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Optimizations of the Skip-Gram Model with negative Sampling

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Contents

Abstract

The Skip-gram Model with negative sampling (SGNS) is an effective algorithm to create word embeddings. SGNS uses Stochastic Gradient Descent (SGD) as it's learning algorithm. While a lot of effort has gone into increasing the throughput of words of SGNS, not much work has gone into optimizing the convergence time. Therefore our work focuses on the latter. We used two techniques to achieve a better convergence time, namely advanced optimizers and input shuffling. We compared our work to the state of the art implementation Gensim. We used the Text8 dataset to train our model and measured the quality of our word embeddings with the wordsim353 dataset, which measures the quality of word embeddings by judging the similarity of different words. We trained our model with multiple advanced optimizers: momentum, Nesterov accelerated gradient, Adagrad, Adadelta, and Adam. We also applied input shuffling to all of the above optimizers. Adam combined with input shuffling outperformed every optimizer. Adam with shuffling also outperformed the current state of the art implementation Gensim. Adam converged to a similarity value of 0.66 (state of the art) in 2 epochs, while Gensim took 4 epochs. We confirmed these results with the enwik9 dataset, as Gensim took 4 epochs to converge and our model (Adam with input shuffling) only 3 epochs. Hence this work shows that advanced optimizers combined with input shuffling do decrease the convergence time of the SGNS. Optimizing our model in terms of throughput, to have the same throughput as Gensim for example, has the potential of further reducing the overall runtime.

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1 Introduction

Word embeddings are the vector representation of words (WE). They can be created in two ways, arbitrarily or with the purpose of capturing the semantic meaning of the word in the vector. To create arbitrarily WE there the most common way is to use the so-called one-hot encoding that is constructed as follows: each word vector will have the numbers of words in the vocabulary as dimension, and every dimension of the vector will be 0 except one that will hold the value 1. Therefore each vector will have one specific dimension where it will be unequal to one. As this representation does not capture any meaning, because each vector has the same distance to each other, a lot of effort went into creating better word embeddings. Those efforts have shown to facilitate a lot of tasks in natural language processing (NLP), such as machine translation or sentence classification. The main problem with creating WE is that there is no real task to learn as there is with more classical ML learning problems. Therefore the approach is to create a fake task, train a neural network on it and then use some weights of the network as WE.

This was also the technique used by Mikolov et al. [**mikolov**] who introduced the Skip Gram Model(SGM), an algorithm to create word embeddings. The SGM used the task of predicting the probability of a word appearing in the context of another word, i.e appearing in a certain window next to the word in a sentence. The SGM gained a lot of attention, as it achieved very good results for a very simplistic model. Therefore a lot of effort went into optimizing it. Most of this effort was trying to improve the throughput of the model, i.e the number of words that are processed per second by the model. Yi et al. tried to optimize it on CPU's [**intel**], by converting vector to vector multiplications into matrix matrix multiplications. Another attempt at optimizing the throughput was made by Seulki and Youngmin [**gpu**] who paralleled the update of each dimension of the embeddings on GPU's. We see that a lot of work went into optimizing the throughput of the model. As this is very interesting, not much work went into improving the convergence time of the model. Therefore one could ask himself if the convergence time of

the SGM can be optimized by the use of advanced optimizers and input shuffling, while at the same time maintaining its accuracy? Therefore our work focused on this task.

This work will first give a short introduction to the Skip-Gram model, then discuss related work and the numerous successful attempts that went into optimizing the throughput of the model. Then we will describe our implementation of the SGM followed by the description of our results. In the Section Results, we will first describe our dataset, the measure we used to compare the quality of word embeddings. And finally, we will discuss our work by comparing it to the state of the art implementation gensim [**gensim**].

2 Background

This section will give an overview of the SGM and related work that was done to optimize it. It will also give an understanding of the used optimizers in our experiments.

2.1 The Skip-Gram Model

The SGM is a very simple model used to learn WE. The idea is to train the model, a neural network, on a fake task and then use the weights as embeddings. The network consists of one input and one output layer. Each of these layers will act as a lookup table for our words, i.e the matrices representing the layers will store word embeddings. The input layer will be a $T \times d$ matrix, whereas the output layer will have dimension $T \times d$, where T is the number of words in our vocabulary and d will be the dimension of our WE. Each row of the input Matrix will store the WE of one word. The same holds for each column of the output layer. Know the question arises, on which task the network is trained? Well, the goal of the SGM is to predict for a given word w the probability of an arbitrary word c to appear next to w in a given window m. The training samples will be all the pairs of words with their context words. m is a hyperparameter of the model. An important thing to notice is that instead of always using the same m, each word will randomly have a number r that is in the range $(1, m)$ as it's window size. The task of the skip gram model is done by maximizing the following equation:

$$\prod_{t=1}^{T} \prod_{-m<j<m} p(w_{t+j}|w_t) \tag{2.1}$$

Where T is the number of words in the corpus data, w_t the tth word in the corpus data and m is the context window. This means that the m nearest words to w are considered

as context words. Equation 2.1 can be transformed into sums by using log probabilities:

$$\sum_{t=1}^{T} \sum_{-m<j<m} log(p(w_{t+j}|w_t)) \tag{2.2}$$

where the parameters are the same as in Equation 2.1.

The basic Skip-Gram Model uses a classical Softmax to calculate the conditional probability $p(w_{t+j}|w_t)$:

$$p(w_{t+j}|w_t) = \frac{exp(\tilde{v}_{w_{t+j}}^T v_{w_t})}{\sum_{w=1}^{v} exp(\tilde{v}_w^T v_{w_t})} \tag{2.3}$$

Here $\tilde{v}_{w_t}$ and v_{w_t} are the vector representations. The model stores vector representations of each word. One for the input words and another for the context word. Here $\tilde{v}_{w_t}$ is the output vector and v_{w_t} the projection layer. There lies a problem in the approach with a classical softmax. As a matter of fact, it is unsuitable to compute the softmax. For the computation of $\sum_{w=1}^{v} exp(\tilde{v}_w{}^T w_t)$, the denominator in Equation 2.1 one has to go over the whole corpus data. As very big data sets are needed to train the model, this is not a solution. Consequently, different solutions were proposed by Mikolov et al. [**mikolov2**]. The first one is to use a Hierarchical softmax introduced by Morin and Bengio [**hsoftmax**]. In this model, the probability distribution of the output nodes is saved in a binary tree which gives one a logarithmic computation time for each of these probabilities and makes it suitable to compute the softmax. Another possibility is the use of negative sampling which we shall discuss in the next section.

2.2 Negative Sampling

An alternative to the Hierarchical Softmax is Noise Contrastive Estimation (NCE) which was introduced by Gutmann and Hyvärinen [**nce-original**], and first applied to NLP by Mnih and Teh [**mnih**]. The idea behind NCE is to distinguish targets words from noise. It does so by reducing the problem to a logistic regression task and does it by maximizing the log probability. The skip-gram Model is only interested in good word representation, hence the probability of the word is not meaningful as long as the quality of the word representations remains high. Mikolov et al. [**mikolov2**] simplified NCE and called it Negative Sampling. Let's dive into it.

The idea behind negative sampling is to only update the output nodes of certain words. This will obviously save an enormous amount of computation time. The idea is that given a pair $(c, w) \in D$, where c is a word in the context window of w and select K random words k_i from the corpus data, more on the random distribution later. We will assume those words do not appear in the context of w. We will denote the score that the (c, w) wasn't drawn at random the following way: $p(y = 1|c, w)$, and if (k, w) is chosen at random this way: $p(y = 0|k, w)$. Now we will use logistic regression to update the weights of the k selected context words and c. By doing so we will only have to update $k + 1$ nodes.

Let's look at how we construct our objective function for a given word w and one of its context words c:

$$
\begin{aligned}
p(c|w) &= p(y = 1|c, w) + \prod_{k \in K} p(y = 0|k, c) \\
&= p(y = 1|c, w) + \prod_{k \in K} 1 - p(y = 1|k, c) \\
&= log((p(y = 1|c, w)) + \sum_{k \in K} log(1 - p(y = 1|k, c)) \\
&= log(\frac{1}{1 + e^{-v_c \tilde{v_w}}}) + \sum_{k \in K} log(1 - \frac{1}{1 + e^{-v_c \tilde{v_k}}}) \\
&= log(\frac{1}{1 + e^{-v_c \tilde{v_w}}}) + \sum_{k \in K} log(\frac{1}{1 + e^{v_c \tilde{v_k}}}) \\
&= log(\sigma(v_c \tilde{v_w}) + \sum_{k \in K} \sigma(log(-v_c \tilde{v_k})) \qquad \text{where, } \sigma(x) = \frac{1}{1 + e^{-x}}
\end{aligned}
$$

Where v_c and $\tilde{v_w}$, can be interpreted as before in Equation 2.1 The goal is know to maximize this objective function. Another way, apart from logistic regression, too look at this function, and assume why it's working so well, is to assume that two vectors are similar if their dot product is high. And therefore we will maximize the dot product of similar words (w, c) and minimize it for dissimilar words (w, k_i). We see that to compute our objective function we will only have to compute the sum over K. Which in practice is very small (2-20). Too put things in perspective lets imagine our data set consists of 100000 words, we set $K = 2$ and let's say that each output neuron has weight vector v

with $|v| = 300$. When updating our weights we would only update $0.2 * 10^{-2}$ of the 300 million weights in the output layer.

