# CORD19 report

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COVID-19 Open Research Dataset Challenge (CORD-19)

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Machine Learning I (DATS 6202), Spring 2020

GitHub Repository

#### 0.0.1 Introduction

Last month, in response to the global COVID-19 pandemic, the White House and other leading research institutions, including the Allen Institute for AI, have prepared the COVID-19 Open Research Dataset (CORD-19): this dataset includes over 57,000 scholarly articles, most of them with full text, about COVID-19, SARS-CoV-2, and related coronaviruses. As literature published keeps increasing in scale, the medical community would need AI tools to quickly gain insights and directions to fight this disease in a timely manner.

Kaggle has issued a competition to develop such tools to help the medical community for this high priority scientific challenge. The public dataset represents a highly readable and clean collection of materials, and it is beeing updated constantly as more publications are released and added to the corpus.

Thanks to the minimal work on pre-processing required by this dataset, we decided to apply a Transformer model to extract sentence embeddings for machine learning task-specific "heads". Given that the pre-trained transformer by the UKPLab uses BERT, we decided to train and fine-tune the same transformer on SciBERT by Allen AI to obtain more relevant embeddings for a scientific and medical corpus.

We then used said embeddings to train different clustering algorithms for unsupervised learning: we used UAMP for dimensionality reduction, and HDBSCAN for density-based clustering while LDA for probability-based clustering. Also, we integrated a semantic search algorithm based on cosine similarity that can take user questions (we recommend to take ideas from Tasks) and provides the top 5 relevant articles from the corpus.

# 1 Data Preprocessing

Luckily the dataset had already been cleaned for the most part, and we only had to create an hashable corpus of text from json files. Once we had the body text and the abstact for each article, and its relevant metadata, in a dataframe, we cleaned the text columns of odd characters using regex. Here we call the preprocessing script to obtain a clean dataframe to use for our machine learning tasks.

```
[1]: import numpy as np
     import pandas as pd
     import os
     import glob
     import json
     # import scispacy
     import spacy
     import tqdm
     import matplotlib.pyplot as plt
     from scripts import preprocessing
```

```
# directories and paths
   root_path = os.getcwd()
   metadata_path = f'{root_path}/data/all_sources_metadata_2020-03-13.csv'
   metadata = pd.read_csv(metadata_path)
   metadata.head()
   metadata.info()
   # read all paths of json file(paper)
   all_json = glob.glob(f'{root_path}/data/**/*.json', recursive=True)
   print(len(all_json))
```

<class 'pandas.core.frame.DataFrame'> RangeIndex: 29500 entries, 0 to 29499 Data columns (total 14 columns):

13229

Dava	COTAMID (COURT II COTAMID).					
#	Column	Non-Null Count	Dtype			
0	sha	17420 non-null	object			
1	source_x	29500 non-null	object			
2	title	29130 non-null	object			
3	doi	26357 non-null	object			
4	pmcid	27337 non-null	object			
5	<pre>pubmed_id</pre>	16730 non-null	float64			
6	license	17692 non-null	object			
7	abstract	26553 non-null	object			
8	<pre>publish_time</pre>	18248 non-null	object			
9	authors	28554 non-null	object			
10	journal	17791 non-null	object			
11	Microsoft Academic Paper ID	1134 non-null	float64			
12	WHO #Covidence	1236 non-null	object			
13	has_full_text	17420 non-null	object			
dtypes: float64(2), object(12)						
memory usage: 3.2+ MB						

