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DEEP LEARNING

Word2vec with PyTorch: Implementing the Original Paper

Covering all the implementation details, skipping highly technical parts. Includes code attached.

Olga Chernytska

Sep 29, 2021 • 16 min read

Thoughts and Theory

ultimately	helped	allowing attempting	required allowed allows	continues pursue achieves	ability desire
visit	went attempted failed forced	willing tried	decided agreed promised	hoped	made needs
them	managed tries forcing	invited asked	chose chosen	leave	give lose learn
sign	returns decides wants	wanted tried	stay perform sing	call accept	carry suppose
escape	struggle save kill try break	go	meet	find prove	
moves	finally shoot freedom	getting bringing come	put get	sold	speak understand fit
cool	tennessee ready	talking let	talk tell	going	believe do happen
looked	looking look	mind ?	hear	things want know say wrong really think	actually
	dog	feel like love me sweet	you i we llve t	got doesnt wasn	
		boy my			

Image by Author

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Word Embeddings is the most fundamental concept in Deep Natural Language Processing. And Word2vec is one of the earliest algorithms used to train word embeddings.

In this post, I want to go deeper into the first paper on word2vec – Efficient Estimation of Word Representations in Vector Space (2013), which as of now has 24k citations, and this number is still growing.

Our plan is the following:

- Review model architectures described in the paper
- Train word2vec model from scratch using PyTorch
- And evaluate the word embeddings that we get

I am attaching my Github project with word2vec implementation through it in this post.

Today we are reviewing only the **first** paper on word embeddings. There are several later papers, describing the evolution of the field.

- Distributed Representations of Words and Phrases and their Compositionality (2013) describes several extensions to the original word2vec to speed up training and improve the quality.
- Distributed Representations of Sentences and Documents (2014) shows how to use the idea behind word2vec to generate sentence and document embeddings. This approach is called Doc2Vec.
- Enriching Word Vectors with Subword Information (2016) introduces even more extensions to word2vec. It no longer operates on the character level (not words and phrases), but known as fastText.

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I believe, if you understand the first paper, you'll easily catch the ideas described in later papers. So let's go!

Disclosure. Word2vec is already an old algorithm and there are more recent options (for instance, [BERT] ([https://en.wikipedia.org/wiki/BERT\(language model\)](https://en.wikipedia.org/wiki/BERT(language model)))). This post is for those, who have just started their journey into Deep NLP, or for those, who are interested in reading and implementing papers.

Contents

- What is word2vec?
- Model Architecture
- Data
- Data Preparation
- Text Processing with PyTorch
- Training Details
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What is word2vec?

Here is my 3-sentence explanation:

1. Word2vec is an approach to create word embeddings.
2. Word embedding is a representation of a word as a vector.

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3. Except for word2vec there exist other methods to create word embeddings, such as fastText, GloVe, ELMO, BERT, GPT-2, etc.

If you are not familiar with the concept of word embeddings, below are the links to several great resources. Read through skipping the details but grasping the intuition behind it. And come back to my post for the word2vec details and coding.

- [Why do we use word embeddings in NLP](#) by Lynn
- [The Illustrated Word2vec](#) by Jay Alammar
- [An introduction to word embeddings for text](#) by Lynn

Better now?

Word embeddings are used literally in every NLP task: classification, named-entity recognition, question answering, summarization, etc. Everywhere. Models do not understand words and letters, they understand numbers. That's where word embeddings come in handy.

Model Architecture

Word2vec is based on the idea that a word's meaning depends on its context. Context is represented as surrounding words.

Think about it. Assume, you are learning a new language by reading a sentence and all the words there are familiar except one. You've never seen this word before, how would you tell its part of speech, right? And sometimes, even its meaning. That's because the information from surrounding words helps you.

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For the word2vec model, context is represented as N words before and N words after the current word. N is a hyperparameter. With larger N we can create better embeddings, but at the same time, such a model requires more computational resources. In the original paper, N is 4–5, and in my visualizations below, N is 2.

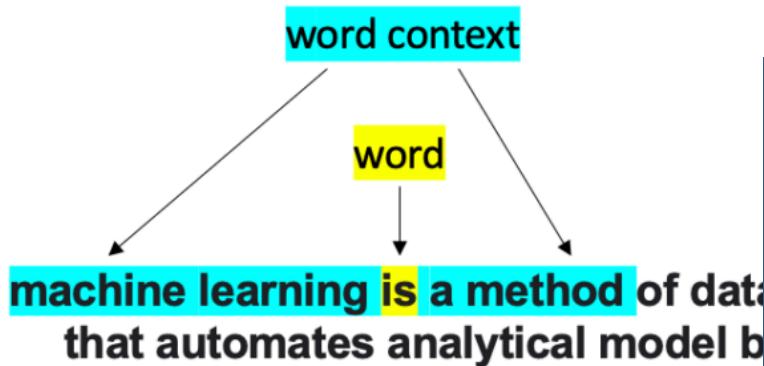


Image 1. A word and its context. Image by Author

There are two word2vec architectures proposed:

- **CBOW** (Continuous Bag-of-Words) – a model that predicts the current word based on its context words.
- **Skip-Gram** – a model that predicts context words based on the current word.

