Autoregressive Modeling is Misspecified for Some Sequence Distributions

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Abstract

Should sequences be modeled autoregressively—one symbol at a time? How much computation is needed to predict the next symbol? While local normalization is cheap, this also limits its power. We point out that some probability distributions over discrete sequences cannot be well-approximated by *any* autoregressive model whose runtime and parameter size grow polynomially in the sequence length—even though their *unnormalized* sequence probabilities are efficient to compute exactly. Intuitively, the probability of the next symbol can be expensive to compute or approximate (even via randomized algorithms) when it marginalizes over exponentially many possible futures, which is in general NP-hard. Our result is conditional on the widely believed hypothesis that $\mathrm{NP} \not\subseteq \mathrm{P/poly}$ (without which the polynomial hierarchy would collapse at the second level). This theoretical observation serves as a caution to the viewpoint that pumping up parameter size is a straightforward way to improve autoregressive models (e.g., in language modeling). It also suggests that globally normalized (energy-based) models may sometimes outperform locally normalized (autoregressive) models, as we demonstrate experimentally for language modeling.

1 Introduction

The expressiveness of modern neural architectures has given rise to successful families of probability models of discrete sequences. Many of the popular models are *autoregressive* [37, 14, 46]. Such models directly define the conditional distribution $q_{\boldsymbol{\theta}}(x_t \mid \mathbf{x}_{1\ldots t-1})$ over each successive symbol in the sequence, conditioning on the history $\mathbf{x}_{1\ldots t-1}$ of previously drawn symbols. Typically $q_{\boldsymbol{\theta}}$ is defined so that these conditional probabilities are efficient to compute, for any parameters $\boldsymbol{\theta}$. As a result, it is efficient to compute the probability of drawing a given sequence $\mathbf{x}$ from the distribution (e.g., during maximum likelihood estimation of $\boldsymbol{\theta}$ from fully observed sequences). It is also efficient to draw a random sequence $\mathbf{x}$ (e.g., in policy gradient training methods [49]). These operations are in general more difficult when using *energy-based models* [29], which directly define the probability of the entire string $\mathbf{x}$ as proportional to $\tilde{q}_{\boldsymbol{\theta}}(\mathbf{x})$ (an *unnormalized probability*) for some non-negative function $\tilde{q}_{\boldsymbol{\theta}}$.

Some of the problems that autoregressive models are used to tackle, such as protein modeling [35], are inherently hard [5]. The success of autoregressive modeling hinges on the capacity of the parametric model $q_{\boldsymbol{\theta}}$. There must exist a parameter vector $\boldsymbol{\theta}^*$ such that $q_{\boldsymbol{\theta}^*}(x \mid \hat{\mathbf{x}}) \approx p(x \mid \hat{\mathbf{x}})$ for all probable histories $\hat{\mathbf{x}}$ and symbols x, where $p(\cdot \mid \hat{\mathbf{x}})$ denotes the true conditional distribution. Modern neural networks provide flexible families $q_{\boldsymbol{\theta}}$ that can often be successfully trained on sufficient data, achieving

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stellar empirical results in many applications [39, 13, 48, 50]. It is well-known that neural networks form families of expressive models: a celebrated result by [44] is that sufficiently large neural networks have the capacity to approximate any desired function. An autoregressive model must specifically approximate the conditional probability function $p(x \mid \hat{\mathbf{x}})$ with a single trained neural network $q_{\boldsymbol{\theta}}$. In other words, training an autoregressive model *compiles* information about the conditional probabilities into the parameters $\boldsymbol{\theta}$, to make computation at *runtime* easy. In contrast, training an energy-based model does not give easy access to the conditional probabilities at runtime. Under the trained energy-based model, $q_{\boldsymbol{\theta}}(x \mid \hat{\mathbf{x}})$ is defined as $q_{\boldsymbol{\theta}}(x \mid \hat{\mathbf{x}}) = {}^{Z(\hat{\mathbf{x}}x)}/_{Z(\hat{\mathbf{x}})}$ where $Z(\hat{\mathbf{x}})$ denotes the total unnormalized probability of all strings starting with $\hat{\mathbf{x}}$, and $\hat{\mathbf{x}}x$ denotes the concatenation of $\hat{\mathbf{x}}$ and x. In the general case, these sums Z must be computed by enumerating exponentially (or infinitely) many strings.

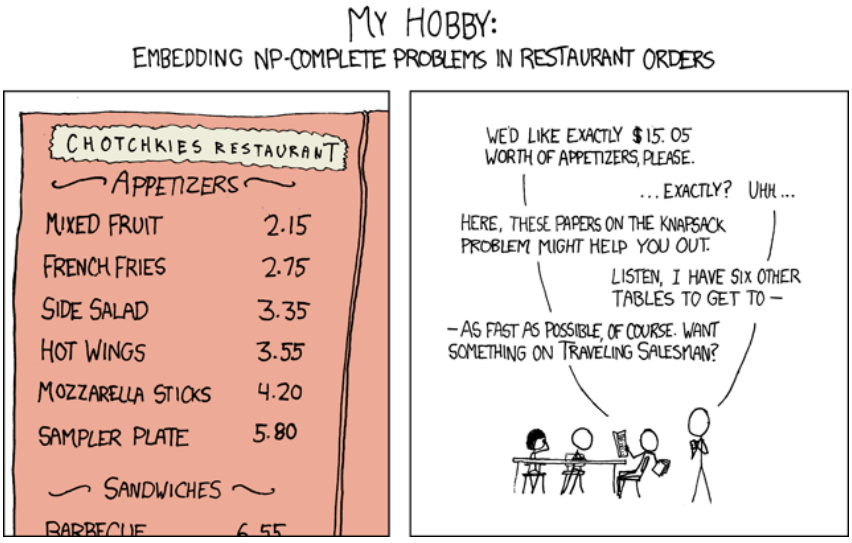

Figure 1: Answers that are backed by reasoning can be difficult to predict with a purely autoregressive model [38]. Natural language inference tasks sometimes require considering exponentially many hypotheses (e.g. the KNAPSACK problem here) to correctly choose the next word, with no known polytime approximation to approximate this. Given a *large enough* neural autoregressive model with correct parameters, any question can be answered correctly, but we show that the required network size can grow superpolynomially in the input length. (The extra size may be used to consider exponentially many hypotheses, or to store the precomputed results of having done so.)

In this paper, we argue that it is not appropriate to model computationally hard problems using autoregressive models. In the worst case, the conditional probabilities are too expensive to compute. An autoregressive architecture such as an RNN [14] or a Transformer [46] allocates a constant or linear amount of computation to each conditional probability. But under common complexity-theoretic assumptions, there exist hard sequence distributions[2] where there simply *do not exist* $O(\text{poly}(n))$-size parameter vectors $\boldsymbol{\theta}_n$ that allow $O(\text{poly}(n))$-time approximation at runtime of all the conditional probabilities $p(x \mid \hat{\mathbf{x}})$ for $\hat{\mathbf{x}} = n$, regardless of the neural architecture design. Thus, even *unlimited training time* and *unlimited training examples* cannot fit any such autoregressive model.

Specifically, we will exhibit a family of sequence distributions whose local conditional distributions cannot (unless $\text{NP} \subseteq \text{P/poly}$) be modeled using any family of computationally tractable parametric models $q_{\boldsymbol{\theta}}$ with parameters $\{\boldsymbol{\theta}^n : n \in \mathbb{N}\}$ whose size grows polynomially in n.

We start by introducing relevant formal definitions in in §2. We provide conditional proofs in §3 that locally normalized (autoregressive) models are not as expressive as globally normalized (energy-based) models. Finally, in §4 we experiment on natural language datasets with one simple alternative to locally normalized (autoregressive) models—*residual energy-based models*, a type of globally normalized sequence model.

[2]E.g., the dialogue completion task in the comic in Figure 1.

2 Background

2.1 Weighted languages

An **unweighted language** $\mathcal{X} \subseteq V^*$ is a set of strings $\mathbf{x}$ over a finite alphabet V. A **weighted language** $\tilde{p}$ is a function $\tilde{p} : V^* \to \mathbb{R}_{\geq 0}$. It may be regarded as specifying an unweighted language $\mathcal{X} = \text{support}(\tilde{p})$ along with positive weights for the strings in $\mathcal{X}$. We say that a weighted language $\tilde{p}$ is **normalizable** if its **global normalizing constant** $Z \triangleq \sum_{\mathbf{x} \in V^*} \tilde{p}(\mathbf{x})$ is strictly positive and finite. When $\tilde{p}$ is normalizable, $p(\mathbf{x}) \triangleq \tilde{p}(\mathbf{x})/Z$ defines a probability distribution over $\mathcal{X}$, in other words, a weighted language with a global normalizing constant of 1.

Let $\hat{\mathbf{x}} \preceq \mathbf{x}$ mean that $\hat{\mathbf{x}}$ is a prefix of $\mathbf{x} \in V^*$ (not necessarily a strict prefix). If $\tilde{p}$ is normalizable, then $Z(\hat{\mathbf{x}}) \triangleq \sum_{\mathbf{x} \in V^* : \hat{\mathbf{x}} \preceq \mathbf{x}} \tilde{p}(\mathbf{x})$ is $\leq Z$ for any $\hat{\mathbf{x}} \in V^*$, yielding a marginal **prefix probability** $Z(\hat{\mathbf{x}})/Z$. If the prefix $\hat{\mathbf{x}}$ has positive prefix probability, then it admits a **local conditional probability** $p(x \mid \hat{\mathbf{x}}) \triangleq Z(\hat{\mathbf{x}}\, x)/Z(\hat{\mathbf{x}})$ for each symbol $x \in V$, where the denominator is interpreted as a **local normalizing constant**. This is the conditional probability that if a random string starts with the prefix $\hat{\mathbf{x}}$, the next symbol is x. There is also a probability $p(\$ \mid \hat{\mathbf{x}}) \triangleq 1 - \sum_{x \in V} p(x \mid \hat{\mathbf{x}}) = \tilde{p}(\hat{\mathbf{x}})/Z(\hat{\mathbf{x}}) \geq 0$ that the string ends immediately after $\hat{\mathbf{x}}$; the special symbol $\$ \notin V$ represents "end of string."

2.2 Computation for weighted languages and associated distributions

We define a weighted language $\tilde{p}$ to be **computable** if it is defined by a Turing machine (also called $\tilde{p}$) that maps any $\mathbf{x} \in V^*$ to $\tilde{p}(\mathbf{x}) \in \mathbb{Q}_{\geq 0}$ in finite time. The Turing machine does not have to compute Z.

While the computable weighted languages allow any computable function as $\tilde{p}$, most architectures for defining weighted languages (e.g., RNNs or Transformers) do only a bounded or linear amount of work per input symbol. As a result, they compute $\tilde{p}(\mathbf{x})$ in time $O(\text{poly}(|\mathbf{x}|))$. That is, $\tilde{p} \in \text{P}$; we refer to such weighted languages as **efficiently computable**. This does not imply that the normalized version p is efficiently computable, since finding the denominator Z requires summing over all of V^*.

If we tried to construct the same normalized distribution p as in the previous paragraph using a autoregressive model architecture, we would model it as a product of local conditional probabilities, $p(\mathbf{x}) = (\prod_{i=1}^{|\mathbf{x}|} p(x_i \mid \mathbf{x}_{1\ldots i-1}))p(\$ \mid \mathbf{x})$. Most such architectures also do only a bounded or linear amount of work per input symbol. Yet one suspects that this may not always be enough work to do the job: as we noted in the introduction, the local conditional probabilities of the original $\tilde{p}$ are expensive to compute (unless $\tilde{p}$ has some special structure making $Z(\hat{\mathbf{x}})$ tractable).

Indeed, the observation of this paper is that for some efficiently computable weighted languages $\tilde{p}$, the local conditional probabilities are expensive to compute or even to approximate well. More precisely, autoregressive models cannot fit the local conditional probabilities unless they are superpolynomial in either their runtime or in their number of parameters (where the parameters may be precomputed at training time). We now explain how to formalize these notions.

2.3 Compact parameters

In the machine learning approach to sequence modeling, we usually do not manually design the Turing machine behind $\tilde{p}$. Rather, we design a parametric model $M^{\tilde{\text{P}}}$ with *parameters* $\boldsymbol{\theta}$. Formalizing this in a general way, $M^{\tilde{\text{P}}}$ is a general-purpose Turing machine that reads $\boldsymbol{\theta}$ (expressed as a string in $\mathbb{B}^*$ where $\mathbb{B} \triangleq \{0, 1\}$) and outputs a specialized Turing machine $\tilde{p}_{\boldsymbol{\theta}} \triangleq M^{\tilde{\text{P}}}(\boldsymbol{\theta})$ that defines a weighted language. For each $\boldsymbol{\theta}$, we obtain a potentially different weighted language.

Strings vary in length, and accurate modeling of longer strings may sometimes require more complex computations with more parameters. For example, when V is a natural language alphabet, a recurrent neural network may require more hidden units to model sentences of the language rather than individual words, and even more units to model whole documents. To accommodate this, we allow an *infinite sequence* of parameter vectors $\boldsymbol{\Theta}^{\tilde{\text{P}}} = \{\boldsymbol{\theta}_n^{\tilde{\text{P}}} \in \mathbb{B}^* \mid n \in \mathbb{N}\}$, which yields an infinite sequence of Turing machines $\{\tilde{p}_n \mid n \in \mathbb{N}\}$ via $\tilde{p}_n \triangleq M^{\tilde{\text{P}}}(\boldsymbol{\theta}_n^{\tilde{\text{P}}})$. We then define $\tilde{p}_{\boldsymbol{\Theta}^{\tilde{\text{P}}}}(\mathbf{x}) \triangleq \tilde{p}_{|\mathbf{x}|}(\mathbf{x})$, so a string of length n is scored by the $\tilde{p}_n$ machine. Of course, it is legal (and common) for all of the $\boldsymbol{\theta}_n^{\tilde{\text{P}}}$ to be equal, or empty, but if desired, we can obtain more power by allowing the number of parameters to grow with n if needed.

We can now consider *how rapidly* the parametric and runtime complexity may grow.