One question remains: how do we choose our random words? Mikolov et al. [**mikolov2**] used the following unigram distribution:

$$P(w) = \frac{f(w)^{\frac{3}{4}}}{\sum_{t=0}^{T} f(w_t)^{\frac{3}{4}}} \tag{2.4}$$

where $f(w)$ is the frequency of w_t. The value of $\frac{3}{4}$ is set empirically. By raising the unigram distribution to power of $\frac{3}{4}$ it makes it less likelier for a word to be drawn if it appears often in the dataset in comparison to the basic unigram distribution. See figure 2.1 for an example. It's quite easily observable that this approach will outperform the
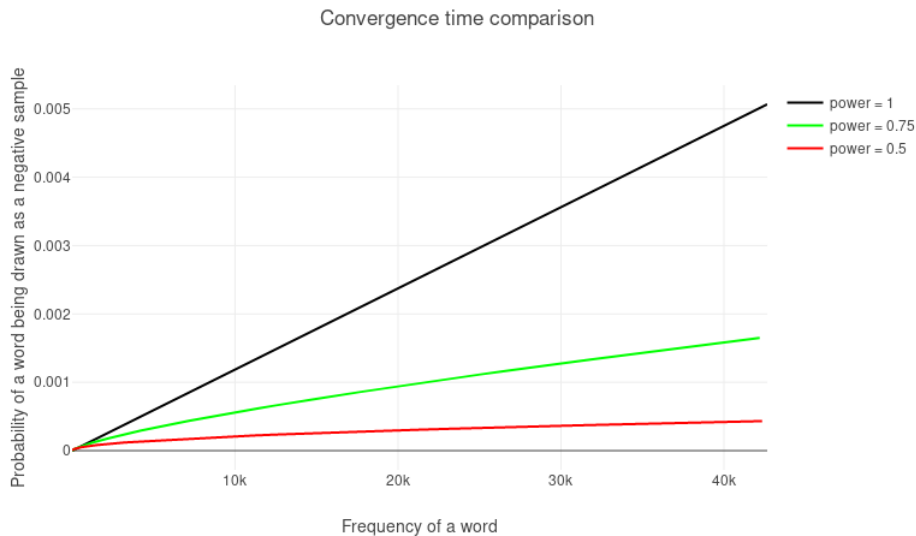
Figure 2.1: Probabililty of a word, of the text8 dataset (sampled), to be chosen at random according to its frequency and the power to which the unigram distribution is raised

classical softmax in computation time. Now the question arises if the accuracy is good enough but according to Mikolov et al. [**mikolov2**] the negative sampling method "is an extremely simple training method that learns accurate representations". As a matter of fact, Mikolov et al. [**mikolov2**] reported a 6% accuracy improvement in comparison to a Hierarchical Softmax model. We now have enough background knowledge about the SGM to look at how it can be optimized. In the next section, we are going to cover what has already be done.

2.3 Optimization of the Skip Gram Model

Due to the popularity of the skip gram model, a lot of research went into optimizing it. This research can actually be divided into two categories, optimization of the throughput and the optimization of the accuracy of the algorithm by allowing words to have multiple meanings. For our work, the optimization of the throughput is of big interest while the semantic optimization is aimed at given the reader a more holistic comprehension of the possible research directions. This section will first give an overview of the optimization of the throughput and then present one paper that focused on context-sensitive word embeddings.

2.3.1 Optimization of the throughput

In the original model, the optimization is done with Stochastic Gradient Descent (SGD), which is a sequential algorithm. This process does not favor a parallelization. To deal with this specific problem Mikolov et al.[**mikolov2**] used a Hogwild tree proposed by Recht et al.[**hogwild**]. The approach is to allow multiple threads to access a shared memory, in this case, the single model. Therefore overwriting errors are bound to happen. But according to Recht et al.[**hogwild**] the overwriting errors won't lead to a significant accuracy loss if the data access isn't too frequent. But in the case of NLP, the problem seems to be a bit more significant, and especially for word embedding, as many words share the same context words. There were several attempts at solving this issue, and we are going to cover a few of them in the following subsections.

Parallelization by the use of caching

This idea was proposed by Vuurens et al. [**efficient**]. The architecture used here is the basic skip gram model with a hierarchical softmax. The general idea is to cache the most frequently used nodes of the binary tree used to memorize the probability distribution and update them on the shared single model after a certain amount of seen words (the paper used the number 10). The paper produced interesting results as they managed to increase execution time by increasing the number of cores used for the calculation. This is very powerful because in the original implementation the execution time regressed after 8 cores, this seems to indicate that too much overwriting was happening, as the

number of concurrent threads surpasses a certain threshold. This can be seen in Figure 2.2, where c31 is the model proposed by Vuurens et al.[**efficient**]. The model did not suffer any accuracy loss in comparison to the original SGM model. This work proposes a
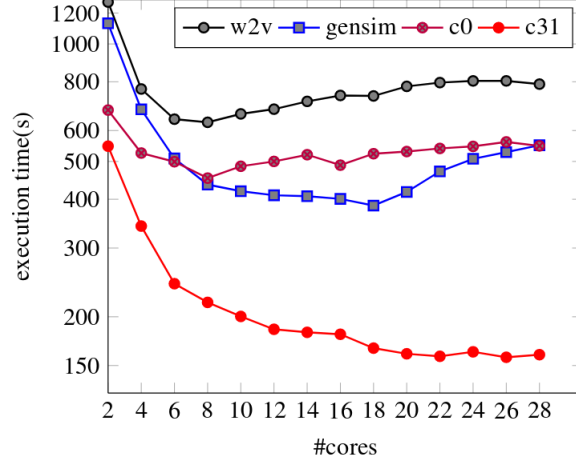
Figure 2.2: Comparasion of the execution time in relation to the number of used cores [**efficient**]

very good way to parallelize the SGM, as in particular, it allows to use more cores during the computation. While this is very interesting, this model focuses on the hierarchical softmax approach. As we implemented the approach using negative sampling this is of less use. Therefore we will look at what has been done with negative sampling in the next section.

Parallization in shared and Distributed Memory

The first parallelized solution which was proposed by Ji et al. [**intel**], is to try to reduce the cost of our vector multiplication. The main idea in this paper is to convert the level 1-BLAS vector to vector operations to a level-3 BLAS matrix multiplication operation. This is achieved, by using the same negative samples for each context word of a given word w. Instead of using for each context word a vector to vector multiplication we can transform this, under the assumption that we will not lose accuracy by sharing the same negative samples, into a matrix multiplication. The matrix multiplication can be

represented in the following way.

$$
\begin{bmatrix} w \\ w_{n_1} \\ \vdots \\ w_{n_k} \end{bmatrix} * \begin{bmatrix} w_{c_1} \\ \vdots \\ w_{c_{2m}} \end{bmatrix}
$$

where w is our given word, $w_{n_1}...w_{n_k}$ are the shared negative samples, with $k \in [5, 20]$, and $w_{c_1}...w_{c_{2m}}$ are the words inside of the context window m of w, with $m \in [10, 20]$, also called a batch of input context words. After each batch the model updates the weights of the used vectors. This model achieves a 3.6 fold increase in throughput, by only losing 1% of accuracy. Those results are interesting but cannot be considered earth-shattering. Another aspect that is not as useful to us is that the experiments were done on Cpu, as modern GPU's are often used in many machine learning libraries, as with Cuda for example, there still need work to be done to optimize it with GPUs. This was attempted by Seulki and Youngmin 2016 [**gpu**], which will be described in the next section.

Accelleration of word2vec by Using GPU's

This work [**gpu**] focused on getting a better throughput on the SGM when using Gpu's. As the skip gram model is a sequential algorithm, one cannot parallelize a lot, there is as explained in the next section the possibility to split the dataset. But we cannot parallelize those splits. Therefore the idea of Seulki and Youngmin was to parallelize the update of a feature. Each Cuda block will be used for one split. And each thread of this block will be used to update one dimension of the word. We, therefore, have a parallelization on the level of the dimension of the embeddings. They achieved very good results as achieved a 20x speedup compared to a single threaded CPU execution. The problem with this and all the above optimization is that the code is not easily available and of use for us. Therefore we need an optimized implementation of the SGM, which Gensim [**gensim**] provides.

2.3.2 Gensim

Gensim [**gensim**] is a pure Python library that holds a state of the art implementation of the SGM. As it was written in Cython, it shows an interesting speed up. Furthermore, with the use of BLAS and precomputed sigmoid tables, it achieves a 3 fold speed increase in comparison to the original w2vec code. Gensim is an important tool as it allows us to compare our data rather easily. It was also used in related work [**intel**] and is therefore of value. This will conclude our overview of the optimizations of the throughput of the SGM. In the next section, we will give a quick outlook of what has been done when trying to improve the semantics of the SGM.

2.3.3 Context sensitive word embedding

A word does not always have the same meaning according to its context. This is a problem that is not addressed by the SGM. Some new models, that have taken this issue into consideration, were proposed. A lot of work has been done in this direction, Liu et al.[**topicalWE**], Bartunov et al.[**breaking**] for example, but the one reporting the best results is Liu et al. [**contextWithTensor**]. The main idea is to change the way we compute the objective function and variables we use in our conditional probability. The idea is to look if a word given a certain context word matches to a topic. Bank would match to finance given the context word money. Bank would also match to nature if river was the given context word. But Bank would not match to nature with the context word money. Now one could ask himself how to achieve such a context sensitive word embedding? First, we have to introduce new variables, therefore let's look at the objective function used: First, let's take a look at the objective function:

$$J(\Omega) = \sum_{(w,t,c)\in D} \sum_{(w,\tilde{t},\tilde{c}\in \tilde{D})} max(0, 1 - g(w,t,c) + g(w,\tilde{t},\tilde{c}))\lambda ||\Omega||_2^2 \qquad (2.5)$$

This approach uses the same negative sample technique as described in the previous sections, D is the corpus data and $\tilde{D}$ is the set of negative samples and λ is the hyperparameter used for the standard L_2 standarization. What is interesting here is the function $g(w,c,t)$, where w is a word, c the context word, and t the context in which the word

appears, g is defined as follows:

$$g(w, c, t) = u^T \sigma(w^T M^{[1:k]} t + V_c^T (w \oplus t) + b_c) \tag{2.6}$$

where, u, V_c, b_c are standard parameters for a neural network, $\oplus$ is the vector concatenation, while the most important parameter is $M^{[1:k]}$, which a tensor layer, the tensor layer is used because of its ability to model multiple interactions in the data, as this will be useful for multiple contexts. They used SGD for the optimization of this objective function. They achieved really interesting results as shown in 2.3.

