Abstract

The softmax function on top of a final linear layer is the de facto method to output probability distributions in neural networks. In many applications such as language models or text generation, this model has to produce distributions over large output vocabularies. Recently, this has been shown to have limited representational capacity due to its connection with the rank bottleneck in matrix factorization. However, little is known about the limitations of linear-softmax for quantities of practical interest such as cross entropy or mode estimation, a direction that we theoretically and empirically explore here. As an efficient and effective solution to alleviate this issue, we propose to learn parametric monotonic functions on top of the logits. We theoretically investigate the rank increasing capabilities of such monotonic functions. Empirically, our method improves in two different quality metrics over the traditional softmax-linear layer in synthetic and real language model experiments, adding little time or memory overhead, while being comparable to the more computationally expensive mixture of softmaxes.

1. Introduction

Most of nowadays deep learning architectures produce a low dimensional data representation that is important both from a computational (parameter reduction) and generalization (less overfitting) perspective. The underlying assumption is that data lies on a small dimensional manifold. These compressed representations are then used for classification or generation. In the discrete case, they are usually fed to a linear layer to produce the so-called “logits”, followed by a softmax function to output a probability distribution over the desired class labels. We refer to this setup as the linear-softmax layer. However, there are situations when the output vocabulary or class label set is (much) larger than the dimension of the data embedding. Typical examples are text models such as neural language models (Zaremba et al., 2014) or sequence to sequence generative models (Sutskever et al., 2014; Graves, 2013; Pascanu et al., 2013) for problems such as machine translation (Bahdanau et al., 2015; Cho et al., 2014), text summarization (Chopra et al., 2016; Rush et al., 2015) or conversational agents (Vinyals & Le, 2015). These models need to approximate different distributions over the full large vocabulary of words generally of size $\Theta(10^5)$. Recent work (Yang et al., 2017; Kanai et al., 2018) has revealed that, in these cases, the linear-softmax layer has limited representational power. They show the connection between this problem and the classic low-rank matrix factorization framework, concluding that the rank deficiency prevents linear-softmax to exactly match in representation almost all probability distributions.

To address the softmax bottleneck issue, (Yang et al., 2017) propose to use a mixture of softmax distributions (MoS) which achieves state-of-the-art language model perplexity on PennTreeBank (PTB) and WikiText2 (WT2) datasets. However, this method has no theoretical guarantees, being also several orders of magnitude more computationally expensive than linear-softmax as we show in section 5.

A different model was proposed by (Kanai et al., 2018) that replace the exponential in softmax by a product between exponential and sigmoid. This model called Sigsoftmax can be reformulated as applying the pointwise nonlinearity $ss(x) := 2x - log(1 + exp(x))$ to the logits before they are fed to the softmax function. Unfortunately, there is no theoretical guarantee that sigsoftmax can convert low-rank to full-rank matrices. In addition, this model raises a few questions that we seek to explore here: i) what other non-linearities are suitable for breaking the softmax bottleneck? ii) can we theoretically understand and guarantee which pointwise functions will break the softmax bottleneck by increasing the matrix rank? iii) can we efficiently learn the best non-linearity for the task of interest jointly with the rest

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of the model?

For the above reasons, we here propose to learn continuous increasing pointwise functions that would beneficially distort the logits before being fed to the softmax layer. Our model is called **Linear-Monotonic-Softmax** (**LMS**). We constrain our functions to be increasing since we want this transformation to be rank preserving, but we theoretically show that if there exists any other pointwise non-linearity to make our matrix full rank, then there is also an increasing continuous and differentiable function with the same property.

We now summarize our contributions:

- We propose the novel **Linear-Monotonic-Softmax** (**LMS**) model to break the softmax bottleneck. It generalizes the approach in (Kanai et al., 2018) by learning parametric pointwise increasing functions to optimally distort the logits before feeding them to the final softmax. Theoretically, we prove that if there exists any pointwise function to remove the rank-deficiency problem, then an analogue LMS model exists.

- We show additional insights into the linear-softmax bottleneck by analyzing some metrics of practical utility such as cross-entropy or mode matching. Theoretically, we make an interesting connection between minimizing the cross entropy of this model and the principle of maximum entropy with linear constraints.

- Empirically, we show that, in a synthetic setting, linear-softmax and MoS (Yang et al., 2017) are (sometimes significantly) worse than LMS for cross-entropy minimization or mode matching. In the real task of language modeling, LMS applied to state-of-the-art models improves the test perplexity over vanilla linear softmax (Merity et al., 2017) and sigsoftmax (Kanai et al., 2018) on standard benchmark datasets, with very little GPU memory or running time overhead, being comparable to the significantly more expensive MoS model.

### 2. Language Modeling

We first briefly explain a representative task for the softmax bottleneck problem, namely language modeling (**LM**). However, this issue concerns any models that produce probability distributions over large output vocabularies. Thus, we will keep the theoretical exposure rather generic.

**LMs** are the simplest fully unsupervised generative models for natural language text which are actively used to improve state-of-the-art results in various natural language processing tasks (Peters et al., 2018; Devlin et al., 2018). Formally, assume we are given a vocabulary of words in a language $V = \{x_1, \ldots, x_M\}$ and a text corpus represented as a sequence of words $X = (X_1, \ldots, X_N)$, where typically $N >> M$. We would like to learn an autoregressive probabilistic model to predict the next word given a context of past words, i.e. we would like to model $P^*(X_i|X_{i-1}, \ldots, X_1) = P^*(X_i|C_i)$, where $C_i = X_{<i}$ and $P^*$ is the true probability distribution of our corpus. We make use of the standard chain rule formula for conditional probability which gives: $P^*(X) = \Pi_{i=1}^n P^*(X_i|C_i)$.