2

```
[3]: preprocessing.nan_checker(metadata)
[3]:
                                       proportion
                                                      dtype
                                  var
     0
         Microsoft Academic Paper ID
                                          0.961559
                                                    float64
     1
                       WHO #Covidence
                                          0.958102
                                                     object
     2
                            pubmed_id
                                          0.432881
                                                    float64
     3
                                          0.409492
                                                     object
                                  sha
     4
                       has_full_text
                                          0.409492
                                                     object
     5
                              license
                                         0.400271
                                                     object
     6
                              journal
                                         0.396915
                                                     object
     7
                         publish_time
                                         0.381424
                                                     object
     8
                                  doi
                                         0.106542
                                                     object
     9
                             abstract
                                         0.099898
                                                     object
     10
                                pmcid
                                         0.073322
                                                     object
     11
                              authors
                                         0.032068
                                                     object
     12
                                title
                                         0.012542
                                                     object
[4]: # drop the rows where abstract is missing
     metadata.dropna(subset = ['abstract'],axis = 0, inplace = True)
     #check dimension of new dataset
     print(metadata.shape)
    (26553, 14)
[4]:
                                               sha source_x \
     2 210a892deb1c61577f6fba58505fd65356ce6636
                                                        CZI
     3 e3b40cc8e0e137c416b4a2273a4dca94ae8178cc
                                                        CZI
     5 0df0d5270a9399cf4e23c0cdd877a80616a9725e
                                                        CZI
     6 f24242580be243d5fc3f432915d86af6854bb8b7
                                                        CZI
     8 e1b336d8be1a4c0ccc5a1bf41e48b3b004d3ece1
                                                        CZI
                                                      title \
     2 Incubation Period and Other Epidemiological Ch...
     3 Characteristics of and Public Health Responses...
     5 An updated estimation of the risk of transmiss...
     6 Real-time forecasts of the 2019-nCoV epidemic ...
     8 COVID-19 outbreak on the Diamond Princess crui...
                                            pubmed_id
                               doi pmcid
                                                           license
     2
               10.3390/jcm9020538
                                     NaN
                                                  NaN
                                                             cc-by
     3
               10.3390/jcm9020575
                                     NaN
                                           32093211.0
                                                              cc-by
       10.1016/j.idm.2020.02.001
                                     NaN
                                                       cc-by-nc-nd
                                                  {\tt NaN}
        10.1016/j.idm.2020.02.002
                                                       cc-by-nc-nd
     6
                                     NaN
                                                  NaN
              10.1093/jtm/taaa030
     8
                                     NaN
                                                  NaN
                                                          cc-by-nc
                                                   abstract publish_time
        The geographic spread of 2019 novel coronaviru...
                                                                   2020
```

```
5 The basic reproduction number of an infectious...
                                                                 2020
     6 The initial cluster of severe pneumonia cases ...
                                                                 2020
     8 Cruise ships carry a large number of people in...
                                                                 2020
                                                   authors \
    2 Linton, M. Natalie; Kobayashi, Tetsuro; Yang, ...
     3
                         Deng, Sheng-Qun; Peng, Hong-Juan
    5 Tang, Biao; Bragazzi, Nicola Luigi; Li, Qian; ...
     6 Roosa, K.; Lee, Y.; Luo, R.; Kirpich, A.; Roth...
                Rocklöv, J.; Sjödin, H.; Wilder-Smith, A.
     8
                             journal Microsoft Academic Paper ID WHO #Covidence \
      Journal of Clinical Medicine
                                                      3.006065e+09
                                                                             #1043
                          J Clin Med
     3
                                                      1.776631e+08
                                                                             #1999
     5 Infectious Disease Modelling
                                                      3.006029e+09
                                                                              #729
     6 Infectious Disease Modelling
                                                      3.006029e+09
                                                                              #865
          Journal of Travel Medicine
                                                      3.006304e+09
                                                                             #2926
       has_full_text
     2
                True
     3
                True
     5
                True
     6
                True
     8
                True
[5]: # remove dupicate with same title
     metadata.drop_duplicates(subset ="title", keep = False, inplace = True)
     #check dimension of new dataset
     print(metadata.shape)
     metadata.head()
    (20224, 14)
[5]:
                                               sha source_x \
     2
         210a892deb1c61577f6fba58505fd65356ce6636
                                                        CZI
     3
         e3b40cc8e0e137c416b4a2273a4dca94ae8178cc
                                                        CZI
                                                        CZI
     6
         f24242580be243d5fc3f432915d86af6854bb8b7
     8
         e1b336d8be1a4c0ccc5a1bf41e48b3b004d3ece1
                                                        CZI
     10 469ed0f00c09e2637351c9735c306f27acf3aace
                                                        CZI
                                                      title \
         Incubation Period and Other Epidemiological Ch...
         Characteristics of and Public Health Responses...
     3
        Real-time forecasts of the 2019-nCoV epidemic ...
     6
         COVID-19 outbreak on the Diamond Princess crui...
     10 First two months of the 2019 Coronavirus Disea...
```

2020

3 In December 2019, cases of unidentified pneumo...

```
pubmed_id
                                                              license \
                                 doi pmcid
     2
                 10.3390/jcm9020538
                                       NaN
                                                    NaN
                                                                cc-by
     3
                 10.3390/jcm9020575
                                       {\tt NaN}
                                             32093211.0
                                                                cc-by
     6
          10.1016/j.idm.2020.02.002
                                       NaN
                                                         cc-by-nc-nd
                                                    NaN
     8
                10.1093/jtm/taaa030
                                       NaN
                                                    NaN
                                                             cc-by-nc
     10
         10.1186/s41256-020-00137-4
                                       NaN
                                                    NaN
                                                                cc-by
                                                    abstract publish time \
     2
         The geographic spread of 2019 novel coronaviru...
                                                                    2020
         In December 2019, cases of unidentified pneumo...
                                                                    2020
     3
         The initial cluster of severe pneumonia cases ...
                                                                    2020
         Cruise ships carry a large number of people in...
                                                                    2020
     10 Similar to outbreaks of many other infectious ...
                                                                    2020
                                                     authors \
     2
         Linton, M. Natalie; Kobayashi, Tetsuro; Yang, ...
     3
                           Deng, Sheng-Qun; Peng, Hong-Juan
     6
         Roosa, K.; Lee, Y.; Luo, R.; Kirpich, A.; Roth...
     8
                 Rocklöv, J.; Sjödin, H.; Wilder-Smith, A.
     10
                                    Chen, Xinguang; Yu, Bin
                                    journal Microsoft Academic Paper ID
              Journal of Clinical Medicine
     2
                                                              3.006065e+09
     3
                                 J Clin Med
                                                              1.776631e+08
     6
              Infectious Disease Modelling
                                                             3.006029e+09
                Journal of Travel Medicine
                                                             3.006304e+09
     10 Global Health Research and Policy
                                                             3.006646e+09
        WHO #Covidence has_full_text
     2
                 #1043
                                 True
     3
                 #1999
                                 True
     6
                  #865
                                 True
                 #2926
                                 True
     10
                 #5595
                                 True
[6]: # read json files
     first_row = preprocessing.FileReader(all_json[0])
     print(first_row)
```