Words	Similar Words
bank	depositor, fdicinsured, river, idbi
bank:1	river, flood, road, hilltop
bank:2	finance, investment, stock, share

Figure 2.3: "Nearest neighbor words model and Skip- Gram. The first line in each block is the results of Skip-Gram; and the rest lines are the results of our model" [**contextWithTensor**]

2.4 Gradient Descent Optimizers

The goal of learning in machine learning is to minimize an objective function $J(\theta)$, where θ is the set of all parameters in our model. This happens by updating the parameters θ at every training time step t. We will denote θ_t as the parameters of our model at the tth time step. In this work, we only examine gradient descent algorithms.

2.4.1 Gradient Descent

The idea in gradient descent optimization is to follow the path of steepest descent in the shape of the objective function. To get information about the shape of the objective function, one has to compute the gradients of all our parameters $\nabla J(\theta_t)$, where J is our objective function, and θ all of our parameters, t denotes the time step at which the parameters are taken. We will define g_t as the gradients of our parameters θ_t according to our objective function J. To follow the path of steepest descent we will have to subtract a portion of this term from our parameter. The magnitude of the portion is

often referred to as the learning rate, denoted as η. For illustration, this means that the gradients will give the direction of the optimization step, whereas the learning rate will give the amplitude of that step. An update at time step t will result in the following equation:

$$\theta_t = \theta_{t-1} - \eta \nabla g_{t-1} \tag{2.7}$$

Where all the variables can be interpreted as above. This will also be the case for further Equations. There are three main variations of Gradient Descent, they differ at the moment they chose to update the parameters.

Stochastic Gradient Descent (SGD)

In this variant the the model will update the parameters after each training sample. The problem with this approach, is that the variance of the direction of the training step will be very high, as each sample will influence the step individually.

Batch Gradient Descent

Here the update of the model happens after having gone through the entire dataset. The problem with this approach is that one updates the model way to infrequently which will lead to a high convergence time.

Mini-Batch Gradient Descent

Update the model after having gone through a specific number of training samples. The idea is that the batch will be representative of the entire dataset. Which will allow the model to learn quicker, as the updates are more frequent (in comparison to batch gradient descent) and less variant (in comparison to SGD).

Problems with Gradient Descent Algorithms

SGD, though it's simplicity, is very limited, therefore some issues appear:

- The learning parameter is yet another hyperparameter to tune, as the optimum setting will largely vary depending on the training task and architecture of the network

- Learning rate schedules, that diminish the learning rate as the training progresses, are commonly accepted technique to improve accuracy. This schedule is most often set at the beginning of the training, and will be completely independent of the training set.

- Every parameter has the same learning rate

To tackle those issues numerous advanced optimizers were developed. They will be covered in the next sections.

2.4.2 Momentum

Momentum is a technique used to address one of SGD weak points. As a matter of fact because SGD can have trouble computing the optimum of objective function that are only steep in one directions. The problem here is that SGD often oscillates in the direction that is not very steep, and only takes small steps in the steep direction. This issue is addressed by SGD with momentum.

It does so by adding a percentage of the last update vector to the current update vector. By doing so the gradient that goes in the same direction will get bigger (building momentum) and gradients that go in different directions will annul themselves. At the update t we will comppute our update vector v_t the following way:

$$v_t = \gamma v_{t-1} + \eta \nabla J(\theta) \tag{2.8}$$

Where v_t and v_{t-1}, respectively are the current and the last update vector. The value 0.9 for γ has shown great results, but this, same as a learning rate, another hyper parameter that need to be tuned according to the specific task. And then we update our weights as usual: $\theta = \theta - v_t$

2.4.3 Nesterov

Momentum can be a powerful tool, but sometimes be its own enemy. With Momentum, the learning algorithm often overshoots and blows by the Optima. Hence it will never converge. This problem was addressed by Nesterov. The idea behind his algorithm is to incorporate the momentum in the computation of our gradients. We will subtract the momentum vector, or just a fraction, from our parameters before computing the gradients. Therefore we will compute the gradients of the position where we would be with momentum, which will allow us to make a step in a better direction. The computation of the update vector will look the following way:

$$v_t = \gamma v_{t-1} + \eta \nabla J(\theta - \gamma v_{t-1}) \qquad (2.9)$$

Where the parameters as the same used with momentum in equation 2.4.2. SGD with momentum and Nesterov accelerated gradient (NAG) has shown tremendous results in RNN's. But some of the earlier mentioned problems still remain. NAG, still treats every parameter the same way. Therefore we need a more complex optimization algorithm, that takes the frequency of a feature into account. Adagrad does just that.

2.4.4 Adagrad

Adagrad first introduced by [**adagrad**] is an optimizer that tries to apply different learning rates to different parameters, according to their frequency. The idea is to give very frequent features a small learning rate, and very sparse features a high learning rate. This can be very important for our task of word embeddings, as rare words in the corpus are more important than very frequent ones. As a matter of fact, Pennigton et al. used this algorithm for their training of Glove [**Glove**], another word embedding system.

Each parameter θ_i, at time step t will have it's own learning rate $\eta_{t,i}$

$$\eta_{t,i} = \frac{\eta_0}{\sqrt{\sum_{i=1}^{t} g_{t,i}^2 \epsilon}} \qquad (2.10)$$

where $g_{t,i} = \nabla J(\theta_{t,i})$ is the partial derivative of the loss function with respect to the parameter θ_i at time step t, and ϵ is a place holder, so that one does not divide by 0, at

the beginning of the computation.

We see that each parameter θ_i has it's one learning rate. For a very frequent feature the sum of the previous gradients will be very high, hence the learning rate low. This is how Adagrad achieves a different learning rate for each feature. Therefore we have $\theta_{t+1,i} = \theta_{t_i} - \eta_{t,i} g_{t,i}$, and we can now construct our global parameter update as follows:

$$\theta_{t+1,i} = \theta_{t_i} - \frac{\eta}{\sqrt{G_{t_{i,i}} + \epsilon}} g_{t,i}, \tag{2.11}$$

with $G_{t_{i,i}}$ being the diagonal Matrix of the sum of the squares of the graditents $(g_{t,i})$. There lies one weakness in this approach: the sum of the squares of the previous gradients grows constantly. This means that after a certain number of epochs the learning rate will be insufficient, to update the model. This issue was addressed by the Adadelta algorithm, that will be covered in the next session.

2.4.5 Adadelta

Adadelta [**adadelta**] not only solves the constantly growing sum problem, but also the fact that one does not have to tune the learning rate by not having one. The gist of Adadelta is that instead of taking all the gradients to compute the sum we will only take a fixed number w of gradients. But instead of inefficiently storing w gradients we will take the exponentially decaying average of the squared gradient, denoted $E[g^2]$. The average at time step t will be computed in the following way:

$$E[g^2]_t = \gamma E[g^2]_{t-1} + (1 - \gamma)g_t^2 \tag{2.12}$$

where γ is a hyperparameter similar to the one used in momentum, that decides how much the past is weighted in contrast to the current gradient. Since Adadelta is an extension of Adagrad the square root of $E[g^2]$ is needed which become the Root Mean Squared Error (RMS):

$$RMS[g]_t = \sqrt{E[g^2]_t + \epsilon} \tag{2.13}$$

Which gives us the following update rule:

$$\theta_t = \theta_{t-1} - \frac{\eta}{RMS[g]_t} g_t \tag{2.14}$$

Here we have two problems, first, the learning rate is still a hyperparameter. And the units do not match. This is a problem xyz wanted to address. That if the parameters would have units the update parameters would have the same parameters. Therefore they define the exponentially decaying average of squared parameter updates:

$$E[\Delta\theta^2]_t = \gamma E[\Delta\theta^2]_{t-1} + (1-\gamma)\Delta\theta_t^2 \tag{2.15}$$

As before we can know us the root mean squared error:

$$RMS[\Delta\theta]_t = \sqrt{E[\Delta\theta^2]_t + \epsilon} \tag{2.16}$$

As at time step t $RMS[\Delta\theta]_t$ is unknown, we approximate it with $RMS[\Delta\theta]_t - 1$. Know we replace η with $RMS[\Delta\theta]_t - 1$ and get the final update rule:

$$\theta_{t+1} = \theta_t - \frac{RMS[\Delta\theta]_{t-1}}{RMS[g]_t}g_t \tag{2.17}$$

2.4.6 Adam

Adaptive Moment Estimation (Adam), is a more recent optimization algorithm. It also computes adaptive learning rates. In comparison to Adagrad and Adadelta, it does not only take into considaration the decaying average of the previous squared gradients but also the decay of the past gradients. Let's introduce :

$$m_t = \beta_1 m_{t-1} + (1-\beta_1)g_t \tag{2.18}$$

as the decaying average of the previous gradients, and

$$v_t = \beta_2 v_{t-1} + (1-\beta_2)g_t^2 \tag{2.19}$$

as the decaying average of the previous squared gradients. Where β is a hyper parameter similar to γ used in the previous optimizers.
One problem arises when using this formula, m_t and tv_t are initialized as vectors of zero. Therefore they are biased towards zero. therofore et al. advised to use a bias corrected version:

$$\tilde{m}_t = \frac{m_t}{1-\beta_1^t} \tag{2.20}$$

$$\tilde{v}_t = \frac{v_t}{1 - \beta_2^t} \tag{2.21}$$

The general update is done exactly in the same way as in Adadelta:

$$\theta_{t+1} = \theta_t - \frac{\eta}{\tilde{v}_t + \epsilon} \tilde{m}_t \tag{2.22}$$

3 Implementation

In this work our goal is to optimize the skip-gram model, we, therefore, implemented our own version of it. As we implemented it in python, computation is slow, we, therefore, altered the original implementation. This chapter will illustrate our proceeding. First, it will give a short introduction to PyTorch, and then cover our implementation. In the latter part, we will talk about the modified version of the skip gram model that we used and the challenging parts of our implementation.

3.1 PyTorch

For our implementation, we chose the open source library PyTorch.[1]. Though it's the simplicity of use it's one of the most used libraries for machine learning. One of the most important features is the calculation of gradients by Pytroch. All gradients are calculated online, therefore there is no need for us to implement the calculation of those gradients. The second important feature that we used, is the large variety of optimizes already implemented in pyTorch. They are proposed in the package `torch.optim`[2]. The last important feature of Pytorch that we used are the classes `Dataset`[3] and `Dataloader`[3]. Both of these classes are meant to work closely together. The Dataset interface has two functions to offer namely: "`__len__`" and "`__getitem__`". Those are then used by a data loader object, that will construct a batch based on those two functions. The loader object will facilitate the training process, as we can simply iterate over it, and get the batches. Furthermore, the data loader can shuffle our dataset before each epoch.

