Why are state-space models more expressive than n-gram models?

Abstract

Recent advancements in recurrent neural networks (RNNs) have reinvigorated interest in their application to natural language processing tasks, particularly with the development of more efficient and parallelizable variants known as state space models (SSMs), which have shown competitive performance against transformer models while maintaining a lower memory footprint. While RNNs and SSMs (e.g., Mamba) have been empirically more successful than rule-based systems based on n-gram models, a rigorous theoretical explanation for this success has not yet been developed, as it is unclear how these models encode the combinatorial rules that govern the next-word prediction task. In this paper, we construct state space language models that can solve the next-word prediction task for languages generated from n-gram rules, thereby showing that the former are more expressive. Our proof shows how SSMs can encode n-gram rules using new theoretical results on their memorization capacity, and demonstrates how their context window can be controlled by restricting the spectrum of the hidden weight matrix. We conduct experiments with a small dataset generated from n-gram rules to show how our framework can be applied to SSMs and RNNs obtained through gradient-based optimization.

1 Introduction

Over the past two decades, breakthroughs in deep learning have revolutionized natural language processing tasks, including language modeling (Radford et al. (2018), Radford et al. (2019)), question-answering (Devlin et al. (2018), Yang et al. (2019)), and machine translation Sutskever et al. (2014). While n-gram models were used widely for next-word prediction before the advent of deep learning, empirically it was found that language models using recurrent neural networks (RNNs) were more effective for complex tasks. Although transformer models, with their attention-based layers, have since led to significant advancements in these tasks Vaswani et al. (2017), recent research has revisited RNN architectures Beck et al. (2024); Feng et al. (2024); Peng et al. (2023), and investigated variants known as state space models (SSMs). Notably, SSMs Gu et al. (2022; 2021); Wang & Xue (2024); Gu & Dao (2024) can be trained efficiently in parallel like transformers, while requiring less memory than transformers for inference.

Recent advances have largely been empirical, with new deep learning architectures developed through experimentation and validated on large datasets Liu et al. (2019); Radford et al. (2018; 2019). A key open problem in natural language processing is to provide a rigorous theoretical framework for the success of deep learning models on next-word prediction tasks. Such a framework could lead to the design of more efficient architectures for SSMs and RNNs, and provide additional insights into the inner workings of these black-box models. A theoretical understanding of how SSMs and RNNs obtained through gradient-based optimization techniques encode the rules governing n-gram languages, and solve the next-word prediction task in this context, would be a first step towards a more rigorous mathematical framework explaining their success in natural language processing.

To theoretically explain the empirical success of these deep learning models, researchers have drawn upon mathematical models based on languages defined by formal grammars Chomsky (1956; 1959); Chomsky & Schützenberger (1963) and universal approximation theory Wang & Xue (2024). While simple examples

of formal grammars like $a^n b^n$ and boolean expressions have been studied with neural networks in Gers & Schmidhuber (2001); Sennhauser & Berwick (2018), these are often too restrictive to capture the nuances of natural language. Another key result is the Turing completeness of RNNs Chung & Siegelmann (2021), which implies that they can solve recognize recursively enumerable languages. However, the proof uses weights that have unbounded precision (or unbounded memory), which does not explain their success in practical applications. While existing results on state space models Wang & Xue (2024) establishes their ability to approximate continuous sequence-to-sequence maps, it cannot be immediately extended to discrete language modelling tasks involving next-word prediction.

In this paper we study the question of why state space models are more expressive than languages based on n-gram rules from a theoretical viewpoint. Given a language generated from a set of n-gram rules, we construct a state space model that can solve next-word prediction for this language. Our construction provides additional insight into the interpretability of SSMs and RNNs, and in particular the role of the hidden weight matrix and the neurons in the hidden layer. The contributions of this work can be summarized as follows.

- Our first key insight is that, in the context of n-gram models, next-word prediction is equivalent to memorizing the n-gram rules. Based on the observation that the embedding layer transforms the sequence of input words into a sequence of vectors, we reduce the problem to demonstrating that SSMs can memorize a set of input-output vectors under mild assumptions.

- Our key technical result provides a theoretical analysis of the memorization capacity of SSMs, extending similar findings in feedforward networks (see Yun et al. (2019)). This result is of independent interest and offers deeper insights into their behaviour.

- We analyze the context window of SSMs, particularly focusing on when the network's output depends solely on the most recent n inputs. We demonstrate that this behaviour is closely related to the spectral decomposition of the hidden-to-hidden weight matrix.

- We conduct experiments with toy data consisting of English sentences generated from n-gram languages, and show how our theoretical insights can be applied to SSMs obtained via gradient-based optimization. We also discuss how our framework can be extended to RNNs, which incorporate a non-linearity into the hidden state update.

The paper is organized as follows. In Section 2, we describe related work on the theoretical underpinnings of language modelling with neural networks. In Section 3, we recall the definition of n-gram languages and state space models, and give an overview of the main results. In Section 4, we state the main results with a construction of SSMs that solve the next-word prediction task, and outline the proof. In Section 5, we apply our theoretical framework to SSMs and RNNs that are trained with gradient-based optimization on a simple dataset from n-gram rules. In Sections 6, we discuss further directions based on our theoretical results. In the Appendix, we present detailed proofs of the main results.