For instance, the CBOW model takes "machine", "method" as inputs and returns "is" as an output. The Skip-Gram model does the opposite.

Both CBOW and Skip-Gram models are multi-class classification models by definition. Detailed visualizations below will make this clear.

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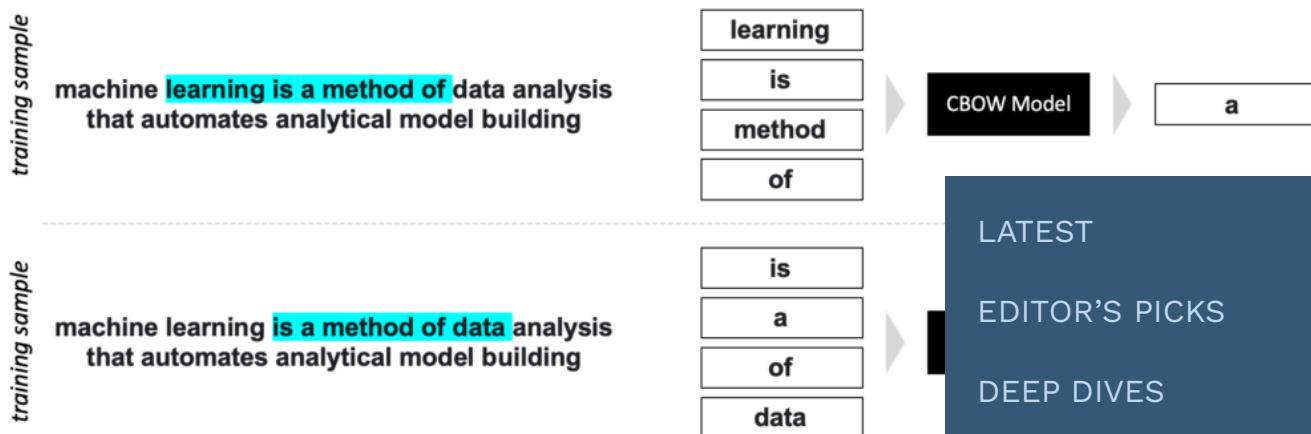
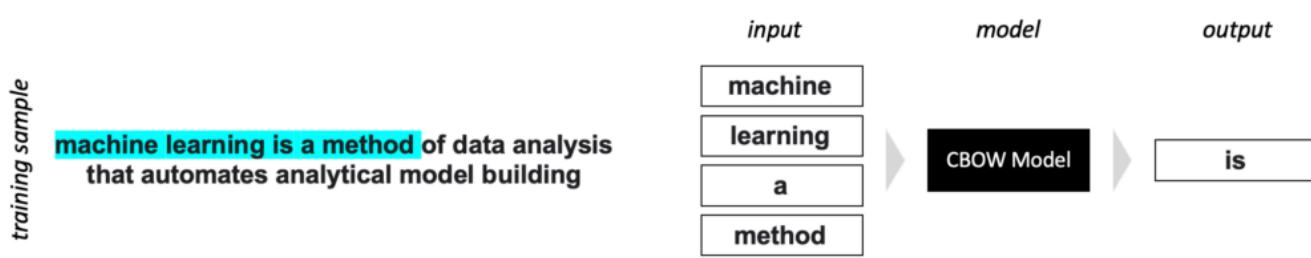


