Cosine Similarity for 1 Trillion Pairs of Vectors

Introducing ChunkDot

Rodrigo Agundez · Following

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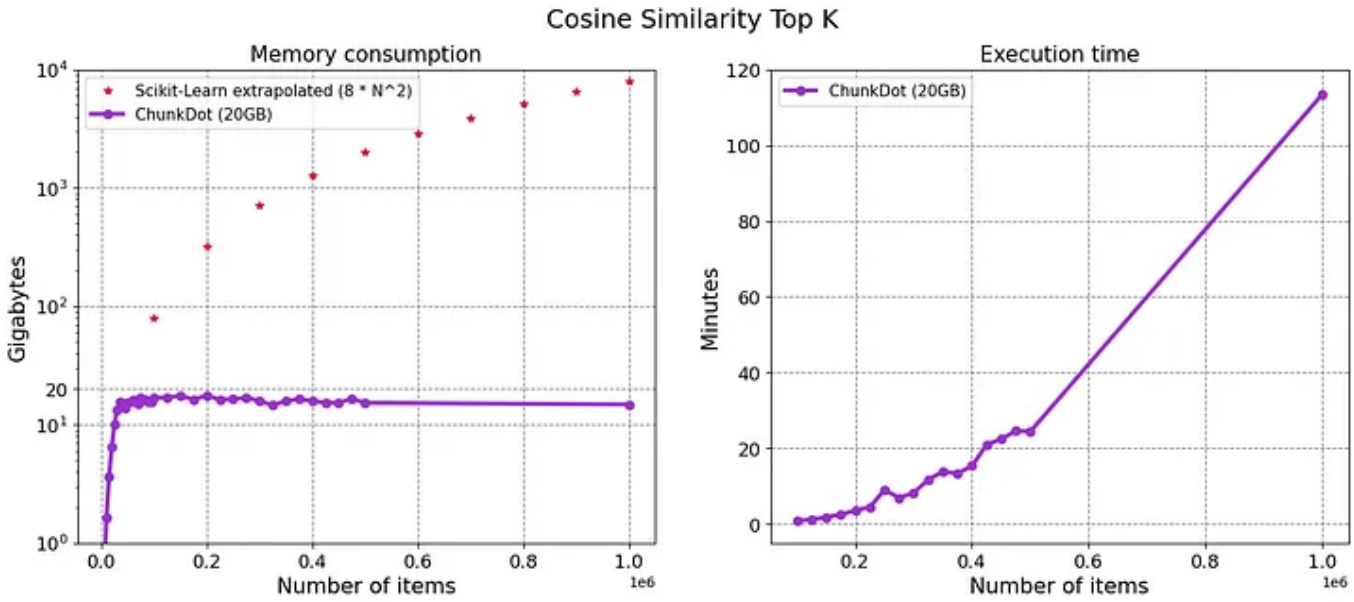
Photo by Tamas Pap on Unsplash

> **UPDATE**
> ChunkDot now supports sparse embeddings, you can read more about it here.

Success! I managed to find vector representations for my 1 million items... I just need to calculate the cosine similarity between all pairs to find the 20 most similar items per item. Then, *from sklearn.metrics.pairwise import cosine_similarity,* throw my 1 million vectorized items into it, and bam! My computer explodes with a *MemoryError* or the kernel of my *Jupyter* notebook dies. The issue, I just tried to hold 1 Trillion (10^{12}) values in memory (~**8000 GB**[1]). Good luck!

This blog post introduces *ChunkDot,* a Python package I built to solve this problem. *ChunkDot* can do this calculation in ~2 hours while keeping the memory consumption under 20 GB, as shown below.



top_k = 100 ; embedding_dim = 256 ; n_threads = 16

If you would like to skip the explanation and jump directly into the usage instructions:

chunkdot

Multi-threaded matrix multiplication and cosine similarity calculations. Appropriate for the calculation of the K most...

pypi.org

Motivation

The first time I encountered this problem was ~6 years ago while working for a client on an entity-matching use case. I was trying to match millions of records saved as free text to create golden records with the aggregated information from similar records[2]. Back then, *Spark* was a new and very shiny tool, so I solved it using *Spark*, with some broadcasting and some *C++* code wrapped in *Cython* wrapped in a *UDF*. I remember feeling that there might be a more elegant and simple way to solve this problem. I finally had time to look into it.