Popular and state of the art language models (Takase et al., 2018; Zolna et al., 2017; Yang et al., 2017; Merity et al., 2017; Melis et al., 2017; Krause et al., 2017; Merity et al., 2016; Grave et al., 2016) use recurrent neural networks (**RNNs**) such as stacked LSTMs (Hochreiter & Schmidhuber, 1997) to represent each context $C_i$ as a vector of fixed dimension $d$ denoted by $h_i \in \mathbb{R}^d$. Words are also embedded in the same continuous space, i.e. word $x_j$ is mapped to vector $w_j \in \mathbb{R}^d$. Typically $d << M$. The RNN cell is a function that allows to express the context vectors recursively: $h_{i+1} = RNN(h_i, x_i)$. Finally, the conditional probability of the next word in a context is given by the **linear-softmax** model which is a standard softmax function on top of the word-context dot-product logits:

$$Q_{\Theta}(X_i|C_j) = \frac{\exp(h_i^\top w_i)}{\sum_{s=1}^{M} \exp(h_s^\top w_s)} \tag{1}$$

$\Theta$ being the model’s parameters. Training is done by minimizing the cross entropy (or its exponential, the **perplexity**)

$$\mathcal{L}(\Theta) = \frac{1}{N} \sum_{i=1}^{N} -\log Q_{\Theta}(X_i|C_j) \tag{2}$$

which is an approximation of the true expected cross entropy

$$\mathcal{L}(\Theta) \approx \mathbb{E}_c \mathbb{E}_{P^{*}(\cdot|c)}[-\log Q(\cdot|c)] = \mathbb{E}_c [H(P^{*}, Q|c)] \tag{3}$$

Active LM research focuses on better context embedding models, optimization, long range dependencies or caching techniques. Inspired by (Yang et al., 2017), we here focus on investigating and alleviating the bottleneck of the **linear-softmax model** (**Eq. 1**). Therefore, we view natural language as a set of conditional distributions $S = \{c_1, P^*(X|c_1), \ldots, c_N, P^*(X|c_N)\}$ where we neglect the dependency between different contexts embeddings (e.g. that they are obtained using a shared neural network).

### 3. Softmax Bottleneck - Problem and Insights

**Main questions.** In the above model (**Eq. 1**) we made the assumption that any (conditional) probability distribution over a large vocabulary $V$ can be "well" parameterized by a single low-dimensional vector $h$ and an exponential family (linear-softmax), while also having access to a set
We further define the context and word matrices: \[ Q_h(X_i) := Q_\Theta(X_i | c) = \frac{\exp(h_i^T w_i)}{\sum_{i'=1}^M \exp(h_{i'}^T w_{i'})} \] (4)

One question we would like to theoretically and empirically investigate is: Is one embedding \( h \) enough to fully represent any distribution of interest, i.e. can we always find \( \Theta \) s.t. \( Q_\Theta(X | c) = P^*(X | c) \) for all distributions of interest \( P^*(\cdot | c) \in \mathcal{S} \)? If not, how "close" can we get in terms of different interesting metrics (e.g. fitting the logits matrix, cross entropy, mode matching)?

We will see that linear-softmax is indeed limited. Next, to alleviate this bottleneck, we will introduce the Linear-Monotonic-Softmax (LMS) model and we will take steps in re-investigating the above question.

**Connection with Matrix Factorization.** We follow the formalism of (Yang et al., 2017) and define the \( \text{log-P matrix} \) associated with any family of conditional probability distributions \( P \) over all possible contexts:

\[ A_P \in \mathbb{R}^{M \times N}, \quad (A_P)_{ij} = \log P(X_i | C_j) \] (5)

We further define the context and word matrices:

\[ H_\Theta = \begin{bmatrix} h_1^T \\ h_2^T \\ \vdots \\ h_N^T \end{bmatrix} \in \mathbb{R}^{N \times d}, \quad W_\Theta = \begin{bmatrix} w_1^T \\ w_2^T \\ \vdots \\ w_M^T \end{bmatrix} \in \mathbb{R}^{M \times d} \] (6)

as well as the **logits matrix** \( W_\Theta H_\Theta^T \). Then, one derives that

\[ A_{Q_{\Theta}} = W_\Theta H_\Theta^T - e_M \cdot \log Z^T \] (7)

where \( e_M = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} \in \mathbb{R}^M \), and \( \log Z = \begin{bmatrix} \log Z_1 \\ \log Z_2 \\ \vdots \\ \log Z_N \end{bmatrix} \in \mathbb{R}^N \) is the vector of log-partition functions in Eq. 1.

Denoting by \( r(\cdot) \) the matrix rank function, one has

\[ r(e_M \cdot \log Z^T) = 1, \quad r(W_\Theta H_\Theta^T) \leq d, \quad r(A_{Q_{\Theta}}) \leq d+1 \] (8)

Where the rightmost inequality is proved using a classic rank inequality\(^2\). Moreover, \( r(A_{Q_{\Theta}}) \geq d - 1 \) if \( r(W_\Theta H_\Theta^T) = d \), which shows that the log-partition functions cannot change the final rank by more than 1. Since \( A_{P^*} \) is likely of full rank \( M \) for real distributions, (Yang et al., 2017) note that \( A_{P^*} \neq A_{Q_{\Theta}} \) when \( d < M - 1 \), meaning that the linear-softmax model has a representational bottleneck.

**Quantifying the Error.** The above exposure shows one face of the coin, but, in practice, we might also be interested to know how "bad" this bottleneck can be. This depends on the choice of the distance function between discrete probability distributions. Such functions may be explicitly minimized in order to learn the parametric distribution \( Q_\Theta \) closest to the true (unknown) data distribution.

a) **Mean Squared Error.** Assuming we remain in the matrix factorization setting, one natural choice of such a distance is mean square error (MSE):

\[ \mathcal{L}_{\text{MSE}}(\Theta) = \frac{1}{N} \| A_{P^*} - A_{Q_{\Theta}} \|^2_F \] (9)

A simple consequence of the Eckart-Young-Mirsky theorem is the following result:

**Theorem 1.** \( \forall \Theta, \| A_{P^*} - A_{Q_{\Theta}} \|^2_F \geq \sum \sigma_{d+2} + \ldots + \sigma_M^2 \) where \( \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_M \) are the singular values of matrix \( A_{P^*} \).

Proof is in Appendix A. This result shows that, under the MSE distance, we cannot find a model arbitrary close to our true distribution if we have a rank deficiency on \( A_{Q_{\Theta}} \). In section 4, we will also investigate the rank deficiency for the Linear-Monotonic-Softmax (LMS) model.

