Biased Importance Sampling for Deep Neural Network Training

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Abstract

Importance sampling has been successfully used to accelerate stochastic optimization in many convex problems. However, the lack of an efficient way to calculate the importance still hinders its application to Deep Learning.

In this paper, we show that the loss value can be used as an alternative importance metric, and propose a way to efficiently approximate it for a deep model, using a small model trained for that purpose in parallel.

This method allows in particular to utilize a biased gradient estimate that implicitly optimizes a soft max-loss, and leads to better generalization performance. While such method suffers from a prohibitively high variance of the gradient estimate when using a standard stochastic optimizer, we show that when it is combined with our sampling mechanism, it results in a reliable procedure.

We showcase the generality of our method by testing it on both image classification and language modeling tasks using deep convolutional and recurrent neural networks. In particular, our method results in 30% faster training of a CNN for CIFAR10 than when using uniform sampling.

Introduction

The dramatic increase in available training data has made the use of Deep Neural Networks feasible, which in turn has significantly improved the state-of-the-art in many fields, in particular Computer Vision and Natural Language Processing. However, due to the complexity of the resulting optimization problem, computational cost is now the core issue in training these large architectures.

When training such models, it appears to any practitioner that not all samples are equally important; many of them are properly handled after a few epochs of training, and most could be ignored at that point without impacting the final model. To this end, we propose a novel importance sampling scheme that accelerates the training, in theory, of any Neural Network architecture.

For convex optimization problems, many works (Bordes et al. 2005; Zhao and Zhang 2015; Needell, Ward, and Srebro 2014; Canévet, Jose, and Fleuret 2016; Richtárik and Takáč 2013) have taken advantage of the difference in importance among the samples to improve the convergence speed of stochastic optimization methods. However, only recently, researchers (Alain et al. 2015; Loshchilov and Hutter 2015) have shifted their focus on using importance sampling for training Deep Neural Networks. Compared to these works, we propose an importance sampling scheme based on the loss and show that our method can be used to improve the convergence of various architectures on realistic text and image datasets, while at the same time using a minimal number of hyperparameters.

Zhao and Zhang (2015) prove that sampling with a distribution proportional to the gradient norm of each sample, is optimal in minimizing the variance of the gradients; thus resulting in a convergence speed-up for Stochastic Gradient Descent (SGD). However, using the gradient norm requires computing second-order quantities during the backward pass, which is computationally prohibitive. We show, theoretically, that using the loss, we can construct an upper bound to the gradient norm that is better than uniform. Nevertheless, computing the loss still requires a full forward pass, hence using it directly on all the samples remains intractable. In order to reduce the computational cost even more, we propose to use the prediction of a small network, trained alongside the deep model we want to eventually train, to predict an approximation of the importance of the training samples. The complexity of this surrogate allows us to modulate the cost / accuracy trade-off.

Finally, we also show a relationship between importance sampling and maximum-loss minimization, which can be used to improve the generalization ability of the trained Deep Neural Network.

In summary, the contributions of this work are:

- We show that using the loss, we can construct a sampling distribution that reduces the variance of the gradients compared to uniform sampling
- The creation of a model able to approximate the loss for a low computational overhead
- The development of an online algorithm that minimizes a soft max-loss in the training set through importance sampling

Related Work

Importance sampling for convex problems has received significant attention over the years. Bordes et al. (2005) developed LASVM, which is an online algorithm that uses importance sampling to train kernelized support vector machines.

Later Needell, Ward, and Srebro (2014) and more recently Zhao and Zhang (2015) developed more general importance sampling methods that improve the convergence of Stochastic Gradient Descent. In particular, the latter has crucially connected the convergence speed of SGD with the variance of the gradient estimator and has shown that the target sampling distribution is the one that minimizes this variance.

Alain et al. (2015) are the first ones, to our knowledge, that attempted to use importance sampling for training Deep Neural Networks. They sample according to the exact gradient norm as computed by a cluster of GPU workers. Even with a cluster of GPUs they have to constrain the networks that they use to fully connected layers in order to be able to compute the gradient norm in a reasonable time. Compared to their approach, the proposed method achieves wall-clock time speed-up, for any architecture, requiring the same resources as plain uniform sampling.

Loshchilov and Hutter (2015) looked towards the loss value to build a sampling distribution for mini-batch creation for Deep Neural Networks. Their method provides the Neural Network with samples that have been previously seen to have high loss. The most important limitation of their work is the introduction of several hard to choose hyperparameters that also impede the generalization of their method to datasets other than MNIST. On the other hand, we conduct experiments with more challenging image and text datasets and show that our method generalizes well without the need to choose any hyperparameters.

Canévet, Jose, and Fleuret (2016) worked on improving the sampling procedure for importance sampling. They imposed a prior tree structure on the weights, and use a sampling procedure inspired by the Monte Carlo Tree Search algorithm, that handles properly the exploration / exploitation dilemma and converges asymptotically to the probability distribution of the weights. However, this method fully relies on the existence of the tree structure, that should reflect the regularity of the importance on the samples, which is in itself a quite complicated embedding problem.

Finally, there is another class of methods related to importance sampling that can be perceived as using an importance metric quite antithetical to most common methods. Curriculum learning (Bengio et al. 2009) and its evolution self-paced learning (Kumar, Packer, and Koller 2010) present the classifier with easy samples first (samples that are likely to have a small loss) and gradually introduce harder and harder samples.

Importance Sampling

Importance sampling aims at increasing the convergence speed of SGD by reducing the variance of the gradient estimates. In the following sections, we analyze how this works and present an efficient procedure that can be used to train any Deep Learning model. Moreover, we also show that our importance sampling method has a close relation to maximum loss minimization, which can result in improved generalization performance.

Exact Importance Sampling

Let x_i, y_i be the i-th input-output pair from the training set, $\Psi(\cdot;\theta)$ a Deep Learning model parameterized by the vector θ, and $L(\cdot,\cdot)$ the loss function to be minimized during training. The goal of training is to find

$$\theta^* = \arg\min_\theta \frac{1}{N} \sum_{i=1}^N L(\Psi(x_i;\theta), y_i) \tag{1}$$

where N corresponds to the number of examples in the training set. Using Stochastic Gradient Descent with learning rate η, we iteratively update the parameters of our model, between two consecutive iterations t and $t+1$, with

$$\theta_{t+1} = \theta_t - \eta \alpha_i \nabla_{\theta_t} L(\Psi(x_i;\theta_t), y_i) \tag{2}$$

where i is a discrete random variable sampled according to a distribution P with probabilities p_i and α_i is a sample weight. For instance, plain SGD with uniform sampling is achieved with $\alpha_i = 1$ and $p_i = \frac{1}{N}$ for all i.