2 Related work

Comparison between neural networks and n-gram models. The experiments in Bengio et al. (2003) using the Brown corpus and the Associated Press News corpus show that language models based on feedforward neural networks achieve lower perplexity scores compared to n-gram models (here the perplexity metric quantifies the model's ability to predict the next word in a sequence). In Chelba et al. (2017), empirical comparisons between RNNs and n-gram models have demonstrated the superior performance of RNNs for next-word prediction, based on experiments conducted using the UPenn TreeBank corpus and the One Billion Words benchmark. In Svete & Cotterell (2024), the authors theoretically analyze how transformer models can solve next-word prediction for datasets generated from n-gram rules, but their choice of query-key matrices only retain information about the positional encoding and not the word embedding, limiting their applicability to models trained using gradient-based optimization. In Jelassi et al. (2024), the authors theoretically analyze the effectiveness of transformers and SSMs on copying tasks that involve n-gram rules, but their experiments do not provide insights into the inner workings of these models. Our work complements these empirical

findings by providing a rigorous theoretical framework explaining how SSMs encode n-gram rules, which can be used to derive insights about the hidden layers and weights of SSMs and RNNs trained on simple datasets with stochastic gradient descent.

Memorization and learning. While memorization refers to the model's ability to fit pre-specified input-output pairs, learning involves capturing the underlying patterns or distributions present in the data, enabling the model to make accurate predictions on new, unseen inputs. The differences between memorization and learning have been analyzed through an empirical lens with gradient-based optimization in Arpit et al. (2017). The memorization capacity of feedforward neural networks has been studied theoretically in Yun et al. (2019); Zhang et al. (2017); Huang & Huang (1991), but their work does not extend to SSMs or RNNs. Our work builds on these theoretical results by analyzing the memorization capacity of SSMs, and illustrates how memorization enables deep learning models to encode n-gram rules for next-word prediction.

On the expressiveness of RNNs and SSMs. In Wang & Xue (2024), it is shown SSMs with layer-wise nonlinear activation can approximate any continuous sequence-to-sequence function with arbitrarily small error, building on analogous results for RNNs. It has also been theoretically demonstrated that both RNNs and transformers are Turing complete, meaning they have the computational power to simulate any Turing machine given sufficient time and resources Pérez et al. (2021); Chung & Siegelmann (2021). The connection between RNNs and formal languages can be viewed through the lens of the Chomsky hierarchy, Chomsky (1956), which classifies formal languages into four categories — regular, context-free, context-sensitive, and recursively enumerable — based on their generative power. RNNs, due to their Turing completeness, can theoretically recognize languages across this entire hierarchy Chung & Siegelmann (2021), but the construction there uses weights that have unbounded precision or unbounded memory, which are not realistic in practice. Our work complements these studies by presenting a theoretical framework showing how SSMs can model languages generated from n-gram rules without imposing any unrealistic assumptions, and we show how our theory can be applied to models trained via gradient-based optimization on simple datasets.

Learning formal languages with stochastic gradient descent. There has been a line of work using special cases of formal languages to investigate how they can be learnt with stochastic gradient descent using commonly used neural network architectures, such as LSTMs to transformers Ackerman & Cybenko (2020). The effectiveness of LSTM models on the languages $a^n b^n$ (and variants thereof) was established in Gers & Schmidhuber (2001), Bodén & Wiles (2000), while similar results for Dyck languages were obtained in Sennhauser & Berwick (2018). In the latter context, LSTM models require exponential memory in terms of the input length, and do not learn the underlying combinatorial rules perfectly. Analogous experiments with Dyck languages were carried out with transformer-based models in Ebrahimi et al. (2020), and the inner workings of these models were studied. However, the simple examples of formal languages studied in these papers do not model the English language effectively, and are less realistic than languages based on n-gram rules. While an extensive empirical evaluation was conducted in Delétang et al. (2023) by training a variety of neural network models on more complex formal languages, a theoretical understanding of these models is lacking. Our work complements these studies by presenting a theoretical framework showing how SSMs and RNNs can encode n-gram rules, as we demonstrate with experimental results using stochastic gradient descent.

3 Preliminaries on language modelling.

In this section we recall the definitions of n-gram languages and state space models, describing how they can be used for next-word prediction. We then give an overview of the main results in our work.

3.1 n-**gram languages**

In this section, we rigorously define the mathematical linguistics models used in our work, focusing on *n-gram language*. An n-gram language generates sequences by estimating the probability of each word based on the preceding words, capturing local dependencies within a sequence Katz (1987); Goodman (2001). These models, widely used in natural language processing, can approximate real-world sentences but struggle with long-range dependencies Goldberg & Orwant (2013). They may be viewed as a special case of a formal

grammar, which provide a more general mathematical framework for generating strings based on a set of combinatorial rules Chomsky (1956).

Definition 3.1. An *n-gram language* $\overline{\mathcal{L}}$ consists of the components $(\mathcal{W}, \mathcal{P}, \mathcal{I})$ (the integer n is also fixed).

- Let $\mathcal{W}$ be a finite set, consisting of all words occurring in the language. Let $\mathcal{W}^* := \mathcal{W} \cup \{\emptyset\}$, and $d = |\mathcal{W}|$.

- Let $\mathcal{P} \subset (\mathcal{W}^*)^n$ be the set of all valid n-grams, i.e., the set of all valid sequences of n consecutive words.

- Let $\mathcal{I} \subset (\mathcal{W}^*)^n$ be the set of all valid initial sequences of n words that can precede any word in $\mathcal{W}$ to form an n-gram.