Image 2. CBOW Model: High-level Overview. Image by

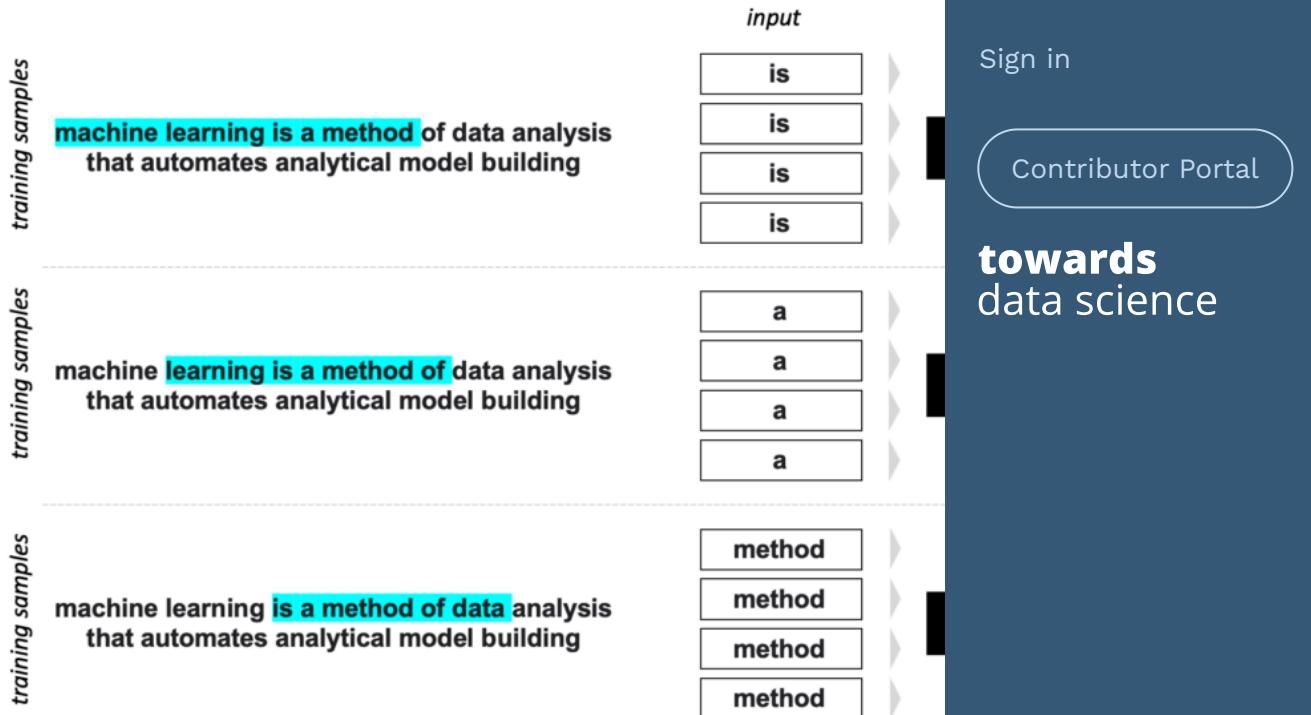


Image 3. Skip-Gram Model: High-level Overview. Image

What is happening in the black box?

The initial step would be to encode all words with an integer (index) that identifies word position in the "Vocabulary" is a term to describe a set of unique

This set may be all words in the text or just the most frequent ones. More on that in Section "Data Preparation".

Word2vec model is very simple and has only two layers:

- **Embedding layer**, which takes word ID and returns its 300-dimensional vector. Word2vec embeddings are 300-dimensional, as authors proved this number to be the best in terms of embedding quality and computational costs. It can be implemented about embedding layer as a simple lookup table with pre-trained weights, or as a linear layer without bias and learnable weights.
- Then comes the **Linear (Dense) layer** with a single output neuron. We create a model for a multi-class classification problem, so the number of classes is equal to the number of words in our vocabulary.

The difference between CBOW and Skip-Gram models is the number of input words. CBOW model takes several words as input and processes them through the same Embedding layer, and then word vectors are averaged before going into the Linear layer. Skip-Gram model takes a single word instead. Detailed comparison of both models is provided in the images below.

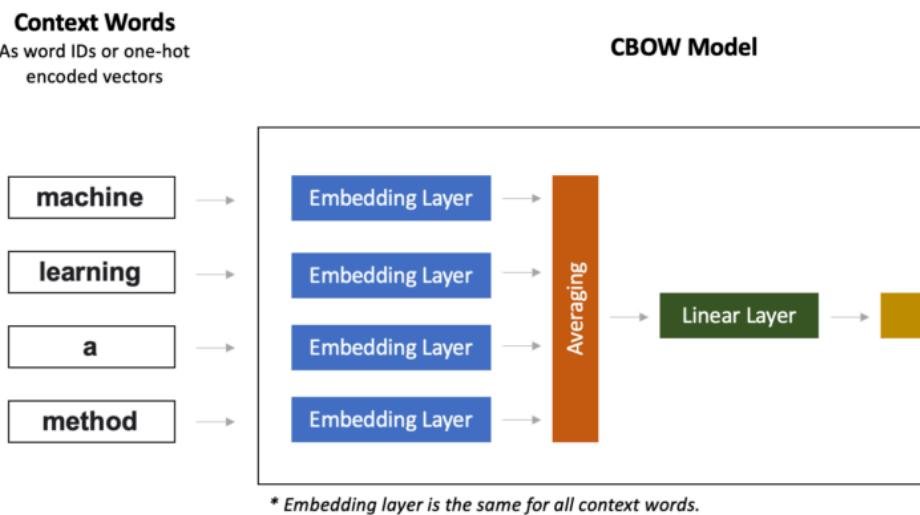


Image 4. CBOW Model: Architecture in Details. Image by [Sudhanshu](#).