If we define the convergence speed S of SGD as the reduction of the distance of the parameter vector θ from the optimal parameter vector θ^* in two consecutive iterations t and $t+1$

$$S = -\mathbb{E}_P \left[\|\theta_{t+1} - \theta^*\|_2^2 - \|\theta_t - \theta^*\|_2^2 \right], \tag{3}$$

and if we have

$$\mathbb{E}_P \left[\alpha_i \nabla_{\theta_t} L(\Psi(x_i;\theta_t), y_i) \right] = \nabla_{\theta_t} \frac{1}{N} \sum_{i=1}^N L(\Psi(x_i;\theta_t), y_i), \tag{4}$$

and set $G_i = \alpha_i \nabla_{\theta_t} L(\Psi(x_i;\theta_t), y_i)$, then we get (this is a different derivation of the result by Wang et al. (2016))

$$\begin{aligned}
S &= -\mathbb{E}_P \left[(\theta_{t+1} - \theta^*)^T (\theta_{t+1} - \theta^*) - (\theta_t - \theta^*)^T (\theta_t - \theta^*) \right] \\
&= -\mathbb{E}_P \left[\theta_{t+1}^T \theta_{t+1} - 2\theta_{t+1}\theta^* - \theta_t^T \theta_t + 2\theta_t \theta^* \right] \\
&= -\mathbb{E}_P \left[(\theta_t - \eta G_i)^T (\theta_t - \eta G_i) + 2\eta G_i^T \theta^* - \theta_t^T \theta_t \right] \\
&= -\mathbb{E}_P \left[-2\eta (\theta_t - \theta^*) G_i + \eta^2 G_i^T G_i \right] \\
&= 2\eta (\theta_t - \theta^*) \mathbb{E}_P [G_i] - \eta^2 \, \mathbb{E}_P [G_i]^T \, \mathbb{E}_P [G_i] - \\
&\quad \eta^2 \mathrm{Tr} \left(\mathbb{V}_P [G_i] \right)
\end{aligned} \tag{5}$$

From the last expression, we observe that it is possible to gain a speedup by sampling from the distribution that minimizes $\mathrm{Tr}(\mathbb{V}_P[G_i])$. Alain et al. (2015) and Zhao and Zhang (2015) show that this distribution has probabilities $p_i \propto \|\nabla_{\theta_t} L(\Psi(x_i;\theta_t), y_i)\|_2$. However, computing the norm of the gradient for each sample is computationally intensive. Alain et al. (2015) use a distributed cluster of workers and constrain their models to fully connected networks while Zhao and Zhang (2015) only consider convex problems and sample according to the Lipschitz constant of the loss of each sample, which is an upper bound of the gradient norm.

To mitigate the computational requirement, we propose to use the loss itself as the importance metric instead of the gradient norm. Although providing the network with a larger number of confusing examples makes intuitive sense, we show that the loss can be used to create a tighter upper bound to the gradient norm than plain uniform sampling using the following theorem.

Theorem 1. *Let $G_i = \|\nabla_{\theta_t} L(\Psi(x_i;\theta_t), y_i)\|$ and $M = \max G_i$. There exist $K > 0$ and $C < M$ such that*

$$\frac{1}{K} L(\Psi(x_i;\theta_t), y_i) + C \geq G_i \quad \forall i \tag{6}$$

The above theorem is derived using the fact that the ordering of samples according to the loss is reflected by their ordering according to the gradient norm. A complete proof of the theorem is provided in the supplementary material. Despite the fact that theorem 2 only proves that sampling using the loss is an improvement compared to uniform sampling, in our experiments we show that it exhibits similar variance reducing properties to sampling according to the gradient norm thus resulting in convergence speed improvement compared to uniform sampling.

To sum up, we propose the following importance sampling scheme that creates an unbiased estimator of the gradient vector of Batch Gradient Descent with lower variance:

$$p_i \propto L(\Psi(x_i;\theta_t), y_i) \tag{7}$$

$$\alpha_i = \frac{1}{N p_i}. \tag{8}$$

Relation to Max Loss Minimization

Minimizing the average loss over the training set does not necessarily result in the best model for classification. Shalev-Shwartz and Wexler (2016) argue that minimizing the maximum loss can lead to better generalization performance, especially if there exist a few “rare” samples in the training set. In this section, we show that introducing a minor bias inducing modification in the sample weights α_i, we are able to focus on the high-loss samples with a variable intensity up to the point of minimizing the maximum loss.

Instead of choosing the sample weights α_i such that we get an unbiased estimator of the gradient, we define them according to

$$\alpha_i = \frac{1}{N p_i^k}, \text{ with } k \in (-\infty, 1]. \tag{9}$$

Using $L_i = L(\Psi(x_i;\theta), y_i)$ and $p_i \propto L_i$, we get

$$\mathbb{E}_P\left[\alpha_i \nabla_\theta L_i\right] = \sum_{i=1}^{N} p_i \alpha_i \nabla_\theta L_i \tag{10}$$

$$= \sum_{i=1}^{N} \frac{p_i^{1-k}}{N} \nabla_\theta L_i \tag{11}$$

$$\propto \sum_{i=1}^{N} \frac{L_i^{1-k}}{N} \nabla_\theta L_i \tag{12}$$

$$\propto \sum_{i=1}^{N} \frac{1}{N} \nabla_\theta L_i^{2-k}, \tag{13}$$

which is an unbiased estimator of the gradient of the original loss function raised to the power $2-k \geq 1$. When $2-k \gg 1$ we essentially minimize the maximum loss but as it will be analyzed in the experiments, smaller values can be helpful both in increasing the convergence speed and improving the generalization error.

Approximate Importance Sampling

Although by using the loss instead of the gradient norm, we simplify the problem and make it straightforward for use with Deep Learning models, calculating the loss for a portion of the training set is still prohibitively resource intensive. To alleviate this problem and make importance sampling practical, we propose approximating the loss with another model, which we train alongside our Deep Learning model.