Given the above data, the language $\overline{\mathcal{L}}$ can be generated as follows. For convenience, we augment sentences with $\emptyset$ symbols so that all sentences have a fixed length N.

- A *valid sequence* is a sequence of words $(w_1, \cdots, w_l)$ such that each subsequence of n consecutive words $(w_i, \cdots, w_{i+n-1})$ for $1 \leq i \leq l - n + 1$ is an element of $\mathcal{P}$.

- A *valid sentence* is a sequence $(w_1, \cdots, w_N)$ such that $(w_1, \cdots, w_l)$ is a valid sequence, and $(w_{l+1}, \cdots, w_N) = (\emptyset, \cdots, \emptyset)$, for some $l \leq N$. The set $\overline{\mathcal{L}} \subset (\mathcal{W}^*)^N$ consists of all valid sentences. ∎

Example. We start with the following example of a language generated from n-gram rules, based on text from J.K.Rowling's "Harry Potter". We use the following two sentences as a starting point: *"Harry woke at five o'clock and was too excited to go back to sleep.", "He got up and pulled on his jeans because he didn't want to walk into the station in his robes."*

Intuitively our language consists of sentences which resemble these, in the following sense. In the first sentence, the words "Harry", "five", "excited" and "sleep" can be replaced with variants to create valid sentences (eg. "Ron", "seven", "angry" and "bed", respectively). See Table 1 for a partial list of n-gram rules that can be used to generate this language; we refer the reader to the Appendix for a full list. Below we list examples of sentences from the language $\overline{\mathcal{L}}$ (the $\emptyset$ symbols are omitted).

- "Ron woke at seven o'clock and was too upset to go back to bed."

- "He rose up and pulled on his denims because he didn't want to saunter into the platform in his trunks."

- "Draco woke at three o'clock and was too elated to go back to sleep."

- "He got up and pulled on his slacks because he didn't want to run into the platform in his boxers."

3.2 Language models

In this section, we formalize the language modelling task, which has been studied extensively in empirical work Radford et al. (2018), Radford et al. (2019) (it is often referred to as "text generation" or "text completion"). The input is a sequence of words $(w_1, \cdots, w_k)$, where the length k can vary (with $k < N$). The desired output is a sequence of words $(w_{k+1}, \cdots, w_N)$ with length $N - k$, so that the composite sequence $(w_1, \cdots, w_N)$ is a valid sentence. We restrict our attention to those input sequences which can be completed to obtain a valid sentence; see below for a precise formulation.

Definition 3.2. Given a sequence of words $\underline{w} = (w_1, \cdots, w_N) \in (\mathcal{W}^*)^N$, define $I(\underline{w})$ as follows.

$$I(\underline{w}) = \begin{cases} 1 \text{ if } (w_1, \cdots, w_N) \in \overline{\mathcal{L}} \\ 0 \text{ otherwise} \end{cases}$$

Fred woke at	George woke at	Harry woke at	He didn't want	He got up
and pulled on	and put on	and was too	apartment in his	at five o'clock
at six o'clock	back to bed.	back to sleep.	because he didn't	building in his
didn't want to	elated to go	excited to go	five o'clock and	go back to
his denims because	his pants because	his slacks because	house in his	in his boxers.
in his trunks.	in his underpants.	into the apartment	into the building	into the house
jog into the	nine o'clock and	on his denims	on his pants	on his slacks
pants because he	platform in his	pulled on his	put on his	rose up and
saunter into the	six o'clock and	slacks because he	sprint into the	stroll into the
the building in	the house in	the platform in	to go back	to jog into
to saunter into	to sprint into	to stroll into	too elated to	too excited to
up and put	want to jog	want to run	want to saunter	want to sprint
was too elated	was too excited	woke at five	woke at nine	woke at six

Table 1: List of n-gram rules, with $n = 3$

Given $1 \leq i < j \leq N$, define the truncated sequence $\underline{w}_{i:j} = (w_i, \cdots, w_j)$.

We say that sequence of words $\underline{w}' = (w_1, \cdots, w_k) \in \mathcal{W}^k$ is *valid starting sequence* if there exists another sequence $(w_{k+1}, \cdots, w_N)$ such that $(w_1, \cdots, w_k, w_{k+1}, \cdots, w_N) \in \overline{\mathcal{L}}$. Let $\overline{\mathcal{L}_k} \subset \mathcal{W}^k$ denote the set of all valid starting sequences. ∎

A language model takes as an input a sequence of words with variable length, and its output is a probability distribution that can be used to determine which words are likely to appear next in the sequence (see Goodman (2001), Katz (1987)). Given a valid starting sequence $(w_1, \cdots, w_k)$ with $n \leq k \leq N - 1$, we can use the language model f to generate the next word w_{k+1}, using the probability distribution associated with $f(w_1, \cdots, w_k)$. This process can be iterated to generate an output sentence $(w_{k+1}, \cdots, w_N)$, as described below. We evaluate how well f models the language $\overline{\mathcal{L}}$ using the risk $R(f)$, which is closely related to the perplexity metric that is used in empirical studies (Zaremba et al. (2014)).

Definition 3.3. A *language model* is a function f that takes in an input sequence $\underline{w} \in (\mathcal{W}^*)^k$, for some k, and outputs a vector of probabilities $f(\underline{w}) = (\hat{f}(w|\underline{w}))_{w \in \mathcal{W}^*}$. Here $\hat{f}(w|\underline{w})$ denotes the probability that the model f will output the word w given the input sequence $\underline{w}$.