However, the MSE error has a major drawback when used to quantify how well two distributions match: it puts emphasis on matching the tail of the distributions rather then their means or modes. To see this intuitively, we use the inequality:

\[ \frac{1}{x + \epsilon} < \frac{\log(x + \epsilon) - \log(x)}{\epsilon} < \frac{1}{x}, \quad \forall x, \epsilon > 0 \] (10)

which, since \( \lim_{x \to 0} 1/x = \infty \), shows that mis-matching the small values of \( \log P(x) \) incurs a much higher error compared to the large values. This behavior can be highly undesirable in practical settings such as prediction of the most likely next word or class, especially since a wide variety of real-world distributions exhibit a power law (e.g. Zipf’s law for natural language (Manning & Schütze, 1999)).

b) **Cross Entropy.** The most used loss for discrete data is cross entropy, so it is natural to analyze the softmax bottleneck in terms of its minimum value.

For a single true distribution \( P^*(X) \) and a parametric model \( Q_h(X_i) \propto \exp(\langle w_i, h \rangle) \) with fixed word embeddings \( W \) and variable (learnable) context vector \( h \), this loss is:

\[ H(P^*, Q_h) = \mathbb{E}_{P^*} \left[ - \log Q_h \right] = -\langle \mathbb{E}_{P^*}[w], h \rangle + \log Z^{(h)} \]

where \( \mathbb{E}_{P^*}[w] = \sum_{j=1}^M P^*(X_j) w_j \in \mathbb{R}^d \) and the partition function \( Z^{(h)} = \sum_{j=1}^M \exp(\langle w_j, h \rangle) \).
A question is: What is the minimum achievable cross-entropy for a learnable vector \( h \in \mathbb{R}^d \)?

Towards this direction, we make the connection with the Maximum Entropy Principle under Linear Constraints via the following theorem.

**Theorem 2.** Let \( H(R) = -\sum_{i=1}^{M} R(X_i) \log R(X_i) \) be the entropy of the discrete distribution \( R \). Then:

1. \( H(P^*, Q_h) \geq H(P^*) \), for any probability distribution \( Q \) (not necessarily from the linear-softmax/exponential family).
2. \( \min_{h} H(P^*, Q_h) = \max_{R} H(R) \), where \( P^* := \{ R \mid R \succeq 0, \sum_{i=1}^{M} R(X_i) = 1, \mathbb{E}_{R}[w] = \mathbb{E}_{P^*}[w] \} \) is a convex polytope defined by \( d+1 \) linear constraints.

A proof is given in Appendix B. One can see that increasing the word embedding dimension and assuming the word embedding matrix \( W \) has full rank (i.e. the new constraints cannot be derived from the previous constraints) implies that the polytope \( P^* \) "shrinks", i.e. the maximum entropy becomes lower. Thus, the following hold.

**Corollary 2.1.** The minimum achievable cross-entropy \( H(P^*, Q_h) \) becomes lower as the word embedding dimension increases, if \( W \) keeps having full rank.

**Corollary 2.2.** If \( d = M \) and the word embedding matrix \( W \) has full rank, then \( P^* = \{ P^* \} \) and the lowest possible cross entropy is achieved: \( \min_{h} H(P^*, Q_h) = H(P^*) \).

**c) Mode Matching.** In classification or generative models for discrete data we are often interested in predicting the modes of the true data distributions, e.g. the most likely next word given a context. Thus, we hope that a parametric model trained with our loss of choice (e.g. cross entropy) also exhibits a high accuracy at matching the modes. In our setting, this is represented by the success percentage:

\[
\frac{1}{N} \# \{ i : \arg \max_j P^*(X_i|C_j) = \arg \max_j Q_{\Theta}(X_i|C_j) \} \tag{11}
\]

We will empirically estimate this quantity for a synthetic experiment in Section 5.

**Breaking the Bottleneck via Mixture of Softmaxes (MoS).** (Yang et al., 2017) propose to use a MoS to alleviate this bottleneck. Concretely, they move from single point context embeddings to \( K \) embeddings as

\[
Q_{\Theta}^{MoS}(X_i|C_j) = \sum_{k=1}^{K} \pi_{j,k} \frac{\exp(g_{j,k}^T w_i)}{\sum_{s=1}^{M} \exp(g_{j,s}^T w_s)} \tag{12}
\]

where \( \pi_{j,k} = \frac{\exp(v_k^T h_j)}{\sum_{k'=1}^{K} \exp(v_{k'}^T h_j)} \) are mixture priors, and \( g_{j,k} = \text{tanh}(U_k h_j) \) are the \( K \) embeddings representing the context \( j \). Here, \( v_k \) and \( U_k \) are the model parameters, shared across all contexts.

While effective and achieving state-of-the-art LM perplexities, this model is several orders of magnitude more expensive than linear-softmax, having no theoretical guarantees to the best of our knowledge.

**4. Monotonic Pointwise Functions**

Our main contribution is to analyse and learn pointwise non-linearities \( f(\cdot) \) that would alleviate the softmax bottleneck. We are thus interested in the **linear-monotonic-softmax** (LMS) layer defined as

\[
Q(X_i) = \frac{\exp(f(h^T w_i))}{\sum_{s=1}^{M} \exp(f(h^T w_s))} \tag{13}
\]

We desire to restrict to pointwise functions that have the following properties:

- **non-linearity**: to break the softmax bottleneck, i.e. to not limit the rank of \( f(W_0 H_0^\top) \) to \( d \)
- **increasing**: to preserve the ranking/order of logits
- **bijectivity on \( \mathbb{R} \)**: \( \lim_{x \to \pm \infty} f(x) = \pm \infty \) to have no obvious limitation in modeling sparse or other distributions
- **continuous and (piecewise) differentiable**: to be learned using backpropagation
- **fast and memory efficient**: to add little overhead compared to linear-softmax and unlike MoS

We will show in Thm. 3 that the above first 4 conditions are not limiting the expressiveness of our models in terms of matrix rank deficiency. Moreover, in Thm. 7 we show that the class of continuous piecewise linear increasing functions is a universal approximator for all differentiable increasing functions with bounded derivative that are defined on a finite interval. Related to the last property, we will explain why these functions are fast and memory efficient.

A particular example of a function with the above properties is \( 2x - \log(1 + \exp(x)) \). This is the main focus of (Kanai et al., 2018), but here we generalize their approach by investigating and learning generic parametric pointwise increasing functions.