Since then, I have seen this issue pop up in one-to-many use cases. The idea of having items as vector representations and then trying to find the K most similar or dissimilar items per item appears in numerous use cases in Machine Learning. Some of these use cases are:

- Similar product recommendations.
- Name and Entity matching.
- Forecasting cold-start problem.
- Recommendation systems cold-start problem.
- User segmentation.

ChunkDot

The core of the problem is that the number of calculations scales with the square of the number of items. If we have N items, then the number of item pairs scales as N^2.
There is a silver lining, though, we only need the K most similar items per item. To determine which are the most similar K, we need to calculate all similarity pairs, but what if we do the calculation in batches (or chunks)? Keep the K most similar items for each batch, discard the rest, and then continue with the next batch until we have processed all items. This is the idea behind *ChunkDot*.

Let's go over an example, suppose I have 10^6 items, and I only require the top 100 most similar items per item. Then the number of similarity values I need is not 10^{12} but 10^6 x 100 = 10^8, a reduction of 99.99%.[3] This does not mean that the memory consumption will be reduced by 99.99%. It means the memory is no longer set by the output matrix but by the memory consumption of the algorithm itself.

Cosine Similarity Top K

Let's go over how *ChunkDot* works. Even though the core of the implementation is in `chunkdot._chunkdot`, I'll focus on the `chunkdot.cosine_similarity_top_k` function as shown below.

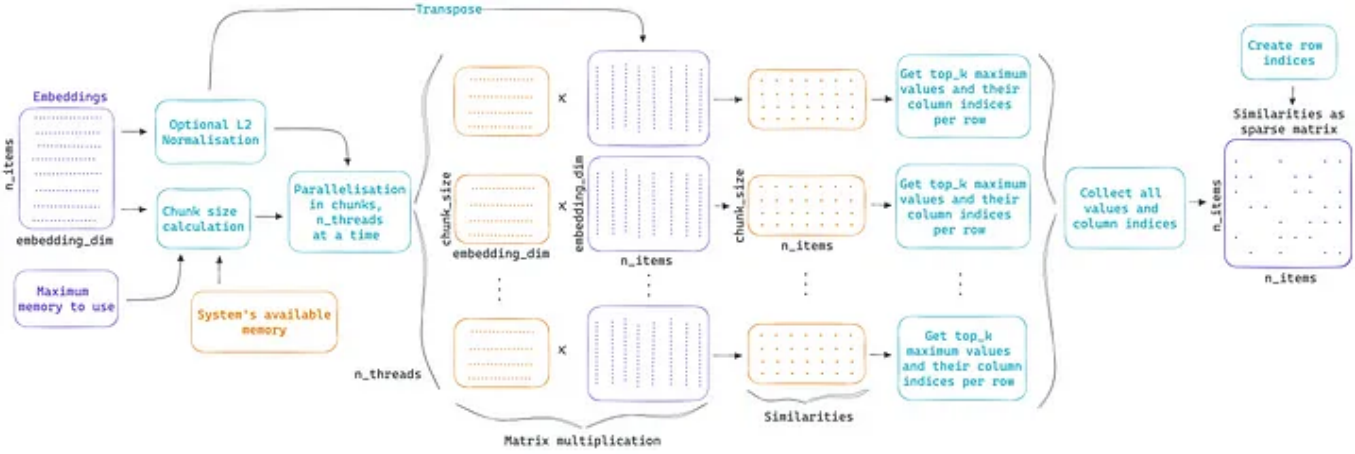
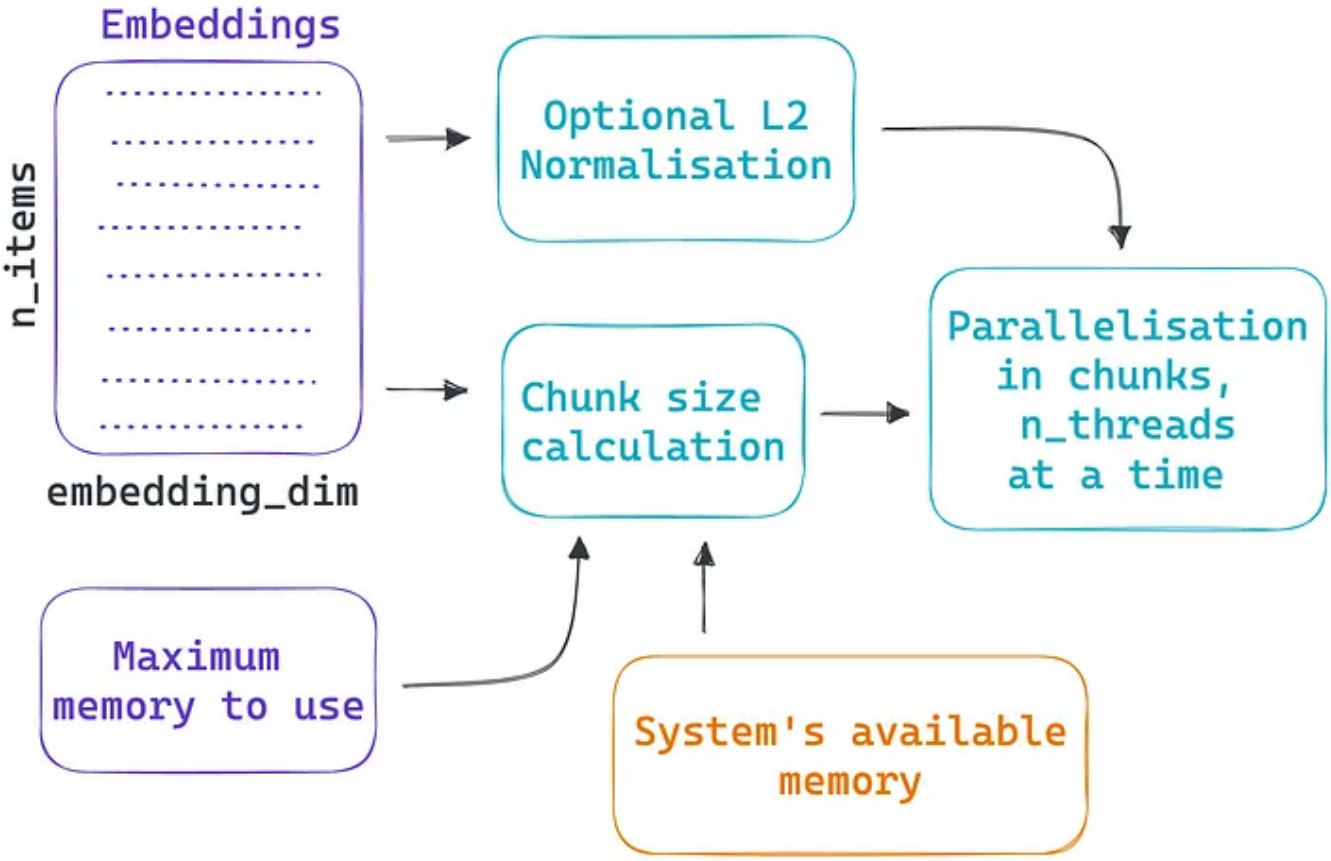