- If $|\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}}|$ is permitted to grow exponentially, then one can exactly fit *any* weighted language $\tilde{p}$ (even an uncomputable one). Simply use $\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}}$ to encode a trie with $O(|V|^{n+1})$ nodes that maps $\mathbf{x} \mapsto \tilde{p}(\mathbf{x})$ for any $|\mathbf{x}|$ of length n, and design $M^{\tilde{\mathrm{p}}}$ such that the Turing machine $\tilde{p}_n = M^{\tilde{\mathrm{p}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}})$ has a (large) state transition table that mirrors the structure of this trie. The resulting collection of Turing machines $\{\tilde{p}_n \mid n \in \mathbb{N}\}$ can then compute $\tilde{p}(\mathbf{x})$ exactly for any $\mathbf{x}$, with only linear runtime $O(|\mathbf{x}|)$ (which is used to traverse the trie).
- Separately, if unbounded runtime is permitted for $M^{\tilde{\mathrm{p}}}$, then one can exactly fit *any computable* weighted language $\tilde{p}$. Simply have $M^{\tilde{\mathrm{p}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}})$ *compute* and return the large trie-structured Turing machine $\tilde{p}_n$ that was mentioned above. In this case, $M^{\tilde{\mathrm{p}}}$ need not even use the parameters $\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}}$, except to determine n.
- Finally, if unbounded runtime is permitted for $\tilde{p}_n$, then again one can exactly fit *any computable* weighted language $\tilde{p}$. In this case, $M^{\tilde{\mathrm{p}}}$ trivially returns $\tilde{p}_n = \tilde{p}$ for all n.
- However, if the parameters $\boldsymbol{\Theta}^{\tilde{\mathrm{p}}}$ are "compact" in the sense that $|\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}}|$ grows only as $O(\mathrm{poly}(n))$, and also $\tilde{p}_n = M^{\tilde{\mathrm{p}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}})$ is constructed by $M^{\tilde{\mathrm{p}}}$ in time $O(\mathrm{poly}(n))$, and $\tilde{p}_n$ scores any $\mathbf{x}$ of length n in time $O(\mathrm{poly}(n))$, then we say that the resulting weighted language $\tilde{p}_{\boldsymbol{\Theta}^{\mathrm{p}}}$ is **efficiently computable with compact parameters**.[3]

  A neural parametric model $M^{\tilde{\mathrm{p}}}$ of a weighted language will typically guarantee this property. The construction and execution of the neural network $\tilde{p}_n$ may perform a polynomial amount of total computation to score the string $\mathbf{x}$. This computation may involve parameters that were precomputed using any amount of effort (e.g., training on data) or even obtained from an oracle (they need not be computable). However, the exponentially many strings of length n must share a polynomial-size parameter vector $\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}}$, which prevents the solution given in the first bullet point.

In practice one obtains a finite prefix of $\boldsymbol{\Theta}^{\tilde{\mathrm{p}}}$ by training. However, we do not consider whether such parameters are easy to estimate or even computable. We simply ask, for a given parametric model $M^{\tilde{\mathrm{p}}}$, whether a polynomially growing sequence $\boldsymbol{\Theta}^{\tilde{\mathrm{p}}}$ of good parameter vectors exists. If not, then there can be no scheme for estimating arbitrarily long finite prefixes of such a sequence—even if unlimited data, computation, pretraining (e.g., BERT [17]), and access to training oracles are allowed at training time.

2.4 Locally normalized parametrization

Many parameter estimation techniques and inference methods specifically work with local conditional probabilities $p(x \mid \hat{\mathbf{x}})$. Thus, it is common to use parametric models where such quantities can be computed efficiently (given the parameters). Here we formalize such parametrization in terms of weighted languages: for any weighted language $\tilde{p}$, we say that the Turing machine M^{q} **efficiently locally normalizes** $\tilde{p}$ **with compact parameters** $\boldsymbol{\Theta}^{\mathrm{q}} = \{\boldsymbol{\theta}_n^{\mathrm{q}} \mid n \in \mathbb{N}\}$ if

- $\tilde{p}$ is normalizable (so p exists)
- the specialized Turing machine $q_n \triangleq M^{\mathrm{q}}(\boldsymbol{\theta}_n^{\mathrm{q}})$ (similar to $\tilde{p}_n$ in §2.3) maps $\hat{\mathbf{x}}x \mapsto p(x \mid \hat{\mathbf{x}})$ for all $x \in V \cup \{\$\}$ and all prefixes $\hat{\mathbf{x}} \in V^*$ with $|\hat{\mathbf{x}}| \leq n$.
- the parameter size $|\boldsymbol{\theta}_n^{\mathrm{q}}|$ grows only as $O(\mathrm{poly}(n))$.
- $q_n = M^{\mathrm{q}}(\boldsymbol{\theta}_n^{\mathrm{q}})$ is constructed by M^{q} in time $O(\mathrm{poly}(n))$
- the worst-case runtime of q_n (on inputs $\hat{\mathbf{x}}x$ of length $\leq n+1$) is $O(\mathrm{poly}(n))$.

If there is M^{q} that efficiently locally normalizes a weighted language $\tilde{p}$ with compact parameters $\boldsymbol{\Theta}^{\mathrm{q}}$, then it is not hard to see that $p = \tilde{p}/Z$ is efficiently computable with compact parameters. More formally:

Lemma 1. *Let M^{q} be a Turing machine that efficiently locally normalizes a weighted language $\tilde{p}$ with compact parameters $\boldsymbol{\Theta}^{\mathrm{q}} = \{\boldsymbol{\theta}_n^{\mathrm{q}} \mid n \in \mathbb{N}\}$. Then p is efficiently computable with compact parameters.*

[3] Since we require $M^{\tilde{\mathrm{p}}}$ to run in polytime, it can only look at a polynomial-sized portion of $\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}}$. Hence it is not really crucial for the parameters $\boldsymbol{\theta}_n^{\mathrm{p}}$ to be compact, but we nonetheless include this intuitive condition, without loss of generality.

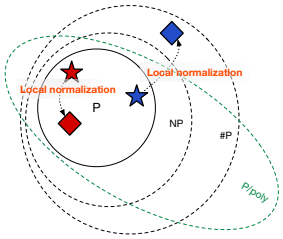

Figure 2: Local normalization of some efficiently computable weighted languages is hard: the stars denote two efficiently computable weighted languages. Their locally normalized parametrizations (denoted by diamonds) define sequence weights as $p(\mathbf{x}) = \left(\prod_t^{|\mathbf{x}|} p(x_t \mid \mathbf{x}_{1\ldots t-1})\right) p(\$ \mid \mathbf{x})$, where for certain prefixes $\mathbf{x}_{1\ldots t-1}$ and some p, computing and approximating $p(\cdot \mid \mathbf{x}_{1\ldots t-1})$ are both NP-hard as we see in §3. Since it's widely believed that $\mathrm{NP} \not\subseteq \mathrm{P/poly}$, and that all efficient approximating algorithms with compact parameters are in $\mathrm{P/poly}$, a locally normalized parametrization (blue diamond) cannot always efficiently approximate the distribution using compact parameters.

Proof. It is simple to define a Turing machine M^{r} that maps each parameter string $\boldsymbol{\theta}_n^{\mathrm{q}}$ to a Turing machine r_n, where $r_n(\mathbf{x})$ simply computes $(\prod_{t=1}^{n} q_n(x_t \mid \mathbf{x}_{1\ldots t-1})) \cdot q_n(\$ \mid \mathbf{x})$. Then $r_n(\mathbf{x}) = p(\mathbf{x})$ for all $\mathbf{x}$ of length n, by the definition of local normalization.

M^{r} can be constructed by incorporating the definition of M^{q}, so that $r_n = M^{\mathrm{r}}(\boldsymbol{\theta}_n^{\mathrm{q}})$ can include $q_n = M^{\mathrm{q}}(\boldsymbol{\theta}_n^{\mathrm{q}})$ as a subroutine. This allows r_n to query q_n for local conditional probabilities and multiply them together.

- Since M^{q} runs in polytime, it is straightforward for this construction to ensure that M^{r} runs in polytime as well.
- Since $q_n(\cdot \mid \hat{\mathbf{x}}) \in O(\mathrm{poly}(n))$, this construction can ensure that r_n runs in polytime as well.
- We were given that $|\boldsymbol{\theta}_n^{\mathrm{q}}| \in O(\mathrm{poly}(n))$ (compact parameters).

Since $\tilde{p}$ is the weighted language defined by $(M^{\mathrm{r}}, \boldsymbol{\Theta}^{\mathrm{q}})$, and M^{r} and $\boldsymbol{\Theta}^{\mathrm{q}}$ have the properties just discussed, we see that $\tilde{p}$ is efficiently computable with compact parameters. □

This result demonstrates that locally normalized models do not provide any extra power. The same distributions can always be captured by globally normalized models (of an appropriate architecture that we used in the proof). But we will see in Theorem 1 that the converse is likely not true: provided that $\mathrm{NP} \not\subseteq \mathrm{P/poly}$, there are efficiently computable weighted languages that cannot be efficiently locally normalized (Figure 2).

2.5 P and P/poly

Our definitions above of efficiently computable weighted languages, and efficiently computable weighted languages with compact parameters, are weighted generalizations of complexity classes P and $\mathrm{P/poly}$, respectively. An unweighted language L is in P iff there is a deterministic Turing machine that decides in $O(\mathrm{poly}(|\mathbf{x}|))$ time whether $\mathbf{x} \in L$. And an unweighted language L' is in $\mathrm{P/poly}$ iff[4] there exist Turing machines $\{M_n : n \in \mathbb{N}\}$ such that M_n decides in $O(\mathrm{poly}(n))$ time whether $\mathbf{x}$ of length n is in L', where each M_n can be constructed in $O(\mathrm{poly}(n))$ time as $M(\boldsymbol{\theta}_n)$, for some Turing machine M and some sequence of polynomially-sized **advice strings** $\{\boldsymbol{\theta}_n \mid n \in \mathbb{N}\}$ with $|\boldsymbol{\theta}_n| \in O(\mathrm{poly}(n))$.

It is easy to show that $\mathrm{P} \subseteq \mathrm{P/poly}$. But $\mathrm{P/poly}$ is larger than P: it contains all sparse languages, regardless of their hardness—even sparse undecidable languages—as well as many dense languages. The extra power of $\mathrm{P/poly}$ comes from its access to compact advice strings that do not have to be efficient to compute (or even computable). This corresponds to statistical modeling, where the trained model has a computationally efficient architecture plus access to parameters that do not have to be efficient to find.

2.6 SAT problems

Although $\mathrm{P/poly}$ is large, it is widely believed that no NP-complete languages are in $\mathrm{P/poly}$. Otherwise we would have all of $\mathrm{NP} \subseteq \mathrm{P/poly}$ (as is easy to see) and the polynomial hierarchy

[4] Our characterization of P/poly [27] is a variant of the standard "advice string" definition [4, §6]. We have replaced the standard call $M(\boldsymbol{\theta}_n, \mathbf{x})$ with the "curried" expression $M(\boldsymbol{\theta}_n)(\mathbf{x})$, which we still require to execute in polynomial total time. In our setting, the intermediate result $M_n = M(\boldsymbol{\theta}_n)$ corresponds to a trained runtime system for inputs of length n.

would collapse at the second level [25]. In particular, it is believed that SAT $\notin$ P/Poly. Given a boolean formula ϕ, SAT accepts ϕ iff ϕ can be satisfied by some value assignment. For example, the formula $(A_1 \vee \neg A_2 \vee A_3) \wedge (A_1 \vee \neg A_4)$ is in SAT, since there is a satisfying assignment $A_1 = 1, A_2 = 1, A_3 = 0, A_4 = 1$. We denote the number of satisfying assignments to ϕ as $\#(\phi)$.

3 Problem with local normalization: the model capacity problem

We claim there exists an efficiently computable and normalizable weighted language $\tilde{p}$ over alphabet $\mathbb{B} \triangleq \{\mathtt{0}, \mathtt{1}\}$ that cannot be efficiently locally normalized with compact parameters. The reason is that under widely held beliefs, computing $p(x \mid \hat{\mathbf{x}})$ is NP-hard for this weighted language (and has no polynomial-time approximation scheme).

3.1 Exact computation of local probabilities is NP-hard (hence not in P/poly)

We prove our claim by defining a certain weighted language $\tilde{p}$ and reducing SAT to computing certain local conditional probabilities of $\tilde{p}$ (as defined in §2.1). Each decision SAT(ϕ) (where ϕ ranges over formulas) corresponds to a particular local conditional probability, implying that there is no polytime scheme for computing all of these probabilities, even with polynomially sized advice strings (i.e., parameters).

Without loss of generality, we consider only formulae ϕ such that the set of variables mentioned at least once in ϕ is $\{A_1, \ldots, A_j\}$ for some $j \in \mathbb{N}$; we use $|\phi|$ to denote the number of variables j in ϕ. We say that $\mathbf{a}$ **satisfies** ϕ if $\mathbf{a} \in \mathbb{B}^{|\phi|}$ and $(A_1 = a_1, \ldots, A_{|\phi|} = a_{|\phi|})$ is a satisfying assignment. Finally, let boldface $\boldsymbol{\phi} \in \mathbb{B}^*$ denote $\mathrm{enc}(\phi)$ where enc is a prefix-free encoding function. We can now define the unweighted language $\mathcal{X} = \{\boldsymbol{\phi}\mathbf{a} \mid \phi \text{ is a formula and } \mathbf{a} \in \mathbb{B}^{|\phi|} \text{ and } \mathbf{a} \text{ satisfies } \phi\}$ over alphabet $\mathbb{B}$, which contains each possible SAT problem concatenated to each of its solutions. For example, $\mathcal{X}$ contains the string $\boldsymbol{\phi}\mathbf{a}$ where $\boldsymbol{\phi} = \mathrm{enc}((A_1 \vee \neg A_2 \vee A_3) \wedge (A_1 \vee \neg A_4))$ and $\mathbf{a} = \mathtt{1101}$.

We now convert $\mathcal{X}$ to a weighted language $\tilde{p}$, defined by $\tilde{p}(\mathbf{x}) = \tilde{p}(\boldsymbol{\phi}, \mathbf{a}) = (\frac{1}{3})^{|\mathbf{x}|+1}$ for $\mathbf{x} \in \mathcal{X}$ (otherwise $\tilde{p}(\mathbf{x}) = 0$). $\tilde{p}$ is normalizable since Z is both finite ($Z = \sum_{\mathbf{x} \in \mathbb{B}^*} \tilde{p}(\mathbf{x}) \leq \sum_{\mathbf{x} \in \mathbb{B}^*} (\frac{1}{3})^{|\mathbf{x}|+1} = 1$) and positive ($Z > 0$ because the example string in the previous paragraph has positive weight). The conditional distribution $p(\mathbf{a} \mid \boldsymbol{\phi})$ is uniform over the satisfying assignments $\mathbf{a}$ of $\boldsymbol{\phi}$, as they all have the same length $|\phi|$.

