

# Knowledge Graph Project (by FORWARD Datalab)



## Part 1. ETL Pipeline

### Load libraries ¶

```
In [1]: import pyspark as sp
import numpy as np
import string
import re
```

### Set environment variable (optional)

```
In [2]: import os
os.environ["PYSPARK_PYTHON"]="/usr/local/bin/python3"
os.environ["PYSPARK_DRIVER_PYTHON"]="/usr/local/bin/python3"
```

### Setup cluster

```
In [3]: from pyspark.sql import SparkSession

spark = SparkSession \
    .builder \
    .appName("Python Knowledge Graph Project") \
    .master("local[*]") \
    .config("spark.some.config.option", "some-value") \
    .getOrCreate()
```

## Load dataset

- Documents: 1.7m documents (arXiv dataset)
- Keyword list: 100,000 keywords (FORWARD Data Lab)
- Download your documents here: <https://www.kaggle.com/Cornell-University/arxiv>  
(<https://www.kaggle.com/Cornell-University/arxiv>).

```
In [4]: df_keywords = spark.read.csv("./mag_cs_keywords.csv", header=True)
df_arxiv = spark.read.json("./original/arxiv-metadata-oai-snapshot.json")
```

```
In [5]: df_keywords = df_keywords.repartition(8)
df_arxiv = df_arxiv.repartition(8)
```

```
In [6]: df_keywords.rdd.getNumPartitions()
```

```
Out[6]: 8
```

```
In [7]: df_keywords.count()
```

```
Out[7]: 104654
```

```
In [8]: abstracts = df_arxiv.select("id", "abstract")
keywords = df_keywords.select("normalizedName")
```

## Cleaning & Normalization

```
In [9]: from pyspark.sql.functions import udf, col
from pyspark.sql import Row
from pyspark.sql.types import ArrayType, StructField, StructType, StringType, IntegerType

# get only lowercase alphabets
def strip_non_ascii(data_str):
    ''' Returns the string without non ASCII characters'''
    stripped = (c.lower() for c in data_str if 96 < ord(c.lower()) < 123 or ord(c)==32) #alphabets

    return ''.join(stripped)
# setup pyspark udf function
strip_non_ascii_udf = udf(strip_non_ascii, StringType())
```

```
In [10]: abstracts = abstracts.withColumn('normalized', strip_non_ascii_udf(abstracts['abstract']))
abstracts = abstracts.select("id", "normalized")
```

```
In [11]: abstracts.show()
```

```
+-----+-----+
|      id|      normalized|
+-----+-----+
|0809.3647| in this paper w...|
|0809.1984| quantum fluctua...|
|0710.3204| we show how com...|
|0704.3898| we give two cla...|
|0807.4706| let g be a grou...|
|0809.2915| the h and zeus ...|
|0803.3905| when designing ...|
|0807.0026| radio telescope...|
|0804.1504| in an internat...|
|0802.4266| we study group ...|
|0802.3187| the role of neu...|
|0710.2708| given a project...|
|0706.0677| this is the thi...|
|0707.1652| the pierre auge...|
|0809.1051| we present a ve...|
|0704.3951| ramification in...|
|0805.4670| based on firstp...|
|0710.4428| an asymptotic m...|
|0712.1683| recently the in...|
|0810.0015| experiments in ...|
+-----+-----+
only showing top 20 rows
```

## Keyword List for Query

- `keywords_dict` : Hash table is used to find whether documents contain keywords
- My first attempt was using regular expression (`re.findall()`).
- When using regular expression, there could be a time complexity issue due to unnecessary computational overhead
- To prevent optimize algorithm, we should search from document to word.

```
In [12]: keywords_list = list(keywords.select('normalizedName').toPandas()['normalizedName'])
keyword_dict = {word:0 for word in keywords_list}
```

## Extract Keyword from the keyword list

```
In [13]: import re

# Define the function you want to return
def extract(s):
    all_matches = set()
    for word in s.split(" "):
        if keyword_dict.get(word, -1) >= 0:
            keyword_dict[word] += 1
            all_matches.add(word)
    return ','.join(all_matches)

# Create the UDF, note that you need to declare the return schema matching the returned type
extract_udf = udf(extract, StringType())

# Apply it
df = abstracts.withColumn('extracted', extract_udf(abstracts['normalized']))
```

```
In [14]: df.show()
```