Let $\mathcal{H}_t = \{(j, \tau, L_j^\tau) \mid j \in \{0, 1, \ldots, N\}, \tau \leq t\}$ be the history of the losses where the triplet (j, τ, L_j^τ) denotes the sample index j, the iteration index τ and the value of the loss for sample j at iteration τ (samples seen in the same mini-batch appear in the history as triplets with the same τ.).

Our goal is to learn a model $M(x_i, y_i, \mathcal{H}_{t-1}) \approx L(\Psi(x_i;\theta_t), y_i)$ that has negligible computational complexity compared to $\Psi(x_i;\theta_t)$. The above formulation can be used to define any model, including approximations of the original neural network $\Psi(\cdot)$. In order to create lightweight models, that do not impact the performance of a single forward-backward pass (or impact it minimally), we focus on models that use the class information and the history of the losses. Specifically, we consider models that map the history and the class to two separate representations that are then combined with a simple linear projection.

To generate a representation for the history, we run an LSTM over the previous losses of a sample and return the hidden state. The use of an LSTM allows the history of other samples to influence the representation through the shared weights. Let this mapping be represented by $M_h(j, \mathcal{H}_{t-1}; \pi_h)$ parameterized by π_h. Regarding the class mapping, we use a simple embedding, namely we map each class to a specific vector in $\mathbb{R}^D$. Let this mapping be $M_y(y_j; \pi_y)$ parameterized by π_y.

Algorithm 1 Approximate importance sampling

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1: Assume inputs $\eta$, $\pi_0$, $\theta_0$, $k \in (-\infty, 1]$, $X = \{x_1, x_2, \ldots, x_N\}$ and $Y = \{y_1, y_2, \ldots, y_N\}$
2: $t \leftarrow 0$
3: repeat
4:     $S \sim$ Uniform$(1, N)$        ▷ Sample a portion of the dataset for further speedup
5:     $p_i \propto M(i, y_i, \mathcal{H}_t)\ \forall i \in S$
6:     $s \sim$ Multinomial$(P)$
7:     $\alpha \leftarrow \frac{1}{N p_s^k}$
8:     $\theta_{t+1} \leftarrow \theta_t - \eta \alpha \nabla_{\theta_t} L(\Psi(x_s;\theta_t), y_s)$
9:     $\pi_{t+1} \leftarrow \pi_t - \eta \nabla_{\pi_t} M(s, y_s, \mathcal{H}_t; \pi_t)$
10:    $\mathcal{H}_{t+1} \leftarrow \mathcal{H}_t \cup \{(s, t, L(\Psi(x_s;\theta_t), y_s))\}$
11:    $t \leftarrow t + 1$
12: until convergence
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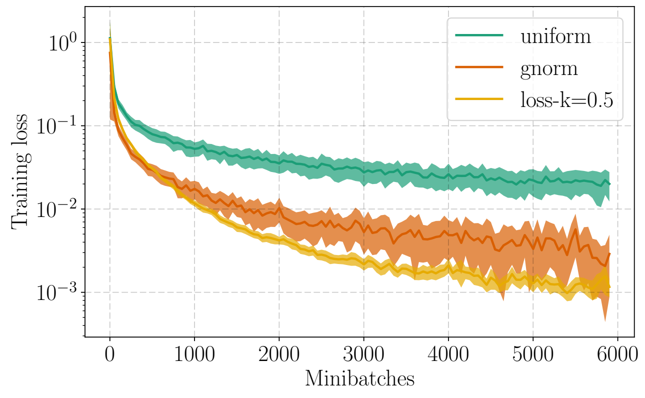
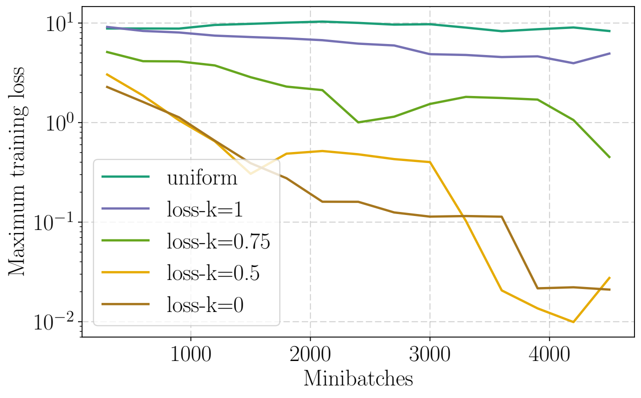


(a) Variance reduction



(b) Effect of k

Figure 1: Averaged results of 10 independent runs on MNIST. Solid lines in Figure 1a show the moving average of the training loss and shaded areas show the moving standard deviation. Figure 1b shows the 5 point moving average of the *maximum* training loss for different values of the hyperparameter k. Smaller values of k minimize the maximum loss in contrast to $k = 1$, which corresponds to unbiased importance sampling, that behaves similar to uniform sampling.

Finally, we solve the following optimization problem and learn a function that predicts the importance of each sample for the next training iteration.

$$\begin{aligned}
M_i &= M\big(M_h(i, \mathcal{H}_{t-1}; \pi_h), M_y(y_i; \pi_y); \pi\big) \\
L_i &= L\big(\Psi(x_i; \theta_t), y_i\big) \\
\pi^*, \pi_h^*, \pi_y^* &= \operatorname*{arg\,min}_{\pi, \pi_h, \pi_y} \frac{1}{N} \sum_{i=1}^{N} (M_i - L_i)^2
\end{aligned} \tag{14}$$

The precise training procedure is described in pseudocode in algorithm 1 where, for succinctness, we use $M(\cdot; \pi)$ to denote the composition and the parameters of the models $M(\cdot)$, $M_h(\cdot)$ and $M_y(\cdot)$.

Smoothing Modern Deep Learning models often contain stochastic layers, such as Dropout, that given a set of constant parameters and a sample can result into vastly different outputs for different runs. This fact, combined with the inevitable approximation error of our importance model, can result into pathological cases of samples being predicted to have a small importance (thus large weight α_i) but ending up having high loss.

To alleviate this problem we use *additive smoothing* to influence the sampling distribution towards uniform sampling. We observe experimentally, that a good rule of thumb is to add a constant c such that $c \leq \frac{1}{2N} \sum_{i=1}^{N} L(\Psi(x_i; \theta_t), y_i)$ for all iterations t.