We will show that computing the local conditional probabilities of $\tilde{p}$ is NP-hard. In particular, we show that SAT can be reduced to computing certain local probabilities, namely the ones that condition on prefixes $\hat{\mathbf{x}}$ that consist only of a formula: $\hat{\mathbf{x}} = \boldsymbol{\phi}$ for some ϕ.

Lemma 2. *Let* LocalProb$(\hat{\mathbf{x}}, c_1)$ *be the decision problem of deciding whether* $p(\mathtt{1} \mid \hat{\mathbf{x}}) > c_1$*, for* $\hat{\mathbf{x}} \in \mathbb{B}^*$ *and* $c_1 \in [0, 1] \cap \mathbb{Q}$*. And let* SAT$(\phi)$ *be the decision problem of deciding whether formula* ϕ *is satisfiable.* SAT $\leq_m^P$ LocalProb.

Proof. We will show that SAT can actually be reduced to LocalProb instances with $c_1 = 0$.

Suppose we would like to answer SAT(ϕ) where ϕ is a formula with variables $A_1, \ldots, A_j$. Define Shift(ϕ) to be a version of ϕ in which A_i has been renamed to A_{i+1} for all $1 \leq i \leq j$. Define a new formula $\phi' = (\neg A_1 \wedge \neg A_2 \wedge \ldots \wedge \neg A_j \wedge \neg A_{j+1}) \vee (A_1 \wedge \mathrm{Shift}(\phi))$.

As usual, boldface $\boldsymbol{\phi}' = \mathrm{enc}(\phi') \in \mathbb{B}^*$ denotes the encoding of ϕ' as a string. The strings in $\mathcal{X}$ that begin with $\boldsymbol{\phi}'$ are precisely the strings of the form $\boldsymbol{\phi}'\mathbf{a}'$ where $\mathbf{a}'$ is a satisfying assignment of ϕ'. This is achieved precisely when $\mathbf{a}' = \mathtt{0}^{j+1}$ or $\mathbf{a}' = \mathtt{1}\mathbf{a}$ where $\mathbf{a}$ is a satisfying assignment of ϕ.

Every string in $\mathcal{X}$ has positive weight under $\tilde{p}$. At least one string in $\mathcal{X}$ begins with $\boldsymbol{\phi}'$, namely $\boldsymbol{\phi}'\mathtt{0}^{j+1}$, so $Z(\boldsymbol{\phi}') > 0$. Therefore the local probability $p(\mathtt{1} \mid \boldsymbol{\phi}') = Z(\boldsymbol{\phi}'\mathtt{1}) \,/\, Z(\boldsymbol{\phi}')$ is defined (see §2.1). Considering the numerator, we see that $p(\mathtt{1} \mid \boldsymbol{\phi}') > 0$ iff $Z(\boldsymbol{\phi}'\mathtt{1}) > 0$ iff ϕ has any satisfying assignments. We can therefore write SAT$(\phi) =$ LocalProb$(\boldsymbol{\phi}', 0)$, which is a polytime reduction. □

Lemma 2 implies that assuming NP $\not\subseteq$ P/poly, no $(M^{\mathrm{q}}, \boldsymbol{\Theta}^{\mathrm{q}})$ can efficiently locally normalize $\tilde{p}$ with compact parameters. Granted, the restriction of $\tilde{p}$ to the finite set $\{\mathbf{x} \in \mathbb{B}^* : |\mathbf{x}| \leq n\}$ can be locally normalized by some polytime Turing machine q_n, using the same trie trick sketched in §2.3. But such

tries have sizes growing exponentially in n, and it is not possible to produce a sequence of such machines, $\{q_n : n \in \mathbb{N}\}$, via a single master Turing machine M^{q} that runs in $O(\mathrm{poly}(n))$.

Theorem 1. *There exists an efficiently computable weighted language $\tilde{p}$ that cannot be efficiently locally normalized with compact parameters, assuming* $\mathrm{NP} \not\subseteq \mathrm{P/poly}$.

Proof. We take $\tilde{p}$ to be the weighted language that was defined above. Suppose there does exist a Turing machine M^{q} that efficiently locally normalizes $\tilde{p}$ with compact parameters $\boldsymbol{\Theta}^{\mathrm{q}} = \{\boldsymbol{\theta}^{\mathrm{q}}_n \mid n \in \mathbb{N}\}$. We will show that this leads to a contradiction since then $\textsc{Sat} \in \mathrm{P/poly}$, implying $\mathrm{NP} \subseteq \mathrm{P/poly}$, contradicting an assumption of the theorem.

For convenience, we will use a version of SAT whose inputs are encoded using the same encoding function enc that was used by our definition of $\mathcal{X}$ in §3.1.[5]

To show that the existence of M^{q} implies $\textsc{Sat} \in \mathrm{P/poly}$, we must use M^{q} to construct an appropriate pair $(M, \boldsymbol{\Theta})$ such that $(M(\boldsymbol{\theta}_n))(\boldsymbol{\phi}) = \textsc{Sat}(\phi)$ if $|\boldsymbol{\phi}| = n$. By Lemma 2, we know that $\boldsymbol{\phi}$ can be transformed in time $\leq f(n) \in O(\mathrm{poly}(n))$ to a string $\hat{\mathbf{x}}$ such that $\textsc{Sat}(\boldsymbol{\phi}) = \textsc{LocalProb}(\hat{\mathbf{x}}, 0)$. Notice that $f(n)$ is an upper bound on the length of $\hat{\mathbf{x}}$ when $|\boldsymbol{\phi}| = n$. Define $\boldsymbol{\Theta}$ by $\boldsymbol{\theta}_n = \boldsymbol{\theta}^{\mathrm{q}}_{f(n)}$, and observe that $|\boldsymbol{\theta}_n| \in O(\mathrm{poly}(n))$ (thanks to compactness of the parameters $\boldsymbol{\Theta}^{\mathrm{q}}$ and the fact that f is polynomially bounded). Finally, define $M(\boldsymbol{\theta}_n)$ to be a Turing machine that maps its input $\boldsymbol{\phi}$ of length n to $\hat{\mathbf{x}}$ of length $\leq f(n)$, then calls $M^{\mathrm{q}}(\boldsymbol{\theta}_n) = M^{\mathrm{q}}(\boldsymbol{\theta}^{\mathrm{q}}_{f(n)})$ on $\hat{\mathbf{x}}\mathtt{1}$ to obtain $p(\mathtt{1} \mid \hat{\mathbf{x}})$, and returns true or false according to whether $p(\mathtt{1} \mid \hat{\mathbf{x}}) > 0$ (i.e., it returns $\textsc{LocalProb}(\hat{\mathbf{x}}, 0)$ which $= \textsc{Sat}(\boldsymbol{\theta})$ as desired). Constructing $M^{\mathrm{q}}(\boldsymbol{\theta}_{f(n)})$ and calling it on $\hat{\mathbf{x}}$ each take time polynomial in n (thanks to efficiency of M^{q}). This completes the proof by contradiction.

It remains to be shown that the unweighted language $\tilde{p}$ is efficiently computable. The following algorithm outputs $\tilde{p}(\mathbf{x}), \forall \mathbf{x} \in \mathbb{B}^*$: If $\mathbf{x}$ has a prefix that encodes a formula ϕ, and the remainder of $\mathbf{x}$ is a satisfying assignment $\mathbf{a}$ to the variables of ϕ, then return $(\frac{1}{3})^{|\mathbf{x}|+1}$. Otherwise return 0. This algorithm can be made to run in polynomial time because whether an assignment satisfies a formula can be determined in polynomial time (i.e., $\textsc{Sat} \in \mathrm{NP}$. □

Remark on RNNs. The above proof showed that $\tilde{p}$ is efficiently computable, though p cannot be efficiently computed by any locally normalized architecture with compact parameters. Because this paper is in part a response to popular neural architectures, we now show that $\tilde{p}$ can in fact be computed efficiently *by recurrent neural networks (RNNs)* with compact parameters. Thus, this is an example where a locally normalized RNN parameterization is fundamentally less efficient (in runtime or parameters) than a globally normalized one.

Since we showed that $\tilde{p}$ is efficiently computable, the existence of an RNN implementation is established in some sense by the ability of finite rational-weighted RNNs to simulate Turing machines [44]. However, it appears straightforward to give a concrete construction, for each $n \in \mathbb{N}$, for a simple RNN that maps each string $\mathbf{x} \in \mathbb{B}^n$ to $\tilde{p}(\mathbf{x})$. Here $\tilde{p}(\mathbf{x})$ will be either $(\frac{1}{3})^{n+1}$ or 0, according to whether $\mathbf{x}$ has the form $\boldsymbol{\phi}\mathbf{a}$ where $\boldsymbol{\phi}$ encodes a 3-CNF-SAT formula ϕ that is satisfied by $\mathbf{a}$.[6] The basic idea is that $\boldsymbol{\phi}$ has $j \leq n$ variables, so there are only $O(n^3)$ possible 3-CNF clauses. The RNN allocates one hidden unit to each of these. When reading $\boldsymbol{\phi}\mathbf{a}$, each clause encountered in $\boldsymbol{\phi}$ causes the corresponding hidden unit to turn on, and then each successive encountered in $\mathbf{a}$ turns off the hidden units for all clauses that would be satisfied by that literal. If any hidden units remain on after $\mathbf{x}$ has been fully read, then $\boldsymbol{\phi}$ was not satisfied by $\mathbf{a}$, and the RNN's final output unit should return 0. Otherwise it should return $(\frac{1}{3})^{n+1}$, which is constant for this RNN. To obtain digital behaviors such as turning hidden units on and off, it is most convenient to use ramp activation functions for the hidden units and the final output unit, rather than sigmoid activation functions. Note that our use of a separate RNN for each input length n is an example of using more

[5] We must require that this version of SAT is NP-complete. This is true provided that we have chosen enc not only to be prefix-free, but to be concise in the sense that $\boldsymbol{\phi} \triangleq \mathrm{enc}(\phi)$ can be converted to and from the conventional encoding of ϕ in polynomial time. In that case, our version of SAT is $\leq^P_m$-interreducible with the conventional version and hence NP-complete.

[6] The restriction to 3-CNF-SAT formulas is convenient, but makes this a slightly different definition of $\mathcal{X}$ and $\tilde{p}$ than we used in the proofs above. Those proofs can be adjusted to show that this $\tilde{p}$, too, cannot be efficiently locally normalized with compact parameters. The only change is that in the construction of Lemma 2, ϕ' must be converted to 3-CNF. The proof of Lemma 2 then obtains its contradiction by showing that 3-CNF-$\textsc{Sat} \in \mathrm{P/poly}$ (which suffices since 3-CNF-SAT is also NP-complete).

hidden units for larger problems, a key idea that we introduced in §2.3 in order to look at asymptotic behavior. The RNN's parameter sequence $\boldsymbol{\Theta}^{\text{RNN}} = \{\boldsymbol{\theta}_n^{\text{RNN}} \mid n \in \mathbb{N}\}$ is obviously compact, as $\boldsymbol{\theta}_n^{\text{RNN}}$ only has to store the input length n. With our alphabet $\mathbb{B}$ for $\tilde{p}$, $|\boldsymbol{\theta}_n^{\text{RNN}}| \in O(\log n)$.

3.2 Approximate computation of local probabilities is also NP-hard

Here we show local probabilities likely cannot be *approximated* well with compact parameters—even with the additional help of randomness. Using our example weighted language $\tilde{p}$ and our $\boldsymbol{\phi}'$ construction introduced in §3.1, it is straightforward to show that approximating $p(\mathtt{0} \mid \boldsymbol{\phi}')$ within *any* multiplicative error, for *all* $\boldsymbol{\phi}'$s, is NP-hard. We see that $p(\mathtt{0} \mid \boldsymbol{\phi}') = 0$ iff a formula ϕ has at least one solution. So we could efficiently solve SAT problems if we could efficiently approximate $p(\mathtt{0} \mid \boldsymbol{\phi}')$ for all $\boldsymbol{\phi}'$s within some multiplicative error, as this would tell us which $p(\mathtt{0} \mid \boldsymbol{\phi}') = 0$ exactly.

However, this demonstration hinges on the difficulty of multiplicative approximation of zeroes, which is unsurprisingly hard. Below we further show that it is also hard to approximate non-zero probabilities. We give two proofs. As in Theorem 1, our results depend on the assumption that $\text{NP} \not\subseteq \text{P/poly}$.

3.2.1 Approximating nonzero local probabilities is hard

First we show superpolynomiality results (i.e. there does not exist a sequence of compact parameters) similar to Theorem 1 for randomized algorithms (and ultimately probabilistic Turing machines) that approximate locally normalized probabilities:

Theorem 2. *Given $\lambda \geq 1$. Assuming $\text{NP} \not\subseteq \text{P/poly}$, there exists an efficiently computable weighted language $\tilde{p} : V^* \to \mathbb{R}_{\geq 0}$ such that there is no $(M^{\text{q}}, \boldsymbol{\Theta}^{\text{q}}, \lambda)$ where $\boldsymbol{\Theta}^{\text{q}} = \{\boldsymbol{\theta}_n^{\text{q}} \mid n \in \mathbb{N}\}$ that satisfies all of the following properties (similar to §2.4):*

- *the parameter size $|\boldsymbol{\theta}_n^{\text{q}}|$ grows as $O(\text{poly}(n))$.*
- *$M^{\text{q}}(\boldsymbol{\theta}_n^{\text{q}})$ runs in time $O(\text{poly}(n))$ and outputs a probabilistic Turing machine $q_n : V^n \to \mathbb{Q} \cap [0, 1]$.*
- *the worst-case runtime of q_n (on inputs of length $\leq n + 1$) is $O(\text{poly}(n))$.*
- *with probability $> 2/3$, the probabilistic computation $q_n(\hat{\mathbf{x}}x)$ approximates $p(x \mid \hat{\mathbf{x}})$ to within a factor of λ, whenever $p(x \mid \hat{\mathbf{x}}) > 0$ and also $x \in V \cup \{\$\}$, $\hat{\mathbf{x}} \in V^*$, and $|\hat{\mathbf{x}}| \leq n$.*

Proof. We take $\tilde{p}$ to be the weighted language that was defined in §3.1, which was already shown to be efficiently computable in the proof of Theorem 1. Suppose $(M^{\text{q}}, \boldsymbol{\Theta}^{\text{q}}, \lambda)$ is a counterexample to Theorem 2. Choose integer $k \geq 1$ in a manner (dependent on λ) to be described at the end of the proof.