Diagram describing ChunkDot's Cosine Similarity Top K algorithm

The algorithm consists of 3 parts, splitting the embeddings matrix into the optimal number of chunks, performing the parallelized operations over the chunks, and collecting the data from each parallel thread to form the similarity matrix.

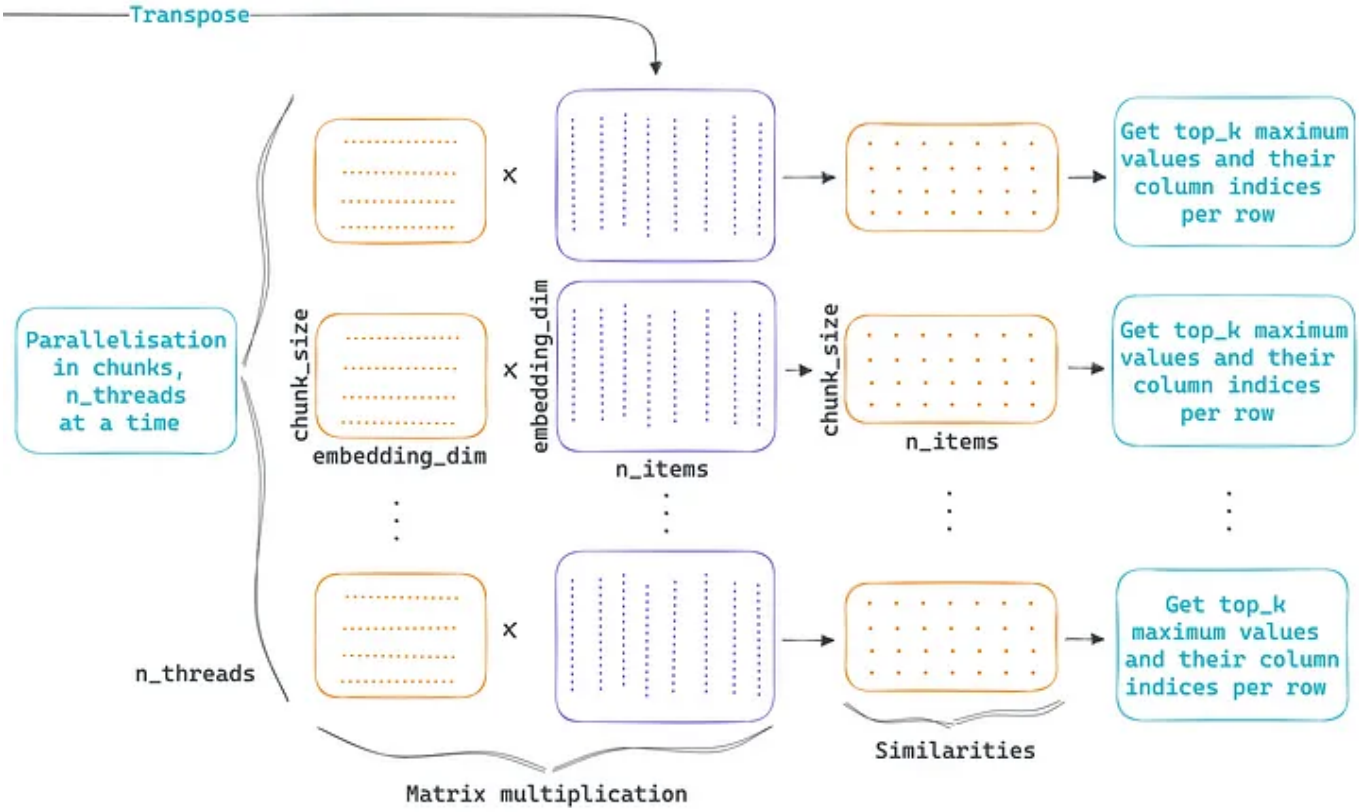
Splitting the input embeddings into chunks



First part of ChunkDot's Cosine Similarity Top K algorithm

The first part of the algorithm receives as input a matrix of embeddings where each row is the vector representation of an item. Then it calculates the optimal chunk size to use during the parallelization. The optimal chunk size is the maximum number of rows to process per thread without exceeding the given maximum memory to use. If no maximum memory to use is given, then the system's available memory is used. In parallel, an optional L2 normalization of the rows can be done. Finally, the normalized embeddings matrix gets split into pieces where each piece contains the number of rows equal to the chunk size. Now the data is ready to be parallelized.

Divide and conquer



Second part of ChunkDot's Cosine Similarity Top K algorithm

The second part of the algorithm performs all the parallel computations; each parallel thread calculates the cosine similarity between the chunk of items vs. all the items. As shown in the figure above, matrix multiplication is sufficient since rows are L2 normalized. Then, only the indices and values of the K most similar items are retrieved so that the density matrix is garbage collected to free up memory.

There is no free lunch; the price to pay for the parallelization and memory footprint reduction is that instead of having one big matrix multiplication, we have thousands of smaller ones plus the overhead of parallelization. This added complexity can raise the execution time to a non-usable level in practice. To manage the parallelization overhead efficiently and to perform these calculations as fast as possible *ChunkDot* uses *Numba*.

> “Numba generates optimized machine code from pure Python code using the LLVM compiler infrastructure. With a few simple annotations, array-oriented and math-heavy Python code can be just-in-time optimized to performance similar as C, C++ and Fortran, without having to switch languages or Python interpreters.”

To take the most out of *Numba,* the code to optimize needs to be supported in no-python mode. At the moment of this writing, the `numpy.argpartition` function is not supported, which is why there is a `numba_argpartition.py` file in *ChunkDo*t’s source code. I submitted this implementation to *Numba* via the PR below, which has been merged. The support should become native on *Numba’s* next release.