8f8eb4f004c2002face0723f2f58cc411954d36e: Bordetella bronchiseptica isolate KM22 has been used in experimental infections of swine as a model of clinical B. bronchiseptica infection and to study host-to-host transmission. The draft genome sequence of KM22 was reported in 2014. Here, we report the complete genome sequence of KM22... 20-kb insert library preparation protocol (https://www.pacb.com/wp-content/uploads/ Procedure-Checklist-20-kb-Template-Preparation-Using-BluePippin-Size-Selection -System.pdf). The 20-kb library was

sequenced with a PacBio RS II platform using two single-molecule real-time (SMRT) cells, resulting in 283,436 total reads and an average read length of 7,600 bp. Reads were subsequently assessed for quality using FastQC (https://www.bioinformatics.babraham.ac.uk/projects/fastqc/). Whole-genome assemb...

```
[7]: # build dataframe
     df_covid = preprocessing.read_directory_files(all_json, metadata)
     df covid.head()
[7]:
                                        paper_id \
     0 8f8eb4f004c2002face0723f2f58cc411954d36e
     1 63f7049d200896290b38b38711113054f7ea1b50
     2 4df45b8404d9de0b376a8ae3c282a517df36fe51
     3 3c3572ba243d61e7631725669c8f88347fdbd5bc
     4 4cb9c6ef889605b3149ab8b59c8258074067ba04
                                                 abstract \
     O Bordetella bronchiseptica isolate KM22 has bee...
     1
     2 The influenza A nucleoprotein (NP) is an attra...
     3 The prevalence of feline herpesvirus-1 (FHV-1)...
     4 The epidemic of severe acute respiratory syndr...
                                                body_text \
     0 20-kb insert library preparation protocol (htt...
     1 I nfectious diseases have been an ever-present...
     2 The transmission of a pathogenic avian H5N1 vi...
     3 Feline herpesvirus type 1 (FHV-1) is the most ...
     4 E merging diseases are frequently zoonoses cau...
                                                  authors \
     O ['Nicholson, Tracy L.', 'Bayles, Darrell O.', ...
     1 ['Fauci, Anthony S.', 'Touchette, Nancy A.', '...
     2 ['Cheung, Ying-Kit', 'Cheng, Samuel Chak-Sum',...
                 ['Kang, Byeong-Teck', 'Park, Hee-Myung']
     3
     4 ['Dominguez, Samuel R.', 'O'Shea, Thomas J.', ...
                                                                             journal
                                                     title
     O Complete Genome Sequence of Bordetella bronchi... Microbiol Resour Announc
     1 Emerging Infectious Diseases: a 10-Year Perspe...
                                                                  Emerg Infect Dis
     2 Two novel HLA-A*0201 T-cell epitopes in avian ...
                                                                           Vet Res
     3 Prevalence of feline herpesvirus 1, feline cal...
                                                                         J Vet Sci
     4 Detection of Group 1 Coronaviruses in Bats in ...
                                                                 Emerg Infect Dis
[8]: # clean abstract and body_text
     cleaned_abstract = []
```

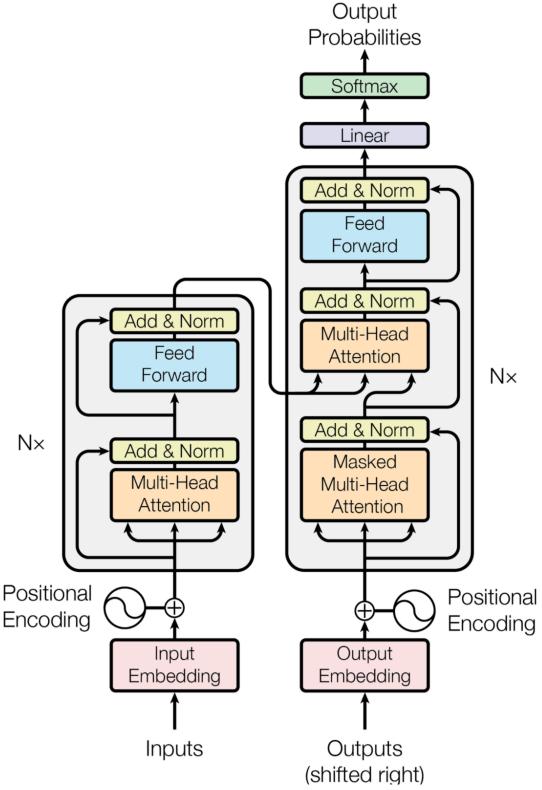
```
for item in df_covid['abstract']:
          item = preprocessing.clean text(item)
          cleaned_abstract.append(item)
      df covid['abstract'] = cleaned_abstract
      #clean body_text
      cleaned body = []
      for item in df_covid['body_text']:
          item = preprocessing.clean text(item)
          cleaned_body.append(item)
      df_covid['body_text'] = cleaned_body
 [9]: pd.DataFrame([[df_covid.shape[0], df_covid.shape[1]]], columns=['# rows', '#_
       [9]:
         # rows
               # columns
          9657
[10]: # save dataframe
      df_covid.to_pickle(f'{root_path}/data/sample_preprocessed_dataframe.pkl')
```

## 2 Train Sentence Transformer on sciBERT

#### 2.0.1 Transformers

When it comes to natural language processing, the most recent developments have seen attention mechanisms prevailing versus more traditiona RNN models. These models use an architecture called Transformer, much faster and easier to parallelize than other networks. This is where these models revolutionize the field: an attention mechanism looks at an input sequence and decides at each step which other components of the sequence are important 1 - meaning it can replicate the way we actually process text, i.e. not only focusing on single words but also considering what's around it to make sense of the language.

Transformers are architectures for transforming a sequence into another by using Encoder and Decoder; yet, they only imply attention mechanisms without any Recurrent Networks (previously the go-to models for many NLP tasks). Here's an image2 to illustrate such Transformer architecture, with the Encoder part on the left and the Decoder on the right.