Define its risk $R(f)$ as follows. Here the quantity $\overline{f}(\underline{w}'|\underline{w})$ below denotes the probability that the model f iteratively generates the output sequence $\underline{w}' = (w_{k+1}, \cdots, w_N)$ given an input sequence $\underline{w} = (w_1, \cdots, w_k)$, and $\underline{w} \oplus \underline{w}'$ denotes the concatenation of the two sequences. If the risk $R(f)$ is close to zero, this means that the language model f can accurately model the language $\overline{\mathcal{L}}$.

$$\overline{f}(\underline{w}'|\underline{w}) = \prod_{j=k}^{N-1} \mathbb{P}(w_{j+1} \mid w_1, \cdots, w_j) = \prod_{j=k}^{N-1} \hat{f}(w_{j+1} \mid w_1, \cdots, w_j)$$

$$R(f) = \frac{1}{N-n} \sum_{k=n}^{k=N-1} \frac{1}{|\overline{\mathcal{L}_k}|} \sum_{\underline{w} \in \overline{\mathcal{L}_k}, \underline{w}' \in (\mathcal{W}^*)^{N-k}} \hat{f}(\underline{w}'|\underline{w})(1 - I(\underline{w} \oplus \underline{w}')) \qquad ∎$$

3.3 State space language models

We start by recalling the definition of a state space model with a single hidden layer, following Section 4 of Zhang et al. (2018b). Below σ denotes the ReLU function applied to each coordinate of the corresponding vector. While it is almost the same as a recurrent neural network, in this setting the σ non-linearity is applied while computing the output, and not during the hidden state update. We note that while the bias term b_y is often not used in state space models, here we add it to the output to increase the expressiveness of the model.

Definition 3.4. A *one-layer state space model* $\mathcal{S}$ consists of an input layer, a hidden layer, and an output layer. The network is characterized by n_0 input neurons, n_h hidden neurons, and n_L output neurons. The weight

matrices are denoted by A, B, and C, where $A \in \mathrm{Mat}_{n_h, n_h}(\mathbb{R})$ is state transition matrix, $B \in \mathrm{Mat}_{n_0, n_h}(\mathbb{R})$ is the input-to-hidden matrix, and $C \in \mathrm{Mat}_{n_h, n_L}(\mathbb{R})$ is the hidden-to-output matrix. We omit the input-output matrix D, which is sometimes used to implement a skip connection.

It gives rise to a function $f_{\mathcal{S}} : (\mathbb{R}^{n_0})^T \to (\mathbb{R}^{n_L})^T$; the state space model processes a sequence of inputs $(x_1, x_2, \ldots, x_T)$, produces a sequence of hidden states $(h_1, h_2, \ldots, h_T)$ and yields outputs $(y_1, y_2, \ldots, y_T)$ via the following equations. Here $x_t \in \mathbb{R}^{n_0}$ is the input vector, $h_t \in \mathbb{R}^{n_h}$ is the hidden state vector, $y_t \in \mathbb{R}^{n_L}$ is the output vector, and b_y is a bias term.

$$h_t = A h_{t-1} + B x_t \quad y_t = C \sigma(h_t + b_y) \quad \blacksquare$$

We recall how state space models can be used for next-word prediction in language modelling tasks (see also Section 4.3 of Gu et al. (2022)). The two key components that we need are a state space model and an embedding layer. The input to the state space language model is a sequence of words, so we start with a preprocessing step that converts a sequence of words to a sequence of one-hot vectors. The dimension of the vector $\theta^*(\underline{w})$ is proportional to the number of words in $\mathcal{W}$, which is usually quite large. In order to reduce the dimension of the vector before feeding it into the state space model, we define an embedding layer as follows.

Definition 3.5. Let $\bar{i} : \mathcal{W}^* \to \{0, 1, \cdots, d\}$ be a bijective map such that $i(\emptyset) = 0$, where $d = |\mathcal{W}|$. We define the word representation $\theta : \mathcal{W}^* \to \mathbb{R}^{d+1}$ as the map which sends $w \in \mathcal{W}^*$ to the corresponding one-hot vector in $\mathbb{R}^{d+1}$ (i.e. with a 1 in the $i(w)$-th position and 0-s elsewhere). Given an embedding matrix $W_0 \in \mathrm{Mat}_{e, d+1}(\mathbb{R})$ with pairwise distinct columns, denote by $\phi_{W_0} : \mathbb{R}^{(d+1)} \to \mathbb{R}^e$ the induced function. The embedding function $\overline{E}$ is defined as below; we say that the embedding layer has dimension e.

$$\underline{w} = (w_1, \cdots, w_N); \qquad \overline{E}(\underline{w}) = [\phi_{W_0}\theta(w_1) \mid \cdots \mid \phi_{W_0}\theta(w_N)] \qquad \blacksquare$$

After the preprocessing step using the embedding layer, which sends $\underline{w}$ to $\overline{E}(\underline{w})$, the resulting vector can in turn be fed into a state space model, which then outputs a vector of probabilities by applying a softmax layer at the end.