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[1]pytorch
[2]https://pytorch.org/docs/stable/optim.html
[3]https://pytorch.org/docs/stable/data.html

3.2 Implementation

This section will give an overview of our implementation. First, it will give a broad overview of the implementation idea and process. Then it will go into detail, explaining the forward process of our model and the construction of our dataset, by the use of the `Dataset` class.

3.2.1 Batched SkipGramModel

As we implemented the SGNS in python, computation time was slow. We, therefore, altered the original implementation to get a faster computation, while taking the risk to have slightly less good quality. Our idea was, to compute the loss for multiple words and context pairs at the same time. Therefore some overwriting may happen at the backpropagation. The exact process will be described in the following paragraph.

Forwarding

Input:
The forwarding method will take two vectors v and c, and a matrix A as an input. The first vector represents all the center words in a batch, the second one the context words. The Matrix represents the negative samples. The two vectors need to have the same length, defined as n. Our training batch X can be seen as in the following way: $X = \{(v_i, c_i) \| 1 \in \{1, ..., n\}, n = |v|\}$. Where (v_i, c_i) is a context pair. The matrix must be of dimension $n \times k$, with k, being the number of negative samples per pair. This means the ith row will store the negative samples for the ith word context pair.
Concatenation of samples:
First, we will concatenate w and our Matrix A. This will result in a Matrix $\tilde{A}$.
Embeddings:
Know we need to get our Embeddings. Therefore we will create a Matrix E_v of dimensionality $n \times d$ where d is the dimension of our word embedding which will store the word embedding of the ith word from our input vector v in it's i^{th} row. We will do the same for the our Matrix $\tilde{A}$ This will result in a $n \times k + 1 \times d$ Array E_v.
Batch Multiplication and negation of samples:
To compute the dot product of each word vector with it's pair and the negative samples,

exactly as done as in the original loss function of Mikolov et al. shown in Equation 2.2, we will need some definitions: let A_j be the jth row of the matrix A, know let $E_c(i, j)$ be the d dimensional embedding of the word stored in $\tilde{A}(i, j)$. To know compute the dot product we will do a so-called batch multiplication[4] which will result in a matrix S where $S(i, j) = E_c(i, j) \cdot A_j$. This will result in a $n \times k + 1$ Matrix S. Know we only have to multiply the last k rows with minus one. The sum of each row represents the loss computed in Equation 2.2, for each word context pair. But this is not what we are wishing to do as the computation time would be too long, therefore we construct our own loss function.

Loss function:

We sum the resulting matrix of and multiply it with -1 hence we get a less for our entire batch, as some words may appear more then once in the batch this will more be an average of it then as with Mikolov et al the exact update per pair.

The process can be best understood with an example, let our training batch be:

$X = (v_1, c_1), (v_2, c_2), (v_3, c_3)$ Input:

$$v = \begin{bmatrix} v_1 & v_2 & v_3 \end{bmatrix}, c = \begin{bmatrix} c1 \\ c2 \\ c3 \end{bmatrix} \text{ and } A = \begin{bmatrix} k_{1,1} & k_{2,1} & k_{3,1} \\ k_{1,2} & k_{2,2} & k_{3,2} \\ k_{1,3} & k_{2,3} & k_{3,3} \end{bmatrix}$$

We then concatenate c and A, resulting in:

$$\tilde{A} = \begin{bmatrix} c_1 & k_{1,1} & k_{2,1} & k_{3,1} \\ c_2 & k_{1,2} & k_{2,2} & k_{3,2} \\ c_3 & k_{1,3} & k_{2,3} & k_{3,3} \end{bmatrix}$$

Embeddings:

$$E_v = \begin{bmatrix} \tilde{v}_{11} & \dots & \tilde{v}_{1d} \\ \tilde{v}_{21} & \dots & \tilde{v}_{2d} \\ \tilde{v}_{31} & \dots & \tilde{v}_{3d} \end{bmatrix}, \text{ where } \tilde{v}_i = \begin{bmatrix} \tilde{v}_{i1} & \dots & \tilde{v}_{id} \end{bmatrix} \text{ is the embedding of } v_i.$$

$$E_c = \begin{bmatrix} \tilde{c}_1 & \tilde{k}_{1,1} & \tilde{k}_{2,1} \\ \tilde{c}_2 & \tilde{k}_{1,2} & \tilde{k}_{2,2} \\ \tilde{c}_3 & \tilde{k}_{1,3} & \tilde{k}_{2,3} \end{bmatrix}, \text{ where each entry of the matrix is a vector of dimension } d$$

Batch multiplication and negation of samples:

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[4]https://pytorch.org/docs/stable/torch.html#torch.bmm

$$S = \begin{bmatrix} \tilde{v}_1 \cdot \tilde{c}_1 & -\tilde{v}_1 \cdot \tilde{k_{1,1}} & -\tilde{v}_1 \cdot \tilde{k_{2,1}} & -\tilde{v}_1 \cdot \tilde{k_{3,1}} \\ \tilde{v}_2 \cdot \tilde{c}_2 & -\tilde{v}_2 \cdot \tilde{k_{1,2}} & -\tilde{v}_2 \cdot \tilde{k_{2,2}} & -\tilde{v}_2 \cdot \tilde{k_{3,2}} \\ \tilde{v}_3 \cdot \tilde{c}_3 & -\tilde{v}_3 \cdot c_3\tilde{k_{1,3}} & -\tilde{v}_3 \cdot c_3\tilde{k_{2,3}} & -\tilde{v}_3 \cdot \tilde{k_{3,3}} \end{bmatrix}$$

Loss computation:

$\mathrm{L} = -\sum_{(i,j)\in k\times n} S(i,j)$

As we now have a way to compute our loss, we need to access the context-pairs, therefore we also had to create our own way of doing it. We will explain the process in the next paragraph.

3.2.2 Creating the context pairs

We needed to provide a way for the `dataloader` to access each word context pair. The straight forward way would be to go once over the whole dataset and create a list that stores all those pairs. The Problem with this approach is that it would not be possible to do so for a very large dataset. The amount needed to store a list of all the possible pairs for a small dataset (text8 dataset, more on the dataset in Section 4.1) is roughly 4GB. As some used datasets are 100x bigger in practice, this is not a suitable solution. Therefore we propose a way to compute the ith word-context pair of the dataset, by only storing the dataset in the RAM. Here we had two tasks, compute the number of possible pairs in our dataset, and given an index i return the wanted pair. Both of these task were respectively done in the methods `__len__` and `__getitem__`.

Number of pairs in the dataset

For the first task, calculating the number of pairs in the dataset, we knew that every sentence except the last one had a length of 20 words (more on this in Section 4.1). As the number was fixed we only needed to compute once the number of pairs in a sentence of length 20. This was done in the following way. We will distinguish two types of words in a sentence: first center words, those have the maximum amount of possible context words, and the border words that do not have this property because they are too close to the start or end of the sentence. We know that every center word has exactly 2 times the amount of the window size as context words. To compute the number of border

pairs in a sentence one only has to subtract the length of the sentence with the double of the window size. The border pairs can be computed by the following equation.

$$\sum_{i=0}^{ctx\_window-1} ctx\_window + i \tag{3.1}$$

Finally, we have to compute the number of pairs in the last sentence, here the challenge is to compute it if the sentence is shorter then twice the length of our window because then the equation described previously does not work. A pseudo-code description can be found in Algorithm 1. We will iterate over the length and add each time step we will compute the number of context pairs the given word has. First, we check if the index is smaller then our window. If this is the case we have to distinguish one special case, namely if our sentence is smaller then where we would be if we added the maximum number of the window. If this is the case we add the length of our sentence -1 to the number of pairs (line 4). A short explanation: Instinctively one would first add the j pairs that are left of our word, and then compute the number of pairs right of the word. For this one would do $len\_last\_sen - 1 - j$ because len_last_sen -1 is the index of the last word in our sentence and to get the number of words between the last and the current j^{th} word one needs to subtract j. Therefore the number of pairs is $len\_last\_sen - 1 - j + j = len\_last\_sen - 1$.

Then we have to check if our word is to close to the end of the last sentence (line 7) to add the context pairs. Here we apply the same procedure as above, add the window amount context pairs from the left, we can do this because we know that $j \geq window$ from line2, we also need to add the words right to the current word, therefore, we take the same difference as before: $len\_last\_sen - 1 - j$. The final case is simply calculating the number of pairs per center word if there are any.

Know we can simply add the number of pairs in our last sentence to the previously computed number, and return the number of pairs in our dataset.

Accessing each pair individually

Now we need to provide a way for the dataloader to access each pair individually, a pseudo code description can be found in 2. Given an item index idx we need to find in which sentence the pair is. Because we know how many pairs there are in each sentence, except the last one, we only have to divide idx by the number of pairs that can be built

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Algorithm 1 Computing the number of pairs in the last sen

1: **for** $j = 0$ **to** len_last_sen -1 **do**
2:    **if** $j < window$ **then**
3:       **if** $j + window \geq len\_last\_sen$ **then**
4:          pairs_last_sen += len_last_sen-1
5:       **else**
6:          pairs_last_sen += j+window
7:    **else if** $j \geq len\_last\_sen - window$ **then**
8:       pairs_last_sen += len_last_sen -1 -j + window
9:    **else**
10:       pairs_last_sen += 2*window
11: **return** pairs_last_sen

---

within one sentence (line2). This division also holds true for the last sentence, as it's the only one with a different number of words in it and is the last one. Once this is done we have access to the sentence where our pair is located. (line3). We have to find the index of our pair within our sentence. We know the number of pairs in all sentence before our sentence (this also holds true if our sentence is the last one), therefore we can subtract the number of pairs that are in all the sentences before our sentence from idx, and will get the index of our pair within it's sentence (line4). Once this is done we only have to iterate over all the possible pairs in our sentence keep count and return when we find the correct pair (line 6-15).