Experiments

In this section, we analyze experimentally the behaviour of the proposed importance sampling schemes. In the first subsection, we show the variance reduction followed by a comparison with the sampling using the gradient norm and an analysis of the effects of the hyperparameter k (from equation 9), which controls the bias. In the following subsections, we present the attained improvements in terms of training time and test error reduction compared to uniform sampling. For our experiments, we use three well known benchmark datasets, MNIST (LeCun, Cortes, and Burges 1998), CIFAR10 (Krizhevsky 2009) and Penn Treebank (Marcus, Marcinkiewicz, and Santorini 1993).

We compare the proposed sampling strategies, **loss**, which uses the actual model to calculate the importance and **approx**, which uses our approximation defined in the previous sections to **uniform** sampling which is our baseline and **gnorm** that uses the gradient norm as the importance.

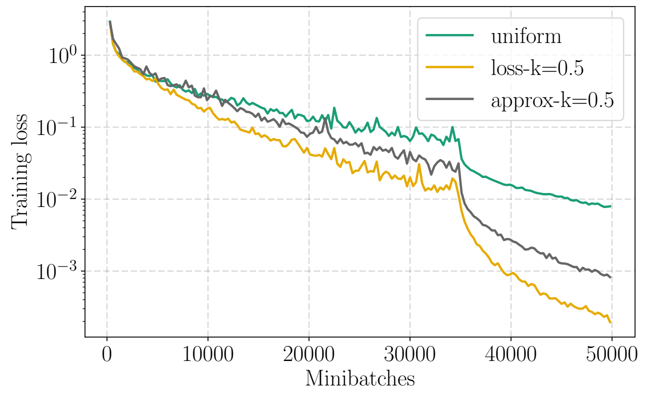
In particular, the **approx** is implemented using an LSTM with a hidden state of size 32. The input to the LSTM layer is at most the 10 previously observed loss values of a sample (features of one dimension). Regarding the class label, it is initially projected in $\mathbb{R}^{32}$ and subsequently concatenated with the hidden state of the LSTM. The resulting 64 dimensional feature is used to predict the loss with a simple linear layer.

In all the experiments, we deviate slightly from our theoretical analysis and algorithm by sampling mini-batches instead of single samples in line 6 of Algorithm 1, and using the Adam optimizer (Kingma and Ba 2014) instead of plain Stochastic Gradient Descent in lines 8 and 9 of Algorithm 1.

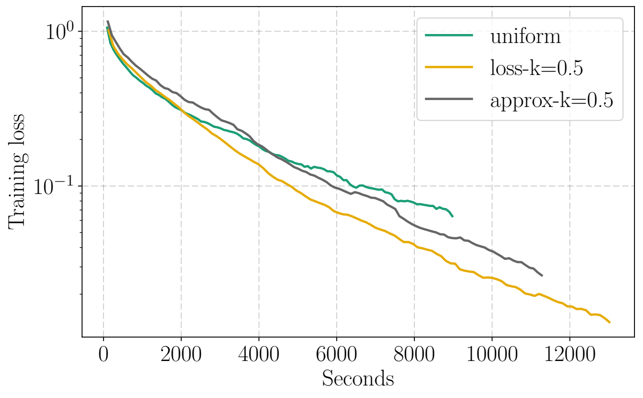
Experiments were conducted using Keras (Chollet and others 2015) with TensorFlow (Abadi et al. 2016), and the code to reproduce the experiments will be provided under an open source license when the paper will be published. When wall clock time is reported, the experiment was run using an Nvidia K80 GPU and the reported time is calculated by subtracting the timestamps before starting one epoch and after finishing one; thus it includes the time needed to transfer data between CPU and GPU memory.

Behaviour of loss-based Importance Sampling

In this section, we present an in-depth analysis of our *biased importance sampling*, by performing experiments on the



(a) Speed-up per epochs



(b) Wall-clock time Speed-up

Figure 2: Training evolution results for CIFAR10 (average of 3 runs). Figure 2a depicts the speed-up achieved with importance sampling in terms of epochs while Figure 2b shows the wall-clock time improvement achieved with importance sampling for the first $35,000$ iterations of training (before the learning rate reduction). Figure 2b shows an 11-point moving average.

well know hand-written digit classification dataset, MNIST. Given the simplicity of the dataset, we choose a down-sized variant of the VGG architecture (Simonyan and Zisserman 2014), with two convolutional layers with 32 filters of size 3×3, a max-pooling layer and a dropout layer with a dropout rate of 0.25, without batch normalization, followed by the same combination of layers with twice the number of filters. Finally, we add two fully connected layers with 512 neurons and dropout with rate 0.5, and a final classification layer. All the layers use the ReLU activation function.

Comparison with the gradient norm The first experiment of this section compares the loss to the gradient norm as importance metrics. We train each network for $6,000$ iterations with a mini-batch size of 128. For each set of parameters we run 10 independent runs with different random seeds and report the average. For the pre-sampling of Algorithm 1 we use $2B$ where B is the size of the mini-batch, so in this case the importance is computed for 256 randomly selected samples per parameter update.

In Figure 1a, we observe that our importance sampling scheme accelerates the training in terms of epochs by $6\times$. It is also evident that the variance is reduced compared to uniform sampling. In this experiment, we observed that sampling with the gradient norm is more than 100 times slower, with respect to wall-clock time, than sampling using the loss. Moreover, compared to the optimal sampling using the gradient norm, we show that gradient norm is very sensitive to randomness introduced by the Dropout layers and thus performs a bit worse than our proposed method. The above could be one of the reasons why no other work has ever used the gradient norm to train Deep Neural Network models with Dropout or Batch Normalization.