As in the proof of Lemma 2, suppose we would like to answer SAT where ϕ is a formula with variables $A_1, \ldots, A_j$. Define $\phi' = (\neg A_1 \wedge \neg A_2 \wedge \ldots \wedge \neg A_j \wedge \neg A_{j+1} \wedge A_{j+k}) \vee (A_1 \wedge \text{Shift}(\phi))$. For $k = 1$, this is the same construction as in Lemma 2, but more generally, it introduces $k - 1$ additional variables into the formula. Let $n = |\boldsymbol{\phi}'|$ and note that n is polynomial in the size of ϕ.

The strings in $\mathcal{X}$ that begin with $\boldsymbol{\phi}'$ are precisely the strings of the form $\boldsymbol{\phi}'\mathbf{a}'$ where $\mathbf{a}'$ is a satisfying assignment of ϕ'. This is achieved precisely when $\mathbf{a}' = \mathtt{0}^{j+k}$ or $\mathbf{a}' = \mathtt{1}\mathbf{a}\vec{b}$ where $\mathbf{a}$ is a satisfying assignment of ϕ and $\vec{b} \in \mathbb{B}^{k-1}$.

All strings in $\mathcal{X}$ that begin with $\boldsymbol{\phi}'$ have equal weight under $\tilde{p}$. Call this weight w.[7]. Clearly $Z(\boldsymbol{\phi}'\mathtt{0}) = w$, and $Z(\boldsymbol{\phi}'\mathtt{1}) = w \cdot 2^{k-1} \cdot (\text{number of satisfying assignments of } \phi)$.

Recall that $p(\mathtt{0} \mid \boldsymbol{\phi}') = Z(\boldsymbol{\phi}'\mathtt{0})/(Z(\boldsymbol{\phi}'\mathtt{0}) + Z(\boldsymbol{\phi}'\mathtt{1}))$. It follows that if ϕ is unsatisfiable, then $p(\mathtt{0} \mid \boldsymbol{\phi}') = 1$, but if ϕ is satisfiable, then $p(\mathtt{0} \mid \boldsymbol{\phi}') \leq 1/(1+2^{k-1})$. By hypothesis, we can compute $q = (M^{\text{q}}(\boldsymbol{\theta}^{\text{q}}_{|\boldsymbol{\phi}'|}))(\boldsymbol{\phi}'\mathtt{0})$ in time $O(\text{poly}(n))$. And by hypothesis, q approximates p (with probability $> 2/3$) to within a factor of λ, meaning that $p \in [q/\lambda, \lambda q]$. By choosing k large enough[8] such that $[q/\lambda, \lambda q]$ cannot contain both 1 and $1/(1+2^{k-1})$, we can use q to determine whether $p = 1$ or $p \leq 1/(1+2^{k-1})$, which allows us to determine $\text{SAT}(\phi)$ in polynomial time (with error probability

[7] Each such string has length $n + j + k$, so $\tilde{p}$ gives it a weight of $w = (\frac{1}{3})^{n+j+k+1}$.

[8] It suffices to ensure that $1 + 2^{k-1} > \lambda^2$, so take any $k > 1 + \log_2(\lambda^2 - 1)$.

$< 1/3$). This shows that SAT $\in$ BPP/poly $=$ P/poly, implying NP $\subseteq$ P/poly, contrary to our assumption. (BPP/poly is similar to P/poly but allows M^{q} to be a bounded-error probabilistic Turing machine.) $\square$

3.2.2 Approximating nonzero local probabilities is hard even for "nice" distributions

The local probability $p(x \mid \hat{\mathbf{x}}) \triangleq Z(\hat{\mathbf{x}}x)/Z(\hat{\mathbf{x}})$ in general may involve *infinite* summations in energy-based models. One might wonder if this is the source of the difficulty.

The example language $\tilde{p}$ used in our proof in Theorem 2 did not have support on all of V^*. Some conditional probabilities were zero. As a result, $\tilde{p}$ more resembles a transition-based parser's action sequence distribution, where certain actions can only be taken in certain contexts, rather than a language model, which is usually smoothed to allocate positive probability to every string in V^*. Again, one might wonder if this is the source of the difficulty.

In fact, even when these situations are not present, local conditional probabilities cannot always be efficiently computed with compact parameters.

Theorem 3.

(a) Theorem 2 remains true even when the approximation guarantee is only required to hold for $\hat{\mathbf{x}}$ such that $\{\mathbf{x} : \hat{\mathbf{x}} \preceq \mathbf{x}\}$ is finite (so that $p(x \mid \hat{\mathbf{x}})$ is computable by brute force).

(b) Theorem 2 remains true even for weighted languages $\tilde{p}$ that have support on all of V^*: that is, $\tilde{p}(\mathbf{x}) > 0 \iff \mathbf{x} \in V^*$.

Proof. For part (a), the proof of Theorem 2 suffices, since it reduces SAT to approximate local probability queries of the stated form. That is, the true local probabilities $p(x \mid \hat{\mathbf{x}})$ that can be computed with finite summations, thanks to the structure of our example language $\tilde{p}$, which guarantees that the prefix $\hat{\mathbf{x}}$ can only continue with suffixes of a fixed length that is easily determined from $\hat{\mathbf{x}}$.

For part (b), again let $V = \{\mathtt{0}, \mathtt{1}\}$. Choose some $\epsilon > 0$ (any choice will do), and let

$$\tilde{p}_1(\mathbf{x}) = \begin{cases} (\frac{1}{3})^{|\mathbf{x}+1|} & \text{if } \mathbf{x} = \boldsymbol{\phi}\mathbf{a} \text{ where } \boldsymbol{\phi} = (\phi) \text{ and } \mathbf{a} \text{ satisfies } \phi \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

$$\tilde{p}_2(\mathbf{x}) = \epsilon \cdot (\tfrac{1}{9})^{|\mathbf{x}+1|} > 0 \tag{2}$$

$$\tilde{p}(\mathbf{x}) = \tilde{p}_1(\mathbf{x}) + \epsilon \cdot \tilde{p}_2(\mathbf{x}) \tag{3}$$

We use Z_1, Z_2, and Z respectively to denote normalizing constants of these three weighted languages. Note that $\tilde{p}_1$ is the weighted language that was previously used in the proofs of Theorems 1 and 2. Our new $\tilde{p}$ is intended to be very similar while satisfying the additional condition of Theorem 3. It is easy to show that $\tilde{p}$ is efficiently computable, much as we showed for $\tilde{p}_1$ in Theorem 1. Also, $\tilde{p}$ is normalizable, since $Z = Z_1 + \epsilon \cdot Z_2$, where $Z_1 \leq (\frac{1}{3})/(1 - \frac{2}{3}) = 1$ and $Z_2 = (\frac{1}{9})/(1 - \frac{2}{9}) = \frac{1}{7}$ are both finite.

The proof proceeds as in Theorem 2, with ϕ' constructed from ϕ as before. Recall that ϕ has j variables, ϕ' has $j + k$ variables, and $|\boldsymbol{\phi}'| = n$. We may assume WLOG that the encoding function enc is such that an encoded formula always has at least as many bits as the number of variables in the formula, so $n \geq j + k$.

Notice that $Z_1(\boldsymbol{\phi}')$ sums over the satisfying assignments of $\boldsymbol{\phi}'$; when there is only one satisfying assignment, it will be small for large j. By contrast, $Z_2(\boldsymbol{\phi}')$ sums over an infinite number of continuations with positive probability. The faster decay rate of $\frac{1}{9}$ in $\tilde{p}_2$ was chosen to keep $Z_2(\boldsymbol{\phi}')$ small relative to $Z_1(\boldsymbol{\phi}')$ despite this. Specifically,

$$Z_1(\boldsymbol{\phi}'\mathtt{0}) = (\tfrac{1}{3})^{n+j+k+1} \tag{4}$$

$$Z_1(\boldsymbol{\phi}'\mathtt{1}) = (\tfrac{1}{3})^{n+j+k+1} \cdot 2^{k-1} \cdot (\text{number of satisfying assignments of } \phi) \tag{5}$$

$$Z_2(\boldsymbol{\phi}'\mathtt{0}) = (\tfrac{1}{9})^{n} \cdot \tfrac{1}{9} \cdot (\tfrac{1}{9}/(1 - \tfrac{2}{9})) \tag{6}$$

$$= \tfrac{1}{7} \cdot (\tfrac{1}{3})^{2(n+1)} \tag{7}$$

$$< \tfrac{1}{7} \cdot Z_1(\boldsymbol{\phi}'\mathtt{0}) \text{ (because } 2(n+1) > n + j + k + 1) \tag{8}$$

$$Z_2(\boldsymbol{\phi}'\mathtt{1}) = Z_2(\boldsymbol{\phi}'\mathtt{0}) \tag{9}$$

As in the proof of Theorem 2, we will show that $p(0 \mid \phi')$ is much larger when ϕ is unsatisfiable. Recall that $Z(\hat{\mathbf{x}}) = Z_1(\hat{\mathbf{x}}) + \epsilon \cdot Z_2(\hat{\mathbf{x}})$. When ϕ has zero satisfying assignments,

$$p(0 \mid \phi') = \frac{Z(\phi'0)}{Z(\phi'0) + Z(\phi'1)} = \frac{Z(\phi'0)}{Z_1(\phi'0) + Z_2(\phi'0) + Z_2(\phi'1)} > \frac{Z(\phi'0)}{Z_1(\phi'0) + 2 \cdot \frac{\epsilon}{7} \cdot Z_1(\phi'0)} \tag{10}$$

whereas if ϕ has at least one satisfying assignment, then

$$p(0 \mid \phi') = \frac{Z(\phi'0)}{Z(\phi'0) + Z(\phi'1)} < \frac{Z(\phi'0)}{Z_1(\phi'0) + Z_1(\phi'1)} \leq \frac{Z(\phi'0)}{Z_1(\phi'0) + 2^{k-1} Z_1(\phi'0)} \tag{11}$$

This rewrites both probabilities in terms of $Z.(\phi'0)$ quantities, which do not depend on the number of satisfying assignments. So now we can see that the first probability is at least $(1 + 2^{k-1}) \;/\; (1 + \frac{2\epsilon}{7})$ times as large as the second probability. Choose k large enough[9] such that $[q/\lambda, \lambda q]$ cannot contain both probabilities, and complete the proof as in Theorem 2. □

3.3 SAT Experiments

The results in §§ 3.1 and 3.2 are worst-case analyses: no efficiently computable model with compact parameters can be expected to correctly predict on all formulas ϕ whether $p(0 \mid \phi'_k) = 0$, whether exactly or approximately. To demonstrate the effect in practice, we conducted basic supervised learning experiments with actual formulas ϕ (drawn from a distribution over random 3-CNF formulae that favors hard examples), to confirm that popular autoregressive models stumble with their default settings.[10] We found that SEQ2SEQ architectures using LSTMs [21] and Transformers [46] in general fail to learn $p(\cdot \mid \phi')$. That is, they cannot reliably decide whether the encoded formula ϕ is satisfiable, across formulae and networks of different sizes. However they have some success predicting some variable assignments given that ϕ is indeed satisfiable. Details of experimental setup and findings are in Appendix D.

4 Modeling Real-Life Datasets with Globally Normalized Models

4.1 Finite growth of parameter string sizes

Efficiently computable languages with compact parameters, such as $\tilde{p}$ which we discussed in §3, by definition have *infinite* parameter strings (which may not be recursively enumerable). In general, we can only hope to learn the first T parameter strings for some $T \in \mathbb{N}$, and therefore can only accurately approximate weights of sequences up to length T, which form a finite language $\mathcal{X}_{\leq T} = \{\mathbf{x} \mid \mathbf{x} \in \mathcal{X}, |\mathbf{x}| \leq T\}$. We would like to stress that our analysis on parameter (in)efficiency in §3 still holds in such finite approximations: let M^p be a fixed Turing machine that (approximately) locally normalizes weighted language $\tilde{p}$ with parameter strings in the manner of §2.3, and let $\boldsymbol{\Theta}^{\mathrm{p}} = \{\boldsymbol{\theta}^{\mathrm{p}}_n \mid n \in \mathbb{N}\}$ be a sequence of such strings. We know from Theorem 2 that there exists 'hard' efficiently computable weighted languages where there is no $k \in \mathbb{R}$ such that $\forall n \in \mathbb{N}, |\boldsymbol{\theta}^{\mathrm{p}}_n| < n^k$, for any $(M^p, \boldsymbol{\Theta}^{\mathrm{p}})$ pair. However, by the definition of efficiently computable weighted language with compact parameters in §2.3, we know that for any $\tilde{p}_{\boldsymbol{\Theta}} = (M^{\tilde{\mathrm{p}}}, \{\boldsymbol{\theta}^{\tilde{\mathrm{p}}}_n \mid n \in \mathbb{N}\})$, $\exists k' \in \mathbb{R}, \forall n \in \mathbb{N}, |\boldsymbol{\theta}^{\tilde{\mathrm{p}}}_n| < n^{k'}$. For 'hard' weighted languages (such as $\tilde{p}$ in §3) the sum of the first T local normalization parameter strings in $\boldsymbol{\Theta}^{\mathrm{p}}$: $\sum_{t=1}^{T} |\boldsymbol{\theta}^{\mathrm{p}}_t|$ will be superpolynomial in T, in which case $\lim_{T\to\infty} \frac{\sum_{t=1}^{T} |\boldsymbol{\theta}^{\mathrm{p}}_t|}{\sum_{t=1}^{T} |\boldsymbol{\theta}^{\tilde{\mathrm{p}}}_t|} = 0$, and the value of T for which our parameter budget admits good up-to-T approximation with locally normalization parameters $\boldsymbol{\Theta}^{\mathrm{p}}$ is low. With slight abuse of notation, we assume $\tilde{p}_{\boldsymbol{\theta}}$ in §4 to be a finite language, whose parameters $\boldsymbol{\theta}$ encode $\{\boldsymbol{\theta}^{\tilde{\mathrm{p}}}_t \mid 0 \leq t \leq T\} \subset \boldsymbol{\Theta}^{\tilde{\mathrm{p}}}$, with support $\mathcal{X}_{\leq T}$. Specific values of T of datasets used in experiments are listed in Appendix C.1.