Definition 3.6. A state space language model $f_{\mathcal{S}}^*$ is a function obtained by combining an embedding layer $\overline{E}$ as above, a state space model $\mathcal{S}$, and a softmax layer $\overline{\sigma}$. Here $\mathcal{S}$ has e input neurons, $d + 1$ output neurons and one hidden layer. It takes as input a sequence $\underline{w} = (w_1, \cdots, w_k)$ with variable length k, and outputs a probability vector in $\mathbb{R}^{d+1}$.

$$f_{\mathcal{S}}^*(\underline{w}) = \overline{\sigma} \circ f_{\mathcal{S}} \circ \overline{E}(\underline{w}) \qquad \blacksquare$$

4 Main results

4.1 Overview of main results

In deep learning, language models were first constructed by combining a neural network and an embedding layer Bengio et al. (2003); Mikolov et al. (2010); Hochreiter & Schmidhuber (1997). The embedding layer converts the input sequence of words into a vector, which is followed by a neural network component that converts this vector into a vector of output probabilities. This process is then iterated, by adding the new word to the original sequence and feeding it into the language model, until we obtain a sentence.

We use state space models, which build on the computational model of recurrent neural networks, to solve the next-word prediction task for a dataset generated from an n-gram language. More precisely, given any n-gram language $\overline{\mathcal{L}}$, we establish the existence of a state space model f which can solve the next-word prediction problem for $\overline{\mathcal{L}}$. Our proof is constructive, and gives insight into the role of memorization in language modelling tasks, and the context window of state space models.

Our proof relies on an analysis of the memorization capacity of state space models, extending analogous results on feedforward neural networks. We use this result to construct a language model that encodes all of the n-gram rules used to define the language $\mathcal{L}$. Our proof also analyses the context window of state space models, and shows that the model's output only depends on the last n input vectors when the hidden weight matrices satisfy a nilpotency constraint. We refer the reader to Appendix **??** for detailed proofs of all results.

4.2   Statement: overview

We present a framework for analyzing the next-word prediction problem for data generated from n-gram languages using state space models. In particular, we show the existence of a state space model which can solve the sentence completion problem with arbitrarily small error for any n-gram language $\overline{\mathcal{L}}$ (see above for the definition of $(\mathcal{W}, \mathcal{P}, \mathcal{I})$; noting in particular that $\mathcal{P}$ is the set of n-gram rules).

Theorem 4.1. *Let $\overline{\mathcal{L}}$ be an n-gram language generated from the datum $(\mathcal{W}, \mathcal{P}, \mathcal{I})$. Given an $\epsilon > 0$, there exists a state space language model $f_{\mathcal{S}}^*$ with the following properties:*

- *The model, $f_{\mathcal{S}}^*$, has error at most ϵ on the language $\overline{\mathcal{L}}$, i.e., $R(f_{\mathcal{S}}^*) < \epsilon$.*

- *The state space model component $\mathcal{S}$ can be chosen so that the number of neurons in the hidden layer is equal to $|\mathcal{P}|$, the number of n-gram rules in the language $\mathcal{L}$.*

- *The embedding layer has dimension e, where $e \geq 1$ is any fixed integer.* ∎

Our proof is constructive by nature. In the next section, we state a more precise version of the above Theorem which specifies the properties that the state space model must satisfy in order for the above to hold. To ensure that the state space model only processes the last n words in the input sequences, we impose a nilpotency restriction on the hidden weight matrix. We present new results on the memorization capacity of state space models, and use them to construct hidden layers that encodes each n-gram as a vector, with different n-grams corresponding to different vectors, which in turn produce output logits that govern next-word prediction. We also explain how our results can be extended to RNN architectures, where the hidden state update is non-linear. Existing results on Turing completeness of RNNs use either unbounded precision or unbounded memory Pérez et al. (2021); Chung & Siegelmann (2021), which limits their application to real-world settings. Our approach does not have these limitations, and in the next section we explain how our insights can be translated to RNNs and state space models trained on toy English datasets.

We note crucially that the number of neurons in the state space model does not depend on the number of sentences in the language $\mathcal{L}$, but only on the number of rules in the n-gram language $\mathcal{L}$. For any language $\mathcal{L}$, we can construct a model that solves next-word prediction by simply memorizing all of its sentences, but such a model would not provide much insight into learning, and the number of neurons would be proportional to the number of sentences in $\mathcal{L}$. The key feature of the above result is that the model does not simply memorize all of the input data, but rather learns the patterns in the data that are specified in the n-gram language. In the next two sections we provide a proof of the result, and formalize this by describing how the state space model learns the patterns.

4.3   Proof: construction of the state space model.

First we introduce some additional notation to specify the algebraic rules that encapsulate the next-word prediction task. Recall that the input to a language model is a sequence of words $\underline{w}'$ that is a valid starting sequence, and the output is a vector that indicates which words can be added to the end, so that the resulting sequence can be completed to obtain a valid sentence. Note that only the last n words are needed for the prediction. We formalize this below, assuming that the sequence $\underline{w}'$ lies in $\mathcal{P}$, the set of all valid n-grams in the language $\mathcal{L}$.