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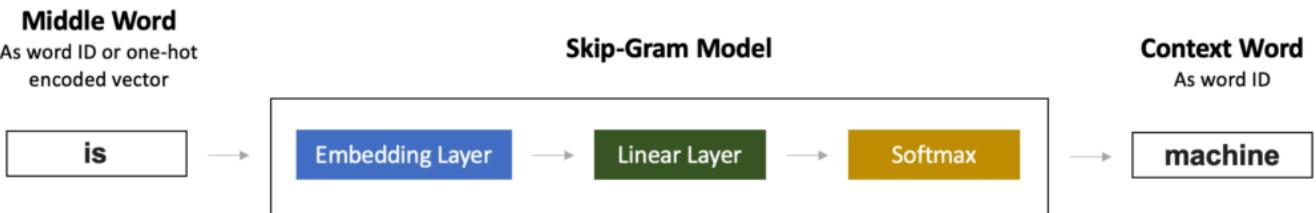


Image 5. Skip-Gram Model: Architecture in Details. Image by Author

Where are the word embeddings?

We train the models that are not going to be used for prediction. Instead, we want to predict a word from its context or content. Instead, we want to get word vectors. It turns out that these vectors are weights of the Embedding layer. More details can be found in the Section "Retrieving Embeddings".

Data

Word2vec is an unsupervised algorithm, so we need a large unlabeled corpus. Originally, word2vec was trained on Google News Corpus, which contains 6B tokens.

I've experimented with smaller datasets available online:

- [WikiText-2](#): 36k text lines and 2M tokens in total (100k words + punctuation)
- [WikiText103](#): 1.8M lines and 100M tokens in total

When training word embedding for the commercial application, you should choose the dataset carefully. For instance, if you're building a recommendation system for Machine Learning papers, train word2vec on scientific papers rather than news from Machine Learning. If you'd like to classify fashion items, a dataset of fashion news would be a better fit. That's because in the original paper, "model" means "approach" and "algorithm" in the machine learning domain, but "person" and "woman" in the fashion domain.

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When reusing trained word embeddings, pay attention to the dataset they were trained on and whether this dataset is appropriate for your task.

Data Preparation

The main step in data preparation is to create a **vocabulary**. The vocabulary contains the words for which embeddings will be created. Vocabulary may be the list of all the unique words in the text corpus, but usually, it is not.

It is better to create vocabulary:

- Either by filtering out rare words, that occur less than N times in the corpus;
- Or by choosing the top N most frequent words.

Such filtering makes much sense because, with a large vocabulary, the model is faster to train. On the other hand, we probably do not want to use embedding for words that appear only once within the text corpus, as these embeddings are probably not good enough. To create good word embeddings the words need to see a word several times and in different contexts.

Each word in the vocabulary has its unique index. The order of the vocabulary may be sorted alphabetically or based on word frequencies, or may not – it should not affect the quality of the embeddings. Vocabulary is usually represented as a dictionary.

```
vocab = {
    "a": 1,
    "analysis": 2,
    "analytical": 3,
```