[9] It suffices to ensure that $(1 + 2^{k-1})/(1 + \frac{2\epsilon}{7}) > \lambda^2$, so take any $k > 1 + \log_2(\lambda^2 \cdot (1 + \frac{2\epsilon}{7}) - 1)$.

[10] Caveats: (1) We did not conduct an extensive search in the hyperparameter space, which could result in better performance. (2) As in other supervised learning settings, our setup confounds (a) the existence of good parameters (model capacity), (b) the ability to find them (search), and (c) the quality of generalization from finite training data (inductive bias). (3) We did not test whether the problem is easier to learn for energy-based models—although a compact solution at least exists in this case (Theorem 1), whether or not easily learnable.

4.2 Residual energy-based models (REBMs)

In practice, energy-based models $p_{\boldsymbol{\theta}}(\mathbf{x}) \triangleq \tilde{p}_{\boldsymbol{\theta}}(\mathbf{x})/Z$ can be difficult to train. A difficulty is that the maximum-likelihood objective involves Z, which in general requires a sum over the support $\mathcal{X}$.

We will assume here that we work with distributions with a finite support $\mathcal{X}_{\leq T} \triangleq \{\mathbf{x} \mid \mathbf{x} \in \mathcal{X}, |\mathbf{x}| \leq T\}$ (i.e., our task will bound the maximum string length T) to ensure that $Z < \infty$ for any value of θ. Consequently, $\tilde{p}$ is normalizable for any value of θ,[11] and we do not have to explicitly restrict the search space to values of θ for which it is.

Even so, exact computation of Z is in general intractable in T. Thus, MLE training methods generally estimate it by sampling. Another approach is to use noise-contrastive estimation (NCE) [19, 20], an alternative objective that avoids explicit computation of Z.

We use the "ranking-based" variant [24] of NCE. However, in pilot experiments we found that globally normalized models in fact achieve *worse* held-out perplexity than locally normalized ones. We attribute this problem to inductive bias (stemming from either the model architecture or the optimization landscape around the initial parameters), rather than to a lack of capacity of the specific globally normalized architecture, although both are possible.

Fortunately, it is possible to infuse a globally normalized architecture with both the inductive bias *and* the capacity of a locally normalized one. We find that this gets better results. Our simple hybrid architecture, the *residual energy-based model* (the name is due to Deng et al. [16], who independently proposed this approach in concurrent work), is a globally normalized distribution:

$$p_{\boldsymbol{\theta}}(\mathbf{x}) \propto \tilde{p}_{\boldsymbol{\theta}}(\mathbf{x}) \triangleq q_0(\mathbf{x}) \cdot \exp g_{\boldsymbol{\theta}}(\mathbf{x}) \tag{12}$$

The *base model* $q_0 : \mathcal{X}_{\leq T} \to (0, 1]$ is a locally normalized neural sequence model that was pretrained on the same distribution. The *discriminator* $g_{\boldsymbol{\theta}} : \mathcal{X}_{\leq T} \to \mathbb{R}$ is a neural function of sequence $\mathbf{x}$, with trainable parameters $\boldsymbol{\theta}$, so that exponentiating it gives a weighted language with support $\mathcal{X}_{\leq T}$.[12]

We use a two-phase training strategy,[13] where we first train the autoregressive base distribution q_0 to approximate p via MLE, then optimize $\boldsymbol{\theta}$ to make $p_{\boldsymbol{\theta}}$ fit the data, so that $g_{\boldsymbol{\theta}}$ is capturing the residuals in log-space. For this second step we use noise-contrastive estimation, using q_0 as an informed noise distribution.

If we make an additional assumption that the autoregressive $q_0(\cdot \mid \mathbf{x}_{1\ldots t})$ is *at most* off by some multiplicative error $\epsilon > 0$, we can bound $g_{\boldsymbol{\theta}}(\mathbf{x}) \in [-T \log \epsilon, T \log \epsilon]$, which may help us learn under limited training samples. Details of the design of base models q_0, discriminators $g_{\boldsymbol{\theta}}$, and training procedure can be found in Appendix B.

4.3 Experiments

We evaluate the effectiveness of REBMs on two different neural architectures (GRU- and Transformer-based) and 3 datasets, on the task of modeling sequence probabilities. An REBM $\tilde{p}_{\boldsymbol{\theta}}$ has two components, $g_{\boldsymbol{\theta}}$ and q_0, and we would like to see how $\tilde{p}_{\boldsymbol{\theta}}$ competes against q_0 itself. We do not further tune q_0 while training $p_{\boldsymbol{\theta}}$. As a fair comparison, we also see how q_0' compares against q_0, where q_0' is simply a version of q_0 that has been trained as many additional epochs as were used to train $p_{\boldsymbol{\theta}}$.

q_0 models are pretrained on moderately large corpora (in GRU cases) or a very large corpus (in the Transformer case).[14] We compare residual energy-based models $\tilde{p}_{\boldsymbol{\theta}}$ to further-fine-tuned base models q_0', on conservatively estimated (at the low end of 95% confidence interval) token perplexity and

[11] Provided that $\tilde{p}$ is also defined to ensure $Z > 0$, for example using an exp function.

[12] A natural extension would be to replace $q_0(\mathbf{x})$ with $q_0(\mathbf{x})^{\beta}$, where $\beta \geq 0$ is a trainable inverse temperature. Now the architecture subsumes the standard energy-based architecture (at $\beta = 0$). A further step in this direction would be to replace $q_0(\mathbf{x})$ for $|\mathbf{x}| = n$ with $\left(\prod_{t=1}^{n} q_0(x_t \mid \mathbf{x}_{1\ldots t-1})^{\beta(\mathbf{x}_{1\ldots t-1})}\right) q_0(\$ \mid \mathbf{x})^{\beta(\mathbf{x})}$, so that the local conditional probabilities that serve as the factors of $q_0(\mathbf{x})$ are raised to different context-dependent β powers according to how trustworthy they are. In both cases, choosing all $\beta = 1$ recovers equation (12). Another extension would provide the neural states of q_0 as additional input to the neural network for $g_{\boldsymbol{\theta}}$.

[13] We provide a more formal argument for such a strategy in Lemma 5.

[14] In the Transformer case we simply take q_0 to be the Grover [50] pretrained language model, which is based on the GPT-2 [41] architecture and performs competitively on news article generation.

bootstrap-sampled log likelihood improvements. The results are in Table 1. Residual energy-based models show consistent perplexity improvement compared to q'_0 that are trained on the same data using the same maximum numbers of iterations. Although the improvement in log-likelihood of $p_{\boldsymbol{\theta}}$ over q_0 is modest (especially for RealNews experiments, where q_0 is a very strong baseline), we verify that these improvements are all statistically significant ($p < 0.05$) using bootstrapped test datasets.

We experiment with different designs of the discriminator $g_{\boldsymbol{\theta}}$, evaluating the effectiveness of bounding $g_{\boldsymbol{\theta}}$ and varying its number of parameters. We find that in Transformer-based experiments, bounding $g_{\boldsymbol{\theta}}$ considerably helps with performance; but the opposite happens for GRU-based models. We speculate that this is due to the base models' performance: the Transformer base models have high parameter count and were trained on a lot of data; and the true distribution p likely is relatively similar to q_0, and benefits from a small hypothesis space—even though we don't know if the at-most-ϵ error assumption in §4.2 holds. On the other hand our GRU-based q_0 has neither the capacity, nor the huge amount of training data. As a result, the unbounded variant $g_{\boldsymbol{\theta}}$ (and $q_{\boldsymbol{\theta}}$) may end up learning a better approximation of p.

Experiment (Architecture)	Model	Best configuration	log likelihood improvement (95% CI)	perplexity improvement
RealNews (Transformer)	$p_{\boldsymbol{\theta}}$	4-layer, $\tanh$	$(-0.18, -0.13), \mu = -0.15$	.03%
RealNews (Transformer)	q'_0	N/A	N/A	.00%
WikiText (GRU)	$p_{\boldsymbol{\theta}}$	1-layer/500, softplus	$(-1.85, -1.54), \mu = -1.69$	1.44%
WikiText (GRU)	q'_0	N/A	N/A	.50%
Yelp (GRU)	$p_{\boldsymbol{\theta}}$	2-layer/500, softplus	$(-1.89, -1.67), \mu = -1.80$	1.82%
Yelp GRU	q'_0	N/A	N/A	.49%

Table 1: Residual energy-based model $\tilde{p}_{\boldsymbol{\theta}}$ improvements over autoregressive base models q_0. The perplexity numbers are per-token, and log likelihood improvements are per sequence (in nats). We only report each dataset's best model (according to validation data) in this table. See Appendix C for experimental details.

5 Related work

5.1 Computational complexity and inference in graphical models

Our work is closely related to the study of inference complexity of graphical models. In particular, [11] showed that if $\mathrm{NP} \not\subseteq \mathrm{P/poly}$—the same assumption we take in this paper—then there is no efficient inference method for any family of graphical models with unbounded treewidth. While we only show superpolynomiality results under the assumption $\mathrm{NP} \not\subseteq \mathrm{P/poly}$, both [11, 26] were able to further sharpen their hardness results under the stronger exponential time hypothesis (ETH) [23]. It is not clear whether assuming ETH would lead to exponential growth of parameter size, which we leave as future work. Our work also implies that general density estimators that rely on autoregressive factoring of joint probability, such as [45], can be misspecified for some distributions.

5.2 Energy-based discrete sequence models

To the best of our knowledge, [42] was the first to introduce the idea of globally normalized discrete sequence models. And [43] first introduced the idea of refining a generative sequence model with a discriminator. Such models have subsequently been neuralized, as in [22, 16]. In particular, the contemporaneous work [16] also proposes to learn a discriminator using NCE, and empirically justifies both qualitative and quantitative improvement. Our work focuses on providing theoretical justification for such energy-based models, on the grounds that they are better at modeling combinatorially hard problems without an explosion of runtime nor of precomputed/pretrained parameters.

It has been widely known that locally normalized taggers conditioned on input prefixes cannot model certain conditional distributions, suffering from so-called *label bias* [28]. [3] pointed out such problems persist for conditional locally normalized models, regardless of model capacity. [28] showed how to avoid label bias using globally normalized feature-based models, taking care to keep the partition function tractable. However tractable partition functions imply efficient local normalization (with compact parameters), and therefore such models are still subject to our model capacity constraints. In contrast, [31, 32] similarly used globally normalized *neural* sequence models, using sequential Monte Carlo to estimate the log-likelihood gradient, and would still work for model families that do not guarantee tractable partition functions. While the label bias problem does not affect fully generative models

$p(\mathbf{y})$ such as the ones shown here, nor conditional models $p(\mathbf{y} \mid \mathbf{x})$ where $\mathbf{x}$ is fully read before any of $\mathbf{y}$ is generated, we show in this paper that such models still lack expressivity unless they have superpolynomial runtime or parameter count.

5.3 *Ad hoc* inference in autoregressive language models

It has been shown that massive autoregressive models [e.g., 41, 8] have had success (to various degrees) on zero- or few-shot inference tasks: these tasks ask a model to execute on-demand inference either by demonstration (few-shot) or by natural language description (zero-shot). But our theoretical results suggest that an autoregressive language model may be parameter-size-inefficient on such tasks (unless $\mathrm{NP} \subseteq \mathrm{P/poly}$), since they generalize the weighted language $\tilde{p}$ we described in §3 (see Figure 1). While it is difficult to tell what capability an autoregressive model has exactly at a given parameter size, preliminary results from GPT-3 [8, Fig. 1.3] show that few-shot accuracy grows logarithmically in parameter size, suggesting that pumping up the number of parameters may not an efficient way to improve performance.

Beyond language modeling, our intuition is that globally normalized models are useful in settings where predicting the future is most naturally done with explicit lookahead that is difficult to compile into a local evaluation function. Such settings occur in game play (famously in chess [10]), where lookahead is still widely used (e.g., via MCTS [9]), as well in low-data regimes where inductive bias has trouble finding the correct local evaluation function [e.g., 15].

6 Conclusion and Future Work

In order to compare sequence modeling architectures, we introduced new characterizations of the modeling task: whether unnormalized probabilities or local conditional probabilities are "efficiently computable with compact parameters." We showed that the class of efficiently computable weighted languages with compact parameters is not closed under local normalization if $\mathrm{NP} \not\subseteq \mathrm{P/poly}$, suggesting that discrete autoregressive sequence models may be parameter-size-inefficient when used to model sequences with complex structure, e.g. natural language. Note that our theoretical results also apply to *any* sequence model where local conditional probabilities can be efficiently computed, such as low-treewidth latent-variable sequence models [47]. Broadly speaking, any sequence model that is easy *both* to evaluate and to sample from is likely susceptible to the model misspecification problem we discuss. To mitigate deficiencies of such models, we have proposed *residual language models*, which fine-tune autoregressive base models with discriminators. We showed this strategy is effective on multiple architectures and datasets.

While *some* efficiently computable weighted languages cannot be locally normalized with compact parameters, we do not know if the same can be said for *most* efficiently computable weighted languages. This problem seems to be closely related to the notion of average complexity of NP-complete languages [30], where the relation between worst-case and average-case complexity has largely remained an open question [7].

We are mostly focused on the theoretical analysis of model capacity of locally and globally normalized models, but do not discuss the hardness of their estimation methods. For locally normalized RNNs there are known sample complexity bounds by reduction to real-valued RNNs [2]. We leave a rigorous analysis for globally normalized ones to future work. Moreover, our proposed residual language models rely on a well-trained base model to help reduce sample complexity, and requires a two-stage training procedure. There may be other ways to regularize globally normalized sequence models without autoregressive models, which we leave as future work.

