A Batch Noise Contrastive Estimation Approach for Training Large Vocabulary Language Models

Youssef Oualil, Dietrich Klakow
Spoken Language Systems (LSV)
Collaborative Research Center on Information Density and Linguistic Encoding
Saarland University, Saarbrücken, Germany
{firstname.lastname}@lsv.uni-saarland.de

Abstract
Training large vocabulary Neural Network Language Models (NNLMs) is a difficult task due to the explicit requirement of the output layer normalization, which typically involves the evaluation of the full softmax function over the complete vocabulary. This paper proposes a Batch Noise Contrastive Estimation (B-NCE) approach to alleviate this problem. This is achieved by reducing the vocabulary, at each time step, to the target words in the batch and then replacing the softmax by the noise contrastive estimation approach, where these words play the role of targets and noise samples at the same time. In doing so, the proposed approach can be fully formulated and implemented using optimal dense matrix operations. Applying B-NCE to train different NNLMs on the Large Text Compression Benchmark (LTCB) and the One Billion Word Benchmark (OBWB) shows a significant reduction of the training time with no noticeable degradation of the models performance. This paper also presents a new baseline comparative study of different standard NNLMs on the large OBWB on a single Titan-X GPU.

1. Introduction
Neural Network Language Models (NNLM) have been shown to significantly outperform standard N-gram LMs on many speech and language technology applications, such as machine translation and speech recognition. The training and evaluation of these models, however, becomes significantly slow and challenging when considering large vocabulary language models. This is mainly due to the explicit normalization of the output layer, which typically requires the evaluation of the full softmax function over the complete vocabulary.

In order to overcome this problem, Schwenk et al. proposed to use a short list of frequent words in combination with N-gram models. The performance of this approach, however, significantly depends on the short list size. In a different attempt, Morin et al. proposed to factorize the output probabilities using a binary tree, which results in an exponential speed-up of the training and evaluation, whereas Mikolov et al. proposed to use an additional class layer as an alternative to the factorization. The performance of these two approaches significantly depends on the design of the binary tree and the class layer size, respectively. As an alternative to modifying the architecture design, the authors of used importance sampling to approximate the output gradient. Unfortunately, this approach requires a control of the samples variance, which can lead otherwise to unstable learning. In a similar work, Mnih et al. proposed to use Noise Contrastive Estimation (NCE) to speed-up the training. NCE treats the learning as a binary classification problem between a target word and noise samples, which are drawn from a noise distribution. Moreover, NCE considers the normalization term as an additional parameter that can be learned during training or fixed beforehand. In this case, the network learns to self-normalize. This property makes NCE more attractive compared to other sampling methods, such as importance sampling, which would still require the use of the softmax function during evaluation.

In batch mode training, however, the implementation of NCE cannot be directly formulated using dense matrix operations, which compromises their speed-up gains.

This paper proposes a new solution to train large vocabulary LMs using NCE in batch mode. The main idea here is to restrict the vocabulary, at each iteration, to the words in the batch and replace the standard softmax function by NCE. In particular, the target words (to predict) in the batch play the role of targets and noise samples at the same time. In doing so, the proposed approach does not require any sampling and can be fully formulated using dense matrix operations, leading to significant speed-up improvements with no noticeable degradation of the performance. Moreover, we can show that this approach optimally approximates the unigram noise distribution, which is widely used in NCE-based LMs.

While applying the proposed batch NCE approach, this paper also presents a new baseline comparative study of different NNLMs on the Large Text Compression Benchmark (LTCB) and the One Billion Word Benchmark (OBWB) on a single Titan-X GPU.