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```

    "automates": 4,
    "building": 5,
    "data": 6,
    ...
}

```

Punctuation marks and other special symbols may be also added to the vocabulary, and we train embeddings for them as well. You may lowercase all the words, or train separate embeddings for `apple` and `Apple`; in some cases, it may be useful to do both.

Depending on what you want your vocabulary (and its corresponding embeddings) to be like – preprocess the text correctly. Lowercase or not, remove punctuation or not, and so on.

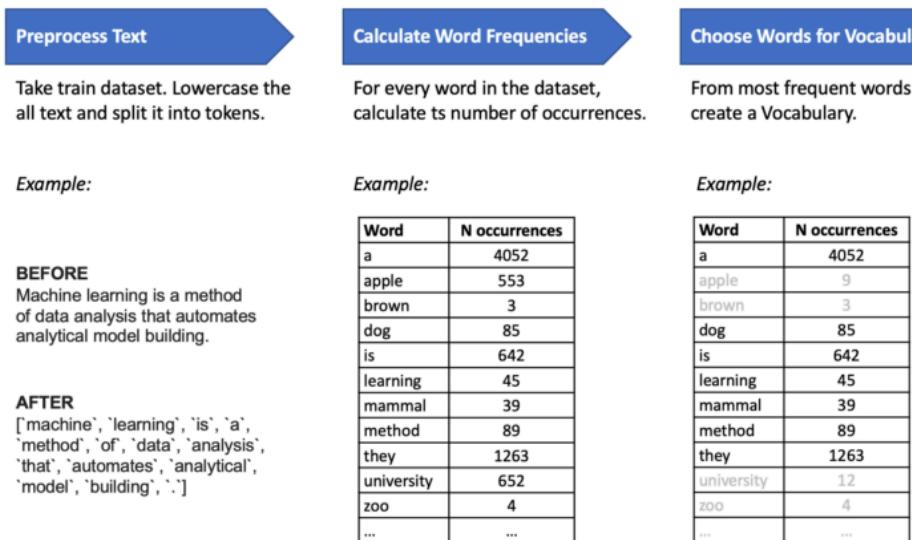


Image 6. How to create Vocabulary from a text corpus. Image by [Sergey Kiselev](#).

For my model:

- I created vocabulary only from the words that appear at least 50 times within a text.
- I used `basic_english` tokenizer from PyTorch to tokenize the text, splits it into tokens by whitespace, but also converts punctuation into separate tokens.

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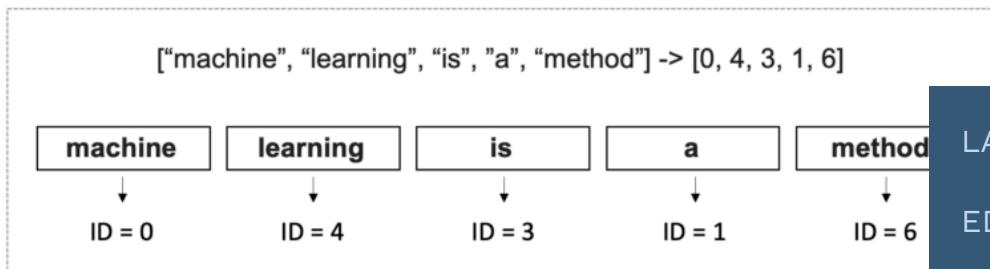
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So, before words go into the model, they are encoded as IDs. The ID corresponds to the word index in the vocabulary. Words that are not in the vocabulary (out-of-vocabulary words) are encoded with some number, for instance, 0.

How to Encode Words



Vocabulary

Word	ID
<unk>	0
a	1

Image 7. How to Encode words with Vocabulary IDs. Image by [Towards Data Science](#).

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Text Processing with PyTorch

The full code for [training word2vec is here](#). Let's look at the important steps.

Models are created in PyTorch by subclassing from `nn.Module`. As described previously, both CBOW and Skip-Gram models consist of two layers: Embedding and Linear.

Below is the model class for CBOW, and [here is the one for Skip-Gram](#).

```
import torch.nn as nn
EMBED_DIMENSION = 300
EMBED_MAX_NORM = 1

class CBOW_Model(nn.Module):
    def __init__(self, vocab_size: int):
        super(CBOW_Model, self).__init__()
        self.embeddings = nn.Embedding(
            num_embeddings=vocab_size,
```

```

        embedding_dim=EMBED_DIMENSION,
        max_norm=EMBED_MAX_NORM,
    )
    self.linear = nn.Linear(
        in_features=EMBED_DIMENSION,
        out_features=vocab_size,
    )
def forward(self, inputs_):
    x = self.embeddings(inputs_)
    x = x.mean(axis=1)
    x = self.linear(x)
    return x

```

Pay attention, there is no Softmax activation in the forward pass. That's because PyTorch CrossEntropyLoss expects raw, unnormalized scores. While in Keras you can pass probabilities to the input to CrossEntropyLoss would be – raw values or unnormalized scores.

Model input is word ID(s). Model output is an N-dimensional vector where N is vocabulary size.

EMBED_MAX_NORM is the parameter to restrict embedding vector norms (to be 1, in our case). It works as a regularization term and prevents weights in Embedding Layer grow uncontrollably. EMBED_MAX_NORM is worth experimenting with. For example, when restricting embedding vector norm, similar words like "king" and "father" have higher cosine similarity, compared to EMBED_MAX_NORM=None.

We create **vocabulary** from the dataset iterator using helper function build_vocab_from_iterator. WikiText-2 and Penn Treebank datasets have rare words replaced with token , which is

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a special symbol with ID=0 and all out-of-vocabulary words also encode with ID=0.

```
from torchtext.vocab import build_vocab_from_iterator MIN_WORD_FREQUENCY

def build_vocab(data_iter, tokenizer):
    vocab = build_vocab_from_iterator(
        map(tokenizer, data_iter),
        specials=["<unk>"],
        min_freq=MIN_WORD_FREQUENCY,
    )
    vocab.set_default_index(vocab["<unk>"])
    return vocab
```

Dataloader we create with collate_fn. This function defines the logic of how to batch individual samples. When loading the PyTorch WikiText-2 and WikiText103 datasets, each sample is a text paragraph.

For instance, in collate_fn for CBOW we "say":

1. Take each text paragraph.

- Lowercase it, tokenize it, and encode it using the text_pipeline.
- If the paragraph is too short – skip it. If it's too long – cut it.
- With the moving window of size 9 (4 history words, 1 target word, and 4 future words) loop through the paragraph.
- All middle words merge into a list – they will be Ys.
- All contexts (history and future words) merge into lists – they will be Xs.

2. Merge Xs from all paragraphs together – they will be the input to the model.

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3. Merge Ys from all paragraphs together – they will be batch Ys.

Pay attention, the number of final batches (Xs and Ys) when we call `collate_fn` will be different from parameter `batch_size` specified in `Dataloader`, and will vary for different paragraphs.

Code for `collate_fn` for CBOW is below, for [Skip-Gram](#) – is here.