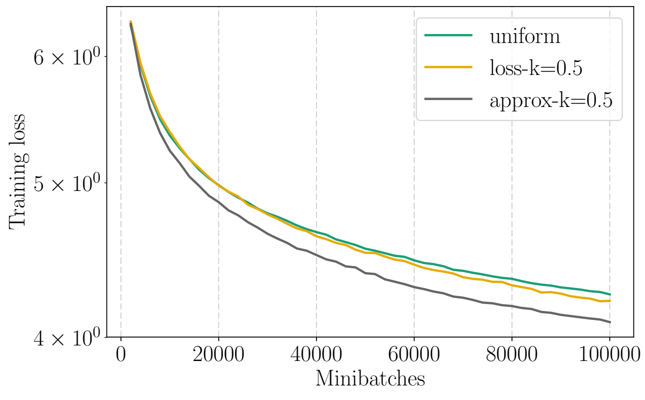
Analysis of the sampling bias Using the loss as the importance metric for sampling our mini-batches allows us to efficiently minimize a surrogate to a soft max-loss, namely the original loss raised to the power $2-k$ (see equation 13). We theorize (based on (Shalev-Shwartz and Wexler 2016)) that minimizing such a loss will be beneficial to the generalization ability of the trained model. Although this will be empirically tested in the last section of the experiments, in this section, we aim to empirically validate our theory that using a small k focuses on the max-loss of the dataset.

For this experiment, we train, again, each network for $6,000$ iterations with $k \in \{0, 0.5, 0.75, 1\}$. Every 300 iterations, we compute the loss for each image in the training set. Figure 1b depicts the moving average of the maximum loss for all the parameter combinations. We observe that smaller values for k, indeed, minimize the maximum loss while $k=1$, which corresponds to unbiased importance sampling, ignores the maximum loss in the same way that uniform sampling does. In addition, using $k<0$ has been observed to result in noisy training, which can be explained by the fact that we increase the gradients of the samples with large gradient norm, thus resulting in very big steps per iteration. Due to the above, we use $k=0.5$ for all subsequent experiments, which has been found to be a good compromise between variance reduction and max-loss minimization.

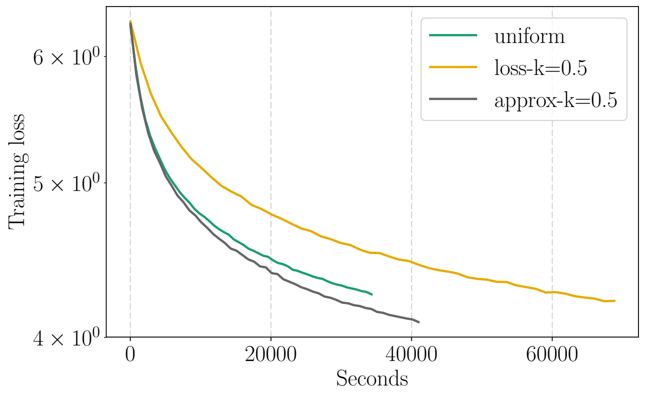
Convergence speed-up

Our second series of experiments aim to show the convergence speed-up achieved by sampling according to the loss (**loss**) and by our fast approximation trained alongside the full model (**approx**). To that end we perform experiments on CIFAR10 (Krizhevsky 2009), an image classification dataset commonly used to evaluate new Deep Learning methods, and Penn Treebank (Marcus, Marcinkiewicz, and Santorini 1993), a widely used word prediction dataset.

Image classification For the CIFAR10 dataset, we developed a VGG-inspired network, with batch normalization, which consists of three convolution-pooling blocks with 64, 128 and 256 filters, two fully connected layers of sizes 1024 and 512, and a classification layer. Dropout is used in a similar manner as for the MNIST network with rates 0.25 after



(a) Speed-up per epochs



(b) Wall-clock time Speed-up

Figure 3: Training evolution results for Penn Treebank for $100,000$ iterations (average of 3 runs). Figure 3a depicts the speed-up achieved with importance sampling in terms of epochs while Figure 3b shows the wall-clock time improvement.

each pooling layer and 0.5 between the fully connected layers. The activation function in all layers is ReLU.

To compare the performance of the methods with respect to training epochs, each network is trained for $50,000$ iterations using a batch size of 128 samples. After $35,000$ iterations we decrease the learning rate by a factor of 10. We perform minor data augmentation by creating $500,000$ images generated by random flipping, horizontal and vertical shifting of the original images. For the importance sampling strategies, we use smoothing as described in the previous sections. In particular, the importance of each sample is incremented by $\frac{1}{2}\bar{L}$, where $\bar{L}$ is the mean of the training loss computed by the exponential moving average of the mini-batch losses. Furthermore, we run each method with 3 different random seeds and report the mean. Similar to the previous experiment, we calculate the importance on a uniformly sampled set twice the batch size and resample with importance (see line 6 Algorithm 1). The results, which are depicted in Figure 2a, show that importance sampling accelerates the training significantly in terms of epochs, resulting in an order of magnitude better training loss after $50,000$ iterations.

In order for our proposed method to be useful as is, we need to achieve speed-up with respect to wall clock time as well as epochs. In Figure 2b, we plot the training loss with respect to the seconds passed for the initial $35,000$ iterations of training for CIFAR10. The experiment shows that our **approx** model is $\sim$ 10% faster than **loss** and $\sim$ 20% slower than uniform per epoch. However, we observe that **approx** reaches the final loss attained with uniform sampling in $\sim$ 15% less time while **loss** in $\sim$ 30% less time shaving off approximately 45 minutes out of the 2.5 hours of training.

One of the reasons that our approximation does not perform as well can be explained by observing the first epochs in Figure 2a or the first seconds in Figure 2b. Our approximation needs to collect information on the evolution of the losses in the set $\mathcal{H}_t$ (see equation 14); thus it does not perform well in the initial epochs. Moreover, the GPU handles very well the small 32×32 images thus the full loss incurs less than 50% slowdown per epoch compared to uniform sampling.

Word prediction To assess the generality of our method, we conducted experiments on a language modeling task. We used the Penn Treebank language dataset, as preprocessed by Mikolov et al. (2011)[1], and a recurrent neural network as the language model. Initially, we split the dataset into sentences and add an "End of sentence" token (resulting in a vocabulary of 10,001 words). For each word we use the previous 20 words, if available, as context for the neural network. Our language model is similar to the small LSTM used by Zaremba, Sutskever, and Vinyals (2014) with 256 units, a word embedding in $\mathbb{R}^{64}$ and dropout with rate 0.5.

In terms of training the language models, we use a batch size of 128 words and train each network for $100,000$ iterations. For the importance sampling strategies, we use constant smoothing instead of adaptive as in the CIFAR10 experiment. To choose the smoothing constant, we experiment with the values $\{0.5, 1, 2.5\}$ and choose 0.5 because it performs better in terms of variance minimization during training. Finally, we run each method with 3 different random seeds and report the mean. Similar to the two previous experiments, we pre-sample uniformly 256 words, namely twice the mini-batch size.