2. Noise Contrastive Estimation
Probabilistic NNLM generally require the normalization of the output layer to produce meaningful probability distributions. Using the softmax function, the probability of the next word \(w\), given the context \(c\) and the model parameters \(\theta\), is given by
\[
p_\theta(w) = p(w|c, \theta) = \frac{\exp(M_\theta(w, c))}{\sum_{v \in V} \exp(M_\theta(v, c))} \tag{1}
\]
\(V\) is the vocabulary and \(M_\theta\) is the neural scoring function. Learning the parameters \(\theta\) generally requires the evaluation of the normalization term for each context \(c\). This evaluation involves the complete vocabulary and therefore, becomes very challenging and resource demanding for large vocabulary corpora. As an alternative solution, proposed to use noise contrastive estimation to train unnormalized probabilistic models. Thus, \(p_\theta(w)\) is approximated as
\[
p_\theta(w) \approx \frac{\exp(M_\theta(w, c))}{Z_c} \tag{2}
\]
distribution \( p \) is a constant value \( Z \) (e.g., \( Z = 1 \) in \([16]\) and \( Z = \exp(h) \) in \([17]\) ). The latter constant will be used in the experiments conducted in Section 4.

The idea behind NCE is to cast the density estimation problem to a binary classification task, which learns to discriminate between real samples drawn from the data distribution \( p_D \) and noise samples drawn from a given noise distribution \( p_N \). Although \( p_N \) is context-dependent, it has been shown (e.g. \([13]\)) that context-independent noise distributions such as unigram, are sufficient to achieve a good performance. Thus, \( p_n = p_n \) in the rest of this paper. If \( K \) denotes the number of noise samples, the probability that the word \( w \) is generated from the data distribution \( (L = 1) \) or noise distribution \( (L = 0) \) are given by

\[
\begin{align*}
p^r_L(w) & \equiv p(L = 1 | w, c) = \frac{p_D(w)}{p_D(w) + K \cdot p_n(w)} \quad (3) \\
p^r_0(w) & \equiv p(L = 0 | w, c) = 1 - p(L = 1 | w, c) \quad (4)
\end{align*}
\]

According to NCE, the model distribution \( p_n \) is expected to converge towards the data distribution \( p_D \) after minimizing the following objective function on the data \( D \)

\[
\mathcal{J}(\theta) = -\sum_{l=1}^{D} \left( \log(p^r_L(w_l)) + \sum_k \log(p^r_k(w_l)) \right) \quad (5)
\]

where \( \{w_k\}_k, k = 1, \ldots, K \) denote the \( K \) noise samples, which are drawn from the noise distribution \( p_n \), to train the model on the target word \( w_l \). The gradient of \( \mathcal{J}(\theta) \) is given by

\[
\frac{\partial \mathcal{J}(\theta)}{\partial \theta} = -\sum_{l=1}^{D} \left( \frac{\partial \log(p^r_L(w_l))}{\partial \theta} + \sum_k \frac{\partial \log(p^r_k(w_l))}{\partial \theta} \right) \quad (6)
\]

NCE training of a neural network follows the standard backpropagation algorithm applied to the objective function \( \mathcal{J} \) and its gradient \( \mathcal{G} \). More details about NCE and its gradient derivation can be found in \([13]\).
Once the error \( E(L') \) at the previous layer according to

\[
\Delta W^t = L^t \cdot \hat{g}^t \quad \text{(9)}
\]

\[
\Delta C^t = \sum_{r \neq j} \hat{g}^t \quad \text{(10)}
\]

\[
E(L') = \hat{g}^t \cdot W^t \quad \text{(11)}
\]

Once the error \( E(L') \) is propagated to the last hidden layer \( L' \) using \( \text{ReLU} \), the learning of the rest of the network follows the standard back-propagation algorithm.

After processing the complete training data, each word \( w \) in the vocabulary will be used exactly \( (B - 1) \times \text{count}(w) \) as a noise. This is strictly equivalent to sampling from a unigram noise distribution, which shows that B-NCE is an optimal implementation of NCE using unigram as noise distribution. We should also mention that some words may occur more than once in the batch. This observation should be taken into consideration before updating the weights and biases.