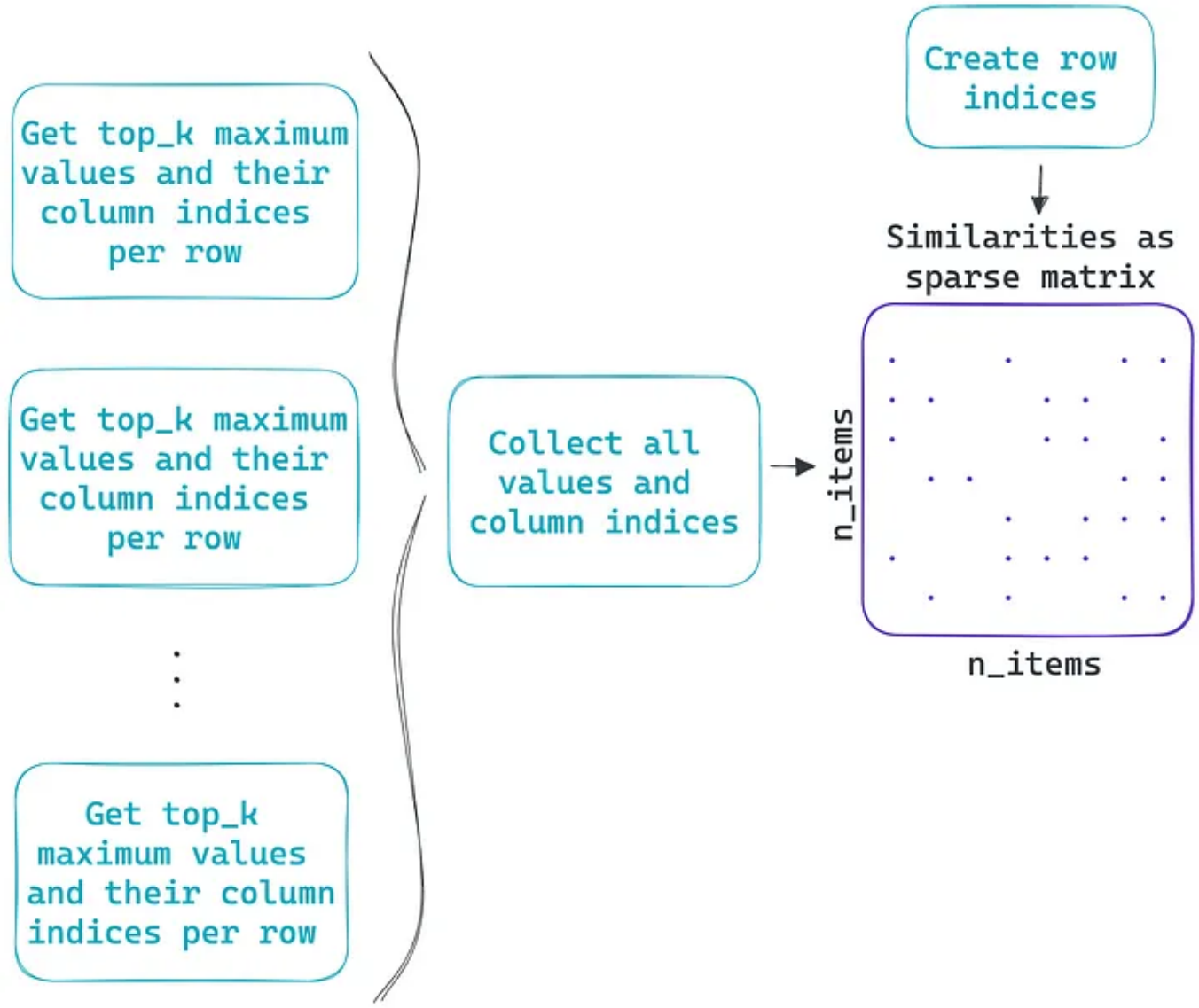
Add numpy argpartition function support by rragundez · Pull Request #8732 · numba/numba

Add numpy argpartition function support. I used some of the implementation of partition. Something to note it that I...

github.com

After the cosine similarity calculations and the retrieval of the K most similar items, we can collect all the values and indices to construct the final sparse similarity matrix.

Similarities as a CSR sparse matrix



Third part of ChunkDot's Cosine Similarity Top K algorithm

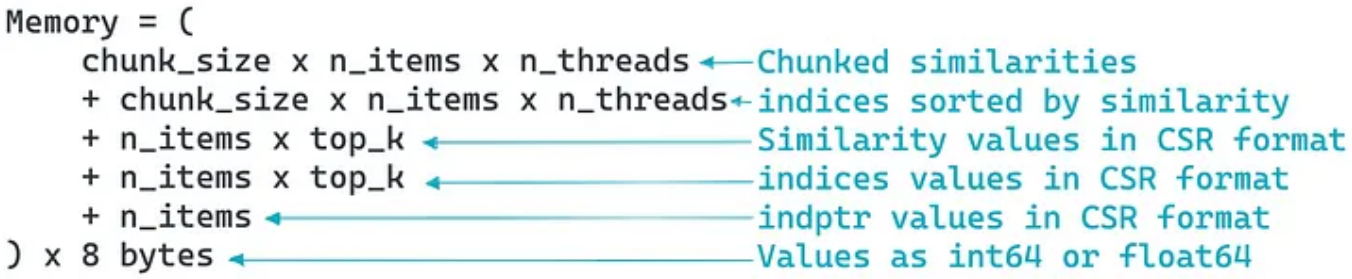
The third part of the algorithm consists of creating the sparse similarity matrix containing the K most similar items per item. This will be a sparse matrix of dimensions *n_items x n_items* containing only *n_items x top_k* non-zero values. The final output will the returned as a SciPy CSR sparse matrix.