The results of the language modeling experiment are presented in Figures 3a and 3b. We observe (from Figure 3a), that using importance sampling indeed improves the convergence speed in terms of epochs. However, using the full **loss** performs marginally better than **uniform** random sampling. The gradient variance is reduced more using the actual model in this case as well, which leads us to the following two explanations:

1. A small amount of noise is beneficial to the training procedure (we could add noise to the **loss** method by increas-

[1] http://www.fit.vutbr.cz/~imikolov/rnnlm/

Table 1: Experimental results across all datasets and methods. The results are averaged over multiple runs (10 for MNIST and 3 for CIFAR10 and Penn Treebank) and we report the mean and the standard deviation. For the Penn Treebank we report the perplexity in the validation set and for the rest the classification error. The learning rate is chosen to maximize the performance of the uniform sampling strategy for all cases. Runs labeled as **loss** use the trained model to predict the loss while **approx** use a smaller model to approximate the loss as defined in the previous sections. An epoch is defined as 300 mini-batches for MNIST/CIFAR10, and 2000 for Penn Treebank respectively.

	Epoch	Method				
		Uniform	Loss k=1	Loss k=0.5	Approx k=1	Approx k=0.5
MNIST	5	0.79% ± 0.11	0.73% ± 0.11	0.56% ± 0.04	0.83% ± 0.06	0.65% ± 0.05
	10	0.64% ± 0.10	0.56% ± 0.07	0.52% ± 0.05	0.60% ± 0.06	0.61% ± 0.04
	20	0.56% ± 0.07	0.53% ± 0.08	0.47% ± 0.04	0.53% ± 0.06	0.54% ± 0.06
CIFAR10	50	12.33% ± 0.39	10.68% ± 0.65	9.58% ± 0.16	11.54% ± 0.55	10.78% ± 0.09
	100	10.19% ± 0.24	9.74% ± 0.44	9.20% ± 0.55	9.71% ± 0.14	9.90% ± 0.47
	150	7.97% ± 0.10	7.77% ± 0.14	7.44% ± 0.14	7.61% ± 0.07	7.64% ± 0.27
PTB	10	184.5 ± 1.56	178.3 ± 2.47	187.2 ± 1.61	179.4 ± 6.20	180.0 ± 4.78
	30	138.6 ± 0.60	137.8 ± 1.53	139.0 ± 0.72	136.2 ± 2.98	134.3 ± 2.19
	50	130.3 ± 0.63	129.9 ± 1.27	130.5 ± 0.21	128.2 ± 2.02	127.4 ± 1.45

ing the smoothing parameter)

2. The slower changes in sample importance between iterations (side effect of using the history for our approximation) are beneficial to importance sampling

Moreover, it is important to note in Figure 3b that even if using the **loss** performed better with respect to epochs than **approx**, it requires twice as much time to train a given number of epochs compared to **uniform**. On the other hand, **approx** is merely $\sim 10\%$ slower per epoch, resulting **20**% less time to achieve the final training loss, shaving almost 2 **hours** from the 9.5 hours required for **uniform** sampling to perform 100, 000 iterations.

We have also attempted to compare our method with the method presented by Loshchilov and Hutter (2015). Although we managed to find a set of hyperparameters that achieve comparable speed-ups for CIFAR10, their method completely fails to converge for Penn Treebank, for the parameters we tested. This behaviour, reflects the experiments of the original paper and can possibly be explained by the ad-hoc aggressive weighting of samples that they employ.

Generalization improvement

In this experimental section we analyze the performance of the previously trained models on unseen data. Our goal is to show that importance sampling does not cause overfitting or affect the performance on the test set in any negative way.

Towards this end, we report the classification error on the test set for experiments conducted using the MNIST and CIFAR10 datasets while for the language modeling task we report the perplexity on the validation set. The results, for all the experiments, are summarized in Table 1, where the values are depicted for the early stages, medium stages and final stages of training.

We observe that the test error is the same or better than using uniform sampling in all cases. More importantly, Table 1 shows that our added bias is indeed helpful in reducing the generalization error, especially in the first stages of training. For MNIST we observe a 0.2% reduction in error at the 5-th epoch when using $k = 0.5$ and for CIFAR10 approximately 1% at the 30-th epoch. For Penn Treebank the case is not as clear although we observe a reduction of 2 at the 30-th epoch when compared to the **approx** method with $k = 1$.

Finally, we have empirically observed that using $k = 0.5$ results in a robust procedure that requires less smoothing and is affected less by noisy importance estimation.

Conclusion

In this paper, we show theoretically and empirically that the loss can be used as an importance metric to accelerate the training of any Deep Neural Network architecture including recurrent ones. In particular, we propose a biased importance sampling scheme (with and without a lightweight approximation), that results in significant speed-up both in terms of wall-clock time and epochs. Using this sampling scheme, we train Deep Neural Networks for image classification and word prediction tasks 20% to 30% faster than using uniform sampling with Adam.

Two important points remain to be investigated thoroughly. The first is the construction of a more principled method to approximate the loss of the full model. Modern neural networks contain hundreds of layers; thus it is hard to imagine that there exists no approximation to their output that can fully take advantage of the cost/accuracy trade-off.

The second point is the exploitation of the reduced variance of the gradient estimator by some other part of the stochastic optimization procedure. Importance sampling, for instance, could be used to perform stochastic line search or improve the robustness of stochastic Quasi-Newton methods.

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Appendix

Justification for sampling with the loss

The goal of this analysis is to justify the use of the loss as the importance metric instead of the gradient norm and provide additional evidence (besides the experiments in the paper) that it is an improvement over uniform sampling.

Initially, we show that sampling with the loss is better at minimizing an upper bound to the variance of the gradients than uniform sampling. Subsequently, we provide additional empirical evidence that the loss is a surrogate for the gradient norm by computing the exact gradient norm for a limited number of samples and comparing it to the loss.

Theoretical justification

Initially, we show in lemma 2 that the most common loss functions for classification and regression define the same ordering as their gradient norm. Subsequently, we use this derivation together with an upper bound to the variance of the gradients and show that sampling according to the loss reduces this upper bound compared to uniform sampling.

Firstly, we prove two lemmas that will be later used in the analysis.

