].T$ 
end procedure

procedure MAPEMBEDDINGS( $W, M$ )
  return  $W \cdot M$ 
end procedure

 $M \leftarrow$  ORTHOGONALIZE( $C$ )
for each word embedding  $w_i$  in  $W$  do
   $E_i \leftarrow$  MAPEMBEDDINGS( $w_i, M$ )
end for
Return  $\{E_1, \dots, E_N\}$ 

```

526 **B.4 The Story Beginnings Used in Our Evaluation**

527 In Table 6, we provide 10 examples over 100 story beginnings we used for our experiments on Tiny
 528 Stories.

529 **B.5 An Example on Multidimensional Scores**

530 As an example, we took the story that appears in the example above and cut it after the word "loud".
 531 We generated a completion of stories using our ARDTs and baselines, then we prompted GPT-4 to
 532 first provide a verbal assessment and then grade the completion. The transcript of interaction is as
 533 follows, with the parts produced by GPT-4 in italic font:

Table 4: Generated Chain-of-Thought data for boolean expression.

Input Prompt	not not (not (False)) is	True and False and not True and True is
Generated Prompt	<p>Let's think step by step.</p> <p>Remember that (i) expressions inside brackets are always evaluated first and that (ii) the order of operations from highest priority to lowest priority is "not", "and", "or", respectively. We first simplify this expression "Z" as follows: "Z = not not (not (False)) = not not (A)" where "A = not (False)". Let's evaluate A: A = not (False) = not False = True. Plugging in A, we get: Z = not not (A) = not not (True) = not not False = True. So the answer is True.</p>	<p>Let's think step by step. Remember that (i) expressions inside brackets are always evaluated first and that (ii) the order of operations from highest priority to lowest priority is "not", "and", "or", respectively. We first simplify this expression "Z" as follows: "Z = True and False and not True and True = A and B" where "A = True and False" and "B = not True and True". Let's evaluate A: A = True and False = False. Let's evaluate B: B = not True and True = not (True and True) = not (True) = False. Plugging in A and B, we get: Z = A and B = False and False = False. So the answer is False.</p>

Table 5: Generated Chain-of-Thought data for navigation.

Input Prompt	If you follow these instructions, do you return to the starting point? Always face forward. Take 2 steps right. Take 9 steps left. Take 7 steps right.	If you follow these instructions, do you return to the starting point? Turn around. Take 1 step. Take 6 steps. Turn around. Take 6 steps. Take 9 steps. Take 1 step.
Generated Prompt	<p>Let's think step by step. We start at the origin (0, 0), facing the positive y-axis. (1) Always face forward: (0, 0), facing the positive y-axis. (2) Take 2 steps right: (0, 2), facing the positive y-axis. (3) Take 9 steps left: (0, -7), facing the positive y-axis. (4) Take 7 steps right: (0, 7), facing the positive y-axis. Since (0, 0) is (0, 0), we are indeed where we started. So the answer is Yes.</p>	<p>Let's think step by step. We start at the origin (0, 0), facing the positive y-axis. (1) Turn around: (0, 0), facing the negative y-axis. (2) Take 1 step: (0, -1), facing the negative y-axis. (3) Take 6 steps: (0, -7), facing the negative y-axis. (4) Turn around: (0, -7), facing the positive y-axis. (5) Take 6 steps: (0, -1), facing the positive y-axis. (6) Take 9 steps: (0, 8), facing the positive y-axis. (7) Take 1 step: (0, 9), facing the positive y-axis. Since (0, 9) is not (0, 0), we are not where we started. So the answer is No.</p>

Table 6: Examples of the story beginnings generated by GPT-4. In the inference phase, we fed these story beginnings generated by GPT-4 into the ARDTs to continue writing the stories.

The beginning of the stories (GPT-4 generated)	
1	Kitty found a bright, lost treasure.
2	Thirsty, they sought a hidden pond.
3	Roxy climbed, seeking icy hill's peak.
4	Billy's idea sparked an unlikely friendship.
5	Leaves underfoot, Roxy ascended triumphantly.
6	Daisy, small yet happy, met Max.
7	Max's playful antics delighted tiny Daisy.
8	Sue's thoughtful gesture warmed her mother.
9	A candle's flame united mother, daughter.
10	The sad cow wished for companionship.

534 the following exercise, the student is given a beginning of a story. The student needs
 535 to complete it into a full story. The exercise tests the student's language abilities and
 536 creativity. The symbol *** marks the separator between the prescribed beginning
 537 and the student's completion:

538 Once upon a time, *** there was a little girl named Lily. She loved to play outside in the
 539 sunshine. One day, she saw a big tree in the garden. She was so excited about it.

540 Please provide your general assessment about the part written by the student (the one
 541 after the *** symbol). Is it grammatically correct? Is it consistent with the beginning
 542 of the story? Pay special attention to whether the student manages to complete the
 543 sentence which is split in the middle by the separator ***.