Definition 4.2. Given a sequence of words $\underline{w}' = \{w_1, \cdots, w_n\} \in \mathcal{P}$, define the set $S_{\underline{w}'}$ as follows.

$$S_{\underline{w}'} = \{w_{n+1} \in \mathcal{W}^* \mid (w_2, \cdots, w_n, w_{n+1}) \in \mathcal{P}\}$$

Define the vector $\overline{s_{\underline{w}'}} \in \mathbb{R}^{d+1}$ as follows, which is a $0 - 1$ vector with 1-s in the indexes corresponding to $S_{\underline{w}'}$. Here $1 \leq j \leq d+1$, and $\bar{i}$ was introduced in Definition 3.5.

$$(\overline{s_{\underline{w}'}})_j = \begin{cases} 1 & \text{if } \bar{i}^{-1}(j) \in S_{\underline{w}'}, \\ \log \epsilon - N \log(d+1) & \text{otherwise.} \end{cases} \quad \blacksquare$$

The combinatorial rules for next-word prediction map the sequence $\underline{w}'$ to the set $S_{\underline{w}'}$, which is represented by the vector $\overline{s_{\underline{w}'}}$. We note that the values of the co-ordinates of $\overline{s_{\underline{w}'}}$ corresponding to the indexes in $S_{\underline{w}'}$ have been set to 1 for simplicity, but other positive values are also valid. We refer the reader to the proof of Theorem 4.1 in Appendix **??** to justify the choice of the coordinate $\log \epsilon - N \log(d+1)$. Our state space model processes a given input sequence $\underline{w}$ by converting it to the vector representation $\overline{E}(\underline{w})$ using the embedding layer. Intuitively, we expect that the state space model $\mathcal{S}$ solves the next-word prediction task if it maps the vector $\overline{E}(\underline{w})$, corresponding to a given valid starting sequence $\underline{w}'$, to the vector $\overline{s}_{\underline{w}_{k-n+1:k}}$ specifying the set of possible next words. This will in turn imply that the state space language model $f_{\mathcal{S}}^*$ will have risk less than ϵ. We formalize this below, noting that only $\underline{w}_{k-n+1:k}$, the last n words in the input sequence, are needed to predict the next word.

Theorem 4.3. *Let $\mathcal{S}$ be a one-layer state space model, such that the following holds, where $\underline{w} = (w_1, \cdots, w_k)$ is any valid starting sequence, and $\overline{E}$ is any embedding function.*

$$f_{\mathcal{S}}(\overline{E}(\underline{w})) = \overline{s}_{\underline{w}_{k-n+1:k}}$$

Let $f_{\mathcal{S}}^*$ be the state space language model obtained by concatenating the state space model $\mathcal{S}$ with an embedding layer $\overline{E}$. Then $f_{\mathcal{S}}^*$ has error at most ϵ, i.e. $R(f_{\mathcal{S}}^*) < \epsilon$. ■

Proposition 4.4. *There exists a state space model $\mathcal{S}$ with e input neurons, one hidden layer containing $|\mathcal{P}|$ neurons, and $d+1$ output neurons. such that the following holds (here $\underline{w} = (w_1, \cdots, w_k)$ is any valid starting sequence).*

$$f_{\mathcal{S}}(\overline{E}(\underline{w})) = \overline{s}_{\underline{w}_{k-n+1:k}}$$

To prove these results, we outline the two key Propositions that are needed in Sections 4.4 and 4.5; see Appendix **??** for detailed proofs.

4.4 Proofs: on the memorization capacity of state space models.

To construct a state space models which satisfies this property, we analyse their memorization capacity in the below proposition. This is an extension of existing results on the memorization capacity of feedforward neural networks Zhang et al. (2017), which show that they can fit an arbitrary finite set of input-output vectors (see also Huang & Huang (1991), Yun et al. (2019)). Our approach is constructive in nature, with the parameters constructed algebraically so that the equalities are satisfied. The key technical step is to show that, for a suitable choice of parameters, the images of the input vectors in the hidden layers are linearly independent. In this context, the proof is more subtle than the analogous step for feedforward neural networks. See Appendix **??** for a detailed proof.

Proposition 4.5. *Given any finite set of input-output pairs $(x_i, y_i)_{i=1}^K$ where $x_i = (x_{i,1}, \cdots, x_{i,l})$ are pairwise distinct with $x_{i,j} \in \mathbb{R}^p$, and $y_i \in \mathbb{R}^q$, there exists a state space model $\mathcal{S}$ with a single hidden layer with K neurons that can memorize this data. Specifically, there exist weight matrices $B \in \mathbb{R}^{p \times K}$, $A \in \mathbb{R}^{K \times K}$, $C \in \mathbb{R}^{K \times q}$ and bias vectors $b_y \in \mathbb{R}^q$ such that for each sequence of input x_i, the state space model produces the corresponding output y_i.*

4.5 Proofs: on the context window of state space models.

Our second key result establishes how we can restrict the state space model's memory to a finite context window by imposing restrictions on the hidden weight matrix. This is crucial for modeling n-gram languages, where the prediction of the next word only depends on the preceding n tokens. The result is formalized in Proposition 4.6 below: if the hidden weight matrix of the state space model is nilpotent of order n, then the state space model's output at any time step depends only on the last n input tokens. Our proof involves a linear algebra calculation with powers of the hidden weight matrix, obtained by using the convolutional view of the state space model. We note that restrictions on the eigenvalues of the weight matrix has been explored as means of mitigating exploding/vanishing gradients in Helfrich & Ye (2020); Kerg et al. (2019).