In this paper, we have argued that probability models have limited expressivity when they perform only a limited amount of computation to predict the next symbol in a string. In particular, standard autoregressive models have less expressivity than comparable energy-based models (whose predictive distributions are harder to compute). Although these models can lean on the unlimited work that may have gone into precomputing the parameters (e.g., training), we showed that this crutch does not save them when the parameters are compact. However, given an autoregressive architecture with limited computation per time step, one could consider using multiple time steps to predict the next symbol—adaptively allocating more time steps (as humans may) for hard prediction instances [18]. For example, a language model for Figure 1 could "talk through its reasoning" by generating a long

sequence of symbols that terminates in the answer. Indeed, GPT-3 [8] seems to deliver better responses when it is prompted to "think aloud" in this way before answering [6]. An autoregressive model can evade our result if it invests superpolynomial computation in predicting the next symbol—whether by deterministically taking superpolynomially many intermediate steps, or by marginalizing over all possible stochastic choices for a linear number of intermediate steps. We leave the design and training of such reasoning policies as a suggestion for future investigation.

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A Lemmata and Proofs in §4

The following two lemmata show that given three weighted languages $\tilde{p}, \tilde{q}, \tilde{r}$ such that $\forall \mathbf{x} \in V^*, \tilde{p}(\mathbf{x}) = \tilde{q}(\mathbf{x}) \cdot \tilde{r}(\mathbf{x})$, then given any of two of the three are efficiently computable with compact parameters, the remaining weighted language is also efficiently computable with compact parameters.

Lemma 3. *Let $\tilde{p}, \tilde{q}, \tilde{r}$ be weighted languages, and $\forall \mathbf{x} \in V^*, \tilde{p}(\mathbf{x}) = \tilde{q}(\mathbf{x}) \cdot \tilde{r}(\mathbf{x})$. $\tilde{p}$ is efficiently computable with weighted parameters if $\tilde{q}$ and $\tilde{r}$ are both efficiently computable with compact parameters.*

Proof. If both $\tilde{q}$ and $\tilde{r}$ are efficiently computable with compact parameters, we label $\tilde{q} = (M^{\tilde{\mathrm{q}}}, \mathbf{\Theta}^{\tilde{q}})$ and $\tilde{r} = (M^{\tilde{\mathrm{r}}}, \mathbf{\Theta}^{\tilde{r}})$. We can design $\mathbf{\Theta}^{\tilde{p}} = \{\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}} \mid n \in \mathbb{N}\}$, where $\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}} = [\boldsymbol{\theta}_n^{\tilde{\mathrm{q}}}, \boldsymbol{\theta}_n^{\tilde{\mathrm{r}}}]$, and an $M^{\tilde{\mathrm{p}}}$ that upon reading $\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}}$ builds two Turing machines $M^{\tilde{\mathrm{q}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{q}}})$ and $M^{\tilde{\mathrm{r}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{r}}})$, and additional states and transitions, to be glued together as a single Turing machine that upon input $\mathbf{x}$ of length n, computes $M^{\tilde{\mathrm{q}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{q}}})(\mathbf{x}) \cdot M^{\tilde{\mathrm{r}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{r}}})(\mathbf{x})$. Since both $M^{\tilde{\mathrm{q}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{q}}})$ and $M^{\tilde{\mathrm{r}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{r}}})$ have runtime $O(\mathrm{poly}(n))$, and $|\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}}| \in O(\mathrm{poly}(n))$, $\tilde{p}$ is efficiently computable with compact parameters by definitions in §2.3. □

Lemma 4. *Let $\tilde{p}, \tilde{q}, \tilde{r}$ be weighted languages. If $\tilde{p}$ and $\tilde{q}$ are both efficiently computable with compact parameters, then there exists an efficiently computable weighted language with compact parameters $\tilde{r}$ such that $\forall \mathbf{x} \in V^*, \tilde{p}(\mathbf{x}) = \tilde{q}(\mathbf{x}) \cdot \tilde{r}(\mathbf{x})$.*

Lemma 5. *If $\exists k > 0$ such that $\frac{\mathbb{E}_{\mathbf{x} \sim q_0'}[\exp g_{\boldsymbol{\theta}}(\mathbf{x})]}{\mathbb{E}_{\mathbf{x} \sim q_0''}[\exp g_{\boldsymbol{\theta}}(\mathbf{x})]} > \exp(-k)$ and $\mathrm{KL}[p||q_0'] - \mathrm{KL}[p||q_0''] > k$ then $\mathrm{KL}[p||q_{\boldsymbol{\theta}}'] > \mathrm{KL}[p||q_{\boldsymbol{\theta}}'']$.*

Proof. The proof is similar to that of Lemma 3. If both $\tilde{p}$ and $\tilde{q}$ are efficiently computable with compact parameters, we label $\tilde{p} = (M^{\tilde{\mathrm{p}}}, \mathbf{\Theta}^{\tilde{p}})$ and $\tilde{q} = (M^{\tilde{\mathrm{q}}}, \mathbf{\Theta}^{\tilde{q}})$. We can design $\mathbf{\Theta}^{\tilde{r}} = \{\boldsymbol{\theta}_n^{\tilde{\mathrm{r}}} \mid n \in \mathbb{N}\}$, where $\boldsymbol{\theta}_n^{\tilde{\mathrm{r}}} = [\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}}, \boldsymbol{\theta}_n^{\tilde{\mathrm{q}}}]$, and an $M^{\tilde{\mathrm{r}}}$ that upon reading $\boldsymbol{\theta}_n^{\tilde{\mathrm{r}}}$ builds two Turing machines $M^{\tilde{\mathrm{p}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}})$ and $M^{\tilde{\mathrm{q}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{q}}})$, and additional states and transitions, to be glued together as a single Turing machine that upon input $\mathbf{x}$ of length n, first computes $M^{\tilde{\mathrm{p}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}})(\mathbf{x})$. If the output is 0, return 0. Otherwise, compute $M^{\tilde{\mathrm{q}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{q}}})(\mathbf{x})$ and return $\frac{M^{\tilde{\mathrm{p}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}})(\mathbf{x})}{M^{\tilde{\mathrm{q}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{q}}})(\mathbf{x})}$. $(M^{\tilde{\mathrm{r}}}, \mathbf{\Theta}^{\tilde{r}})$ meets our requirement for $\tilde{r}$. Moreover, since both $M^{\tilde{\mathrm{p}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{p}}})$ and $M^{\tilde{\mathrm{q}}}(\boldsymbol{\theta}_n^{\tilde{\mathrm{q}}})$ have runtime $O(\mathrm{poly}(n))$, and $|\boldsymbol{\theta}_n^{\tilde{\mathrm{r}}}| \in O(\mathrm{poly}(n))$, $\tilde{r}$ is efficiently computable with compact parameters by definitions in §2.3. □

B Implementation Details of Residual Language Models

B.1 Design of base models q_0

q_0 can be any distribution over $\mathcal{X}_{\leq T}$[15] provided that we can sample from it, and evaluate $q_0(\mathbf{x}), \forall \mathbf{x} \in \mathcal{X}_{\leq T}$, both in $O(\mathrm{poly}(|\mathbf{x}|))$. In this work, we experiment with two designs of q_0: GRU- and Transformer-based locally normalized language models. GRU-based models are used in WikiText and Yelp experiments. The GRU-based q_0's are parametrized with 2-layer GRUs with 500 hidden units, and word embeddings of dimension size 500.

As for Transformer-based q_0's, we make use of Grover models [50], which effectively are GPT-2 models trained on the aforementioned REALNEWS dataset. In this work, we experiment with the 'base' variant of public available weights, which are 12-layered Transformers, with 12 heads, and 768 hidden units.

B.2 Design of discriminators $g_{\boldsymbol{\theta}}$

We formulate $g_{\boldsymbol{\theta}}(\mathbf{x})$ as a summation of scores at positions $1 \ldots |\mathbf{x}|$, passed through an activation function f:

$$g_{\boldsymbol{\theta}}(\mathbf{x}) = f\left(\sum_{i=1}^{|\mathbf{x}|} g_t(\mathbf{x}; \boldsymbol{\theta})\right). \tag{13}$$

[15] Note that since q_0 does not have support over $\mathcal{X}$, it has to assign $p(\$ \mid \mathbf{x}_{1\ldots T}) = 1$, which is generally not an issue.

To verify whether lower-bounding $g_{\boldsymbol{\theta}}$ would help with learning, as we discuss in §4.2, we experiment with two variants of f:

- **tanh**: $f(x) = 2 \cdot \tanh(x)$
- **softplus**: $f(x) = -\log(1 + \exp(x + s))$

The former one is bounded between $(-2, 2)$, while the second one has range $(-\infty, 0)$. The offset term s in the softplus activation function determines initial values of $Z_{\boldsymbol{\theta}}$. In this paper we set $s = 20$.

The design of $g_t(\mathbf{x}; \boldsymbol{\theta})$ follows their base model counterparts: we use Bi-GRU discriminators for GRU base models; and bi-directional Transformer discriminators for Transformer ones. For GRUs $g_t(\mathbf{x}; \boldsymbol{\theta}) = \mathbf{h}_t \cdot x_t$, For Transformers $g_t(\mathbf{x}; \boldsymbol{\theta}) = \sum \mathbf{h}_t$ where $\mathbf{h}_t$ are the hidden states at time step t. In both cases, the discriminators have access to information of the whole sequence $\mathbf{x}$ at any timestep: the Bi-GRU discriminators achieve this through the bi-directional RNNs, and the Transformers through the attention mechanism without directional masking.

B.3 Training procedure

As we note in §4.2, MLE-based training methods are generally not feasible for globally normalized models. We therefore opt to train our model using the ranking variant of noise contrastive estimation (NCE) [34], which does not require samples from q_0 and has a simple form for residual LMs. Using q_0 as a *noise distribution*, NCE training requires minimizing the following single-sequence loss, in expectation over the true distribution p:

$$\mathcal{L}_{\text{NCE}}(\boldsymbol{\theta}, \mathbf{x}, q_0, K) = -\log \frac{\frac{\tilde{p}_{\boldsymbol{\theta}}}{q_0}(\mathbf{x})}{\sum_{k=0}^{K} \frac{\tilde{p}_{\boldsymbol{\theta}}}{q_0}(\mathbf{x}^{(k)})}, \tag{14}$$

where $\mathbf{x}^{(0)} \triangleq \mathbf{x}$, $\frac{\tilde{p}_{\boldsymbol{\theta}}}{q_0}(\mathbf{x}) \triangleq \frac{\tilde{p}_{\boldsymbol{\theta}}(\mathbf{x})}{q_0(\mathbf{x})}$, and $\mathbf{x}^{(1)} \dots \mathbf{x}^{(K)} \sim q_0$. Since $\tilde{p}_{\boldsymbol{\theta}}(\mathbf{x}) = q_0(\mathbf{x}) \cdot \exp g_{\boldsymbol{\theta}}(\mathbf{x})$, we have $\frac{\tilde{p}_{\boldsymbol{\theta}}}{q_0}(\mathbf{x}) = \exp g_{\boldsymbol{\theta}}(\mathbf{x})$. The NCE minimization objective (14) now reduces to the simple form

$$\mathcal{L}_{\text{NCE}}(\boldsymbol{\theta}, \mathbf{x}, q_0, K) = -g_{\boldsymbol{\theta}}(\mathbf{x}) + \log(\exp g_{\boldsymbol{\theta}}(\mathbf{x}) + \sum_{k=1}^{K} \exp g_{\boldsymbol{\theta}}(\mathbf{x}^{(k)})). \tag{15}$$

Notice that minimizing the expected loss with stochastic gradient descent methods $\mathcal{L}_{\text{NCE}}$ defined in equation (15) requires only evaluating sequence probabilities under $g_{\boldsymbol{\theta}}$, and tuning its parameters, but not the base model q_0. We only need to generate the noise samples $\{\mathbf{x}^{(k)} \sim q \mid k \in [K]\}$ from q_0. This way we do not need to backpropagate through parameters of the base model q_0, which can speed up training considerably when q_0 is backed by a huge network. In fact, the training of $g_{\boldsymbol{\theta}}$ can be completely agnostic to the design of q_0, allowing for the application of finetuning any locally normalized q_0.

Given the same discriminator $g_{\boldsymbol{\theta}}$, the difference of KL-divergence between the true model p and residual language models $\tilde{p}'_{\boldsymbol{\theta}}(\mathbf{x}) = q'_0(\mathbf{x}) \cdot \exp g_{\boldsymbol{\theta}}(\mathbf{x})$, and the KL-divergence between the true model and $\tilde{p}''_{\boldsymbol{\theta}}(\mathbf{x}) = q''_0(\mathbf{x}) \cdot \exp g_{\boldsymbol{\theta}}(\mathbf{x})$, defined with base models q'_0 and q''_0 respectively, can be written as

$$\text{KL}[p||q'_{\boldsymbol{\theta}}] - \text{KL}[p||q''_{\boldsymbol{\theta}}] = \text{KL}[p||q'_0] - \text{KL}[p||q''_0] + \log \frac{Z'}{Z''}, \tag{16}$$

where $Z' = \mathbb{E}_{\mathbf{x} \sim q'_0}[\exp g_{\boldsymbol{\theta}}(\mathbf{x})]$, and Z'' is similarly defined with q''_0. As a direct result of equation (16), we can see that finding q''_0 where $\text{KL}[p||q''_0] < \text{KL}[p||q'_0]$ implies improvement in $\text{KL}[p||q''_{\boldsymbol{\theta}}]$ over $\text{KL}[p||q'_{\boldsymbol{\theta}}]$, under mild conditions:

Lemma 5. *If* $\exists k > 0$ *such that* $\frac{\mathbb{E}_{\mathbf{x} \sim q'_0}[\exp g_{\boldsymbol{\theta}}(\mathbf{x})]}{\mathbb{E}_{\mathbf{x} \sim q''_0}[\exp g_{\boldsymbol{\theta}}(\mathbf{x})]} > \exp(-k)$ *and* $\text{KL}[p||q'_0] - \text{KL}[p||q''_0] > k$ *then* $\text{KL}[p||q'_{\boldsymbol{\theta}}] > \text{KL}[p||q''_{\boldsymbol{\theta}}]$.