id	normalized	extracted
0809.3647	in this paper w...	size,algorithm,pr...
0809.1984	quantum fluctua...	quantum,field,res...
0710.3204	we show how com...	current,scatterin...
0704.3898	we give two cla...	set,metric,functi...
0807.4706	let g be a grou...	product,cluster,q...
0809.2915	the h and zeus ...	scattering,mass,q...
0803.3905	when designing ...	set,art,modelling...
0807.0026	radio telescope...	range,leakage,pos...
0804.1504	in an internat...	imagination,refle...
0802.4266	we study group ...	bimodule,skew,group
0802.3187	the role of neu...	quark,phase,gauge...
0710.2708	given a project...	bundle,decomposit...
0706.0677	this is the thi...	geodesic,link,ser...
0707.1652	the pierre auge...	pose,unit,distrib...
0809.1051	we present a ve...	range,quantum,res...
0704.3951	ramification in...	filtration,struct...
0805.4670	based on firstp...	character,layers,...
0710.4428	an asymptotic m...	structures,dynami...
0712.1683	recently the in...	wave,molecule,dif...
0810.0015	experiments in ...	cell,relation,low...

only showing top 20 rows

**Drop Empty Rows where no keyword exists**

```
In [15]: from pyspark.sql.functions import length
df = df.filter(length('extracted')>2)
```

```
In [16]: df.show()
```

```
+-----+-----+-----+
|      id|      normalized|      extracted|
+-----+-----+-----+
|0809.3647| in this paper w...|size,algorithm,pr...|
|0809.1984| quantum fluctua...|quantum,field,res...|
|0710.3204| we show how com...|current,scatterin...|
|0704.3898| we give two cla...|set,metric,functi...|
|0807.4706| let g be a grou...|product,cluster,q...|
|0809.2915| the h and zeus ...|scattering,mass,q...|
|0803.3905| when designing ...|set,art,modelling...|
|0807.0026| radio telescope...|range,leakage,pos...|
|0804.1504| in an internat...|imagination,refle...|
|0802.4266| we study group ...| bimodule,skew,group|
|0802.3187| the role of neu...|quark,phase,gauge...|
|0710.2708| given a project...|bundle,decomposit...|
|0706.0677| this is the thi...|geodesic,link,ser...|
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|0810.0015| experiments in ...|cell,relation,low...|
+-----+-----+-----+
only showing top 20 rows
```

$$PMI(A, B) = \frac{P(A, B)}{P(A) * P(B)}$$

$$P(A, B) = \frac{c((A, B), C_{\text{pairs}})}{c(C_{\text{pairs}})}$$

$$P(A) = \frac{c(A)}{c(C)}, P(B) = \frac{c(B)}{c(C)}$$

where C stands for word collection

## 1. Get Word Count

- corpus : It is a dictionary of unigram count

```
defaultdict(int,  
            {'conjugate': 4041,  
             'quantum': 162709,  
             'lambda': 18154,  
             'method': 195849,  
             'quantization': 11050,  
             ...  
            })
```

```
In [17]: corpus_temp = df.select("extracted").rdd.repartition(32).flatMap(lambda x: (x["extracted"].split(",")))  
corpus = corpus_temp.countByValue()
```

## 2. Get Cooccurrence Count

- corpus2 : It is a dictionary where key is tuple (pair of unigrams) and value is frequency

```
defaultdict(int,  
            {('conjugate', 'quantum'): 490,  
             ('conjugate', 'lambda'): 60,  
             ('conjugate', 'method'): 606,  
             ('conjugate', 'quantization'): 82,  
             ...  
            })
```

```
In [18]: rdds = df.select("extracted").rdd.repartition(32).map(lambda x: x['extracted'].split(","))
```

```
In [19]: from itertools import combinations  
corpus2_temp = rdds.flatMap(lambda x: combinations(x,2))  
corpus2 = corpus2_temp.countByValue()
```

## 3. How to avoid bottleneck?

- Use clusters! (Amazon EMR, S3)

## 4. Save Result Here

- Uncomment to save to text file

```
In [20]: # corpus_temp.repartition(8).saveAsTextFile("./corpus_final.txt")
# corpus2_temp.repartition(8).saveAsTextFile("./corpus2_final.txt")
```

## 5. Load From File

- Uncomment to load from file

```
In [21]: # corpus = spark.sparkContext.textFile("./corpus_final.txt").countByValue()
# corpus2 = spark.sparkContext.textFile("./corpus2_final.txt").countByValue()

"""
Clean corpus when read from file
Since we are loading from a textfile, tuples are converted into strings
"""
# from collections import defaultdict
# corpus_temp = defaultdict(int)

# corpus = dict(map(lambda x: (x[0].strip(), x[1]), corpus.items()))
# for k, v in corpus2.items():
#     k1, k2 = re.sub("'", "", k.strip('()')).split(",")
#     k2 = k2.strip()
#     w1, w2 = min(k1, k2), max(k1, k2)
#     corpus_temp[(w1, w2)] += v
# corpus2 = corpus_temp
```

```
Out[21]: '\nClean corpus when read from file\nSince we are loading from a textfile, tuples are converted into strings\n'
```