Proposition 4.6. *Let $\mathcal{S}$ be a state space model such that the hidden weight matrix W_{hh} is nilpotent of order n (with respect to the standard basis of $\mathbb{R}^{n_h}$). Then given an input sequence $\underline{x} = (x_1, \cdots, x_T)$, the output $f_{\mathcal{S}}(\underline{x})$ only depends on the last n input values $(x_{T-n+1}, \cdots, x_T)$.*

4.6 Extensions to recurrent neural networks.

Recurrent neural networks (RNNs) and state space models both rely on sequential updates of a hidden state to process input sequences, with the hidden state at each time step is determined by the previous hidden state and the current input. The key difference is that the hidden state update for RNNs uses non-linearity and bias terms from the update, so that $h_t = \sigma(W_x x_t + W_h h_{t-1} + b_h)$ (here h_t is the hidden state, and x_t is the input). Unlike the S3 model which can compute multiple time steps simultaneously due to the linear hidden state update, the output of a RNN cannot be parallelized during training Gu et al. (2021). We now outline how the key results of this section can be extended to recurrent neural networks.

Our results in Proposition 4.6 on the context window of state space layers can be extended to this setting with one key modification. In addition to the hidden weight matrix W_{hh} satisfying the nilpotency constraint $W_{hh}^n = 0$, we also impose a condition that it is block nilpotent with respect to the standard basis formed by the hidden neurons. This is imposed to ensure that the piecewise linear map $\sigma \circ W_h h$ satisfies the same relation; see Appendix **??** for a more precise definition and proof. We expect that Proposition 4.5 can be also be extended to this setting; the key step is to establish the linear independence of the vectors $\sigma(h_t)$ obtained from each of the input sequences, noting that in this setting the ReLU function is applied during the hidden state update.

5 Experimental results: learning n-gram rules with state space models.

In this section, we conduct experiments with state space models trained on datasets generated synthetically from n-gram rules from the example in Section 3, and show that they are capable of predicting the next word with near-perfect accuracies. We study the spectral decomposition of the hidden weight matrices, and use it to analyse the context window of the state space model. We also illustrate how the hidden state vectors in the state space model encode n-gram rules, by visualizing the vectors with a cluster plot using principle component analysis. These results show how our theoretical framework can be used to gain insights into the inner workings of state space models trained on simple datasets using gradient-based optimization.

5.1 Data generation

We generate data using the n-gram language from the example in Section 3.1, with $n = 3$. To generate a sentence using the model, we start with a valid initial sequence from Definition 3.1 (such as "Harry woke at"). At each step, given an input sentence we append a word with the property that the sequence of last n-words is a valid n-gram; when there are multiple such words, we randomly choose one with this property. By iteratively applying these rules, the model generates hundreds of sentences that are grammatically correct. As an example, for the input sentence "He got up and pulled on his", the next word could be "trousers", "denims", "jeans", "pants" or "slacks" (as our set of valid trigrams include "on his trousers", "on his denims", "on his jean", "on his pants" and "on his slacks"). After iterating this process, two valid complete sentences include "He got up and pulled on his trousers because he didn't want to walk into the station in his underpants" and "He got up and pulled on his denims because he didn't want to sprint into the house in his pyjamas".

5.2 Experimental setup

We train a state space language model for next-word prediction on the above dataset. Following the setup in Section 4.3, the model consists of an embedding layer with dimension 10, a hidden layer with 64 hidden neurons, and a fully connected layer that produces the output logits. In our experiment, instead of using a pre-trained word embedding (based on algorithms such as word2vec Mikolov et al. (2013a;b) or GloVe Pennington et al. (2014)), we train the embedding layer jointly with the state space model. The model is trained for 25 epochs with a fixed learning rate of 0.001, using stochastic gradient descent with the cross-entropy loss function. We evaluate the model's accuracy on an unseen test set; each sentence in the test set is truncated to a length of 6, and the model's completion is evaluated by checking if the resulting sentence lies in our dataset. After replicating the experiment 5 times with different random seeds, we find the model consistently achieves near-perfect accuracies when using a training dataset with 40 sentences.

5.3 Spectral decomposition of hidden weight matrices

In this section, we revisit the theoretical framework in Lemma 5.6, and apply these insights to state space models that are obtained through gradient-based optimization. The key feature of our theoretical construction is that the hidden-hidden weight matrix is nilpotent, i.e. that it has zero eigenvalues. The below plot shows the eigenvalues derived from the hidden-hidden weight matrix of the recurrent language model. Each blue dot represents an eigenvalue, plotted in the complex plane with the real part on the x-axis and the imaginary part on the y-axis, while the red dashed circle indicates the unit disk.

In an empirical setting, we note that the nilpotency condition on the matrix must be relaxed; instead of stipulating that a power of W_{hh} is exactly 0, we instead check whether it is approximately equal to 0. Using the eigen-decomposition of a matrix, it is well-known that this condition will hold for n sufficiently large precisely if all of the eigenvalues have norm less than 1. The diagram shows that the eigenvalues all lie within the unit circle, with only one exception, which supports our hypothesis.

To extend Lemma 4.6 to recurrent neural networks, as described in Appendix **??**, we impose the additional condition that the hidden weight matrix W_{hh} is block nilpotent. This implies that $(\sigma \circ W_{hh})^n$ is the zero map; note here $\sigma \circ W_{hh}$ is a piecewise linear function. Unlike the state transition matrix above, we find that the matrix W_{hh} has multiple eigenvalues with values greater than 1. However, by computing the norm of vectors $(\sigma \circ W_{hh})^n \overline{E}(\underline{w})$ for varying input sequences $\underline{w}$, we find that nevertheless the map $(\sigma \circ W_{hh})^n$ approaches 0 as n increases. Using these observations based on the theory in Lemma 4.6, bounding the Lipschitz norm of the map $\sigma \circ W_{hh}$ allows us to estimate the effective context window of an RNN (here we use Lipschitz norm instead of operator norm as this map is non-linear).