Lemma 1. *Let $f(x) : \mathbb{R} \rightarrow \mathbb{R}$ be a strictly convex monotonically decreasing function then*

$$f(x_1) > f(x_2) \iff \left|\frac{\partial f}{\partial x_1}\right| > \left|\frac{\partial f}{\partial x_2}\right| \; \forall \, x_1, x_2 \in \mathbb{R}. \quad (15)$$

Proof. By the definition of $f(x)$ we have

$$\frac{\partial^2 f}{\partial x^2} > 0 \,\forall\, x \quad (16)$$

$$\frac{\partial f}{\partial x} \leq 0 \,\forall\, x, \quad (17)$$

which means that $\frac{\partial f}{\partial x}$ is monotonically increasing and non-positive. In that case we have

$$x_1 < x_2 \iff f(x_1) > f(x_2) \quad (18)$$

$$x_1 < x_2 \iff \frac{\partial f}{\partial x_1} < \frac{\partial f}{\partial x_2} \iff \left|\frac{\partial f}{\partial x_1}\right| > \left|\frac{\partial f}{\partial x_2}\right| \quad (19)$$

therefore proving the lemma. □

Lemma 2. *Let $L(\psi) : D \rightarrow \mathbb{R}$ be either the negative log likelihood or the squared error loss function defined respectively as*

$$\begin{aligned} L_1(\psi) = -y^T log(\psi) \qquad & y \in \{0,1\}^d \; s.t. y^T y = 1 \\ & D = [0,1]^d \; s.t. \; \|\psi\|_1 = 1 \\ L_2(\psi) = \|y - \psi\|_2^2 \qquad & y \in \mathbb{R}^d \quad D = \mathbb{R}^d \end{aligned} \quad (20)$$

where y is the target vector. Then

$$L(\psi_1) > L(\psi_2) \iff \|\nabla_\psi L(\psi_1)\| > \|\nabla_\psi L(\psi_2)\| \quad (21)$$

Proof. In the case of the squared error loss we have

$$\|\nabla_\psi L(\psi)\|_2^2 = \|-2(y-\psi)\|_2^2 = 4L(\psi), \quad (22)$$

thus proving the lemma.

For the log likelihood loss we can use the fact that only one dimension of y can be non-zero and prove it using lemma 1 because $f(x) = -log(x)$ is a strictly convex monotonically decreasing function. □

Main analysis We can now prove theorem 2 which is also written below for completeness.

Theorem 2. *Let $G_i = \|\nabla_{\theta_t} L(\Psi(x_i;\theta_t), y_i)\|$ and $M = \max G_i$. There exist $K > 0$ and $C < M$ such that*

$$\frac{1}{K} L(\Psi(x_i;\theta_t), y_i) + C \geq G_i \quad \forall i \quad (23)$$

Proof. The goal of importance sampling is to minimize

$$\text{Tr}\left(\mathbb{V}\left[\nabla_\theta L(\Psi(x_i;\theta), y_i)\right]\right) = \mathbb{E}\left[\|\nabla_\theta L(\Psi(x_i;\theta), y_i)\|_2^2\right]. \quad (24)$$

To perform importance sampling, we sample according to the distribution P with probabilities p_i and use per sample weights $\alpha_i = \frac{1}{Np_i}$ in order to have an unbiased estimator of the gradients. Consequently, the variance of the gradients is

$$\mathbb{E}_P\left[\|\alpha_i \nabla_\theta L(\Psi(x_i;\theta), y_i)\|_2^2\right] = \quad (25)$$

$$\sum_{i=1}^N p_i \alpha_i^2 \|\nabla_\theta L(\Psi(x_i;\theta), y_i)\|_2^2 = \quad (26)$$

$$\sum_{i=1}^N \frac{1}{Np_i} \frac{1}{N} \|\nabla_\theta L(\Psi(x_i;\theta), y_i)\|_2^2 = \quad (27)$$

$$\sum_{i=1}^N \alpha_i \frac{1}{N} \|\nabla_\theta L(\Psi(x_i;\theta), y_i)\|_2^2. \quad (28)$$

Assuming that the neural network is Lipschitz continuous (assumption that holds when the weights are not infinite) with constant K, we derive the following upper bound to the variance

$$\mathbb{E}_P\left[\|\alpha_i \nabla_\theta L(\Psi(x_i;\theta), y_i)\|_2^2\right] \leq \quad (29)$$

$$\sum_{i=1}^N \alpha_i \frac{1}{N} \|\nabla_\theta \Psi(x_i;\theta)\|_2^2 \left\|\nabla_{\Psi(x_i;\theta)} L(\Psi(x_i;\theta), y_i)\right\|_2^2 \leq \quad (30)$$

$$K^2 \sum_{i=1}^N \alpha_i \frac{1}{N} \left\|\nabla_{\Psi(x_i;\theta)} L(\Psi(x_i;\theta), y_i)\right\|_2^2. \quad (31)$$

Since we have a finite set of samples, there exists a constant C such that

$$\begin{aligned} L(\Psi(x_i;\theta), y_i) + C \geq \left\|\nabla_{\Psi(x_i;\theta)} L(\Psi(x_i;\theta), y_i)\right\| \\ \forall\, i \in \{1, 2, \ldots, N\}. \end{aligned} \quad (32)$$

However, using lemma 2 we know that this upper bound is better than uniform because $L(\Psi(x_i;\theta), y_i)$ and $\left\|\nabla_{\Psi(x_i;\theta)} L(\Psi(x_i;\theta), y_i)\right\|$ grow and shrink in tandem. In particular the following equation holds, where $M = \max \left\|\nabla_{\Psi(x_i;\theta)} L(\Psi(x_i;\theta), y_i)\right\|$ and $C < M$

$$\begin{aligned} &L(\Psi(x_i;\theta), y_i) + C - \left\|\nabla_{\Psi(x_i;\theta)} L(\Psi(x_i;\theta), y_i)\right\| < \\ &M - \left\|\nabla_{\Psi(x_i;\theta)} L(\Psi(x_i;\theta), y_i)\right\| \quad \forall i. \end{aligned} \tag{33}$$

Using equations 31, 32 and 33 and replacing the constants in 31 with K we derive the original claim concluding the proof. □

Empirical justification

In this section, we provide empirical evidence regarding the use of the loss instead of the gradient norm as the importance metric. Specifically, we conduct experiments computing the exact gradient norm and the loss value for the first 20,000 samples during training. The gradient norm is normalized in each mini-batch to account for the changes in the norm of the weights.