Chunk size calculation

The idea behind calculating the biggest possible chunk size is that the bigger the chunk, the fewer threads are needed, therefore reducing the execution time of the algorithm.

To reduce memory utilization, all threads outputs are collected in arrays that

are passed by reference to each thread. *ChunkDot*'s algorithm memory consumption is then described by[4]:



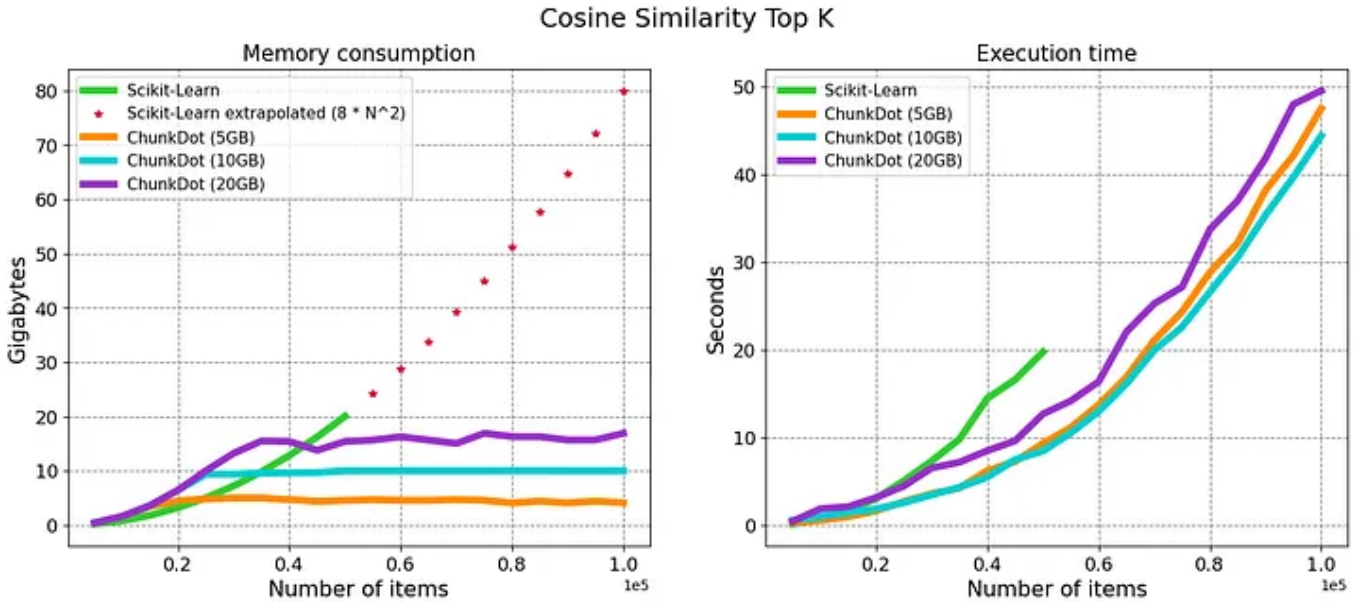
Where the number of threads is given by *Numba*'s `get_num_threads` function. The optimal chunk size is the solution for `chunk_size` in the equation above.

Memory and speed

I made a benchmark comparison with SciKit-Learn's cosine similarity on memory consumption and execution time.

> This is not entirely a fair comparison since the purpose of SciKit-Learn's cosine similarity function is to retrieve the similarities of all pairs of items and not just the K most similar. Having said that, I do not know of any other similar and simple approach that can be executed on a common laptop without a rigorous setup. I also think most of us will be looking first at the SciKit-Learn function to solve this problem. Therefore it seemed appropriate to benchmark against it.