3.2. Adaptive B-NCE

The proposed B-NCE approach as defined above uses a fixed number of noise samples \((B - 1)\), which is dependent on the batch size. In cases where the latter is small (e.g., \( B \leq 100 \)), B-NCE can be extended to use an additional \( K \) noise samples. This can be done by simply drawing an additional \( K \) samples from the noise distribution \( p_n \), and share them across the batch as it was done in \[16\]. The adaptive B-NCE follows the exact same steps described above using the extended output weight sub-matrix \( W_{B+K} \) (\( B \times (B + K) \)), and the extended sub-vector bias \( C_{B+K} \) (\( 1 \times (B + K) \)) to evaluate \( \text{NCE} \), whereas \( \text{S-NCE} \) becomes

\[
Y' = O' \oplus (B + K - 1) \cdot N_{B+K} \quad \text{(12)}
\]

where \( N_{B+K} = [N', N'_{B+K}] \). \( N_{B+K} \) are the probabilities of the additional \( K \) noise samples using the noise distribution \( p_n \).

4. Experiments and Results

To evaluate the proposed B-NCE approach, we conducted a set of LM experiments on two different corpora. Namely, the Large Text Compression Benchmark (LTCB) \[15\], which is an extract of the enwik9 dataset, and the very large One Billion Word Benchmark (OBWB) \[7\].

The data split and processing is the same as the one used in \[19,20\]. In particular, the LTBC vocabulary is limited to the 80K most frequent words with all remaining words replaced by \(<\text{unk}>\). Similarly to RNNLM toolkit \[10\], we add a single \(<\text{sep}>\) tag at the end of each sentence whereas the begin tag \(<\text{start}>\) is not used. The resulting corpus size is 133M with an \(<\text{unk}>\) rate of 1.43\% for the training set and 2.30\% for the test set. The second corpus is the OBWB, which contains \( \approx 0.8B \) tokens with a vocabulary size of \( \approx 0.8M \) words. The data processing follows the description provided in \[7\] leading to an \(<\text{unk}>\) rate of \( \approx 0.3\% \). Similarly to LTBC, a single \(<\text{sep}>\) tag is added at the end of each sentence. In the experiments described below, the first 5 held-out sets are used for validation whereas the remaining 45 sets are used for testing. The obtained results, however, showed that the models perplexity on these two sets is comparable, with an average difference of less than 0.5 points in perplexity.

The primary motive of using LTBC, with its medium vocabulary size (80K), is to be able to compare the performance of LMs trained using NCE to their counterparts that are trained using the full \textit{softmax}. When using NCE to train the models, the evaluation is either performed using the NCE constant \( Z \) for normalization (PPL\(^N\)), in this case the target word probabilities are given by \[2\], or using the \textit{softmax} function (PPL\(^S\)), which calculates these probabilities using \( \hat{g} \). The difference in performance between these metrics will evaluate the ability of the models to learn to self-normalize after training. For a comprehensive comparison of the different models, we also report the Number of Parameters (NoP) required by each model as well as its Training Speed (TS), which is calculated as the number of words processed per second (w/s) during training. All experiments were conducted on a single Titan-X GPU.

4.1. Baseline Models

In order to assess the gap among established NNLMs, this paper also presents a comparative study of different standard architectures with comparable NoPs. That is, we report results for the standard Feed-forward network (FFNN) \[1\], the Recurrent Neural Network (RNN) \[10\] as well as the Long-Short Term Memory network (LSTM) \[21\]. Our RNN implementation uses a projection weight matrix to couple the word embedding and the hidden layer sizes. We also report results after adding a bottleneck fully-connected ReLu layer right before the output layer in the recurrent models. These models are marked with the prefix \textit{ReLu} in the tables below. Each of the models is trained using the proposed B-NCE approach and the shared noise NCE (S-NCE) \[16\]. For the LTBC corpus, we also report results of the models trained with the full \textit{softmax} function. This is the primary motive for using this corpus. We would like also to highlight that the goal of this paper is not about improving LMs performance but rather showing how a significant training speed-up can be achieved without compromising the models performance for large vocabulary LMs. Hence, we solely focus our experiments on NCE as a major approach to achieve this goal \[12,13,16\] in comparison to the reference full \textit{softmax} function. Comparison to other training approaches such as importance sampling will be conducted in future work.