**Notations:** For any matrix \( A \in \mathbb{R}^{M \times N} \) and pointwise function \( f : \mathbb{R} \to \mathbb{R} \), we denote by \( f(A) \) the matrix \( B \in \mathbb{R}^{M \times N} \) with \( B_{ij} = f(A_{ij}) \). In the case \( f(x) = x^p \), we will follow (Amini et al., 2012) and use the notation \( A^\circ p \).

We list our main theoretical results for pointwise functions.

**How powerful are monotonic pointwise non-linearities?**

We prove that the conditions imposed above on pointwise \( f \)'s are not restrictive when concerned about matrix rank increase.
Theorem 3. Let \( A \in \mathbb{R}^{M \times N} \) be any fixed real matrix of any rank. If there exists a pointwise function \( f : \mathbb{R} \to \mathbb{R} \) s.t. \( f(A) \) has rank at least \( K \), then there also exists a bijective, continuous, piecewise differentiable and strictly increasing function \( g : \mathbb{R} \to \mathbb{R} \) s.t. \( g(A) \) has rank at least \( K \).

Proof is in Appendix C.

Making a matrix full-rank via pointwise operators. Thm. 3 shows that we only need to characterize low-rank matrices for which there exists any pointwise operator that increases its rank. In the most useful case, we would like to know when such operators can make it full rank. But, first, we observe that not all matrices can be made full-rank no matter what pointwise function one uses, for example matrices that have the same column repeated, or those that have two columns with constant entries. Next, we state a simple, but practically useful result for our language model formalism. Proof is in Appendix D.

Lemma 4. Let \( A \in \mathbb{R}^{M \times N}, M \leq N \) be any fixed real matrix of rank at most \( d \), i.e. \( A = WH^T \) where \( W \in \mathbb{R}^{M \times d} \), \( H \in \mathbb{R}^{N \times d} \). Denote by \( h_i \) and \( w_i \) the \( i \)-th rows in \( H \) and \( W \). If one can find \( M \) distinct rows \( j_1, \ldots, j_M \) in \( H \) s.t. the values \( \langle w_i, h_{j_i} \rangle \) are distinct from all the other entries of matrix \( A \), then there exists a pointwise function \( f : \mathbb{R} \to \mathbb{R} \) s.t. \( f(A) \) has full rank \( M \).

Next, we focus on simple power operators \( A^{\odot p} \) and cite a previous result that shows a limitation: small \( p \) values cannot make the matrix rank arbitrarily large.

Theorem 5. (Amini et al., 2012) Let \( A \in \mathbb{R}^{N \times M} \) be a rank \( d \) matrix. Let \( p \) be any positive integer. Then

\[
r(A^{\odot p}) \leq \min \left\{ N, M, \left( d + p - 1 \right) \right\}
\]

(14)

However, \( \lim_{p \to +\infty} \left( \frac{d+p-1}{p} \right) = \infty, \forall d > 1 \), so there is still hope we can find monomials that make a matrix full rank if we look at sufficiently large powers. The following novel result proved in Appendix E confirms in a particular case that this is almost surely achieved. Let \( O^N_K = \{ A \in \mathbb{R}^{N \times N} : r(A) = k \} \) be the submanifold of \( \mathbb{R}^{N \times N} \) consisting of rank \( k \) matrices.

Theorem 6. For \( N > 1 \), the pointwise function \( f(x) = x^2 \) makes matrices in \( O^N_{N-1} \) to almost surely become full rank.

Architecture(s) of Learnable Monotonic Functions. Even though some particular pointwise functions such as monomials/polynomials can make a low-rank matrix to be full-rank and, thus, remove the rank deficiency bottleneck, it is not guaranteed that this new matrix is close to the true data matrix. For this reason, we propose to learn parametric pointwise functions together with our model. For the reasons previously described, we design these functions to be bijective on full \( \mathbb{R} \), increasing, continuous and (almost everywhere) differentiable. We note that the problem of learning parametric monotonic functions was analyzed by (Sill, 1998), but here we use the architecture proposed in (Daniels & Velikova, 2010), namely:

\[
f(x) = \sum_{i=1}^{K} v_i \sigma(u_i x + b_i) + b, \text{ s.t. } u_i, v_i \geq 0, \forall i
\]

(15)

This corresponds to a one hidden neural network with \( K \) hidden units and positively constraint weights (but not the biases). (Daniels & Velikova, 2010) prove that this class of functions is universal approximator for all continuous increasing functions. However, in practice, one has to use a large number of hidden units \( K \) in order to achieve a good approximation. While for our synthetic experiments in Section 5 this was not an issue, for the real language modeling experiments this results in a heavy computational overhead. To understand why, in language modeling one has to process at a time large minibatches of contexts, meaning that matrices of size \( N \times M \) have to be stored in the GPU memory. If one uses the above architecture or the MoS architecture (Yang et al., 2017), one has to store in the GPU memory and process intermediate tensors of dimension \( N \times M \times K \), which can result in a significant running time and memory overhead even for small values of \( K \) such as 10 or 15. Moreover, one is forced to use smaller batch sizes to accommodate the additional factor, which is a problem for the data hungry large scale training of language models.

To address the above computation problem, we propose to use an efficient class of parametric piecewise linear increasing functions called PLIF = Piecewise Linear Increasing Functions. An example is shown in Fig. 1. Formally, we fix a (large enough) interval \([−T, T]\) and \( K + 1 \) equally distant knots in this interval: \( l_i = −T + \frac{2T}{K}, \forall 0 \leq i \leq K \). We define our function to be piecewise linear, meaning that

\[
f(x) = s_i x + b_i, \forall x \in [l_i, l_{i+1}],
\]

where \( s_i \) is the slope of the linear function on the interval \([l_i, l_{i+1}]\). To strictly enforce monotonicity, we desire that \( s_i > 0 \) which we achieve with a softplus function (i.e. \( \log(1 + \exp(x)) \)) on top of unconstrained slope values. Moreover, we need the

\[M\] is the vocabulary size, \( N \) is the number of contexts in a minibatch.
We first explore a synthetic experimental setting that has the following advantages:

- allows to separate the softmax bottleneck from other potential bottlenecks, e.g. in the RNN context embedding layer.