Algorithm 2 Getting the context pair from the id

1: n_pairs_in_sen = border_pairs + center_pairs
2: id_sen = $\lfloor \frac{idx}{n\_pairs\_in\_sen} \rfloor$
3: sen = dataset[id_sen]
4: pair_id_in_sen = $idx - id\_sen * (n\_pairs\_in\_sen)$
5: counter = 0
6: **for** $i = 0$ **to** len_sen **do**
7:    **for** $j = 0$ **to** $window$ **do**
8:       **if** $i + j < len\_sen$ **then**
9:          **if** counter == pair_id_sen **then**
10:            **return** (word2idx[sen[i]], word2idx[sen[i+j]])
11:          counter += 1
12:       **if** $i - j \geq 0$ **then**
13:          **if** counter == pair_id_sen **then**
14:            **return** (word2idx[sen[i]], word2idx[sen[i-j]])
15:          counter += 1

Adaptability to other datasets

The above described implementation is limited to datasets formatted as ours, namely having all sentences except the last of the same length. But our model can be quickly modified to achieve the same results on any given dataset. To compute the length of the dataset one would have to use Algorithm 2 to compute the length of each sentence, and take the sum over all the length of each sentence. To access the context-pairs the challenge lies in getting the id of the sentences. Therefore one would have to go over the dataset and compute the numbers of pairs for each sentence, sum them up and wait until the sum is greater than the searched pair. Once this is done the algorithm stays the same.

4 Results

This section will give an overview over the used datasets, the used metric to evaluate our models, the configuration of our model and finally the experimental results achieved.

4.1 Dataset

In this implementation we mainly used the text8 [1] dataset. We chose this dataset for two reasons. First of all, it's a very small dataset, more on exact numbers later, that allowed us to do a lot of computations. Secondly, this data set was used in a lot of related work (cite GPU, CPU,caching) hence giving us a very good benchmark. The text8 dataset consists of 1702 lines of 1000 words, with a vocabulary of roughly 63000 words, there is no punctuation in the dataset. Therefore we had to choose between building arbitrary sentences and keeping the dataset as it is. We chose the first option because it gives us a faster computation time, and did not show any significant loss in quality empirically, as shown in Table 4.1. We chose a sentence's length of 20. Furthermore, we applied a technique called subsampling that reduces the data set size. We needed a second larger dataset to confirm our results. We, therefore, chose the enwik9 dataset[2].This dataset needed more preprocessing as it's plain HTML. We, therefore, used a preprocessing script.[3]. We also split this dataset into sentences of length 20 and applied subsampling. The next section will give an explanation on the sampling process. A comparison of the two used datasets can be found in Table 4.2.

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[1]http://mattmahoney.net/dc/enwik8.zip
[2]http://mattmahoney.net/dc/enwik9.zip
[3]http://mattmahoney.net/dc/textdata.html, Appendix A

Length of Sentences	20	1 Document
Training Time for one batch	10min	18min
Convergence Time	3 epochs	3 epochs
Word Similarity	0.66	0.66

Table 4.1: Training and Convergence time according to choice of the length of sentences in text8 dataset

Dataset	Text8	Text8 sampled($10^{-}4$)	enwik9	enwik9 sampled($10^{-}4$)
Number of Words in Dataset	17mio	8mio	125mio	57mio
Vocabulary Size	250k	63k	800k	195k

Table 4.2: Comparison of the text8 and enwik9 dataset

4.1.1 Subsampling

Subsampling is a technique introduced by Mikolov et al. [**mikolov**] to reduce the dataset size while at the same time increasing the quality of the dataset, i.e getting better word embeddings with it. The idea behind subsampling is that words appear very frequently in the dataset such as: "the, as, it, of" but do not give an intrinsic value to the words that appear in its context. Therefore the goal of subsampling is to delete such words from the dataset. This will decrease the computation time, as it will reduce the number of training samples, and should, in theory, increase the accuracy of the model. The increase in accuracy can also be explained by the fact that words that would not have appeared in the context of each other, may know to do because words between have been deleted. Know the question arises, how one chooses to delete a word. Mikolov et al. chose the following equation to compute the deletion of a word w in the data set:

$$P(w) = 1 - \sqrt{\frac{t}{f(w)}} \tag{4.1}$$

where $f(w)$ is the frequency of w, and t is a threshold set empirically. As Equation 4.1 is a probability, subsampling is not a deterministic procedure, words that may have been deleted with a threshold of $10^{-}2$, may stay in the Dataset with a lower threshold, as can be seen on the example on Table 4.4. Mikolov et al. recommend a value between 0 and 10^{-5}, depending on the size of the dataset. We experimented with different values and 10^{-4} seemed the most suited. We did this by simply looking at a random set of sentences and humanly judging the results. An example of the first sentence with

different sampling thresholds can be found in Table 4.4. The table shows the first 20 words of our dataset, without the words that were subsampled according to a threshold sample. Stats about subsampling can be found in Table 4.3.

Sampling Treshhold	0	10^{-1}	10^{-2}	10^{-3}	10^{-4}
Number of words in Dataset	16 mio	15mio	11 mio	8mio	4 mio

Table 4.3: Size of preproccessed text8 dataset according to sampling treshold

Min count

We also deleted every word that did not appear more than 5 times in our dataset. We got this technique from gensim [**gensim**], that introduced this parameter into their training. This is a good technique because of three reasons: first certain words of our data sets do not appear in a common lexicon (twigleg, melqu), or come from a foreign language (Volksvereinigung), or are names and acronyms. Secondly, each document often has spelling mistakes, those (as long as the same spelling mistake does not appear too often, what should be avoided in practice) would be deleted by sampling too, as the words do not have any meaning. Lastly, a word that only appears one time in our dataset will be very dependent on its original initialization. This is the case because it will only be updated with its context pairs once, which is only a dozen of times in practice, and then wont be updated any more. For all of the above reasons we applied this technique. It should, such as subsampling, in theory, improve the quality of the word embeddings and will decrease the computation time.

Sampling Treshold	First sentence of Dataset
10^{-1}	Anarchism originated as a term of abuse first used against early working class radicals including the diggers of the english
10^{-2}	Anarchism originated as a term of abuse first used against early working class radicals including diggers of english
10^{-3}	Anarchism originated a term abuse first used against early working class radicals including diggers the english
10^{-4}	Anarchism originated abuse used against working class radicals diggers english
10^{-5}	against radicals diggers

Table 4.4: Example of a sentence with different sampling tresholds

4.2 Evaluating word embedings

Evaluating word embedding is not an easy task. We cannot split our data set into train and test set. As the task that the network is learning is of no interest to us. Therefore we need to verify that our embedding is of quality with other techniques. To define quality we first need to define a measure of similarity between two vectors. Let us introduce the cosine distance for this task.

4.2.1 Cosine distance

The cosine similarity, this is not the cosine distance, of vectors v and w is the cosine of the angle between the two vectors It can be calculated by taking the dot product of v and w and dividing it by the magnitude of v and w multiplied with each other. We get:

$$cos\_sim(v, w) = \frac{v \cdot w}{|v||w|} \tag{4.2}$$

The cosine of 0°is 1, it's 0 for two vectors that are orthogonal to each other and vectors that point in the opposite direction will have a cosine of their angle of -1. This is not a good distance measure as -1 is smaller than 0, and therefore two vectors pointing away from each other would be closer than two orthogonal vectors, but by subtracting 1 from the cosine of the angle we can create a good distance measure between the two vectors. This distance does not take into account any order of magnitude. Hence for our tasks, two vectors will be considered equal if they are of different magnitude but point in the same direction. This technique apart from being shown empirically to work very well to measure the quality of word embedding has another advantage. By normalizing the vectors the calculation of the cosine angle becomes the dot product of the two vectors. Which can be computed very fast on modern GPU's. Know that we have a measure to compute the similarity of two vectors let us introduce a way to rate the quality of our embeddings.

Word1	Word2	Score
"FBI"	"Investigation"	"8.31"
"Mars"	"scientist"	"5.63"

Table 4.5: Example of pairs and their rating in wordsim353

4.2.2 Word similarity and wordsim353

To measure the quality of our word embedding we will need a dataset to compare our results too. We chose wordsim353[4] for this task, as it's the most used in the related literature. The data set consists of 353 pairs of words rated by humans on their similarity. The similarity score is in the range of 1 and 10, an example for two of such pairs can be found in Figure 4.5. We will rank our embeddings on the Pearson correlation coefficient between the cosine distance and the scores attributed by humans, as again this is what is done in the literature.

4.3 Configuration of the network

The skip gram model has a lot of possible parameters, that can be tuned. We experimented with different models and finally decided for one that we tried to optimize. This section will give a short overview of each parameter, where we will explain the process in which we chose the value of the given parameter. The explanation of the parameters will be structured as follows: `Parameter` - Description and tuning - *Value*

- `Negative Samples` Here we have to find a trade-off between, setting the parameter too high which will result in increased accuracy but a longer computation time. For smaller data sets a higher number of negative samples is often needed. In their original paper Mikolov et al. recommend a value of 5-20. We tested a few values in the range of 5 to 15, as 10 yielded state of the art results we chose this value. - *10*

- `Context Window:` The bigger the window the more training examples the network will have, but if the window is too big the semantic meaning of the window will be erased. Mikolov et al. proposed a setting between 2-10, as all our sentences are of size 20 we chose 5. - *5*

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[4]http://www.cs.technion.ac.il/ gabr/resources/data/wordsim353/wordsim353.zip

- **`Dimension of the embedding`**: Here the choice is less obvious, as the dimension needs to be high enough to capture the meaning, but cannot be too high as this leads to a decrease in performance as shown by Yin and Shen [**dimensions˙size**]. We therefore used Gensim to find the best embedding possible. - *100*

- **`Batch size`**: As described in section 3.2.1, there is a tradeoff to find between quality and training time. We first used a batch size of 5000, but then decide after non conclusive results (see 5.3.2) that 2000 would be better - *2000*

- **`Alpha`**: learning rate, this hyper parameter was tuned in every optimizer therefore only the range will be indicated - *(1e-5,1)*

4.4 Input Shuffling

We used input shuffling as a technique to optimize the skip gram model. We will first describe input shuffling in a general way and then explain why we suppose that input shuffling could work well on the skip gram model.