We won't bore you with the details of the model and its mathematical aspects, but we can point out two main characteristics of Transformers: - the Multi-Head Attention layers treat each word's relationship with every other word in the same sentence, basically paying attention to more words than just one when processing sequences. These layers will ap-

ply to every (input/target, depending on encoder/decoder) sentence the following equation:

Attention 
$$(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \operatorname{softmax} \left( \frac{\mathbf{Q}\mathbf{K}^{\mathsf{T}}}{\sqrt{d_{keys}}} \right) \mathbf{V}$$

- the positional encodings of words are dense vectors (some extra word embeddings) representing the position of a word within the sentencem and are added to each word's embeddings.

#### 2.0.2 BERT & SciBERT

A 2018 paper3 published by various Google researchers brought to life a nowadays state-of-the-art application of a Transformer-based architectures for self-supervised pretraining on large corpus, BERT (*Bidirectional Encoder Representations from Transformers*). BERT is a method of pretraining language representations, so that we can train a general-purpose model on an immense corpus and then use said model for downstream NLP tasks - its bidirectional characteristic allows to represent each word within its context (i.e. other words in the sentence, both on the left and right of represented word).

If the original BERT trained a large (12-layer to 24-layer) Transformer on a large corpuse of Wikipedia and BookCorpus, more recent BERT-alike models have trained the same architecture on specific corpuses for domain-relevant tasks. For instance, in 2019 Allen AI released SciBERT,4 a BERT model trained on huge corpus of scientific papers (82% of which from biomedical domain) from semanticscholar.org, which significantly improves BERT performance on downstream NLP tasks specific to scientific problems. We believe that using SciBERT for this project will yield much better results than the generic original BERT model given the specificity of our data.

#### 2.0.3 Sentence-BERT

BERT-alike models described above have set a new bar for sentence-pair regressions tasks, but unfortunately they need both sentences to be fed in the Transformer, causing such a computational overhead that makes unsupervised tasks virtually impossible.

Thus, in 2019 researchers at UKPLab released SBERT,5 a modification of pre-trained BERT to derive semantic sentence embeddings easily comparable for similarity and clustering. SBERT fine-tunes BERT-alike models with a siamese or triplet network structure to obtain such embeddings. Such a revolutionary paper proposed a model that still maintains BERT-level accuracy, while scaling down time complexity from 65 hours to 5 seconds for specific unsupervised NLP tasks, including similarity comparison, semantic search and clustering. (ah! exactly what we are trying to do here!) Here's an illustration of the SBERT architecture as described in the paper (the structure would not change if the objective function was different, as it may be for different tasks):

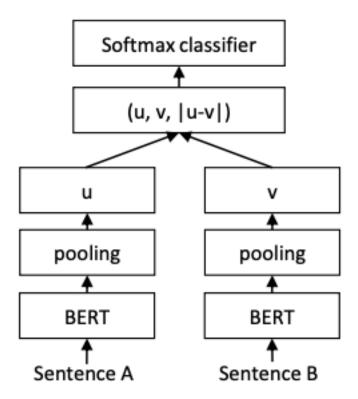


Figure 1: SBERT architecture with classification objective function, e.g., for fine-tuning on SNLI dataset. The two BERT networks have tied weights (siamese network structure).

# 3 Sentence embeddings for analysis

Now, we intend to perform some clustering as well as semantic search on the CORD-19 dataset. To do so, we need SBERT sentence embeddings so that we can accomplish these tasks in reasonable time. We decided that pre-trained embeddings on BERT would have not provide the SOTA outcome we were looking for, thus we fine-tuned our sentence embedding method on SciBERT to get science-specific sentence embeddings.

The SBERT library provides the code to tune any BERT-like model (in our case, SciBERT) on the Natural Language Inference (NLI) data, published by Allen AI. The following script trained SciBERT on the NLI dataset using a Softmax Classifier as training loss and the STS (Semantic Text Similarity) dataset as benchmark for evaluation, and provided us a file-tuned sentence embedder to derive embeddings for our clustering and search tasks on the CORD-19 dataset.

```
# select one Transformer
model_name = 'allenai/scibert_scivocab_uncased'

# Use sciBERT model for mapping tokens to embeddings
word_embedding_model = models.BERT(model_name)
```

```
# Apply mean pooling to get one fixed sized sentence vector
pooling_model = models.Pooling(word_embedding_model.get_word_embedding_dimension(),
                            pooling_mode_mean_tokens=True,
                            pooling_mode_cls_token=False,
                            pooling_mode_max_tokens=False)
model = SentenceTransformer(modules=[word_embedding_model, pooling_model])
# Convert the dataset to a DataLoader ready for training
train_data = SentencesDataset(nli_reader.get_examples('train.gz'), model=model)
train_dataloader = DataLoader(train_data, shuffle=True, batch_size=batch_size)
dev_data = SentencesDataset(examples=sts_reader.get_examples('sts-dev.csv'), model=model)
dev_dataloader = DataLoader(dev_data, shuffle=False, batch_size=batch_size)
evaluator = EmbeddingSimilarityEvaluator(dev_dataloader)
num_epochs = 2
warmup_steps = math.ceil(len(train_dataloader) * num_epochs / batch_size * 0.1) #10% of train
# Train the model
model.fit(train_objectives=[(train_dataloader, train_loss)],
         evaluator=evaluator,
         epochs=num_epochs,
         evaluation_steps=1000,
         warmup_steps=warmup_steps,
         output_path=model_save_path
```

The training of the sentence transformer took eventually around 5 hours when performed on Kaggle notebook with GPU.