To this end, we repeatedly sample \( N \) different "true" discrete distributions over a fixed synthetic word vocabulary of size \( M \). We use a Dirichlet prior with all concentration parameters equal to \( \alpha \):

\[
P^* (\cdot | c_j) \sim \text{Dir}(\alpha), \text{ for } j = 1, \ldots, N 
\]

The effect of \( \alpha \) is shown for \( M = 3 \) in Fig. 2 and for larger values of \( M \) in Fig. 5 from Appendix G.

We learn parametric models \( Q_\Theta (\cdot | c_j) \) to match the true \( P^* \) distributions. We learn a set of word embeddings shared across all contexts and a separate context embedding per each distribution \( Q_\Theta (\cdot | c_j) \). All embeddings have dimension \( D \). We use the linear softmax model as defined by Eq. 1, the Mixture of Softmaxes (MoS) model defined in (Yang et al., 2017), and our LMS model given by Eq. 13 with a pointwise monotonic function parameterized using the \( K \) hidden units architecture shown in Eq. 15. Learning the models’ parameters is done by minimizing the cross entropy which is equivalent to minimizing the divergence \( K L (P^* | Q_\Theta) \) for each context \( c_j \).

Results. We present the results for different Dirichlet parameter \( \alpha \), vocabulary sizes \( M \), embedding sizes \( D \) and evaluation metrics (mode matching and cross entropy / KL divergence) in Figures 3 and 4, but also show additional results in Appendix H in Figures 6, 7 and 8. In all the settings, we used \( N = 10^5 \) contexts, where \( N \) is the number of different distributions \( P^* (\cdot | c_j) \).

Discussion. We observe that, in the vast majority of the presented settings, LMS outperforms Linear-Softmax and MoS on both the task of mode matching and on the minimum achievable cross-entropy (KL divergence). Especially in the "low D - large M" setting, the difference is significantly large showcasing both the existence of the softmax bottleneck, as well as the merits of our proposed LMS model.

However, we note that there is still room for future work and improvements, for example mode matching still largely suffers for low \( D \) and large \( M \).
Figure 3. Percentage of contexts $j$ for which the modes of true and parametric distributions match, i.e. $\arg\max_i P^*(X_i|c_j) = \arg\max_i Q_{\Theta}(X_i|c_j)$. Higher the better. Dirichlet concentration $\alpha = 0.1$.

Figure 4. Average $KL(P^*||Q_{\Theta})$ (across all contexts). Lower the better. Dirichlet concentration $\alpha = 0.1$. 
Table 1. Single model perplexities on validation and test sets on Penn Treebank and WikiText-2 datasets. For a fair comparison, baseline results are obtained by running the respective open-source implementations locally, however, being comparable to the published results. We also show the training time per epoch when using a single Tesla P100 GPU.

|                  | PENN TREEBANK | WikiText-2 |
|------------------|---------------|------------|
|                  | #Param | Valid ppl | Test ppl | #sec/ep | #Param | Valid ppl | Test ppl | #sec/ep |
| Linear-Softmax w/ AWD-LSTM, w/o finetune (Merity et al., 2017) | 24.2M   | 60.83     | 58.37    | ∼60    | 33M    | 68.11     | 65.22    | ∼120    |
| Ours LMS-PLIF, 10^6 knots w/ AWD-LSTM, w/o finetune (YANG ET AL., 2017) | 24.4M   | 59.45     | 57.25    | ∼70    | 33.2M  | 67.87     | 64.86    | ∼150    |
| MoS, K = 15 w/ AWD-LSTM, w/o finetune (YANG ET AL., 2017) | 26.6M   | 58.58     | 56.43    | ∼150   | 33M    | 66.01     | 63.33    | ∼550    |
| MoS(15 comp) + OUR PLIF (10^6 knots) w/ AWD-LSTM, w/o finetune | 28.6M   | 58.20     | 56.02    | ∼220   | -      | -         | -        | -        |

5.2. Language Model Experiments

We now move to the real setting of language modeling. At this step, due to computational reasons discussed in section 4, we will use our PLIF architecture introduced in the same section.

Datasets. Following previous work (Mikolov; Inan et al., 2016; Kim et al., 2016; Zoph & Le, 2016), we use the two most popular LM datasets: Penn TreeBank (Mikolov et al., 2010) and WikiText-2 (Merity et al., 2016). Word vocabulary sizes for these datasets are 10,000 and 33,000, respectively.

Baselines. We integrate our PLIF layer on top of the state of the art language models of AWD-LSTM (Merity et al., 2017) and AWD-LSTM+MoS (Yang et al., 2017). We use the AWD-LSTM open source implementation \(^4\). All the models in Tab. 1 \(^5\) were ran locally and we report these results; we did this to understand how different softmax models compare with each other when using the exact same context embedding architecture. We note that (Yang et al., 2017) redo architecture search after integrating their MoS model, their goal being to reduce the number of parameters to the same size as AWD-LSTM. We also note that, locally, the SigSoftmax model (Kanai et al., 2018), which is a particular case of our LMS model, did not improve the perplexity compared to linear-softmax for none of the datasets; we thus do not include it in our results.

We note that our PLIF architecture can also be combined with MoS instead of standard softmax. We call this model “MoS + PLIF” and report results in Tab. 1. We use embedding dimension 400 for all the models in Tab. 1. For optimization, we rely on the strategy described in (Merity et al., 2017) consisting of running stochastic gradient descent (SGD) with constant learning rate (20.0) until the cross entropy loss starts stabilizing, and then switching to averaged SGD. This strategy was shown to improve state of the art language models (Takase et al., 2018) and to consistently and by a large margin outperform popular adaptive methods such as ADAM (Kingma & Ba, 2015).

Results and Discussion. Table 1 shows the results. We note that our LMS-PLIF layer consistently improves over linear-softmax when combined with the same state-of-the-art AWD-LSTM context embedding architecture. The computational prices (memory and training time) we pay for using LMS-PLIF are negligible compared to linear-softmax. However, while MoS outperforms our simple LMS-PLIF model, it is computationally several orders of magnitude more expensive, which is a practical advantage of our method. Finally, combining MoS and our PLIF model gives the best Penn TreeBank result, outperforming all baselines (but at the highest computational cost).