Subsequently, we plot the loss sorted by the gradient norm. If there exists C such that $L(\Psi(x_i;\theta), y_i) = C \left\|\nabla_\theta L(\Psi(x_i;\theta), y_i)\right\|$ we should see approximately a line. In case of order preservation we should see a monotonically increasing function.

In figure 4, we observe a correlation between the gradient norm and the loss. In all cases, samples with high gradient norm also have high loss. In the Penn Treebank dataset, (Figure 4c), there exist some samples with high loss but very low gradient norm. This can be explained because LSTMs use the $\tanh(\cdot)$ activation function which can have very low gradient but incorrect output. We note that this cannot hurt performance, it just means that we waste some CPU/GPU cycles on samples that are incorrectly classified but will not affect the parameters heavily.

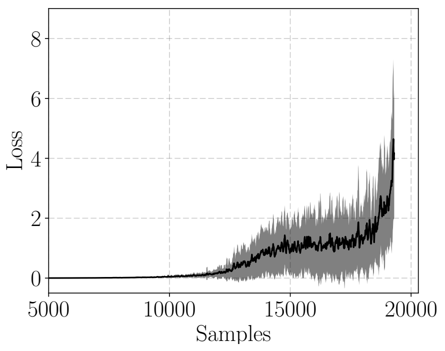
Loss tracking by our approximation

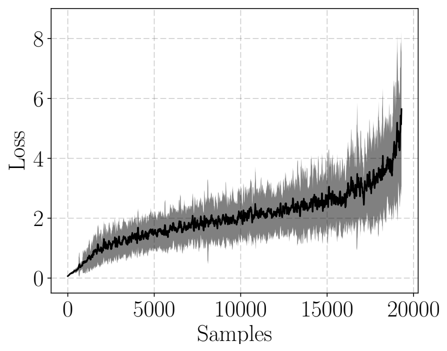
In this section, we present empirical evidence that the proposed approximate model predicts the loss with reasonable accuracy. In order to describe the experiment, we introduce the following notation. Let $\hat{L}_i$ be the loss value computed for the i-th sample and used as importance in the sampling procedure. In addition, let L_i be the loss computed in the forward pass of the optimization procedure, with the same parameters and for the same sample. As mentioned in the paper, L_i and $\hat{L}_i$ can differ even if we use the full network to compute $\hat{L}_i$, due to stochasticity introduced by Dropout layers and Batch Normalization.

To compute how well $\hat{L}_i$ "tracks" L_i we solve the following least squares problem for every minibatch. The value of the coefficient a shows how well $\hat{L}_i$ approximates L_i.

$$a^*, b^* = \underset{a,b}{\arg\min} \sum_{i \in B} \left(a\hat{L}_i + b - L_i\right)^2 \tag{34}$$

In Figure 5, we present the evolution of the coefficient a for the experiments in CIFAR10 and Penn Treebank. Regarding CIFAR10, we observe that the loss is really hard to track, even using the full Neural Network. However, the approximation presents a positive correlation with L_i which appears to be enough for reducing the variance of the gradients. Moreover, after $15,000$ mini-batches the approximation "tracks" the loss with the same accuracy as the full network. On the other hand, in the Penn Treebank experiment, there seems to be less noise and L_i is predicted accurately by both methods. Once again, we observe, that as the training progresses our approximation seems to converge towards the same quality of predictions as using the full network.


(a) MNIST


(b) CIFAR10

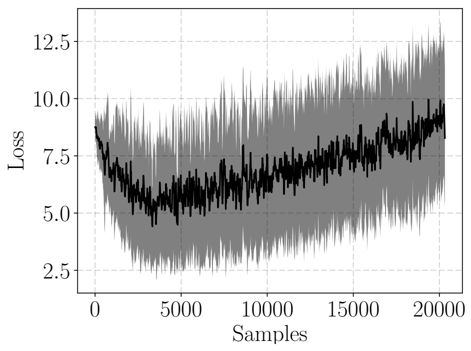
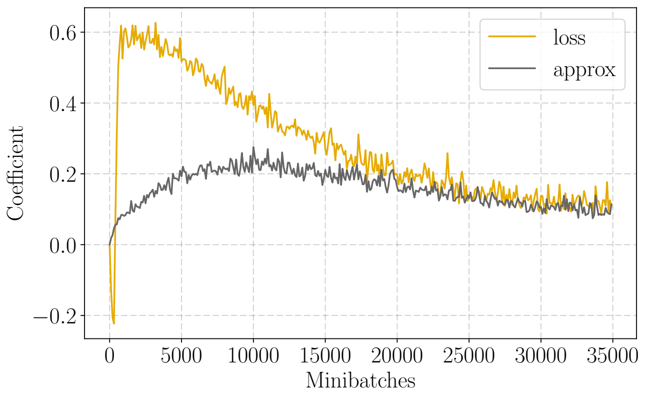

(c) Penn Treebank

Figure 4: Loss values sorted by gradient norm. The solid line is a moving average (50 samples window) and the shaded area denotes one standard deviation.


(a) CIFAR10

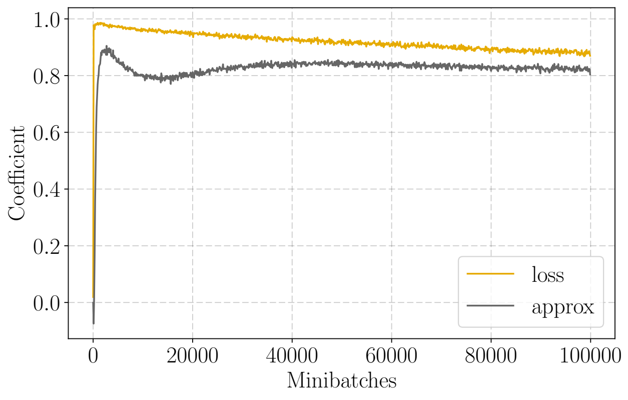

(b) Penn Treebank

Figure 5: The coefficient a from equation 34 is plotted for **loss** and **approx**. A coefficient value of 1 means that the loss is tracked perfectly while 0 means almost uniform sampling. Due to randomness introduced by layers such as Dropout and Batch Normalization, even using the full network (**loss**) does not mean perfect prediction.