Let $X = x_1...x_n$ be our input data set. Input Shuffling describes the process of taking a random permutation of the dataset as input at each epoch. The idea behind this technique is to present our optimizer with different loss surfaces so that it's able to find the best optimum. Therefore it's easier for the neural network to escape a local minimum. As for example if a network had converged to a local minimum after one epoch it could not escape it as all the parameters are the same. But if we change the shape of the loss function, by input shuffling, then there would be a greater probability for the network to escape the local minimum.

There are two reasons why we think that input shuffling is particularly well suited for the skip gram model. The first one has to do with the fact that when we read our words sequentially that words that only appear very early will not benefit from the context words being already updated from others. The second idea is that we used the special batch technique described in Section 3.2.1. When using this technique and not using shuffling we will always have words that appear next to each other in a batch and will, therefore, update the same words at the same time. We, therefore, lose some quality. But if instead, we would use input shuffling then in one batch the words would likely not be similar and therefore only taking the average of a small part of pairs with the same words will be less likely.

4.5 Convergence time

To optimize convergence time we have to define it first. Therefore we used the already available implementation Gensim [**gensim**]. Gensim is an open source software that proposes an implementation of the SGNS in python. It is also written in cython, therefore it has a fast computation time, but can be used inside a python implementation. Together with the knowledge from Ji et al.[**intel**] that a score of 0.66 in the task of word similarity, with the text8 dataset, is the state of the art, we tested Gensim (more on this process in Chapter 5 and found out that it took 4 epochs to converge. Therefore we defined the following criteria for convergence:

$\rho - \rho_{prev} < 0.009 \vee \rho = 0.66$

where ρ is the Pearson coefficient on the wordsim353 task. We also stopped computation, if it took more then 20 epochs to converge.

4.6 Results by optimizer

We ran multiple experiments for each optimizer. This section will only give an overview of the achieved results. Each section will give an explanation over the achieved result with a specific optimizer.

4.6.1 SGD

The first challenge for each optimizer was to find a correct learning rate. As SGD is the optimizer used in Gensim [**gensim**] we first tried the same learning rate as Gensim [**gensim**] and then performed a random search to find a better one. As expected a bell curve shape resulted, a learning rate that is too high leads to diversion and a learning rate that is too low leads to a training time that is too slow. The best value that we found for the learning rate is 0.0075. With this setting SGD converged in 11 epochs. The second experiment was to add input shuffling. As seen in figure 4.1, for almost every learning rate the convergence time decreased. Our model, with the best setting, know converges in only 7 epochs. Another interesting fact to point out from Figure 4.1 is that with input shuffling we achieved better results with higher learning rates. As for

learning rates of 0.01 and 0.025 we did converge in 11 epochs with input shuffling but did not converge in 20 epochs without it.
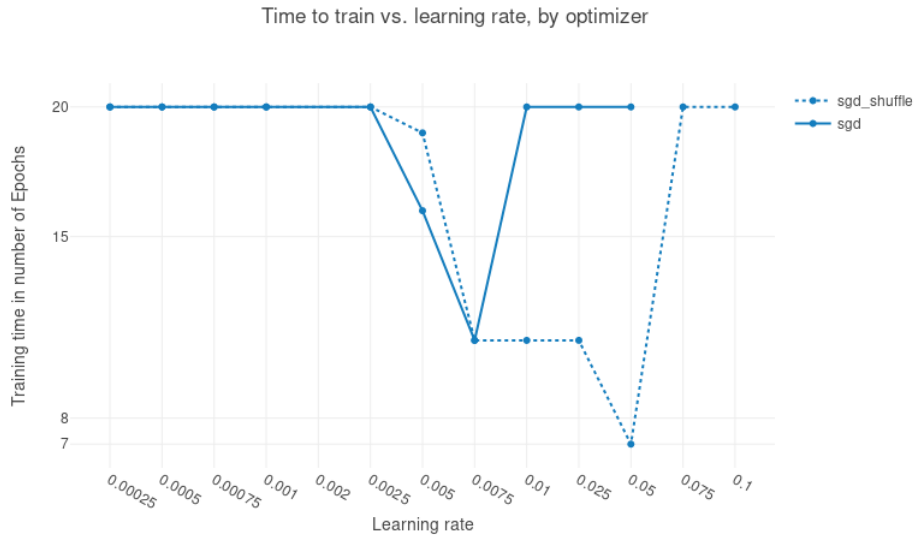

Figure 4.1: Training time Stochastic Gradient Descent with input Shuffling

4.6.2 Momentum and Nesterov

Momentum[**momentum**] and NAG [**nag**] both have an additional hyper parameter γ, that, as described in Section 2.4, defines the percentage of the previous gradient that will be added to the current gradients. We set $\gamma = 0.9$ as this is the typical value and did not alter it during our experiments. Momentum and Nesterov alone respectively only slightly decrease or increase the convergence time. As the first one optimally converges in 9 epochs and the second one in 13. If we combine these optimizers with input shuffling, interestingly the same phenomena as with plain SGD appear. The convergence time gets better, 8 epochs for Momentum and 3 epochs for NAG. The phenomena that a higher learning rat yields better results also happens with both of the optimizers. As Momentum does not converge in 20 epochs with a learning rate of 0.002 but does in 8 with input shuffling.
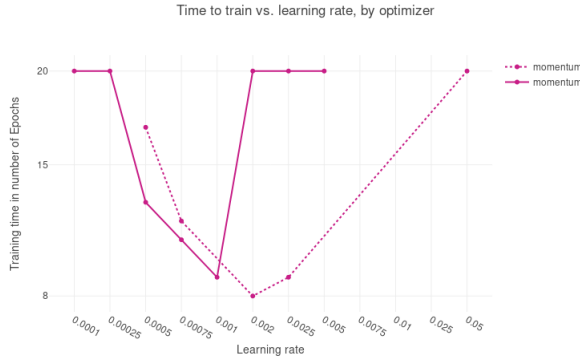
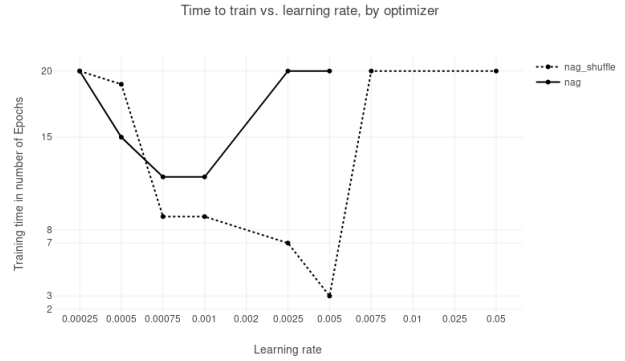Figure 4.2: Training time Momentum with input Shuffling

Figure 4.3: Training time Nesterov with input Shuffling

4.6.3 Adagrad

Adagrad [**adagrad**] is a very interesting tool for learning word embeddings as it decreases the learning rate for very frequent occurring features, and vice versa (this is explained in detail in Section 2.4.4). Because words that appear very frequently often do not have a semantic gain that is as important as words that appear less frequently to their context words, it's good to have a lower learning rate. So, in theory, Adagrad is particularly well suited for our task. This was confirmed empirically as our model converged in 4 epochs. When combined with shuffling adagrad only took 3 epochs to converge. This shows the tendency of the skip gram model to converge faster with input shuffling and the big impact of having different learning rate for each feature. Here it's interesting to notice that a higher learning rate combined with input shuffling did not yield better results than without shuffling. Both of our best results happened with a learning rate of 0.1, as can be seen in Figure 4.4.

4.6.4 Adadelta

In theory Adadelta [**adadelta**] should outperform Adagrad as it's an extension of the former. Because it didn't have any learning rate to tune, we only did 2 experiments, with and without input shuffling. We are aware of the fact that there are additional hyperparameters by did, for simplicity reason, and because their effect is not as high as the learning rate in other optimizers, decide no to tune it. We left it to it's default value $\rho = 0.9$. This parameter defines the percentage taken when calculating the exponentially
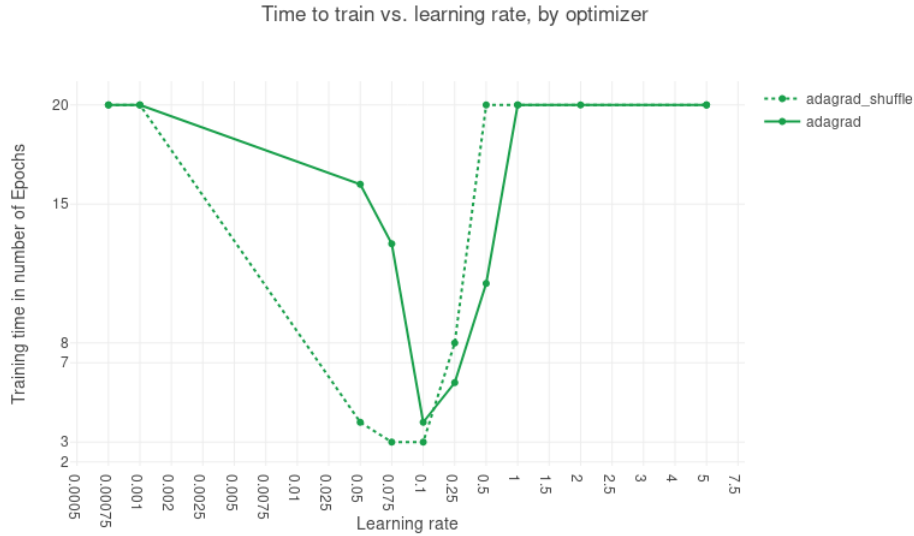
Figure 4.4: Training time Adagrad with input Shuffling

decaying average of past gradients, as explained in 2.4.5Adadelta did not manage to achieve a word similarity of 0.66. It only converged to a similarity of 0.59. It did this in 20 epochs without input shuffling and in 3 with input shuffling, as can be seen in Table 4.6

Adadelta Model	Convergence Time	Word similarity
Without Shuffling	20	0.59
With Shuffling	3	0.59