Table 2. Statistics on the slope values of the PLIF pointwise function trained on WikiText-2.

|            | MEAN | STD  | MIN  | MAX  |
|------------|------|------|------|------|
|            | 1.10 | 0.62 | 0.02 | 5.16 |

To give further insights into our method, we also show in table 2 statistics on the slope values of a learned PLIF function, revealing its highly non-linear nature.
6. Conclusion

We re-analyzed the softmax bottleneck here from multiple perspectives and confirmed, both theoretically and empirically, that the widely used softmax layer is not flexible enough to model arbitrarily distributions over large vocabularies. We proposed LMS-PLIF, a model that learns parametric monotonic functions to make softmax more flexible, and show some of its capabilities. There are several exciting future directions, including better theoretical understanding of the representational power of the LMS-PLIF layer and, empirically, exploring other supervised and unsupervised discrete problems with large number of classes.

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A. Proof of Theorem 1

Proof. Using Eq. 8, we know that \( r(A_{Q_B}) \leq d + 1 \). However, Eckart-Young-Mirsky theorem gives:

\[
\|A - B\|^2_F \geq \sqrt{\sigma_{d+2}^2 + \ldots + \sigma_M^2},
\]

\[
\forall B \in \mathbb{R}^{M \times N} \text{ s.t. } r(B) \leq d + 1
\]

Thus, our result follows for \( B = A_{Q_B} \). \( \square \)

B. Proof of Theorem 2

Proof. i) Using the non-negativity property of the KL divergence, one derives:

\[
KL(R||Q) = H(R, Q) - H(R) \geq 0 \tag{17}
\]

for any probability distribution \( R \). The result follows easily by taking \( R = P^* \).

ii) Let \( Q_h(X_i) \propto \exp(\langle w_i, h \rangle) \). Then, for any probability distribution \( R \), it is straightforward to derive that

\[
H(R, Q_h) = -\langle E_R[w], h \rangle + \log Z(h) \tag{18}
\]

Moreover, if \( R \in \mathcal{P}^* \) is any distribution satisfying the d-dimensional linear constraints, one derives from Eq. 18 that

\[
H(P^*, Q_h) = H(R, Q_h), \forall R \in \mathcal{P}^* \tag{19}
\]

combining Eqs. 19 and 17, we get:

\[
H(P^*, Q_h) \geq H(R), \forall R \in \mathcal{P}^* \tag{20}
\]

thus

\[
H(P^*, Q_h) \geq \max_{R \in \mathcal{P}} H(R) \tag{21}
\]

which, since \( Q_h \) is arbitrary in the above exponential family, implies that

\[
\min_h H(P^*, Q_h) \geq \max_{R \in \mathcal{P}} H(R) \tag{22}
\]

We are only left with proving the reverse, namely that \( \min_h H(P^*, Q_h) \leq \max_{R \in \mathcal{P}} H(R) \). We use the standard derivations for the Maximum Entropy Principle, namely we form the Lagrangian:

\[
L(\lambda, \beta, h) := H(R) + \beta \left( \sum_{i=1}^{M} R(X_i) - 1 \right) + \langle \lambda, E[R[w] - E_{P^*}[w]] \rangle \tag{23}
\]

Setting its derivatives to 0, one gets that \( R^* = \arg \max_{R \in \mathcal{P}} H(R) \) has the form

\[
R^*(X_i) \propto \exp(\langle w_i, \lambda^* \rangle) \tag{24}
\]

for some \( \lambda^* \in \mathbb{R}^d \) that is chosen by solving the d-linear system \( E_{R^*}[w] - E_{P^*}[w] = 0 \). One can observe that \( Q_{\lambda^*} = R^* \), getting

\[
\min_h H(P^*, Q_h) \leq H(P^*, Q_{\lambda^*}) = H(P^*, R^*)
\]

Finally, using Eq. 19, we get:

\[
H(P^*, R^*) = H(R^*, R^*) = H(R^*) = \max_{R \in \mathcal{P}} H(R)
\]

which concludes the proof. \( \square \)

C. Proof of Theorem 3

Proof. Since \( f(A) \) has rank at least \( K \), there exists at least one submatrix \( M \in \mathbb{R}^{K \times K} \) of \( A \) such that \( \det(f(M)) \neq 0 \). Let \( b_1 < b_2 < \ldots < b_T \) be all the distinct values of \( M \). Denote by \( \epsilon = \frac{1}{4}\min_{i>1}|b_i - b_{i-1}| \). We first prove the following lemmas.

Lemma 8. Let \( P \in \mathbb{R}[X_1, \ldots, X_T] \) be a multivariate polynomial with real coefficients. Assume there exist infinite sets \( S_1, \ldots, S_T \) such that \( P \) vanishes on all the points of \( S_1 \times S_2 \times \ldots \times S_T \). Then \( P \) vanishes on any point of \( \mathbb{R}^T \).

Proof. We prove this by induction over \( T \). The result easily holds for \( T = 1 \), since a real univariate non-zero polynomial can only have a finite set of roots. Assume now that the result holds for any polynomial in \( T - 1 \) variables. We can write \( P(X_1, X_2, \ldots, X_T) \) as a univariate polynomial in \( X_1 \) with coefficients polynomials in \( \mathbb{R}[X_2, \ldots, X_T] \) as follows:

\[
P(X_1, X_2, \ldots, X_T) = \sum_{i=1}^{d_1} Q_i(X_2, \ldots, X_T) X_1^i
\]

where \( d_1 \) is the maximum degree of \( X_1 \). For any arbitrary \( x_2, \ldots, x_T \in S_2 \times \ldots \times S_T \), we know from the hypothesis that \( P(c, x_2, \ldots, x_T) = 0, \forall c \in S_1 \). Since \( S_1 \) is infinite we have that the univariate polynomial in \( X_1 \) is identical 0, i.e. \( P(X, x_2, \ldots, x_T) \equiv 0 \), which implies that \( Q_i(x_2, \ldots, x_T) = 0 \). However, \( x_2, \ldots, x_T \in S_2 \times \ldots \times S_T \) were chosen arbitrarily, thus \( Q_i(x_2, \ldots, x_T) = 0, \forall x_2, \ldots, x_T \in S_2 \times \ldots \times S_T \). Applying the induction hypothesis for \( T - 1 \), one gets that all \( Q_i \) vanish on the full \( \mathbb{R}^{T-1} \). Thus, \( P(X, x_2, \ldots, x_T) \equiv 0, \forall (x_2, \ldots, x_T) \in \mathbb{R}^{T-1} \), which implies that \( P(x_1, x_2, \ldots, x_T) = 0, \forall (x_1, x_2, \ldots, x_T) \in \mathbb{R}^T \). \( \square \)

Lemma 9. There exist \( c_i \in [b_i - \epsilon, b_i + \epsilon], \forall i \in \{1, \ldots, T\} \) s.t. given any pointwise function \( h \) satisfying \( h(b_i) = c_i, \forall 1 \leq i \leq T \), we have \( \det(h(M)) \neq 0 \).