544 This is a charming and whimsical story about a little girl named Lily who feels excited upon
 545 discovering a big tree in the garden.

546 The grammar is generally correct.

547 Overall, the student's completion of the story demonstrates adequate language abilities and
 548 creativity. However, adding more details about Lily's exploration, as well as her thoughts
 549 and actions after discovering the tree, could make the story more engaging and vivid.

550 Now, grade the student's completion in terms of grammar, creativity, consistency with the
 551 story's beginning and whether the plot makes sense. Moreover, please provide your best
 552 guess of what the age of the student might be, as reflected from the completion. Choose
 553 from possible age groups: A: 3 or under. B: 4-5. C: 6-7. D: 8-9. E: 10-12. F: 13-16.

554 Grammar: 9/10, Creativity: 4/10, Consistency: 7/10, Age group: E (10-12)

555 C Interpretability

556 One advantage of using decision trees over complex neural networks is the Interpretability of the
 557 computational process. Unlike neural networks, which rely on abstract vector operations in high-
 558 dimensional space, decision trees implement relatively simple logic, computing their output based on
 559 splitting criteria that may be easily displayed to, and interpreted by, humans. That said, recall that
 560 our decision trees operate on aggregations of word vector embeddings, which make interpretability
 561 harder to achieve. Specifically, each splitting rule of the decision tree is based on the value of
 562 a single coordinate, which does not necessarily have an interpretable semantic value when using
 563 rotation-invariant word embedding methods such as Word2Vec.

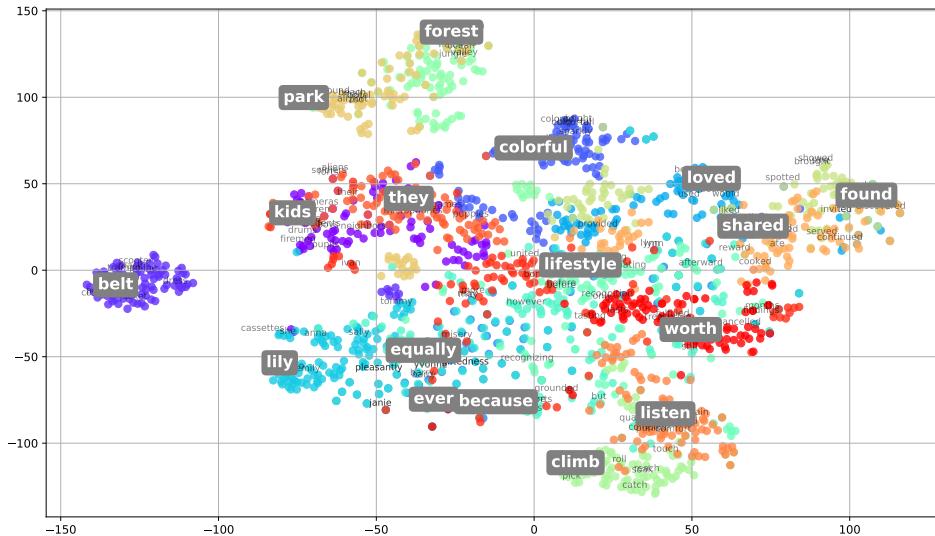


Figure 3: t-SNE van der Maaten (2013) visualization of 20 cluster centers. We selected 20 cluster centers and display 4 words closest to the cluster centers.

564 In order to generate decision trees with meaningful splitting rules, we modify the word embedding
 565 such that single coordinates have specific semantic values. To achieve this, we begin by clustering
 566 all the word vectors from the dataset (over 16K words) into 20 clusters using K-means. We then
 567 choose one representative word for each cluster, by taking the word that is closest to the center of

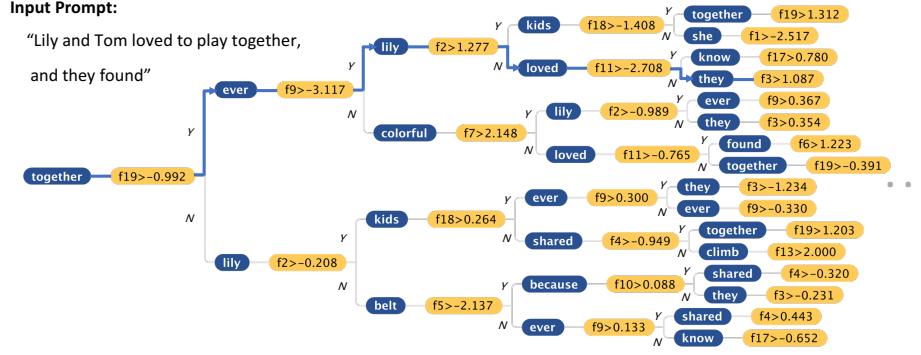


Figure 4: **Track the decision-making process within the decision trees.** We use 'Lily and Tom loved to play together, and they found' as an input prompt and generate the next word using our ARDTs. We visualize part of the process within the decision tree. Specifically, we visualized 31 nodes of the first decision tree.