4.2. LTBC Experiments

For the LTBC experiments, the embedding size is fixed at 200, the 5-gram FFNN has two hidden layers, whereas RNN and LSTM use a single recurrent layer. All non-recurrent layers use ReLu as activation function. More details about the models architectures are shown in Table \[1\] where \“(R)\” stands for recurrent and \“(B)\” for bottleneck. The batch size is fixed at 400 and the initial learning rate is set to 0.4. The latter is halved when no improvement on the validation data is observed for an additional 7 epochs. We also use a norm-based gradient clipping with a threshold of 5 but we do not use dropout. Moreover, B-NCE and S-NCE use the unigram as noise distribution \( p_n \). Following the setup proposed in \[13,16\], S-NCE uses \( K = 100 \) noise samples, whereas B-NCE uses only the target words in the batch (\( K=0 \)). Note that S-NCE will process and update \( B + K \) words at its output layer during each forward-backward pass, whereas B-NCE updates only \( B \) words. Similarly to \[17\], the NCE normalization constant is set to \( Z = \exp(9) \), which approximates the mean of the normalization term using \textit{softmax}.
The LTCB results reported in Table 2 clearly show that B-NCE reduces the training time by a factor of 4 to 8 with a slight degradation in the models performance compared to softmax. Moreover, we can also see that B-NCE slightly outperforms S-NCE while being faster and simpler to implement. In particular, B-NCE does not require the sampling step since it uses the rest of the output words in the batch itself as noise samples to train the model on each target word. This can be efficiently implemented using dense matrix operations (see Sections 3).

Table 2 also shows that PPL is close from PPL\(^\text{L}\), which typically reflects that the models trained using NCE are able to self-normalize, where the normalization term using softmax is, in average, very close from the NCE constant Z. We have also observed in our experiments that the models degradation and the gap between PPL\(^\text{L}\) and PPL\(^\text{L}\) strongly depend on the amount of training data, the vocabulary size as well as the size of the last hidden layer. More particularly, increasing the training data leads to a more stable learning and therefore to a smaller gap between these two metrics and a much lower degradation of the models performance (see OBWB experiments below).

### Table 2: LMs performance on LTCB.

| Model          | PPL\(^\text{L}\) | PPL\(^\text{L}\) | TS (w/s) | NoP |
|----------------|-----------------|-----------------|----------|-----|
| 5-gram FFNN    | 110.2           | 8.4K            | 48.8M    |     |
| RNN            | 125.4           | 29.1K           | 48.8M    |     |
| 5-gram FFNN (B-NCE) | 119.4      | 133.7           | 35.1K    |     |
| RNN\((\text{softmax})\) | 79.7          | 5.9K            | 64.6M    |     |
| RNN (S-NCE)    | 88.7            | 84.2            | 37.8K    | 64.6M|
| RNN (B-NCE)    | 87.6            | 82.5            | 43.7K    | 64.6M|
| ReLu-RNN\((\text{softmax})\) | 69.5          | 6.6K            | 48.8M    |     |
| ReLu-RNN (S-NCE) | 80.2          | 73.3            | 30.9K    | 48.8M|
| ReLu-RNN (B-NCE) | 79.4          | 76.0            | 36.7K    | 48.8M|
| LSTM\((\text{softmax})\) | 62.5          | 8.9K            | 66.0M    |     |
| LSTM (S-NCE)   | 77.4            | 73.1            | 27.2K    | 66.0M|
| LSTM (B-NCE)   | 70.9            | 68.3            | 37.1K    | 66.0M|
| ReLu-LSTM\((\text{softmax})\) | 59.2          | 8.2K            | 50.3M    |     |
| ReLu-LSTM (S-NCE) | 68.4          | 67.1            | 26.9K    | 50.3M|
| ReLu-LSTM (B-NCE) | 64.9          | 62.4            | 32.0K    | 50.3M|

We can also conclude from Table 2 that the additional ReLu layer improves the performance while significantly decreasing the number of parameters (NoP). This conclusion is valid for both, RNN and LSTM. These results confirm that adding a fully-connected bottleneck layer can significantly boost the performance of recurrent models. This idea has been previously used in computer vision tasks in combination with Convolutional Neural Networks (CNN) [22], as well as in speech recognition [23], where the fully-connected layer is used as part of the LSTM recurrent module.