(a) Eigenvalues of the Hidden-Hidden Weight Matrix

(b) Embeddings Plot

Figure 1: Comparison of Eigenvalues and Embeddings

5.4 Hidden embeddings for n-grams

In this section, we revisit the theoretical framework from Proposition 5.3, and apply these insights to the state space models obtained through gradient-based optimization. The key feature of our theoretical construction there is that given an input sequence of words $\underline{w}$, the image in the hidden layer depends only on the n-gram obtained from the last n words of the sequence; in other words, the n-gram rule is encoded as a vector in the hidden layer. Our findings build on an earlier study in Karpathy et al. (2015), which investigates the internal mechanisms of LSTMs and finds interpretable behaviors in individual neurons that track specific attributes, such as quotes or parenthesis.

To evaluate this hypothesis, below we apply principal component analysis (PCA) to compress the 64-dimensional hidden embedding vectors obtained from the state space model to 2-dimensional vectors that we visualize in Figure 1(b) above. Each point in the scatter plot represents a hidden state corresponding

to a specific input sentence, with the colors of the points correspond to the n-gram consisting of the last three words. This visualization illustrates the state space model's ability to encode n-gram rules, as vectors corresponding to the same n-gram are clustered together. Since input sequences ending in the n-gram rule have similar representations in the hidden layer, the output logits will also have similar values, enabling the state space model to predict the next word accurately.

6 Discussion and further directions.

Generalizations of n-gram languages. The present work shows that using the simplified models based on n-gram languages can provide insights into the workings of state space models and RNNs trained on next-word prediction tasks. However, it is well-known that n-gram languages cannot effectively model the English language in its entirety, as the number of n-gram rules required to do so will be prohibitively large Liu et al. (2024). More intricate models based on formal grammars Chomsky (1956; 1959); Chomsky & Schützenberger (1963), which have been developed by the mathematical linguistics community, are better suited for complex real-world datasets. While existing results on the Turing completeness of RNNs show the existence of recurrent models that can solve next-word prediction for formal grammars Pérez et al. (2021); Chung & Siegelmann (2021), the construction uses unbounded precision (or memory), which does not explain their success in real-world scenarios. It would be interesting to extend our construction to formal grammars and use the framework to gain further insights into the inner workings of state space models and RNNs obtained through gradient-based optimization.

Generalized state space models and transformers. While the state space models we study struggle with maintaining information over long sequences, more recent work on generalized state space models extends this by incorporating the HiPPo matrix Gu et al. (2022), which helps them efficiently represent and update the state information to capture both recent and distant past inputs. Transformers employ self-attention mechanisms, which enable them to directly attend to all tokens in a sequence, making them highly effective for long-context language modeling. While this may not be needed for n-gram languages where the model only needs to consider the most recent tokens, formal grammars require the model to remember recursive relationships between different parts of a sentence and maintain consistency across nested clauses. It is known theoretically that transformers are more expressive than n-gram models Svete & Cotterell (2024), but their construction uses query-key matrices that only use positional encoding and not the word embeddings, and this assumption does not hold in real-world settings with gradient-based optimization. It would be interesting to extend our theoretical framework to generalized state space models Gu et al. (2022); Gu & Dao (2024) and transformers Radford et al. (2018; 2019), and gain a deeper understanding of the interpretability of these models which are obtained through gradient-based optimization.

Stochastic gradient descent and overparametrization. Our empirical results indicate that state space models and RNNs that are trained on synthetic language data generated from n-gram rules can achieve near-perfect accuracies. This leads us to the question of whether we can obtain theoretical guarantees showing that stochastic gradient descent yields state space models and RNNs with near-zero generalization error in this context. There has been existing work on generalization bounds for RNNs using the PAC-Learning framework Chen et al. (2020); Zhang et al. (2018a), and theoretical guarantees for the convergence of stochastic gradient descent with RNNs in the overparametrized setting Allen-Zhu et al. (2019b) (building on earlier work for feedforward neural networks Allen-Zhu et al. (2019a); Zou et al. (2020)). However, these theoretical guarantees are obtained for tasks that involve memorizing input-output pairs, and cannot be directly applied to distributions that model real-world settings, such as data generated from n-grams models. It would be interesting to extend their theoretical guarantees to state space models and RNNs using datasets generated from n-gram languages, and analyze theoretically whether or not overparametrization is required in this setting.

7 Conclusion.

In this paper, we use languages generated from n-gram rules to theoretically understand how neural networks excel at language modelling tasks. We focus on next-word prediction using state space language models, and

show that they can solve the sentence completion task for languages generated from n-gram rules. In our proof, we construct a state space model that encodes the n-gram rules which govern the next-word prediction task, and discuss how our results can be extend to recurrent neural networks. Our key theoretical results include a rigorous analysis of the memorization capacity of state space models, and demonstrate how the context window can be regulated through the spectral decomposition of the hidden weight matrix. We conduct experiments with a small dataset to illustrate how our framework yields insights into the inner workings of state space models obtained through gradient-based optimization. We do not anticipate any negative societal impacts, as the present work is theoretical. Our results shed light on the theoretical underpinnings of language modelling with neural networks, and we expect that it will provide insights into the inner workings of these black-box models.

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