At this point, we can simply use our fine-tuned model (perfect for our biomedical dataset) to encode our corpus. This script provided the embeddings we need, both for the abstract and separately for the full text of each article (the latter process also took around 4-6 hours on GPU to complete). We will then access these embeddings in the dataframe for downstream tasks below.

```
## import embeddings
import pandas as pd
from sentence_transformers import SentenceTransformer
from scripts import embeddings

# download pre-trained model
model = SentenceTransformer('model1') # model we fine-tuned and saved

# import dataframe without embeddings yet
df_covid = pd.read_pickle(f'{root_path}/data/sample_preprocessed_dataframe.pkl')

# add abstract embeddings to dataframe
df_covid['abs_embeddings'] = embeddings.sent_embeddings(df_covid['abstract'], model)
```

```
# add full text embeddings to dataframe
df_covid['body_embeddings'] = embeddings.sent_embeddings(df_covid['body_text'], model)
# save dataframe
df_covid.to_pickle('./data/compelete_dataframe.pkl')
```

## 4 Clustering

#### 4.1 UMAP

Uniform Manifold Approximation and Projection (UMAP)6 is an algorithm for dimension reduction based on manifold learning techniques and ideas from topological data analysis. It provides a very general framework for approaching manifold learning and dimension reduction, but can also provide specific concrete realizations and can preserve more of the global structure with superior run time performance.

```
[13]: import umap.umap_ as umap
    import matplotlib.pyplot as plt
    import pandas as pd
    import numpy as np

[14]: #open pickle file to extract vextorization
    df=pd.read_pickle('data/compelete_dataframe.pkl')

[15]: reducer = umap.UMAP(n_neighbors = 5)

[16]: #for abstract
    numpy_array=df['abs_embeddings'][0]
    for i in range(1,len(df['abs_embeddings'])):
        numpy_array=np.row_stack((numpy_array,df['abs_embeddings'][i]))

[17]: #for body text
    numpy_array2=df['body_embeddings'][0]
    for i in range(1,len(df['body_embeddings'])):
        numpy_array2=np.row_stack((numpy_array2,df['body_embeddings'][i]))
```

### 4.1.1 Visualization

#### Abstract

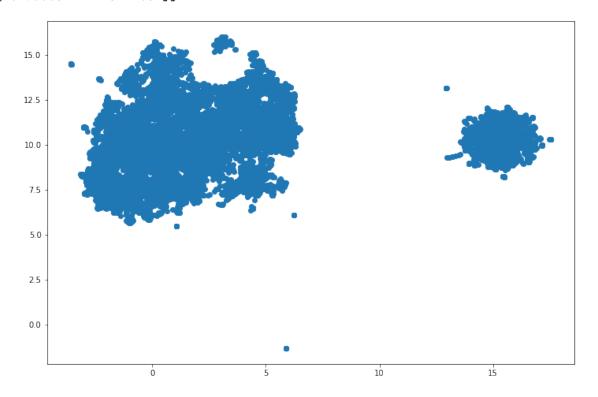
```
[18]: # reduce to two dimentions and plot result
clusterable_embedding = reducer.fit_transform(np.asmatrix(numpy_array))
plt.figure(figsize=(12,8))
plt.scatter(clusterable_embedding[:,0],clusterable_embedding[:,1])
clusterable_embedding.shape
print(clusterable_embedding)
```

/usr/local/lib/python3.7/site-packages/numba/np/ufunc/parallel.py:355: NumbaWarning: The TBB threading layer requires TBB version 2019.5 or later

i.e., TBB\_INTERFACE\_VERSION >= 11005. Found TBB\_INTERFACE\_VERSION = 11000. The TBB threading layer is disabled.

```
warnings.warn(problem)
```

```
[[ 1.3151064 14.963993 ]
[16.357409 10.505647 ]
[-1.4696 7.2187424]
...
[ 3.8887513 7.5552874]
[-1.7892604 10.335872 ]
[-0.76065 12.922169 ]]
```

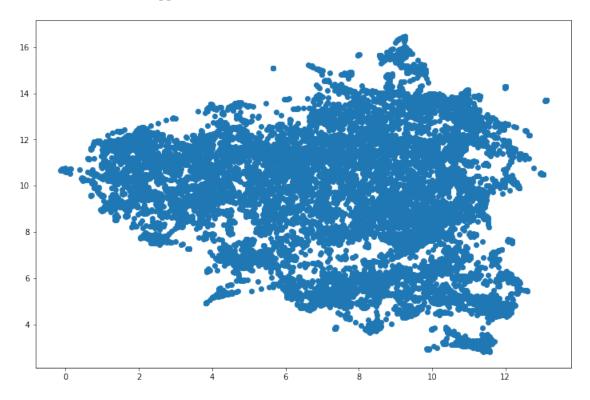


## **Body Text**

```
[19]: clusterable_embedding2 = reducer.fit_transform(np.asmatrix(numpy_array2))
    plt.figure(figsize=(12,8))
    plt.scatter(clusterable_embedding2[:,0],clusterable_embedding2[:,1])
    clusterable_embedding2.shape
    print(clusterable_embedding2)
```

```
[[ 4.8522654 7.29898 ]
[10.4329405 11.176286 ]
```

```
[11.461031 2.9171674] ...
[ 6.1377482 6.2594786] [ 7.7757587 5.3794594] [ 7.9246597 11.538631 ]]
```