## Part 2. Graph Visualization

### Draw Graph

```
In [22]: freq_threshold = 0
PMI_threshold = 10
```

```
In [23]: import networkx as nx
import math
import pdb
G = nx.Graph()

total_word_freq = sum(corpus.values())
total_pair_freq = sum(corpus2.values())
for (n1, n2), cooccurrence in corpus2.items():
    if corpus[n1] > freq_threshold and corpus[n2] > freq_threshold and
cooccurrence:
        pa = corpus[n1] / total_word_freq
        pb = corpus[n2] / total_word_freq
        pab = cooccurrence / total_pair_freq

        pmi = math.log(pab/(pa*pb), 2)
        G.add_edge(n1, n2, weight=pmi)
```

## !! Test Your QUERY Here !!

- Type your query here
- Sample queries include

gene, class, theory, stat, dimension, state

```
In [24]: query = 'colonialism'
sorted(G.adj[query].items(), key=lambda x: x[1]['weight'], reverse=True)
[:10]
```

```
Out[24]: [('patriarchy', {'weight': 21.569935731346103}),
('solidarity', {'weight': 17.400010729903787}),
('meter', {'weight': 11.037579806057254}),
('astronomy', {'weight': 9.556613057920654}),
('white', {'weight': 8.155514749599684}),
('center', {'weight': 7.155382616518959}),
('telescope', {'weight': 6.94331407898773}),
('impact', {'weight': 6.596238365040749}),
('support', {'weight': 6.590599858680719})]
```



- Higher than 10 pmi demonstrates a strong relationship between the two words
- Below is the sample pmi table from the wikipedia dataset.

word 1	word 2	count word 1	count word2	co-occurrence	pmi
puerto	rico	1938	1311	1159	10.0349081703
car	driver	5578	2749	1384	8.41470768304
it	the	283891	3293296	3347	-1.72037278119
of	and	1761436	1375396	1190	-3.70663100173

- Reference: [https://en.wikipedia.org/wiki/Pointwise\\_mutual\\_information](https://en.wikipedia.org/wiki/Pointwise_mutual_information)  
([https://en.wikipedia.org/wiki/Pointwise\\_mutual\\_information](https://en.wikipedia.org/wiki/Pointwise_mutual_information))

## Top 10 Related Words

- Queries and their related keywords are sorted here by pmi.
- Natural science domain seems to working well

```
In [25]: result = list()
for i, q in enumerate(list(G.nodes)):
    weight = sorted(G.adj[q].items(), key=lambda x: x[1]['weight'], reverse=True)[:3]

    if len(weight)==0:
        r1, r2, r3 = 0, 0, 0
        pmi = 0
    elif len(weight)==1:
        r1, r2, r3 = weight[0][0], 0, 0
        pmi = weight[0][1]['weight']
    elif len(weight)==2:
        r1, r2, r3 = weight[0][0], weight[1][0], 0
        pmi = weight[0][1]['weight']
    else:
        r1, r2, r3 = weight[0][0], weight[1][0], weight[2][0]
        pmi = weight[0][1]['weight']

    result.append((q, r1, r2, r3, pmi))

result.sort(key=lambda x: x[4], reverse=True)

for q, r1, r2, r3, _ in result[:10]:
    print("query: {}".format(q))
    print("result: {0}, {1}, {2}\n".format(r1, r2, r3))
```

```
query: spastic
result: hypertonia, reflex, muscle

query: hypertonia
result: spastic, reflex, muscle

query: jatropha
result: endophyte, colonization, crop

query: endophyte
result: jatropha, colonization, crop

query: thrombopoietin
result: thrombopoiesis, megakaryocyte, platelet

query: thrombopoiesis
result: thrombopoietin, megakaryocyte, platelet

query: megakaryocyte
result: thrombopoietin, thrombopoiesis, platelet

query: mamluk
result: terracotta, mesopotamia, lustre

query: terracotta
result: mamluk, mesopotamia, lustre

query: colonialism
result: patriarchy, solidarity, meter
```