Proof.

$$\begin{aligned}
\mathrm{KL}[p||q'_{\boldsymbol{\theta}}] - \mathrm{KL}[p||q''_{\boldsymbol{\theta}}] &= \mathop{\mathbb{E}}_{\mathbf{x}\sim p}[\log q''_{\boldsymbol{\theta}}(\mathbf{x}) - \log q'_{\boldsymbol{\theta}}(\mathbf{x})] \\
&= \mathop{\mathbb{E}}_{\mathbf{x}\sim p}[\log \frac{q''_0(\mathbf{x}) \exp g_{\boldsymbol{\theta}}(\mathbf{x})}{\sum_{\mathbf{x}'\in\mathcal{X}_{\leq T}} q''_0(\mathbf{x}) \exp g_{\boldsymbol{\theta}}(\mathbf{x})} - \log \frac{q'_0(\mathbf{x}) \exp g_{\boldsymbol{\theta}}(\mathbf{x})}{\sum_{\mathbf{x}'\in\mathcal{X}_{\leq T}} q'_0(\mathbf{x}) \exp g_{\boldsymbol{\theta}}(\mathbf{x})}] \\
&= \mathop{\mathbb{E}}_{\mathbf{x}\sim p}[\log \frac{q''_0(\mathbf{x}) \exp g_{\boldsymbol{\theta}}(\mathbf{x})}{\mathbb{E}_{\mathbf{x}'\sim q''_0}[\exp g_{\boldsymbol{\theta}}(\mathbf{x})]} - \log \frac{q'_0(\mathbf{x}) \exp g_{\boldsymbol{\theta}}(\mathbf{x})}{\mathbb{E}_{\mathbf{x}'\sim q'_0}[\exp g_{\boldsymbol{\theta}}(\mathbf{x})]}] \\
&= \mathop{\mathbb{E}}_{\mathbf{x}\sim p}[\log q''_0(\mathbf{x}) - \log q'_0(\mathbf{x})] + \mathop{\mathbb{E}}_{\mathbf{x}\sim p}[\log \mathop{\mathbb{E}}_{\mathbf{x}'\sim q'_0}[\exp g_{\boldsymbol{\theta}}(\mathbf{x})] - \log \mathop{\mathbb{E}}_{\mathbf{x}'\sim q''_0}[\exp g_{\boldsymbol{\theta}}(\mathbf{x})]] \\
&= \mathrm{KL}[p||q'_0] - \mathrm{KL}[p||q''_0] + \log \frac{\mathbb{E}_{\mathbf{x}'\sim q'_0}[\exp g_{\boldsymbol{\theta}}(\mathbf{x})]}{\mathbb{E}_{\mathbf{x}'\sim q''_0}[\exp g_{\boldsymbol{\theta}}(\mathbf{x})]}. \qquad (17)
\end{aligned}$$

Plugging assumptions $\frac{\mathbb{E}_{\mathbf{x}\sim q'_0}[\exp g_{\boldsymbol{\theta}}(\mathbf{x})]}{\mathbb{E}_{\mathbf{x}\sim q''_0}[\exp g_{\boldsymbol{\theta}}(\mathbf{x})]} > \exp(-k)$ and $\mathrm{KL}[p||q'_0] - \mathrm{KL}[p||q''_0] > k$ into equation (17), $\mathrm{KL}[p||q'_{\boldsymbol{\theta}}] - \mathrm{KL}[p||q''_{\boldsymbol{\theta}}] > 0$. □

Lemma 5 suggests a training strategy that we first train the base model q_0, then finetune $g_{\boldsymbol{\theta}}$: under a roughly uniform $g_{\boldsymbol{\theta}}$ (e.g. when $\boldsymbol{\theta}$ is newly initialized), $\mathbb{E}_{\mathbf{x}\sim q'_0}[\exp g_{\boldsymbol{\theta}}]/\mathbb{E}_{\mathbf{x}\sim q''_0}[\exp g_{\boldsymbol{\theta}}] \approx \exp(0)$; so improvements on the inclusive KL-divergence of base model $\mathrm{KL}[p||q_0]$ will mostly translate to improvement in $\mathrm{KL}[p||\tilde{q}_{\boldsymbol{\theta}}]$. Optimizing the base model (i.e. finding q''_0 such that $\mathrm{KL}[p||q''_0] < \mathrm{KL}[p||q'_0]$) is much easier than directly minimizing $\mathrm{KL}[p||q'_{\boldsymbol{\theta}}]$: the former can be done by minimizing empirical cross entropy, which is computationally efficient, while the latter involves an intractable partition function $\sum_{\mathbf{x}\in\mathcal{X}_{\leq T}} \tilde{p}'_{\boldsymbol{\theta}}(\mathbf{x})$.

Pseudocode for fine-tuning $g_{\boldsymbol{\theta}}$ is listed in Algorithm 1.

Algorithm 1: Pseudocode for training $g_{\boldsymbol{\theta}}$

Input:

- Training/validation corpora $\mathcal{D}_{\{\text{train,dev}\}}$
- base model $q_0 : \mathcal{X}_{\leq T} \to [0, 1]$
- initial parameter vector $\boldsymbol{\theta}_0 \in \mathbb{B}^d$
- noise sample size $K \in \mathbb{N}$

Output: unnormalized residual language model $\tilde{q}_{\boldsymbol{\theta}} : \mathcal{X}_{\leq T} \to [0, 1]$

$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}_0$;

`/* ` $\mathcal{L}_{\text{NCE}}$ `is defined in equation (15)` `*/`

while $\sum_{\mathbf{x}\in\mathcal{D}_{dev}} \mathcal{L}_{\text{NCE}}(\boldsymbol{\theta}, \mathbf{x}, q_0, K)$ *is still decreasing* **do**

  foreach $\mathbf{x} \in$ *shuffle*$(\mathcal{D}_{train})$ **do**

    $\nabla_{\boldsymbol{\theta}}\mathcal{L}_{\text{NCE}} = \nabla_{\boldsymbol{\theta}}\mathcal{L}_{\text{NCE}}(\boldsymbol{\theta}, \mathbf{x}, q_0, K)$;

    $\boldsymbol{\theta} \leftarrow$ update-gradient$(\boldsymbol{\theta}, \nabla_{\boldsymbol{\theta}}\mathcal{L}_{\text{NCE}})$;

  end

end

return $\mathbf{x} \mapsto q_0(\mathbf{x}) + \exp g_{\boldsymbol{\theta}}(\mathbf{x})$;

B.4 Computing normalized probabilities

The unnormalized probability $\tilde{q}_{\boldsymbol{\theta}}(\mathbf{x})$ (in equation (12)) can be evaluated easily, and should suffice for (re)ranking purposes (e.g. for ASR and MT applications). However, the *normalized* probability $q_{\boldsymbol{\theta}}(\mathbf{x}) \triangleq \frac{\tilde{q}_{\boldsymbol{\theta}}(\mathbf{x})}{\sum_{\mathbf{x}} \tilde{q}_{\boldsymbol{\theta}}(\mathbf{x})}$ does require computing the partition function $Z_{\boldsymbol{\theta}}$. An unbiased importance sampling

estimate of $\sum_{\mathbf{x} \in \mathcal{X}_{\leq T}} \tilde{q}_{\boldsymbol{\theta}}(\mathbf{x})$ is

$$
\begin{aligned}
Z_{\boldsymbol{\theta}} &= \sum_{\mathbf{x} \in \mathcal{X}_{\leq T}} \tilde{p}_{\boldsymbol{\theta}}(\mathbf{x}) \\
&= \sum_{\mathbf{x} \in \mathcal{X}_{\leq T}} q_0(\mathbf{x}) \exp g_{\boldsymbol{\theta}}(\mathbf{x}) \\
&= \mathop{\mathbb{E}}_{\mathbf{x} \sim q_0} \left[\exp g_{\boldsymbol{\theta}}(\mathbf{x}) \right] \\
&\approx \sum_{m=1}^{M} \frac{\exp g_{\boldsymbol{\theta}}(\mathbf{x}^{(m)})}{M} = \hat{Z}_{\boldsymbol{\theta}\, M},
\end{aligned} \tag{18}
$$

where $\mathbf{x}^{(1)} \ldots \mathbf{x}^{(M)} \sim q_0$.

C Experimental Details

C.1 Datasets

Residual language model experiments are conducted on these datasets:

- **Segmented WikiText**: we take the standard WikiText-2 corpus [36], and segment it into sequences at new line breaks. We discard all empty lines, and any line that starts with the '=' token. In effect, we obtain sequences that are mostly entire paragraphs. We also only keep lines that are shorter than 800 tokens after BPE tokenization. Because of our preprocessing, Segmented WikiText loses much interparagraph context information, and doesn't have the 'simple' header sequences that were in the original WikiText corpus, and is much harder to language-model.
- **Yelp**: the Yelp dataset[16] contains business reviews. As in Segmented WikiText, We keep reviews shorter than 800 tokens.
- **REALNEWS**: we make use of the standard REALNEWS corpus comes from [50], which contains news articles that are up to $1,024$ tokens long.

In all experiments we tokenize with BPE tokenizers derived from the GPT-2 language models: the GRU models use Huggingface's implementation[17] and the Transformers use Grover's[18]. Number of sequences in preprocessed datasets are listed in Table 2.

	Train	Dev	Test
RealNews	$3,855$	$1,533$	$6,158$
WikiText	$18,519$	878	$2,183$
Yelp	$10,951$	$9,964$	994

Table 2: Number of sequences in preprocessed datasets (for training and tuning the discriminators $g_{\boldsymbol{\theta}}$, and evaluation).

C.2 Pretraining base models q_0

We use a pretrained Grover model as the base model in RealNews experiments. For GRU-based experiments, we train base models on WikiText and Yelp datasets using separate training and validation splits than those of the discriminator $g_{\boldsymbol{\theta}}$ (Table 3). The base models are periodically (every $1,000$ iterations) evaluated on the validation split for early stopping, where we stop if there is no improvement on validation perplexity for 10 consecutive evaluations. The base models $q_{\boldsymbol{\theta}}$ achieve 113.98 for Segmented WikiText, and 110.89 in test set perplexity, respectively. Note that these base models are further fine-tuned on additional datasets in our comparison against residual language models.

[16] https://www.yelp.com/dataset
[17] https://github.com/huggingface/transformers
[18] https://github.com/rowanz/grover

	Train	Dev
WikiText	$17,556$	$1,841$
Yelp	$9,954$	$1,000$

Table 3: Number of sequences in preprocessed datasets (for training and tuning the base model q). Note that we do not train our own base models for RealNews, but use one of the pretrained models provided by [50].

C.3 Metrics

We evaluate the relative performance of residual language models against autoregressive models (i.e. fine-tuned base models) on two metrics, log likelihood and perplexity improvement, which are approximated as follows:

- **Log likelihood improvement**: since p, $p_{\boldsymbol{\theta}}$ and q_0 are all distributions over $\mathcal{X}_{\leq T}$, we can quantitatively evaluate their difference in log likelihood. We measure the difference between $\mathrm{KL}[p||p_{\boldsymbol{\theta}}]$ and $\mathrm{KL}[p||q_0]$:[19]

$$\begin{aligned}\mathrm{KL}[p||p_{\boldsymbol{\theta}}] - \mathrm{KL}[p||q_0] &= \mathop{\mathbb{E}}_{\mathbf{x}\sim p}\left[\log p_{\boldsymbol{\theta}}(\mathbf{x}) - \log q_0(\mathbf{x})\right] \\ &= \mathop{\mathbb{E}}_{\mathbf{x}\sim p}\left[\log \tilde{p}_{\boldsymbol{\theta}}(\mathbf{x}) - \log q_0(\mathbf{x})\right] - \log Z_{\boldsymbol{\theta}} \\ &= \mathop{\mathbb{E}}_{\mathbf{x}\sim p}\left[g_{\boldsymbol{\theta}}(\mathbf{x})\right] - \log Z_{\boldsymbol{\theta}} \\ &\approx \frac{\sum_{\mathbf{x}\in\mathcal{D}_{\text{test}}} g_{\boldsymbol{\theta}}(\mathbf{x})}{|\mathcal{D}_{\text{test}}|} - \log \hat{Z}_{\boldsymbol{\theta}\,M}, \end{aligned} \tag{19}$$

  where $\hat{Z}_{\boldsymbol{\theta}\,M}$ is estimated using equation (18). A negative value of log likelihood difference indicates that $\tilde{q}_{\boldsymbol{\theta}}$ approximates p better than q_0 in terms of KL-divergence.

- **Perplexity improvement**: perplexity is a common language modeling metric. Following [42], we compute

$$\text{perplexity improvement of } p_{\boldsymbol{\theta}} = \frac{\exp\frac{|\mathcal{D}|\log \hat{Z}_{\boldsymbol{\theta}\,M}}{w(\mathcal{D}_{\text{test}})}}{\exp\frac{\sum_{\mathbf{x}\in\mathcal{D}_{\text{test}}} g_{\boldsymbol{\theta}}(\mathbf{x})}{w(\mathcal{D}_{\text{test}})}}, \tag{20}$$

  where $w(\mathcal{D})$ is the total token count of dataset $\mathcal{D}$, and $|\mathcal{D}|$ is the number of sequences of $\mathcal{D}$. $\hat{Z}_{\boldsymbol{\theta}\,M}$ is ecomputed Appendix B.4

Both evaluation metrics involve estimating the partition function with $\hat{Z}_{\boldsymbol{\theta}\,M}$. For the perplexity improvement metric, we obtain 32 estimates of $\hat{Z}_{\boldsymbol{\theta}\,M}$[20], which are normally distributed, and compute equation (20) using $\hat{Z}_{\boldsymbol{\theta}\,M}$ the conservative end of a 95% confidence level. To account for variance in our test datasets, we further make use of bootstrapping estimation for log likelihood improvement: we bootstrap-sample $1,000$ subsamples for each test dataset, and compute equation (19) for each datapoint in the Cartesian product ($1,000 \times 32$ in total). We then report results at the 2.5% and 97.5% percentiles.

C.4 Hyperparameters

Transformer experiments. We train our models on 64 GPUs across 8 nodes, with a total batch size of $64 \times 8 \times 2 = 1,024$, and with 1 noise sequence ($K = 1$ in Appendix B.3) per batch. We use an initial learning rate of $5e-5$. The rest of the hyperparameters largely follow settings in [50]. Optimization is done with the Grover implementation of AdaFactor.

[19] Note that q_0 here is the base model component of $\tilde{p}_{\boldsymbol{\theta}}$. While comparing between residual language models and autoregressive models, we also finetune q_0 on additional data to get a new model q_0', which has different parameters than q_0.