Proof. Assume the contrary, that \( \forall c_i \in [b_i - \epsilon, b_i + \epsilon], \det(h(M)) = 0 \).

We note that, using the Leibniz formula of the determinant, one easily sees that \( \det(M) \) can be written as
We now return to the proof of the main theorem. For each $i \in \{1, \ldots, T\}$, let us denote by $c_i \in [b_i - \epsilon, b_i + \epsilon]$ the values to any other real input of $g$ such that $g(b_i) = c_i$. It is obvious that $\det(g(M))$ depends only on the values $g(b_i)$, so we are free to assign any other values to any other real input of $g$ as long as the above constraints on $g$ are satisfied. One example of such $g$ is a piecewise linear function defined to match the following values: $g(b_i) = c_i, g(b_i + 2\epsilon) = b_i + 2\epsilon, \forall 1 \leq i \leq T, g(x) = x, \forall x < b_i - 2\epsilon$ and $g(x) = x, \forall x > b_i + 2\epsilon$. It can be easily seen that such a function is bijective, piecewise differentiable, continuous and strictly increasing.

D. Proof of Lemma 4

Proof. If $(w_i, h_{j_i})$ are distinct from all the other entries in the matrix $A$, one can design the following pointwise function:

$$f(x) = \begin{cases} 1 & \text{if } \exists \text{ s.t. } x = \langle w_i, h_{j_i} \rangle \\ 0 & \text{else} \end{cases}$$

Then, let $B$ be the $M \times M$ submatrix of $A$ consisting of all its M rows and the M columns indexed by $j_i$'s. It is then clear that $f(B) = \mathbb{1}_M$, which is obviously full rank.

E. Proof of Theorem 6

Proof. We will make use of the following folklore lemmas:

Lemma 10. Let $\mathcal{M} = \bigcup_i \mathcal{M}_i$ be a finite union of Riemannian manifolds of dimension $m$, embedded in $\mathbb{R}^k$, with Riemannian metric $g_i$ inherited from $\mathbb{R}^k$. Then, any finite union $S$ of submanifolds of the $\mathcal{M}_i$'s of dimensions strictly smaller than $m$ is a set of null measure. In other words, any point from $M$ is almost surely not in $S$.

Proof. (sketch) any submanifold of $\mathcal{M}$ of strictly smaller dimension than $m$ has volume or measure zero. The result then follows from the fact that a finite union of sets of measure zero has also measure zero.

Lemma 11. The set $O^N_k$ of rank-$k$ matrices of size $N \times N$ with $0 < k < N$ is a Riemannian manifold of dimension $2kN - k^2$ embedded in $\mathbb{R}^{N^2}$.

Proof. See e.g. (Shalit et al., 2012). The Riemannian metric for embedded manifolds is simply the Euclidean metric restricted to the manifold.

We now return to the main proof of the theorem. From lemma 11 we have that $\dim(O^N_{N-1}) = N^2 - 1$. We want to prove that the subset of $O^N_{N-1}$ of rank $N - 1$ matrices for which $x^2$ is not increasing their rank has dimension strictly smaller than $\dim(O^N_{N-1})$. In this case, using lemma 10, the measure of all ill-behaved matrices would be 0, so any matrix from $O^N_{N-1}$ is almost surely well-behaved, i.e. the rank of $A^\otimes 2$ is almost surely full rank $N$ for $A \in O^N_{N-1}$.

We begin by removing from $O^N_{N-1}$ the set of all matrices that have two proportional columns, a set that we name $\Xi^N$. This is a finite union of manifolds of dimension $N(N - 1) + 1$, namely all sets of matrices for which column $i$ is proportional to column $j$, for all $1 \leq i < j \leq N$.

Now, for any arbitrary $A \in O^N_{N-1} \setminus \Xi^N$ with columns $x^{(1)}, \ldots, x^{(N)} \in \mathbb{R}^N$, one can easily derive that $\exists \gamma_i \in \mathbb{R}$, not all equal to 0 s.t. $\sum_{i=1}^{N} \gamma_i x^{(i)} = 0$. We know that at least one $\gamma_i = 0$ from the fact that $A \in O^N_{N-1}$; let us denote by $\Gamma^i$ the set of such matrices $A \in O^N_{N-1}$. Since $O^N_{N-1}$ is the (finite) union of the $\Gamma^i$'s, we want to show that the set of ill-behaved matrices in each $\Gamma^i$ is contained in a manifold of dimension strictly smaller than that of $O^N_{N-1}$, which will conclude, using the fact that a finite union of null measure sets has null measure.

Without loss of generality, let us assume that $A \in \Gamma^N$, i.e. that $\gamma_N \neq 0$. Let us note that

$$\Gamma^N = \{ A \in O^N_{N-1} : \gamma_N = 1 \},$$

by substituting each $\gamma_i$ with $\gamma_i/\gamma_N$ for $1 \leq i \leq N - 1$.

More precisely, of $\frac{N(N-1)}{2}$ manifolds, one per each pair of columns.

The $N(N-1)+1$ dimension comes from the fact that there are N-1 independent columns, plus a scalar, namely the multiplication factor between column $i$ and column $j$.

Footnotes:

1. w.r.t. the volume form of the manifold, i.e. locally w.r.t. to the $m$-dimensional Lebesgue measure.

8. The $N(N-1)+1$ dimension comes from the fact that there are $N-1$ independent columns, plus a scalar, namely the multiplication factor between column $i$ and column $j$. 

Breaking the Softmax Bottleneck via Learnable Monotonic Pointwise Non-linearities
If \( A^{\otimes 2} \) is not full rank, there exist \( \alpha_1, \ldots, \alpha_N \in \mathbb{R} \) such that

\[
\sum_{i=1}^{N-1} \alpha_i (x^{(i)})^{\otimes 2} = \alpha_N \left( \sum_{i=1}^{N-1} \gamma_i x^{(i)} \right)^{\otimes 2}.
\]

For fixed \( \alpha_1, \ldots, \alpha_N \in \mathbb{R} \), denote by \( M_\alpha \) the subset of the solutions \( \{x^{(i)}\}_{1 \leq i \leq N-1} \subset \mathbb{R}^N \) of the above equation.