## 4.2 HDBSCAN

We are trying to run vectorization and separate the literature by two ways, the first one is HDB-SCAN. HDBSCAN is a clustering algorithm developed by Campello, Moulavi, and Sander.7 It extends DBSCAN (a classic density-based spatial algorithm) by converting it into a hierarchical clustering algorithm, and then using a technique to extract a flat clustering based in the stability of clusters.

```
[20]: import hdbscan
  import numpy as np
  import seaborn as sns
  import pandas as pd

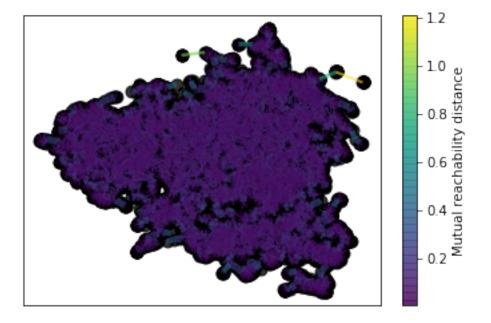
[21]: #Abstract
  clusterer = hdbscan.HDBSCAN(min_cluster_size=2, gen_min_span_tree=True)
  clusterer=clusterer.fit(clusterable_embedding)
```

```
[22]: #Body Text clusterer2=clusterer.fit(clusterable_embedding2)
```

#### 4.2.1 Visualization

#### Abstract

[23]: <matplotlib.axes.\_subplots.AxesSubplot at 0x187927690>



```
[64]: #Build the cluster hierarchy clusterer.single_linkage_tree_.plot(cmap='viridis', colorbar=True)
```

```
[25]: #Condense the cluster tree clusterer.condensed_tree_.plot()
```

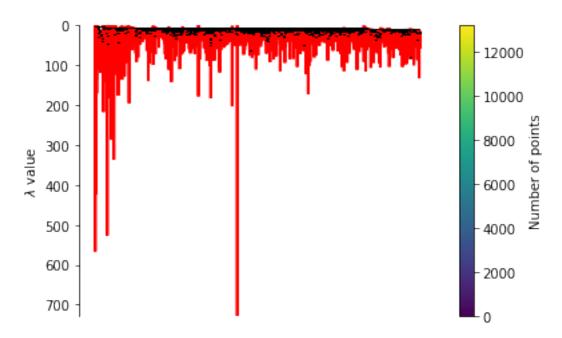
[25]: <matplotlib.axes.\_subplots.AxesSubplot at 0x1e1f44790>



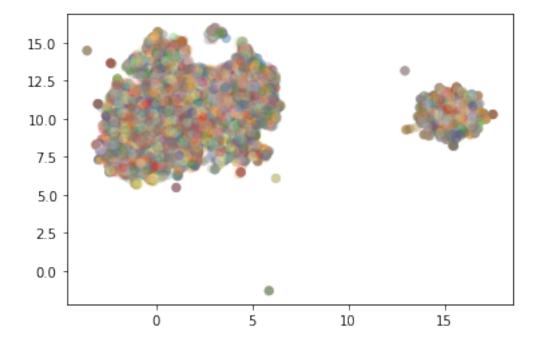
[26]: #Extract the clusters
clusterer.condensed\_tree\_.plot(select\_clusters=True, selection\_palette=sns.

→color\_palette())

[26]: <matplotlib.axes.\_subplots.AxesSubplot at 0x181937990>



## [27]: <matplotlib.collections.PathCollection at 0x23aa19990>

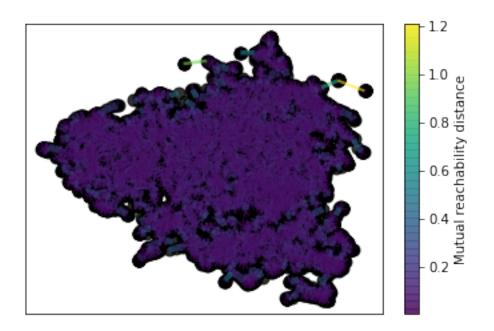


We got more than 1000 clustering groups totally, so HDBSCAN may not be the best way to cluster, and then we will try K-Means.

## **Body Text**

```
[28]: #Build the minimum spanning tree clusterer2.minimum_spanning_tree_.plot(edge_cmap='viridis', edge_alpha=0.6, node_size=80, edge_linewidth=2)
```

[28]: <matplotlib.axes.\_subplots.AxesSubplot at 0x1e2337dd0>



```
[]: #Build the cluster hierarchy clusterer2.single_linkage_tree_.plot(cmap='viridis', colorbar=True)
```

```
[29]: #Condense the cluster tree
clusterer2.condensed_tree_.plot()
```

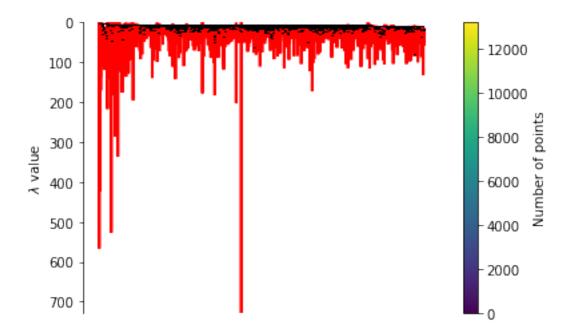
[29]: <matplotlib.axes.\_subplots.AxesSubplot at 0x2401f0f10>



```
[30]: #Extract the clusters
clusterer2.condensed_tree_.plot(select_clusters=True, selection_palette=sns.

→color_palette())
```