Table 4.6: Convergence Time and Quality with Adadelta

4.6.5 Adam

Adam is the most advanced of all the optimizers used in our experiments and did yield the best results as seen in Figure 4.5. Adam converged in 3 epochs without shuffling and 2 with. This is the best result that we got with any optimizer. It's also interesting to note that as same as with Adagrad it did not react to input shuffling the same way as SGD did. In fact, it worked in the opposite direction, as we achieved our best result with input shuffling while having a lower learning rate 0.001 then we used to achieve the best result without input shuffling 0.05.
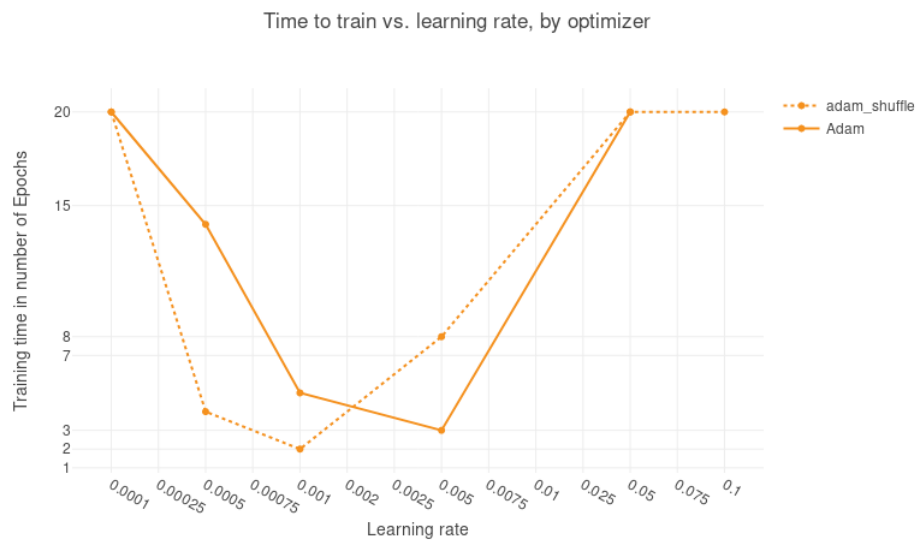
Figure 4.5: Training time Adam with input Shuffling

5 Discussion

In this section, we will shortly discuss our results then extensively compare our work to the existing literature while trying to explain some of the differences. It will follow a section describing the limitations and possible extensions of our work. Finally, we will conclude this chapter with a section that describes the problems we encountered made during the implementation such that they can be avoided by others in the future.

5.1 Our work

In this section, we will quickly discuss our findings, and try to give some explanation to it.

5.1.1 Shuffling and learning rate with SGD

As shown in figures 4.1, 4.2 and 4.3, the model, when using SGD as an optimizer, was able to use a higher learning rate when the input was shuffled as when not. Therefore arises the questions why those this phenomena happen. One possibility is that the model is presented with a slightly different loss function every time, which is closer to the optimal loss function, therefore the steps taken by the optimizer are closer to the optimum and can, therefore, be bigger. Another explanation to why this did not happen to advanced optimizers is that we used a batched version of SGNS. Theretofore when not shuffled the optimizer often has the average value for some words, so that the gradient will be a rough estimation of the true gradient, and can, therefore, be imprecise. This is counter-attacked by advanced optimizers as they have adaptive learning rates.

Large differences with NAG and SGD when using shuffling

As shown in figures 4.1 and 4.3, plain SGD, and Nesterov Accelerated gradient, greatly differ in their convergence time when using shuffling into comparison when not. We attribute these results partially to a good random initialization guess and not only input shuffling. Due to a lack of time these results where not replicate more than once.

5.2 Related Work

In this section, we will compare our work to related work. We will first compare us to the baseline model, the original C implementation from Mikolov et al [**Mikolov**]. As they did not use the same datasets as we, this will hinder the quality of the comparison. We, therefore, compare ourself extensively to Gensim [**gensim**]. Gensim is optimized to have a very high throughput which allowed us to, achieve a lot of computations. Furthermore, Gensim gave us access to the loss and the resulting word embeddings, which facilitated the comparison process.

5.2.1 word2vec

As Mikolov et al. published the original paper which introduced the SGNS, it is, of course, relevant to compare ourselves to their work. The first important thing to take under account is that Mikolov et al. only trained their model on a very large google news dataset incorporating more than 3 billion words. This makes the comparison of our work more difficult. But we will make some assumptions, as they could be of value if true. In their original paper, Mikolov et al. reported results from computations that took 1 and 3 epochs. We accord these good results, which clearly outperformed our SGD model and Gensim, to the very large dataset and furthermore, as a matter of fact, their results are better with 3 than with 1 epoch. We do not have any information about the convergence time or criterion. Hence it would be interesting to use their dataset for comparison.

One thing we can compare is the quality of our word embeddings. Mikolov et al. did not report any results on their model with the text8 dataset, but they, therefore, published their code. Which was then used by Ji et al [**intel**] and they tested the model on the

text8 dataset. They reported a similarity of 0.63 on the wordsim task. This is obviously outperformed by all our models. We did not find any explanation on why those results differ as much.

The final assumption is that an advanced optimizer could maybe outperform SGD in terms of quality on a large data set. This will be discussed in further work.

5.2.2 Gensim

The training with Gensim has a lot of possible parameters an extended list can be found in the appendix. This section we will only describe the parameters we changed from the default setting. The description of each parameter will be done in the following way:
`name` (type) – *Description* – Value
Parameters:

- `sentences` (iterable of iterables) – *Dataset* – text8 document splitted into sentences of 20 words

- `size`(int) – *Dimensionality of the word vectors* – 100

- `window` (int) –*Maximum distance between the current and predicted word within a sentence* – 5

- `min_count` (int) – *Ignores all words with total frequency lower than this* – 5

- `workers` (int) – *Use these many worker threads to train the model (=faster training with multicore machines)* – 4

- `sg` (0, 1) – *Training algorithm: 1 for skip–gram*–1

- `negative` (int) –*Number of negative samples*– 10

- `ns_exponent` (float) – *Exponent in the unigram distribution, when choosing random samples, as shown in Equation 2.4* – 0.75

- `alpha` (float) – *The initial learning rate.* – 0.025

- `min_alpha` (float) – *Learning rate will linearly drop to min_alpha as training progresses.* –0.0001

- `sample` (float) – *Treshold for subsampling as described in Equation 4.1.* – 1e–4

- `iter` (int) – *Number of iterations (epochs) over the corpus.* – 10

- `compute_loss` (bool) –*If True, loss is stored at the end of each batch*– True

- `callbacks` (iterable of CallbackAny2Vec) – *Set of functions that will be executed at given training times, used in order to follow the loss and the progress of the model in word similarity* – see Appendix

Gensim vs. SGD

First, as stated earlier, we are not going to compare ourselves to Gensim in runtime. This does not make any sense as first of all our code is written in pytorch in comparison to Gensim which is implemented in cython[1], which is 23x faster then plain Numpy, we use pytorch that optimizes Matrix multiplication so the difference shouldn't be that big, but still makes a difference. Secondly, we did not use any other runtime optimization technique, as our main goal was to improve the convergence time.

There are a few interesting contradictions to note between Gensim and our own implementation of the SGNS. First of all the convergence time was not the same. There are different possibilities for why this could be the case. First, our batched approach could hinder performance in term of convergence as our loss function is not exactly the same. When a word appears more than once in our batch, the gradient will be an average over the gradients of each pair alone, as it is done by Gensim. Another difference between our implementation is the fact that Gensim checks whether negative samples are not equal to the context word. And if that is the case selects a new random sample. Therefore the learning of the input and output context is optimized. Yet another possibility is the decay of the learning rate used by Gensim. In fact, decaying the learning rate has been proven in a lot of work to decrease the convergence time. Gensim linearly decreases the learning rate, as we did not use this technique, the decay of the learning rate could help explain the noted differences. The first hypothesis may be confirmed by the fact that when combined with input shuffling SGD does perform closer to Gensim, going from 11 to 7 epochs to converge, as input shuffling reduces the number of co-occurences of the same word in a batch. Know the question arises if the 3 epochs, that Gensim is better, can be explained by the selection of better negative samples and the learning rate decay?

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[1]https://rare-technologies.com/word2vec-in-python-part-two-optimizing/

Gensim vs. Adam

The Adam optimizer did outperform the Gensim application in performance (only slightly: 0.01 correlation coefficient better) and convergence time. Adam converged in 2 epochs while Gensim in 4. To be sure of our results we ran each computation 40 times. The results can be seen in Figure 5.1.
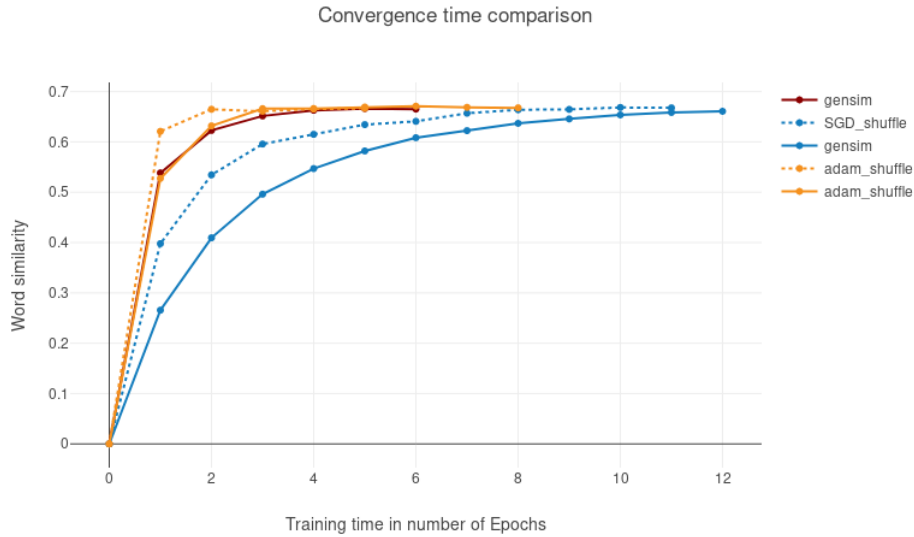

Figure 5.1: Training time Stochastic Gradient Descent with input Shuffling

5.3 Challenges faced

During our implementation we did encounter some problems, this section has the purpose of informing the scientific community to not make the same mistakes.