Define

\[
\varphi : (x^{(1)}, \ldots, x^{(N-1)}) \in \mathbb{R}^{N-1} \mapsto \sum_{i=1}^{N-1} \alpha_i (x^{(i)})^{\otimes 2} - \alpha_N \left( \sum_{i=1}^{N-1} \gamma_i x^{(i)} \right)^{\otimes 2}.
\]

This can be re-written \( \varphi(x) = x^T G x \) with \( G_{ij} = \delta_{ij}(\alpha_i - \alpha_N \gamma_i^2) - (1 - \delta_{ij}) \alpha_N \gamma_i \gamma_j \).

It can be easily shown that since \( A \) is not in \( \Xi^N \), \( G \) is not the null matrix. Indeed, if \( G = 0 \), then either \( \alpha_N = 0 \) and then \( \alpha_i = \alpha_N \gamma_i^2 = 0 \) for all \( i \), which is excluded – or \( \alpha_N \neq 0 \), and then \( \alpha_N \gamma_i \gamma_j = 0 \) for all \( i \neq j \), meaning only one \( \gamma_{i_0} \) is non-zero, i.e. \( x^{(N)} = -\gamma_{i_0} x^{(i_0)} \) and hence \( A \in \Xi^N \).

Note that since \( G \) is not the null matrix, \( \dim(\ker G) < N - 1 \). Furthermore, let \( U := \mathbb{R}^{N-1} \setminus \ker G \). Invoking the Pre-Image theorem, the set \( U \cap \varphi^{-1}(\{0\}) \) is a submanifold of \( \mathbb{R}^{N-1} \) of dimension \( (N - 1) - 1 = N - 2 \). Therefore, \( \varphi^{-1}(\{0\}) \) is a finite union of manifolds of dimensions smaller than (or equal to) \( N - 2 \).

Since Eq. (26) can be written as an intersection of \( N \) equations as the one defined by \( \varphi \) (i.e. one per coordinate), the set \( M_\alpha \) of solutions of Eq. (26) is included in a finite union of manifolds of dimensions smaller than (or equal to) \( N(N - 2) \).

Finally, the total set \( X \) of matrices we are after – i.e. of rank \( N - 1 \) and which cannot be made full ranked by pointwise square – can be defined as the union over \( \alpha \) of all \( M_\alpha \), i.e. \( X = \bigcup_\alpha M_\alpha \). As \( X \) has the structure of a fiber bundle, with base space the set of \( \alpha \)'s (of dimension \( N \)), \( X \) is a subset of submanifolds of dimensions smaller than \( N + N(N - 2) = N^2 - N < N^2 - 1 \) for \( N > 1 \), which concludes the proof.

\[ f_K(i) = h(i), \forall 0 \leq i \leq K. \] Since \( h \) is increasing, one obtains that \( f_K \) is also increasing. It is then easy to see that \( f_K \) is a PLIF function. Moreover, the slopes are given by the formula:

\[
s_i = \frac{h(l_{i+1}) - h(l_i)}{l_{i+1} - l_i}.
\]

We define the additional function \( g_K(x) := f_K(x) - h(x) \). We wish to prove that \( \lim_{K \to \infty} \max_{x \in [-T,T]} |g_K(x)| = 0 \).

For this, we first use Cauchy’s theorem deriving that \( \exists x \in (l_{i+1}, l_i) \) s.t. \( s_i = \frac{h(l_{i+1}) - h(l_i)}{l_{i+1} - l_i} = h'(c_i) \). Thus, since \( h' \) is bounded by \( R \), we get that \( |s_i| < R, \forall i \). This further implies that \( |g_K'(x)| < 2R, \forall x \in [-T,T] \). Moreover, from the definition of \( f_K \) we have that \( g_K(l_i) = 0, \forall i \). Finally, for any \( x \in [-T,T] \), let \( [l_{i+1}, l_i] \) be the interval in which \( x \) lies. We have that:

\[
|g_K(x)| = |g_K(x) - g_K(l_i)| = \frac{|g_K(x) - g_K(l_i)|}{|x - l_i|} |x - l_i| \leq 2R|x - l_i| \leq 2R\frac{2T}{K}
\]

where the first inequality happens from the same argument derived from Cauchy’s theorem as above. It is now trivial to prove that \( \lim_{K \to \infty} \max_{x \in [-T,T]} |g_K(x)| = 0 \), which concludes our proof.

\[ \square \]

\section*{G. Effect of the Dirichlet concentration}

See fig. 5.

\section*{H. Additional Synthetic Experiments}

See fig. 6, 7, 8.

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**F. Proof of Theorem 7**

**Proof.** Let \( h : [-T,T] \) be any increasing function defined on \([-T,T] \). Assume bounded derivatives, i.e. \( \exists R \) s.t. \( |h'(x)| < R, \forall x \in [-T,T] \). Then, for a fixed positive integer \( K \), we consider the knots \( l_i = -T + \frac{2iT}{K}, \forall 0 \leq i \leq K \). Next, using standard linear interpolation, we define a piecewise linear function \( f_K : [-T,T] \to \mathbb{R} \) s.t.
Figure 5. Distribution of M-class discrete distributions sampled from a Dirichlet prior. Larger concentration parameters result in close to uniform distributions, while low values result in sparse or long-tail distributions.
Figure 6. Percentage of contexts $j$ for which the modes of true and parametric distributions match, i.e. $\arg\max_{i} P^*(X_i|c_j) = \arg\max_{i} Q_\Theta(X_i|c_j)$. Higher the better. Dirichlet concentration $\alpha = 0.01$.

Figure 7. Average $KL(P^*||Q_\Theta)$ (across all contexts). Lower the better. Dirichlet concentration $\alpha = 0.01$. 
Figure 8. Percentage of contexts $j$ for which the modes of true and parametric distributions match, i.e \( \arg \max_i P^*(X_i|c_j) = \arg \max_i Q_\Theta(X_i|c_j) \). Higher the better. Dirichlet concentration $\alpha = 1$. 