### 4.3. One Billion Word Benchmark Experiments

The OBWB experiments are similar to LTCB with minor differences. Namely, the embedding size is set to 500 for all models, the batch size is fixed at 500, S-NCE uses \(K = 200\) noise samples and the initial learning rate is set to 1.0. Given that the vocabulary size is \(\approx 0.8M\), it was not possible to train the language models using the full softmax function. Therefore, we only report results for B-NCE and S-NCE. More details about the models configuration are shown in Table 3.

Table 3: LMs performance on OBWB.

| Model          | PPL\(^\text{L}\) | PPL\(^\text{L}\) | TS (w/s) | NoP |
|----------------|-----------------|-----------------|----------|-----|
| 5-gram FFNN    | 125.4           | 123.3           | 10.0K    | 8.8B|
| RNN            | 150.0           | 145.0           | 10.0K    | 8.8B|
| 5-gram FFNN (B-NCE) | 150.0      | 145.0           | 10.0K    | 8.8B|
| RNN\((\text{softmax})\) | 70.8          | 67.6            | 24.9K    | 1.59B|
| RNN (S-NCE)    | 63.4            | 61.4            | 27.8K    | 1.59B|
| RNN (B-NCE)    | 59.6            | 59.1            | 20.1K    | 0.88B|
| LSTM\((\text{softmax})\) | 79.4          | 64.8            | 48.1K    | 1.60B|
| LSTM (S-NCE)   | 48.6            | 48.1            | 13.1K    | 1.60B|
| LSTM (B-NCE)   | 51.0            | 50.9            | 13.0K    | 0.89B|
| ReLu-LSTM\((\text{softmax})\) | 49.2          | 48.8            | 14.7K    | 0.89B|

In comparison to other results on the OBWB. We can see that the small ReLu-RNN achieves a close performance from the very large RNN model (PPL \(= 51.3\) and NoP \(= 208\)B) proposed in [17]. Moreover, the performance of the small ReLu-LSTM is comparable to the LSTM models proposed in [16] and [13] which use large hidden layers. In particular, the first paper trains a large 4-layers LSTM model using S-NCE on 4 GPUs (PPL \(= 43.2\) and NoP \(= 3.4B\)), whereas the second uses a recurrent bottleneck layer [23] and a total of \(K = 8192\) noise samples with importance sampling on 32 Tesla K40 GPUs.

### 5. Conclusions and Future Work

We have presented a batch-NCE approach which allows a fast and simple training of large vocabulary LMs. This approach eliminates the sampling step required in standard NCE and can be fully formulated using dense matrix operations. Experiments on LTCB and OBWB have shown that this approach achieves a comparable performance to a softmax function while significantly speeding-up the training. While the evaluation focused on NCE performance, future experiments will be conducted to evaluate B-NCE in comparison to other alternatives of softmax.

### 6. Acknowledgment

This research was funded by the German Research Foundation (DFG) as part of SFB 1102.
7. References

[1] Y. Bengio, R. Ducharme, P. Vincent, and C. Jauvin, “A neural probabilistic language model,” *Journal of machine learning research*, vol. 3, pp. 1137–1155, Mar. 2003.

[2] T. Mikolov, M. Karafiát, L. Burget, J. Černocký, and S. Khudanpur, “Recurrent neural network based language model,” in *11th Annual Conference of the International Speech Communication Association (INTERSPEECH)*, Makuhari, Chiba, Japan, Sep. 2010, pp. 1045–1048.

[3] R. Rosenfeld, “Two decades of statistical language modeling: Where do we go from here?” in *Proceedings of the IEEE*, vol. 88, 2000, pp. 1270–1278.

[4] R. Kneser and H. Ney, “Improved backing-off for m-gram language modeling,” in *International Conference on Acoustics, Speech, and Signal Processing, (ICASSP)*, Detroit, Michigan, USA, May 1995, pp. 181–184.

[5] D. Bahdanau, K. Cho, and Y. Bengio, “Neural machine translation by jointly learning to align and translate,” in *International Conference on Learning Representations (ICLR)*, 2014.

[6] G. Hinton, L. Deng, D. Yu, G. E. Dahl, A. t. Mohamed, N. Jaitly, A. Senior, V. Vanhoucke, P. Nguyen, T. N. Sainath, and B. Kingsbury, “Deep neural networks for acoustic modeling in speech recognition: The shared views of four research groups,” *IEEE Signal Processing Magazine*, vol. 29, no. 6, pp. 82–97, Nov. 2012.