[30]: <matplotlib.axes.\_subplots.AxesSubplot at 0x246403ed0>



```
[31]: #clusterer = hdbscan.HDBSCAN(min_cluster_size=10, prediction_data=True).

→ fit(clusterable_embedding)

color_palette = sns.color_palette('Paired',max(clusterer2.labels_))

cluster_colors = [color_palette[x] if x >= 0 and x<max(clusterer2.labels_))

else (0.5, 0.5, 0.5)

for x in clusterer.labels_]

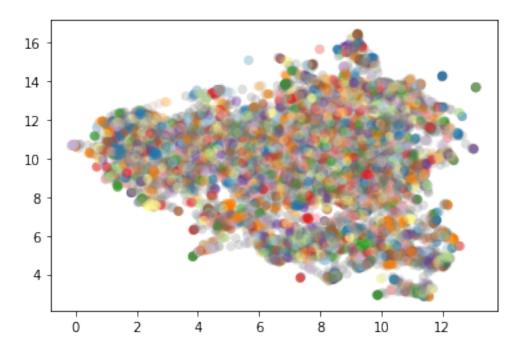
cluster_member_colors2 = [sns.desaturate(x, p) for x, p in

zip(cluster_colors, clusterer2.probabilities_)]

plt.scatter(*clusterable_embedding2.T, s=50, linewidth=0, □

→ c=cluster_member_colors2, alpha=0.25)
```

[31]: <matplotlib.collections.PathCollection at 0x254244b10>



#### 4.3 K-means

Then we will see what k-means clustering to be like and what makes it different from HDBSCAN. First step is finding best k-value. Distortion computes the sum of squared distances from each point to its assigned center. When distortion is plotted against k there will be a k value after which decreases in distortion are minimal. This is the desired number of clusters.

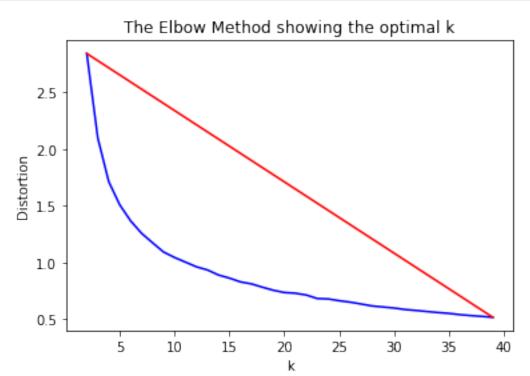
```
[32]: from sklearn.cluster import KMeans
```

#### Abstract

```
[35]: X_line = [K[0], K[-1]]
Y_line = [distortions[0], distortions[-1]]

# Plot the elbow
plt.plot(K, distortions, 'b-')
plt.plot(X_line, Y_line, 'r')
```

```
plt.xlabel('k')
plt.ylabel('Distortion')
plt.title('The Elbow Method showing the optimal k')
plt.show()
```



The best k-value is about 9 to 12, so we determined the best one is 10

```
[36]: kmeans = KMeans(n_clusters=10, random_state=0).

→fit_predict(clusterable_embedding)

kmeans
```

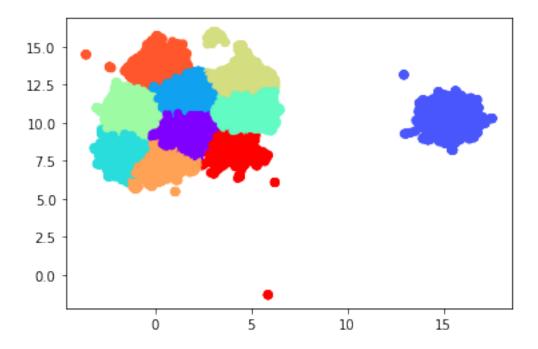
[36]: array([8, 1, 3, ..., 9, 5, 8], dtype=int32)

```
[37]: kmeans_clustering_model=KMeans(n_clusters=10, random_state=0) kmeans_clustering_model.fit(clusterable_embedding) kmeans_label=kmeans_clustering_model.labels_
```

[38]: df['cluster\_']=kmeans\_label

Now we can compare two ways of clustering. Usually K-Means works well for "round" or spherical, and when most dense in the center of the sphere not contaminated by noise/outliers. Our dataset does not centered with arbitrary shapes and too many noises, therefore K-Means works well here.

[39]: <matplotlib.collections.PathCollection at 0x254578190>

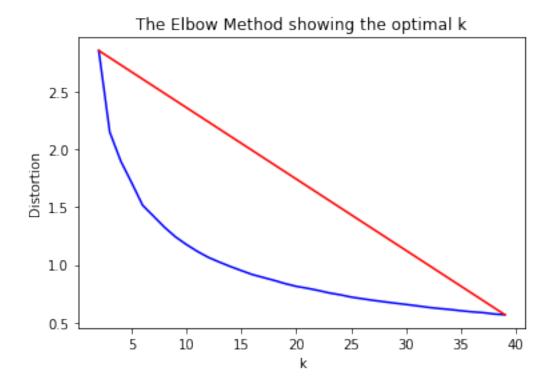


#### **Body Text**

```
[41]: from scipy.spatial.distance import cdist
distortions2 = []
K2 = range(2, 40)
for k in K:
    k_means2 = KMeans(n_clusters=k, random_state=42).fit(clusterable_embedding2)
    k_means2.fit(clusterable_embedding2)
    distortions2.append(sum(np.min(cdist(clusterable_embedding2, k_means2.
    →cluster_centers_, 'euclidean'), axis=1)) / pd.DataFrame(df).shape[0])
```

```
[42]: X_line2 = [K2[0], K2[-1]]
Y_line2 = [distortions2[0], distortions2[-1]]

# Plot the elbow
plt.plot(K2, distortions2, 'b-')
plt.plot(X_line2, Y_line2, 'r')
plt.xlabel('k')
plt.ylabel('Distortion')
plt.title('The Elbow Method showing the optimal k')
plt.show()
```



## 4.4 Topic Modeling

After finding the best clustering model, we will try to label each topic. Most frequent methods of topic modeling, including Latent Dirichlet Allocation.9, a generative statistical model that uses unobserved groups to explain why some parts of a corpus are similar (and non-negative matrix factorization!), do not work with the embeddings method we chose. Indeed, LDA model posits that each document is a mixture of a small number of topics, where each topic is described by a distribution of words and each word's presence in the document can be attributed to one of these topics. As for further work, we could re-preprocess text, using TFIDFVectorizer or CountVectorizer to then find the topics from each model.