[20] We set $M = 512$ in this paper.

GRU experiments. We train our models on 8 GPUs on a single node, with a total batch size of $8 \times 2 = 16$, and with 25 noise sequences ($K = 25$ in Appendix B.3) per batch. We have an initial learning rate of $1e-4$. Upon no improvement on validation data, we half the learning rate, with patience $= 1$. The model parameters are l_2 regularized with a coefficient of $1e-5$. We also apply dropout regularization with $p = 0.5$. Optimization is done with PyTorch-supplied Adam.

C.5 Configurations

We study the effects of these configurations:

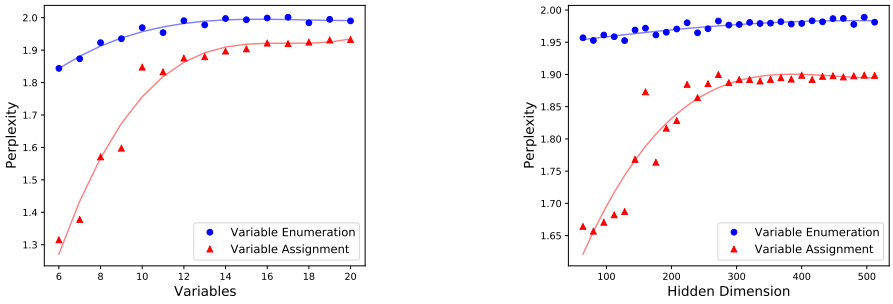
- **Bounding $g_{\boldsymbol{\theta}}$**: we note in §4.2 that with the strong hypothesis that the base model q_0 has bounded error, $g_{\boldsymbol{\theta}}$ will have a bounded range, and leads to a much smaller hypothesis space. In this work we experiment with both bounded and unbounded $g_{\boldsymbol{\theta}}$'s, with ranges $(-\infty, 0)$ and $(-2, 2)$ respectively. More details can be found in Appendix B.2.
- **Model capability of $g_{\boldsymbol{\theta}}$**: we hypothesize that the expressiveness of $g_{\boldsymbol{\theta}}$ does not need to be as rich as the parametrization of q_0, since $g_{\boldsymbol{\theta}}$ essentially only has to tell whether the sequence $\mathbf{x}$ comes from p or q_0. For the GRU + WikiText experiments, we experiment with $\{1, 2\}$-layer GRU models of $g_{\boldsymbol{\theta}}$. For 1-layer models, we additionally experiment with a setup that has only 250 hidden units. For the Transformers/RealNews dataset, we experiment with $\{12, 4\}$-layer Transformer models.

C.6 Log likelihood improvements under different configurations

Model Size	Activation	log likelihood improvement	
		95% CI	μ
RealNews (Transformers)			
12-layer	softplus	$(-0.13, 0.08)$	-0.09
12-layer	tanh	$(-0.14, -0.10)$	-0.12
4-layer	softplus	$(-0.15, 2.62)$	-0.02
4-layer	tanh	$(-0.18, -0.13)$	-0.16
WikiText (GRUs)			
2-layer / 500	tanh	$(-0.00, 0.00)$	-0.00
2-layer / 500	softplus	$(-1.32, -0.85)$	-1.18
1-layer / 500	tanh	$(-0.79, -0.64)$	-0.71
1-layer / 500	softplus	$(-1.85, -1.54)$	-1.69
1-layer / 250	tanh	$(-0.02, 0.02)$	-0.00
1-layer / 250	softplus	$(-1.85, -1.46)$	-1.67
Yelp (GRUs)			
2-layer / 500	tanh	$(-0.03, 0.01)$	-0.02
2-layer / 500	softplus	$(-1.89, -1.67)$	-1.80
1-layer / 500	tanh	$(-0.65, -0.57)$	-0.61
1-layer / 500	softplus	$(-2.62, -2.03)$	-2.43
1-layer / 250	tanh	$(-0.00, 0.00)$	-0.00
1-layer / 250	softplus	$(-2.25, -1.99)$	-2.13

Table 4: Comparison of different configurations.

We also see in Table 4 that using $\tanh$ as the activation function f does better than softplus for Transformers; but performs very poorly for GRUs. We also observe degeneracy problems. We speculate that our Transformer-based base models $q_{\boldsymbol{\theta}}$ have already learned a good approximation of the true distribution; and limiting the model capacity of $g_{\boldsymbol{\theta}}$ in exchange of smaller variance results in a favorable trade-off, and vice versa for GRUs. Regarding discriminator capability: we see that performance is not sensitive to model size. Our best Transformers run actually is from the smaller-model runs. And the 1-layer 500-unit GRU models achieve best performance. Overall, results in Table 4 suggests that performance is sensitive to the choice of model configuration.



(a) Controlling variable count

(b) Controlling parameter size

Figure 3: (LSTM) Average enumeration and variable assignments, controlling variable count (left) and parameter size (right). Trend line uses cubic polynomial regression.

D Empirical results from supervised learning of $q_{\boldsymbol{\theta}}(\cdot \mid \boldsymbol{\phi}')$

We define $L_{\textsc{HardLocalProb}} = \{\boldsymbol{\phi}'\mathbf{a} \mid \boldsymbol{\phi}' = \text{enc}(\text{AddOne}(\phi)), \phi \in \textsc{Hard3Sats}\}$ to be a subset of $\mathcal{X}$ defined in §3, where the encoded formulae ϕ are 'hard' 3-CNF-SAT problems. HARD3SATS is defined as 3-CNF-SAT problems that have clause density close to the empirically found phase transition constant [12]: $\textsc{Hard3Sats} = \{\phi \mid \textsc{NumOfClauses}(\phi) = \lfloor \alpha \cdot \textsc{NumOfVars}(\phi) \rfloor\}$, where NUMOFCLAUSES and NUMOVVARS indicate the numbers of clauses and variables of ϕ respectively. It has been shown[21] that there exists $\alpha \in \mathbb{R}$ such that if $\textsc{NumOfClauses}(\phi)/\textsc{NumOfVars}(\phi) > \alpha$, ϕ tends to have no solution when $\textsc{NumOfVars} \to \infty$; and if $\textsc{NumOfClauses}(\phi)/\textsc{NumOfVars}(\phi) < \alpha$, ϕ tends to have at least one solution when $\textsc{NumOfVars} \to \infty$. It has also been empirically discovered that if $\textsc{NumOfClauses}(\phi)/\textsc{NumOfVars}(\phi) \approx \alpha$, the 3-CNF-SAT formula ϕ is generally 'hard' and has no known efficient deciding algorithms. HARD3SATS is a set of such problems, and we hypothesize that $L_{\textsc{HardLocalProb}}$, to which HARD3SATS reduce, are also hard.

While $L_{\textsc{HardLocalProb}}$ are not real-life problems, they nonetheless share a feature with hard real-life structure prediction problems: the difficulty in computing local probability $p(a_0 \mid \boldsymbol{\phi}')$ for problems in $L_{\textsc{HardLocalProb}}$ is largely due to the absence of known efficient algorithms that marginalizes $\tilde{p}(\boldsymbol{\phi}' a_0)$ over exponentially many suffixes $\mathbf{a} \in \mathbb{B}^{|\phi'|}$, which is precisely the reason #SAT problems are hard.

In our experiments we evaluate the ability of standard sequence-to-sequence models to approximate the conditional distribution $p(\mathbf{a} \mid \boldsymbol{\phi}')$. We randomly sample 3-CNF-SAT formulae, from a distribution over HARDSATS to construct empirical distributions for use in standard machine learning settings. These formulae are encoded in a variant of the DIMACS format [1], with variables sorted by the use count in the formula. Varying the variable count from 6 to 20, we sample 102,000 formulae for each variable length, which are then split into training/validation/test sets with ratio 100:1:1. Since the AddOne operation increases the encoded formula length considerably and does not add useful information in this specific task, we feed into the encoder $\text{enc}(\phi)$ rather than $\text{enc}(\phi')$, which helps with empirical performance. But we still use the satisfying assignments to $\boldsymbol{\phi}'$ as output sequences in both training and evaluation.

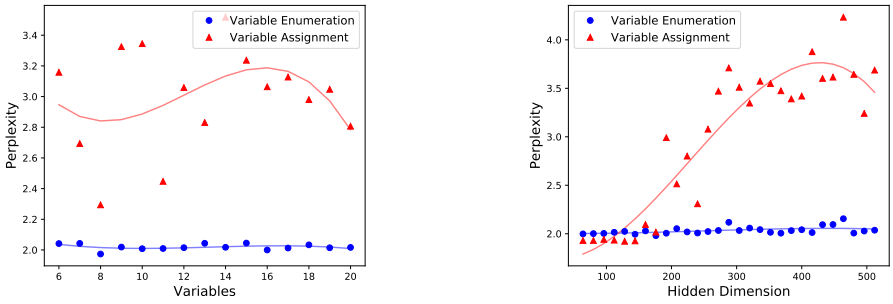
We evaluate $q_{\boldsymbol{\theta}}$ on two metrics:

- **Enumeration Perplexity** is the perplexity of variable a_1 conditioned on $\boldsymbol{\phi}'$ under $q_{\boldsymbol{\theta}}$. Since $p(a_1 = 0 \mid \boldsymbol{\phi}') = \frac{1}{\#(\phi)+1}$, this effectively measures how well $q_{\boldsymbol{\theta}}$ approximates $\#\textsc{Sat}(\phi)$.
- **Variable Assignment Perplexity** is the perplexity of variables $\mathbf{a}_{2\ldots}$ conditioned on prefix $\boldsymbol{\phi}'.1$ under $q_{\boldsymbol{\theta}}$, for ϕ's that are satisfiable. In other words, we would like to see whether the $q_{\boldsymbol{\theta}}$ could generate satisfying variable assignments, given that the formula is satisfiable.

We conduct experiments using the FAIRSEQ package [40]. We make use of two different neural architectures:

- **LSTM** in this configuration, we use the `lstm_luong_wmt_en_de` model template, a standard LSTM Encoder-Decoder architecture with Luong-style attention [33].

[21] α is empirically found to be ≈ 4.2667.



(a) Controlling variable count

(b) Controlling parameter size

Figure 4: (Transformers) Average enumeration and variable assignments, controlling variable count (left) and parameter size (right). Trend line uses cubic polynomial regression.

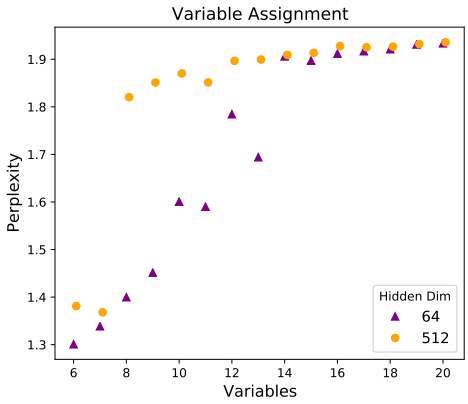


Figure 5: Average variable assignment perplexity for differently sized models (LSTM).

- **Transformers** in this configuration, we use the `transformer_iwslt_de_en` model template, a Transformer architecture.

For both architectures, we vary the hidden state dimension size from 64 to 512 with an increment of 16. The LSTM models have 2 layers, and the Transformers have 4 layers. For each variable count-parameter size configuration, we train a SEQ2SEQ model on the train split and tuned on the validation split, with early stopping (patience= 2). We additionally do 5 random restarts for the LSTM models, and results from different random seeds are aggregated together. We do not tune optimization hyperparameters, and left them as-is, using the templates' suggested values.

We calculate the average enumeration and variable assignment perplexities, controlling variable count and parameter size respectively, and plot the curves in Figures 3 and 4. The first impression is that Transformer-based models in Figure 4 perform poorly, not being able to learn either enumeration and assignments, suggesting that there are learning problems that we have yet diagnosed (e.g. bad hyperparameters, not enough training data). We therefore focus on the LSTM figures in Figure 3. It can be seen that neither varying the variable count, nor the parameter size, has much effect on enumeration perplexities, which remain constantly high across all experiments, suggesting that the RNN encoder has not learned to generalize well to solve the #-SAT problem in all our experiments. On the other hand, we can see in Figure 3b that the variable assignment perplexity increases with the variable count, showing that the RNN architecture does manage to learn (some) conditional dependencies $p(a_t \mid \boldsymbol{\phi}.\mathbf{a}_{1\ldots t-1})$, and overall learning to complete parts of the variable assignment is easier than learning #SAT by comparing Figure 3b to Figure 3a. Regarding parameter size, increasing dimension size does not seem to help with enumeration perplexity. And the models have encountered learning problems on higher variable counts with increased parameter sizes, as can be seen in Figure 5.

```
- 5 1 1 # 1 6 3 # - 5 5 - 4 # - 5 2 - 6 # 2 4 - 1 # - 5 3 1 # - 6 1 1 # - 2
2 - 2 # 3 - 4 1 # - 4 3 - 5 # - 6 - 5 4 # 2 3 - 3 # 2 - 2 2 # 1 - 3 1 # - 6
- 4 2 # - 4 - 4 4 # 4 - 5 - 4 # 6 - 6 6 # - 2 1 5 # 5 2 - 3 # - 6 - 1 - 3 #
                - 6 2 - 5 # - 3 - 1 3 # 1 - 1 - 1 # - 4 - 2 3
```

Figure 6: Sample 3-CNF-SAT formula from HARD3SATS, encoded in a modified DIMACS format. The integers are variable indices: if there is a minus sign '-' preceding an index, the variable is negated (otherwise it isn't). The hash symbol # indicates clause boundaries. This particular formula is satisfiable, with one possible variable assignment `111101`.

To conclude, we find there does exist a family of hard distributions over sequences that RNNs trained using SGD-based methods cannot approximate accurately. While such RNNs do approximate some of the conditional distributions $p(\cdot \mid \mathbf{x}_{1\ldots t})$ well, they all fail to model the conditional distribution $p(A_1 \mid \boldsymbol{\phi}')$, to which #SAT reduces. We also note, while the theoretical results say p can only be approximated by locally normalized $q_{\boldsymbol{\theta}}$'s with a superpolynomially large $\boldsymbol{\theta}$, such $\boldsymbol{\theta}$'s may not be easy to find using SGD-based methods with finitely many samples.