5.3.1 Using the wrong embeddings

To start with, we did not choose the same initialization value as Gensim in our word embeddings. We initialized the input layer with normal distribution between (-1,1), as opposed to Gensim which initializes all the weights to 0. We did this because as we first started, we did indeed do the same thing as Gensim, and initialized the projection layer with 0. But then our model did not seem to train well. Retrospectively we accord this

to a learning rate that was too low. But back then we did not have the clarity of mind to see it, and instead changed the input layer initialization. After a few simulations, we saw that we did not perform as good as Gensim. And as we changed the initialization of the projection layer back to 0, as we already had adjusted the learning rate, we achieved good results. Therefore this is a recommendation to future work to not set the initialization to (-1,1).

5.3.2 Batch size and loss function adjustements

During our experiments, we faced a moment where we needed to us a very high learning rate (50) to achieve good results. As this is the complete opposite of what is standard, we got suspicious. To remedy the problem we made a few changes. First, we needed to find a good batch size. During the above-explained raise of the learning rate, we used a batch size of 5000. We then decided to take a batch size of 2000.

Secondly, at the same time, we did experiment with different loss functions. As our batched model does not have exactly the same loss function as introduced by Mikolov et al. [**mikolov**], we needed to find one that suited our goals the best. At the beginning of our experiment, we took the average of all the scores stored in our final matrix, as explained in 3.2.1. But then chose to take the sum as the training did not seem optimal. With these two changes, we did increase convergence time and word similarity, while at the same time having a usual learning rate.

Know the question arises why this happened? Is this because the shape of the loss function better suits our advanced optimizers? Or because the loss function is closer to its original form? Our hypothesis looks the following way: When taking the average, our loss function is represented as follows:

$$\frac{-1}{b} * \sum_{x \in X} loss(x) \tag{5.1}$$

where X is our batch and $b = |X|$. When taking the partial derivative of each parameter, the constant $\frac{-1}{b}$ will remain the same. Therefore it's the same as taking the sum as the loss function and multiplying each gradient with $\frac{-1}{b}$. As our batch size was really high, i.e 2000 and 5000, this could highly influence the learning rate. This is also the conclusion of Goyal et al. [**fb**], that worked with very high batch sizes, i.e 8000: "When the minibatch size is multiplied by k, multiply the learning rate by k". We, therefore, did a small

experiment to confirm this assumption. The results can be found in Table test. This shows empirically that this could be the main reason for the high learning rate.

5.4 Future Work

This work showed that the convergence time of the SGNS could be improved with the use of input shuffling and advanced optimizers. As with every work, there still exists possible extensions. First and foremost an aspect of our implementation that can be prejudicial is that we only extensively tested our model with one small dataset. Both of these aspects can be seen as problematic. By using a very small dataset we do not use the model in the condition it is most needed for, as the dataset used in practice usually consists of more then 1 billion words. There is a small argument that can be made for machine translation as the use of small parallel corpus is not unusual in this field. But the main issue with using only one data set it that it has been shown that some optimizers perform better with specific shapes of loss functions. To make a compelling argument it's, therefore, necessary to show that our Model with the use of Input shuffling and Adam as it's optimizer also outperform Gensim with other data sets. We did show that this seems to be the case as Adam outperformed Gensim on the enwik9 dataset as well. But first, this experiment needs to be replicated a high number of times, i.e at least 40, so that the claim can hold consistently, and confirmed with other datasets as well. Furthermore, our implementation did not outperform Gensim in runtime, as this was not the goal of our work. Therefore one could improve an already existing, optimized version, with input shuffling and advanced optimizers and should achieve a better runtime than Gensim.

6 Conclusion

This work provides an overview of the Skip Gram Model with negative Sampling (SGNS) and the numerous successful attemps of optimizing the throughput of the model. As this is the case, no effort went into optimizng the convergence time of the SGNS, therefore this work focused on this point. We decided to use advanced optimizers and input shuffling as optimizing techniques. After giving a short overview over Gradient Descent algorithms this work proposes a slighlty altered version of the SGNS. Where the idea is to compute the loss over the sum of a lot of training samples instead of computing it for each invidiually. This allowed us a faster runtime. We did this as it allowed us to compute more models and analyze the convergence time faster. We used the text8 dataset for most of our models. And used the word similarity as a quality measure for the word embeddings (WE). We used the State of the art implementation Gensim to compare ourself. We did achieve a better convergence time then gensim with Adam as an optimizer and the use of input shuffling. Gensim convereged in 4 epochs to a word similairty of 0.66 and our model only took 2 epochs to achieve the same quality. We did confirm these findings with one test run on the enwik9 dataset. As gensim took 5 epochs to converge and our model only 3. Those results still need to be confirmed with more datasets. Finally if this work would combined with an optimized throughput could improve the state of the art runtime of the SGNS.

A Code

A.1 Gensim

```python
from gensim.models.callbacks import CallbackAny2Vec
from gensim.models import Word2Vec
vocab = set(text8_ds1)
gensim_emb = dict()


class EpochLogger(CallbackAny2Vec):
    def __init__(self):
        self.epoch = 0
        self.cum_loss = 0
        self.loss_list = []
        self.ws_list = []
        self.prev_score = -1
        self.no_improvement = 0


    def on_epoch_end(self, model):
        for word in vocab:
            gensim_emb[word] = model.wv[word]

        score = -1*wordsim_task(gensim_emb)[0][1]
        self.ws_list.append(score)

        if(score - self.prev_score < 0.0009):
```

```
        self.no_improvement +=1

    print("Epoch #{} end: cum_loss={}, ws_score={}".format(self.epoch,

    if(self.no_improvement == 2):
        print("No improvement in word similarity early stoppage")


    self.epoch += 1
    self.prev_score = score

def on_batch_end(self, model):
    """Method called at the end of each batch.
    Parameters
    _____

    model : :class:'~gensim.models.base_any2vec.BaseWordEmbeddingsModel
        Current model.
    """
    self.cum_loss += model.get_latest_training_loss()
```

B Math

C Parameters

D Dataset

- `hashfxn` (function) – *Hash function to use to randomly initialize weights, for increased training reproducibility.* – VERIFY

- `hs` (0, 1) – *If 1, hierarchical softmax will be used for model training. If 0, and negative is non–zero, negative sampling will be used.* – 0

- `corpus_file` (str, optional) – None

- `cbow_mean` (0, 1, optional) - Unnecessary since cbow is not used

- seed (int, optional) – Seed for the random number generator. Initial vectors for each word are seeded with a hash of the concatenation of word + str(seed). Note that for a fully deterministically-reproducible run, you must also limit the model to a single worker thread (workers=1), to eliminate ordering jitter from OS thread scheduling. (In Python 3, reproducibility between interpreter launches also requires use of the PYTHONHASHSEED environment variable to control hash randomization). - None

- `max_vocab_size` (int, optional) – Limits the RAM during vocabulary building; if there are more unique words than this, then prune the infrequent ones. Every 10 million word types need about 1GB of RAM. Set to None for no limit. - None

- `max_final_vocab` (int, optional) – Limits the vocab to a target vocab size by automatically picking a matching min_count. If the specified min_count is more than the calculated min_count, the specified min_count will be used. Set to None if not required. - None item `trim_rule` (function, optional) –Vocabulary trimming rule, specifies whether certain words should remain in the vocabulary, be trimmed away, or handled using the default (discard if word count ¡ min_count). Can be None (min_count will be used, look to keep_vocab_item()), or a callable that accepts parameters (word, count, min_count) and returns either gensim.utils.RULE_DISCARD,

gensim.utils.RULE_KEEP or gensim.utils.RULE_DEFAULT. The rule, if given, is only used to prune vocabulary during build_vocab() and is not stored as part of the model.

The input parameters are of the following types: word (str) - the word we are examining count (int) - the word's frequency count in the corpus min_count (int) - the minimum count threshold. - None

- `sorted_vocab` (0, 1, optional) – If 1, sort the vocabulary by descending frequency before assigning word indexes. See sort_vocab(). - None

- `batch_words` (int, optional) – Target size (in words) for batches of examples passed to worker threads (and thus cython routines).(Larger batches will be passed if individual texts are longer than 10000 words, but the standard cython code truncates to that maximum.) - None

Let's examine an example: $(w_1, c_1)(w_2, c_2)(w_3, c_3)$ be our batch. Therefore $pos_u =$

$$\begin{bmatrix} w_1 & w_2 & w_3 \end{bmatrix}, pos_v = \begin{bmatrix} c1 \\ c2 \\ c3 \end{bmatrix} \text{ and } neg_v = \begin{bmatrix} k_{1,1} & k_{2,1} & k_{3,1} \\ k_{1,2} & k_{2,2} & k_{3,2} \\ k_{1,3} & k_{2,3} & k_{3,3} \end{bmatrix}$$

We then concatenate pos_v and neg_v, while negating neg_v resulting in:

$$samples = \begin{bmatrix} c_1 & -k_{1,1} & -k_{2,1} & -k_{3,1} \\ c_2 & -k_{1,2} & -k_{2,2} & -k_{3,2} \\ c_3 & -k_{1,3} & -k_{2,3} & -k_{3,3} \end{bmatrix}$$

We then multiply pos_u and *samples* resulting in:

$$scores = \begin{bmatrix} w_1 \cdot c_1 & -w_1 \cdot k_{1,1} & -w_1 \cdot k_{2,1} & -w_1 \cdot k_{3,1} \\ w_2 \cdot c_2 & -w_2 \cdot k_{1,2} & -w_2 \cdot k_{2,2} & k_{3,2} \\ w_3 \cdot c_3 & -w_3 \cdot c_3 k_{1,3} & -w_3 \cdot c_3 k_{2,3} & k_{3,3} \end{bmatrix}$$ Finnally we sum up the score

and multiply it with minus one to make it a minimizing problem:

$$-\left(\sum_{i=1}^{3} w_i \cdot c_i - \sum_{j=0}^{3} -w_i \cdot -k_i, j\right)$$