The figure below shows the results. For the *SciKit-Learn* implementation, I did not go above 50K items as it was already taking ~20 GB of memory. I did include a projection of the expected memory consumption.

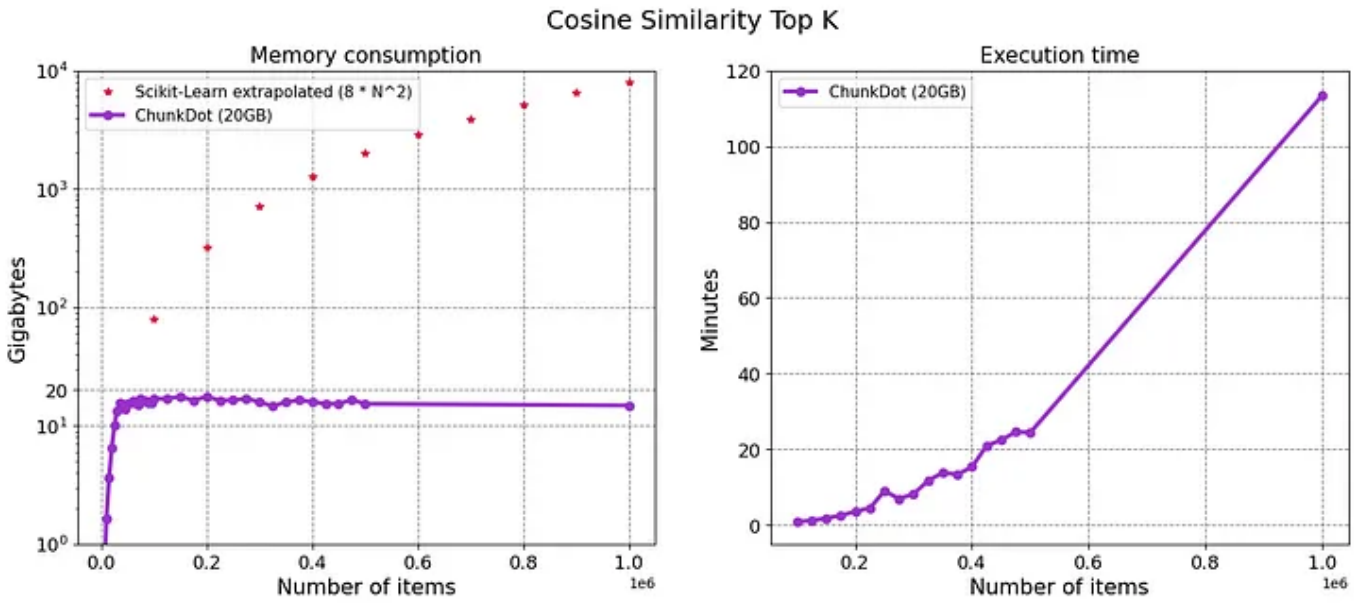


top_k = 100 ; embedding_dim = 256 ; n_threads = 16

The results show that the algorithm works, it can do the calculation for a large number of items while keeping the memory consumption capped. In the above-left figure, *SciKit-Learn*'s implementation is compared with *ChunkDot* using 3 different maximum memories: 5 GB, 10 GB, and 20 GB.

Nowadays is common to have 20 GB of RAM; you can easily compute 100K different items and retrieve their K most similar items in around 1min. Quite unexpectedly, the *ChunkDot* algorithm is also faster, thanks, *Numba*! and it seems that the maximum memory to use does not matter that much for execution time… weird.
I did a thorough review of the results and methodology and reran them several times, but I wouldn't claim that *ChunkDot* is univocally faster. What I do know for certain is that I was able to do the calculation for 100K and 1 million items without a problem.

For 1 million items, which are 1 trillion comparisons, I only had to wait ~2 hours using 20 GB of memory, as shown in the figure below.



top_k = 100 ; embedding_dim = 256 ; n_threads = 16

Usage

```
pip install -U chunkdot
```

Calculate the 50 most similar and dissimilar items for 100K items.

```
import numpy as np
from chunkdot import cosine_similarity_top_k

embeddings = np.random.randn(100000, 256)
# using all you system's memory
cosine_similarity_top_k(embeddings, top_k=50)
# most dissimilar items using 20 GB
cosine_similarity_top_k(embeddings, top_k=-50, max_memory=20E9)
```

```
<100000x100000 sparse matrix of type '<class 'numpy.float64'>'
 with 5000000 stored elements in Compressed Sparse Row format>
```

Conclusion

I hope you find this blog post and *ChunkDot* useful! I enjoyed a lot working on this problem and getting satisfactory results. Some potential improvements:

- Add support for input embeddings as a sparse matrix. This might already be supported, but I just haven't thoroughly unit tested for this. I decided to return a `TypeError` exception to avoid silent errors. This will especially enable NLP use cases where the vectorization of items is done using n-grams, bag-of-words, or similar.