## 5 Semantic search

#### 5.0.1 Cosine similarity

An amazing use of the embeddings we obtained with our fine-tuned Sentence Transformer model is to query the corpus and find the most similar embeddings to the query's embeddings. This can be simply done by calculating cosine similarity among embeddings, and then select the least-distant ones as the most relevant to the query.

Here we propose a semantic search system where the user can input a question about COVID-19 and they will get the top 5 most relevant articles from the corpus. We suggest to interrogate our system with questions taken from the Kaggle's suggested tasks.

```
[4]: ## call searches and get table out
   from scripts import searches
   import pandas as pd
   from sentence_transformers import SentenceTransformer
   import os
   # import model
   embedder = SentenceTransformer('model1') #this or the model we trained and saved
   # load corpus
   df_covid = pd.read_pickle(os.getcwd()+'/data/compelete_dataframe.pkl')
[6]: # asking the user
   query = input('What would you like to know from CORD-19? ')
   print('\nUse abstracts:')
   new_searches.sem_search(query, embedder, df_covid['abstract'].to_list(),_

→df_covid['abs_embeddings'].to_list(),df_covid)
   What would you like to know from CORD-19? coronavirus
   Use abstracts:
   _____
   Top 5 most similar articles in corpus:
   +-----
   ______
   Abstract
                                     Journal | Score |
   ----+
```

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```
[7]: # asking the user (slower)
    print('\nUse full text:')
    new_searches.sem_search(query, embedder, df_covid['body_text'].to_list(),__

→df_covid['body_embeddings'].to_list(),df_covid)
    Use full text:
    Top 5 most similar articles in corpus:
                                       Abstract
                                           - 1
                                                                    | Score |
    Title
                                                     Journal
    Niclosamide Is a Proton Carrier and Targets Acidic Endosomes with Broad
    PLoS Pathog | 0.6462 |
    Antiviral Effects
                                    1
    Comparison of fit factors among healthcare providers working in the
    Medicine (Baltimore) | 0.5974 |
    Emergency Department Center before and after training with three types of
           N95 and higher filter respirators
                                    feline infectious peritonitis fip is a severe fatal immune augmented
```

Biomed

In Vitro Antiviral Activity of Circular Triple Helix Forming

Res Int   0.5784
disease in cat population. it is caused by fip virus fipv , a virulent
Oligonucleotide RNA towards Feline Infectious Peritonitis Virus Replication
prophylactics are not effective. the in vitro antiviral properties of five   
circular triple helix forming oligonucleotide tfo rnas tfo1 to tfo5 ,
which target the different regions of virulent feline coronavirus fcov
strain fipv wsu 79 1146 genome, were tested in fipv infected crandell rees
feline kidney crfk cells. rt qpcr results showed that the circular tfo
rnas, except tfo2, inhibit fipv replication, where the viral genome copy
numbers decreased significantly by 5 fold log 10 from 10 14 in the virus
inoculated cells to 10 9 in the circular tfo rnastransfected cells.
furthermore, the binding of the circular tfo rna with the targeted viral
genome segment was also confirmed using electrophoretic mobility shift
assay. the strength of binding kinetics between the tfo rnas and their
target regions was demonstrated by nanoitc assay. in conclusion, the
circular tfos have the potential to be further developed as antiviral
agents against fipv infection.
"The Duty to Prevent" during an epidemic situation like 2015 Korean MERS   Epidemiol Health   0.5156
l <sup>-</sup>
outbreak

A benchmark driven g	guide to l	oinding si	te comparison	: An exhau	stive	PLoS
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## 6 Conclusion

This project taught us how complex models that are truly applicable and easily transferable can (fairly) quickly yield amazing results on massive and diverse amount of data, in this case natural language data. Transformers model (which we were even able to fine-tune for our domain-specific project) have been perfected to an extent that we can perform both supervised and unsupervised tasks in a timely manner, given the widely available hardware accelerators in the community.

For the CORD-19 challenge, we decided to fine-tuned Sentence-BERT on SciBERT, so that we had our own Sentence-SciBERT to obtain embeddings from our data to use for unsupervised downstream tasks. Thus, we used these embeddings to cluster the articles. HDBSCAN proved quite innefficient, as given the high condensity of the dataset the model did not yield very interpretable results. On the other hand, a classic K-means model performed well on such dense and "spherical" dataset, by learning 10 clusters of articles. Unfortunately, our embeddings could not be used to try topic modeling algorithms, such as LDA.

Finally, we had fun experimenting with a simple algorithm based on cosine similarity to search through the dataset. By using embeddings of articles and of the query, this straightforward application can output the most relevant articles for the user searches in a pretty table. Go ahead and download this notebook from our GitHub Repo to play around with it!

We hope we were able to prove the potentiality and power of these machine learning models and approaches, and we wish that the research community will continue to have such a fundamental impact on current and urgent problems!