## Visualization

- The final plot shows that related words form a group of cluster

```
In [26]: samples = ["spastic", "hypertonia", "reflex", "muscle", "endophyte", "jatropha", "colonization", "crop", "colonialism", "patriarchy", "solidarity", "meter"]
```

```
In [27]: matrix = list()
for i, row in enumerate(samples):
    row_temp = list()
    for j, col in enumerate(samples):
        w1, w2 = samples[i], samples[j]
        if G.adj.get(w1, 0) and G.adj[w1].get(w2, 0) and G.adj[w1][w2].get("weight", 0):
            row_temp.append(G.adj[w1][w2]["weight"])
        else:
            row_temp.append(0)
    matrix.append(row_temp)
```

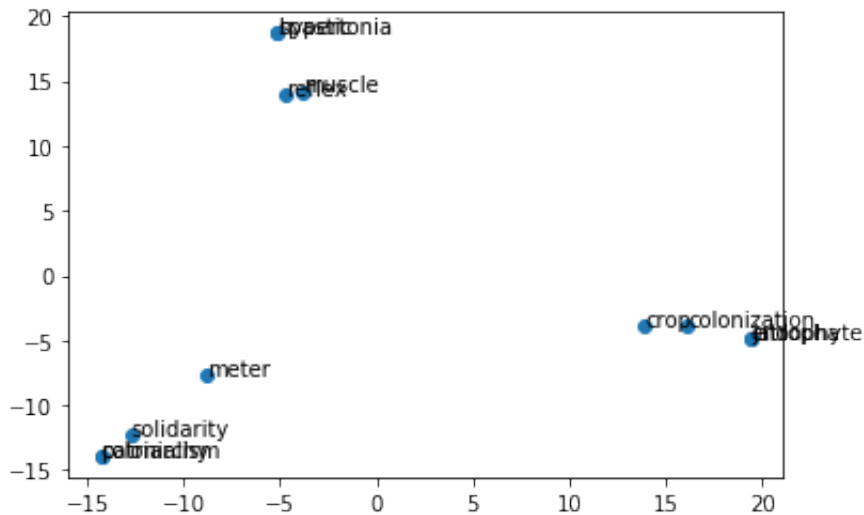
```
In [28]: from sklearn.decomposition import PCA

pca = PCA(n_components=2)
result = pca.fit_transform(matrix)
```

```
In [30]: from matplotlib import pyplot

pyplot.scatter(result[:, 0], result[:, 1])
for i, word in enumerate(samples):
    pyplot.annotate(word, xy=(result[i, 0], result[i, 1]))

pyplot.figure(figsize=(15,15))
pyplot.show()
```



<Figure size 1080x1080 with 0 Axes>

## Future Directions

- Tokenization
  - Include n-gram (2,3,4,...) extractor to extract longer keywords.
  - e.g.) keyword: computer science
  - Phrase mining or Named Entity Recognition can be used during the process
- Embedding
  - Use cooccurrence matrix to train word embeddings (Glove)
  - Or, load word embedding from Glove or Word2Vec and project to 2D plot.
  - Evaluate the similarity of two words by using l1 distance , l2 distance , or cosine similarity .
- Metric
  - We may investigate NPMI

## References

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  - <https://medium.com/@christo.lagali/run-jupyter-notebooks-with-pyspark-on-an-emr-cluster-9630ef54c4e1> (<https://medium.com/@christo.lagali/run-jupyter-notebooks-with-pyspark-on-an-emr-cluster-9630ef54c4e1>)
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- Extract keywords in document
  - <https://stackoverflow.com/questions/48869922/how-to-efficiently-check-if-a-list-of-words-is-contained-in-a-spark-dataframe> (<https://stackoverflow.com/questions/48869922/how-to-efficiently-check-if-a-list-of-words-is-contained-in-a-spark-dataframe>)
  - <https://stackoverflow.com/questions/46410887/pyspark-string-matching-to-create-new-column> (<https://stackoverflow.com/questions/46410887/pyspark-string-matching-to-create-new-column>)
- Useful tutorials
  - <https://spark.apache.org/docs/1.6.3/ml-features.html> (<https://spark.apache.org/docs/1.6.3/ml-features.html>)
- Word embeddings and visualization
  - [https://web.stanford.edu/class/cs224n/assignments/a1\\_preview/exploring\\_word\\_vectors.html](https://web.stanford.edu/class/cs224n/assignments/a1_preview/exploring_word_vectors.html) ([https://web.stanford.edu/class/cs224n/assignments/a1\\_preview/exploring\\_word\\_vectors.html](https://web.stanford.edu/class/cs224n/assignments/a1_preview/exploring_word_vectors.html))
  - <https://machinelearningmastery.com/develop-word-embeddings-python-gensim/> (<https://machinelearningmastery.com/develop-word-embeddings-python-gensim/>)