UPDATE. ChunkDot now supports sparse embeddings, you can read more about it here.

Bulk Similarity Calculations for Sparse Embeddings

ChunkDot support for sparse matrices

pub.towardsai.net

- The cosine similarity between item *i* and *j,* is equal to the similarity between *j* and *i. It is* enough to perform the calculations that render the upper-triangular matrix. This can be done via the Einstein summation function in *Numpy*, unfortunately, is not supported by *Numba* at the moment.

- Instead of returning the K most similar items, return items whose similarity is above/below a certain threshold.
- Add GPU support since *Numba* supports it.

Numba for CUDA GPUs — Numba 0.56.4+0.g288a38bbd.dirty-py3.7-linux-x86_64.egg documentation

Callback into the Python Interpreter from within JIT'ed code

numba.readthedocs.io

[1] These calculations are normally returned as *float64*. Not that it matters, though, with *float32* I would still need ~4000 GB of memory.

[2] The situation was a bit more complex, but this is the part related to this blog post.

[3] Here I have ignored the memory contribution from storing the indexes needed to assign each similarity value to an item pair. Their memory contribution, though, is irrelevant to this conclusion.

[4] Supposing that all threads could be holding the maximum amount of memory at the same time.

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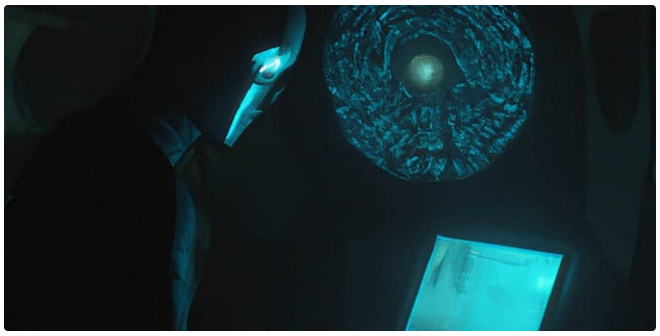

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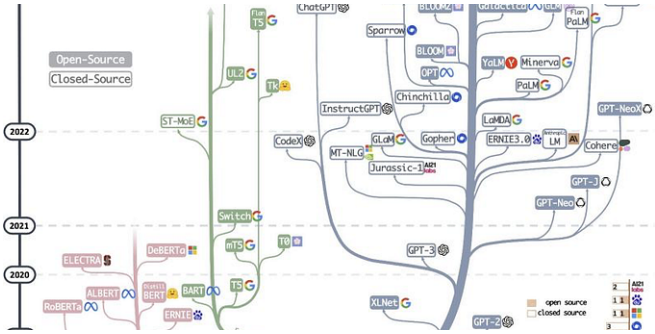

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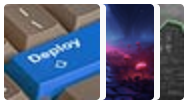

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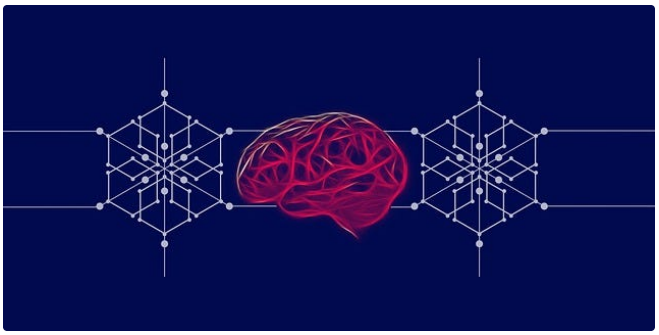

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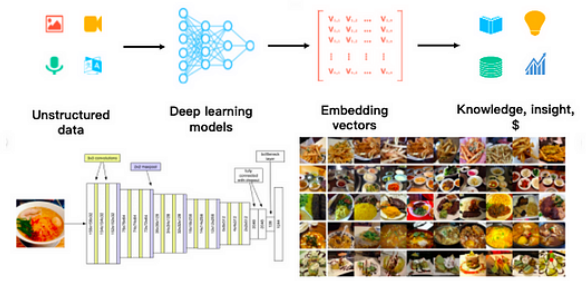

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