```
import torch
CBOW_N_WORDS = 4
MAX_SEQUENCE_LENGTH = 256

def collate_cbow(batch, text_pipeline):
    batch_input, batch_output = [], []
    for text in batch:
        text_tokens_ids = text_pipeline(text)

        if len(text_tokens_ids) < CBOW_N_WORDS * 2:
            continue

        if MAX_SEQUENCE_LENGTH:
            text_tokens_ids = text_tokens_ids[:MAX_SEQUENCE_LENGTH]

        for idx in range(len(text_tokens_ids) - 1):
            token_id_sequence = text_tokens_ids[idx:idx + 2]
            output = token_id_sequence.pop(CBOW_N_WORDS)
            input_ = token_id_sequence
            batch_input.append(input_)
            batch_output.append(output)

    batch_input = torch.tensor(batch_input, dtype=torch.long)
    batch_output = torch.tensor(batch_output, dtype=torch.long)
    return batch_input, batch_output
```

And here is how to used `collate_fn` with PyTorch



```
from torch.utils.data  
import DataLoader  
from functools import partial  
  
dataloader = DataLoader(  
    data_iter,  
    batch_size=batch_size,  
    shuffle=True,  
    collate_fn=partial(collate_cbow, text_p  
)
```

I've also created a class Trainer, that is used for validation. It contains a typical PyTorch train and eval loop. For those who have experience with PyTorch, it will be straightforward.

If you want to understand the code better – I recommend my repository and play with it.

Training Details

Word2vec is trained as a multi-class classification problem using the Cross-Entropy loss.

You choose batch size to fit into the memory. Just like the paper, batch size is the number of dataset paragraphs, which are processed into input-output pairs, and this number can be much larger.

The paper optimizer is AdaGrad, but I've used a much more popular Adam.

I've skipped the paper part with Hierarchical Softmax and used plain Softmax. No Huffman tree was used either.

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vocabulary. Hierarchical Softmax and Huffman tree – are tricks for speeding up the training. But PyTorch has a lot of optimization under the hood, so training is already fast enough.

As recommended in the paper, I've started with a learning rate of 0.025 and decreased it linearly every epoch until it reaches 0 at the end of the last epoch. Here [PyTorch LambdaLR scheduler](#) helps a lot; and [here is how I used it](#).

The authors trained the model for only 3 epochs in their experiments (but on a very large dataset). I've experimented with number smaller and larger and decided to stick with 3.

For WikiText-2 dataset:

- My vocabulary size was about 4k words (the words that occurred in the text at least 50 times).
- Training took less than 20 minutes on GPU for Skip-Gram models.

For WikiText103 dataset:

- My vocabulary size was about 50k words.
- The model trained overnight.

Retrieving Embeddings

The full procedure is described in [this notebook](#).

Word embeddings are stored in the Embedding layer. The layer size is (vocab_size, 300), which means there is an embedding for all the words in the vocabulary.

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When trained on the WikiText-2 dataset both CBOW and Skip-Gram models have weights in the Embedding layer of size (4099, 300), where each row is a word vector. Here is how to get Embedding layer weights:

```
embeddings = list(model.parameters())[0]
```

And here is how to get words in the same order as in the embedding matrix:

```
vocab.get_itos()
```

Before using embedding in your model, it's worth checking if they were trained properly. There are several options:

1. Cluster word embeddings and check if related words lie in separate clusters.
2. Visualize word embedding with t-SNE and check if similar words lie close to each other.
3. Find the most similar words for a random word and check if they form a cluster.

Visualization with t-SN

You may use [sklearn t-SNE](#) and [plotly](#) to create a visualization like the one below. Here numeric strings and they form 2 separate clusters.



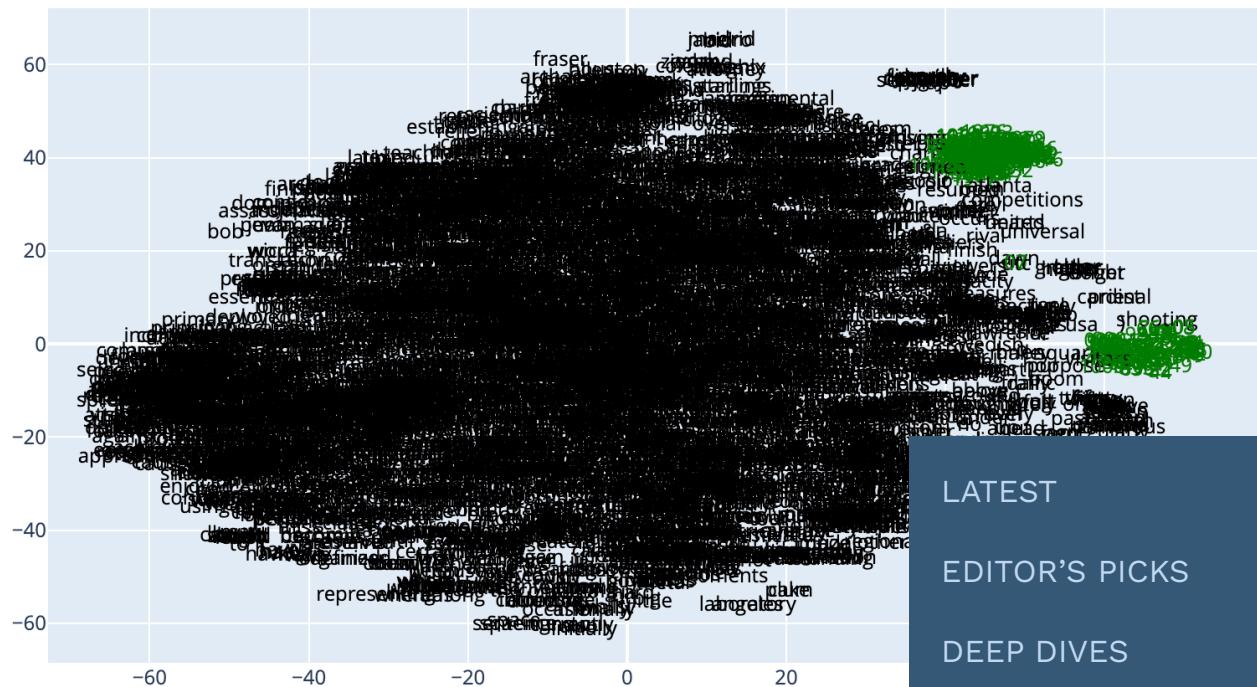


Image 8. Visualization of CBOW embeddings trained on WikiText-2 corpus. 2-clustered words plotted in green.

After zooming in, we may see that this division of words into 2 clusters makes much sense. The top left cluster is from years, while the lower right – from plain numbers.

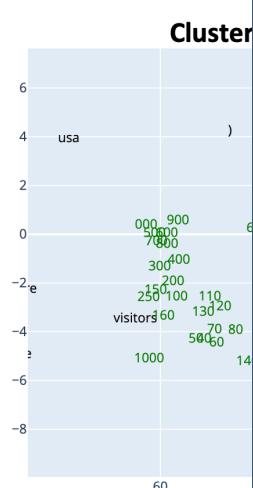
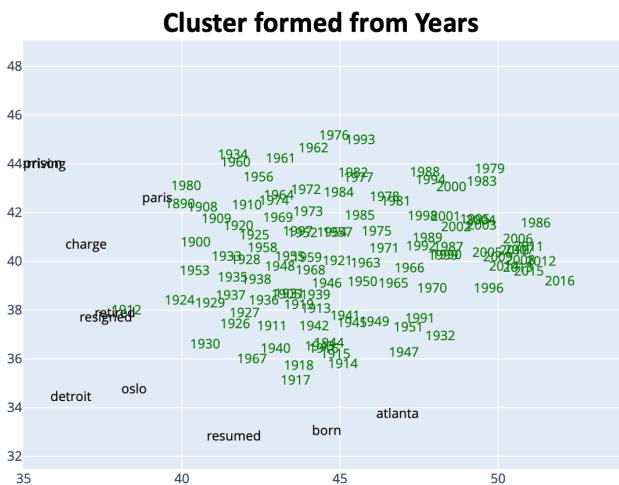


Image 9. Numeric clusters when zoomed in. The top left cluster is formed from years, while the bottom right – from plain numbers.

You may explore [this plotly visualization](#) to find even more interesting relations. And the code for creating [this visualization is here.](#)

Similar Words

Word similarity is calculated as [cosine similarity](#) between word vectors. The higher the cosine similarity, the more similar words are assumed to be, obviously.

For instance, for the word "father" here are the most similar words in the vocabulary:

#CBOW model trained on WikiText-2

mother: 0.842

wife: 0.809

friend: 0.796

brother: 0.775

daughter: 0.773

#Skip-Gram model trained on WikiText-2

mother: 0.626

brother: 0.600

son: 0.579

wife: 0.563

daughter: 0.542

Code for [finding similar words is here.](#)

King – Man + Woman = Queen

According to the paper, a properly trained word2vec model can solve equations "king – man + woman = ?" (answer: "queen").

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big + small = ?" (answer: "smaller"), or "Paris – France + Germany = ?" (answer: "Berlin").

Equations are solved by performing mathematical operations on the word vectors: $\text{vector("king")} - \text{vector("man")} + \text{vector("woman")}$. And the final vector should be the closest to the vector("queen") .

Unfortunately, I could not reproduce that part. My CBOW and Skip-Gram models trained on WikiText-2 and WikiText-103 did not catch this kind of relation ([code here](#)).

The closest vectors to $\text{vector("king")} - \text{vector("man")} + \text{vector("woman")}$ are:

```
#CBOW model trained on WikiText-2 dataset
```

```
king: 0.757
```

```
bishop: 0.536
```

```
lord: 0.529
```

```
reign: 0.519
```

```
pope: 0.501
```

```
#Skip-Gram model trained on WikiText-2 dataset
```

```
king: 0.690
```

```
reign: 0.469
```

```
son: 0.453
```

```
woman: 0.436
```

```
daughter: 0.435
```

```
#CBOW model trained on WikiText103 dataset
```

```
king: 0.652
```

```
woman: 0.494
```

```
queen: 0.354
```

```
daughter: 0.342
```

```
couple: 0.330
```

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The closest vectors to $\text{vector}(\text{"bigger"}) - \text{vector}(\text{"big"}) + \text{vector}(\text{"small"})$ are:

```
#CBOW model trained on WikiText-2 dataset
```

```
small: 0.588
```

```
<unk>: 0.546
```

```
smaller: 0.396
```

```
architecture: 0.395
```

```
fields: 0.385
```

```
#Skip-Gram model trained on WikiText-2 dataset
```

```
small: 0.638
```

```
<unk>: 0.384
```

```
wood: 0.373
```

```
large: 0.342
```

```
chemical: 0.339
```

```
#CBOW model trained on WikiText103 dataset
```

```
bigger: 0.606
```

```
small: 0.526
```

```
smaller: 0.273
```

```
simple: 0.258
```

```
large: 0.258
```

Sometimes, correct words are within the top5, but not top1. I assume there are two possible reasons for this:

1. Some error within a code. To double-check I implemented the equations from scratch and compared them with [Gensim library](#) and on the same dataset (WikiText103). Gensim word embeddings are also trained on these equations.
2. So more probable reason is that the datasets are different. WikiText-2 contains 2M tokens and WikiText103 contains 10M tokens.

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while the Google News corpus used in the paper contains 6B tokens, which is 60 (!!!) times larger.

Dataset size really matters while training word embedding. And authors also mentioned that in the paper.

What's Next?

I hope this post helps you to build a foundation so you can move on to more advanced algorithms. For now, it's interesting to dig deep into the original paper and implement it from scratch. Recommended.

Originally published at <https://notrocketscience.buzz> on April 29, 2021. If you'd like to read more tutorials like this, check out my blog "Not Rocket Science" – [Telegram](#) and [Twitter](#).

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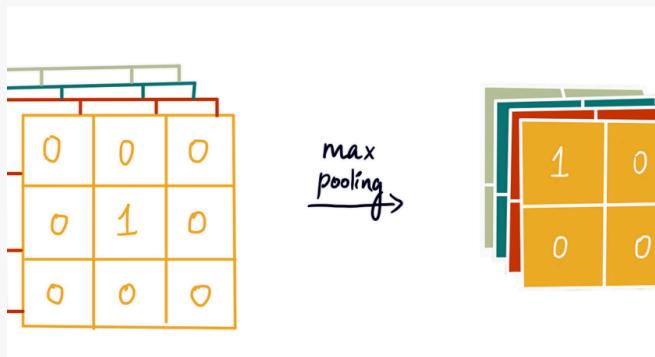
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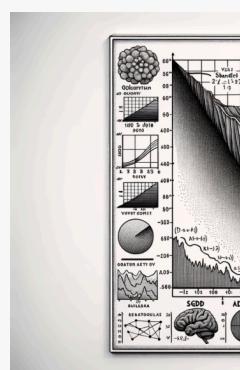
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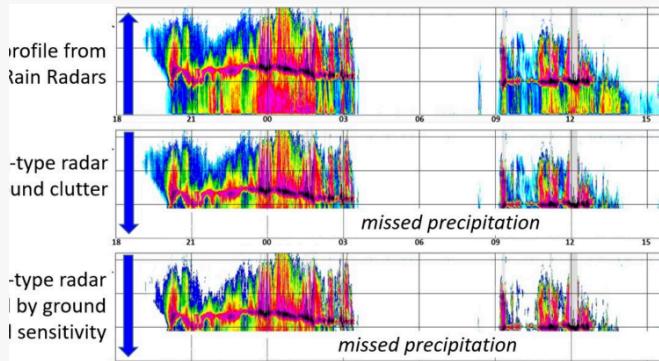
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