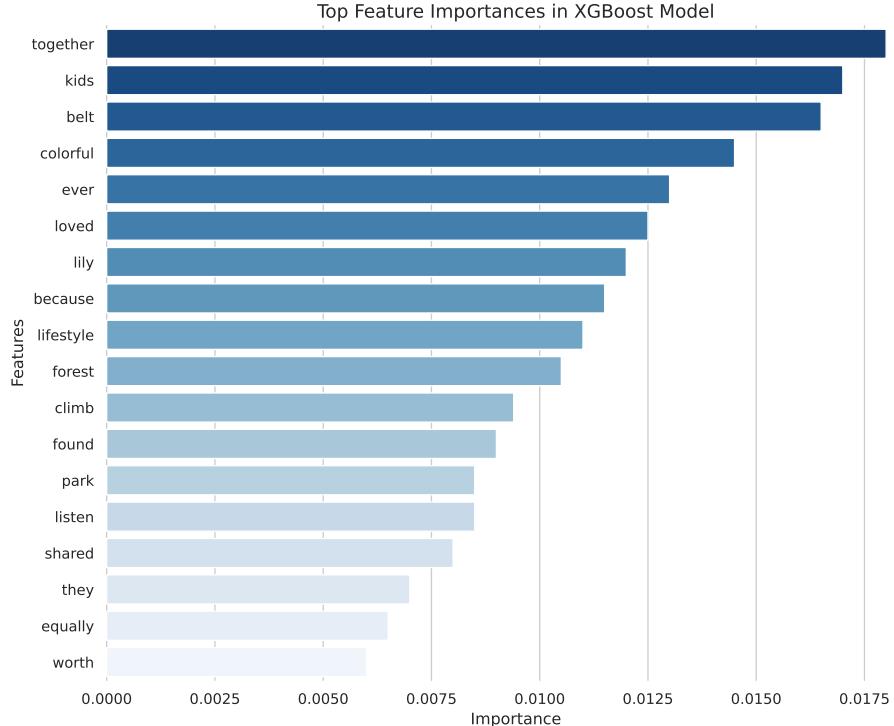


Figure 5: Feature Importance. We present the feature importance of the top 20 words most closely associated with each cluster, based on their average gain.

568 the cluster in the embedding space (see Figure 3 for an illustration of the clusters and representative
 569 words). Now, these words (represented as vectors) form a basis for a new 20-dimensional embedding
 570 space, which is a linear subspace of the original 100-dimensional space of Word2Vec. We use these
 571 basis words to compute the new word embedding, by projecting each vector from the original space
 572 into this subspace, and representing the projection as a linear combination of the basis words.
 573 Mathematically, if x_1, \dots, x_k are the basis words, we define our new embedding Φ into \mathbb{R}^k by:
 574 $\Phi(x) = \arg \min_{z \in \mathbb{R}^k} \|\sum_i z_i \Psi(x_i) - \Psi(x)\|_2$. Observe that each basis word x_i is mapped by Φ to
 575 a unit vector e_i . Intuitively, the i -th coordinate of the embedding Φ now represents words that are
 576 semantically similar to the word x_i . Now, splitting rules based on the coordinate i can be interpreted
 577 as "testing" whether a word similar to x_i appears in the sentence.

578 We visualize one of the decision trees trained on the Tiny Stories Dataset using the new “interpretable”
579 embedding Φ in Figure 1. Note that, unlike complex neural network architectures, which carry out
580 opaque computations, the decision process of the ARDT with the new embedding appears to be
581 semantically meaningful. For example, observe that the word *Lily* appears for three times as the
582 most relevant word during node splits. Considering *Lily* is a frequently occurring name in the Tiny
583 Stories dataset, its frequent appearance in the tree can be deemed reasonable. We further analyze
584 the importance of different features by plotting their importance score. We plot the importance of
585 each cluster, represented by a single word, in Figure 5. We assess the importance of each cluster by
586 calculating its average gain during every split within the model.

587 In Figure 4, we use the input sentence “Lily and Tom loved to play together and they found” as an
588 example to visualize part of the decision-making process of the first decision tree in the ensemble.
589 We note that each feature corresponds to a single cluster, represented by a single word, e.g. the
590 feature f_2 corresponds to the word “Lily”. That is, the word “Lily” will be mapped to the unit vector
591 $e_2 = (0, 1, 0, \dots, 0)$. Note that most words (besides the 20 words used as a basis for the embedding),
592 will be mapped to a linear combination of the basis words, and so can also affect (positively or
593 negatively) the value of the feature f_2 . Since the input vector is a weighted-average of the embedding
594 of all words, the decision when splitting on the feature f_2 may be affected by multiple words in the
595 sentence.