[7] C. Chelba, T. Mikolov, M. Schuster, Q. Ge, T. Brants, P. Koehn, and T. Robinson, “One billion word benchmark for measuring progress in statistical language modeling,” *CoRR*, vol. abs/1312.3005, 2013.

[8] H. Schwenk and J. Gauvain, “Training neural network language models on very large corpora,” in *Proceedings of the Conference on Human Language Technology and Empirical Methods in Natural Language Processing*, Oct. 2005, pp. 201–208.

[9] F. Morin and Y. Bengio, “Hierarchical probabilistic neural network language model,” in *Proceedings of the 10th International Workshop on Artificial Intelligence and Statistics*, 2005, pp. 246–252.

[10] T. Mikolov, S. Kombrink, L. Burget, J. Černocký, and S. Khudanpur, “Extensions of recurrent neural network language model,” in *IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, May 2011, pp. 5528–5531.

[11] Y. Bengio and J.-S. Sénécal, “Quick training of probabilistic neural nets by importance sampling,” in *Proceedings of the conference on Artificial Intelligence and Statistics (AISTATS)*, 2003.

[12] ———, “Adaptive importance sampling to accelerate training of a neural probabilistic language model,” *IEEE Trans. Neural Networks*, vol. 19, no. 4, pp. 713–722, 2008.

[13] A. Mnih and Y. W. Teh, “A fast and simple algorithm for training neural probabilistic language models,” in *Proceedings of the 29th International Conference on Machine Learning*, 2012, pp. 1751–1758.

[14] M. U. Gutmann and A. Hyvärinen, “Noise-contrastive estimation of unnormalized statistical models, with applications to natural image statistics,” *Journal of machine learning research*, vol. 13, pp. 307–361, Feb. 2012.

[15] M. Mahoney, “Large text compression benchmark.” 2011. [Online]. Available: [http://mattmahoney.net/dc/textdata.html](http://mattmahoney.net/dc/textdata.html)

[16] B. Zoph, A. Vaswani, J. May, and K. Knight, “Simple, fast noise-contrastive estimation for large RNN vocabularies,” in *NAACL HLT 2016, The 2016 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, San Diego California, USA, June 12-17, 2016*, pp. 1217–1222.

[17] X. Chen, X. Liu, M. J. F. Gales, and P. C. Woodland, “Recurrent neural network language model training with noise contrastive estimation for speech recognition,” in *IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, 2015, pp. 5411–5415.

[18] R. Józefowicz, O. Vinyals, M. Schuster, N. Shazeer, and Y. Wu, “Exploring the limits of language modeling,” *CoRR*, vol. abs/1602.02410, 2016.

[19] Y. Oualil, C. Greenberg, M. Singh, and D. Klakow, “Sequential recurrent neural networks for language modeling,” in *17th Annual Conference of the International Speech Communication Association (INTERSPEECH)*, San Francisco, CA, USA, Sep. 8-12 2016, pp. 3509–3513.

[20] Y. Oualil, M. Singh, C. Greenberg, and D. Klakow, “Long-short range context neural networks for language modeling,” in *Proceedings of the 2016 Conference on Empirical Methods in Natural Language Processing*, Austin, Texas, USA, Nov. 2016, pp. 1473–1481.

[21] M. Sundermeyer, R. Schlüter, and H. Ney, “LSTM neural networks for language modeling,” in *13th Annual Conference of the International Speech Communication Association (INTER-SPEECH)*, Portland, OR, USA, Sep. 2012, pp. 194–197.

[22] K. Simonyan and A. Zisserman, “Very deep convolutional networks for large-scale image recognition,” *CoRR*, vol. abs/1409.1556, 2014.

[23] H. Sak, A. W. Senior, and F. Beaufays, “Long short-term memory recurrent neural network architectures for large scale acoustic modeling,” in *15th Annual Conference of the International Speech Communication Association (INTERSPEECH)*, Sep. 14-18 2014, pp. 338–342.