Knowledge Graph Project (FORWARD Data Lab)

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/bin/python3"
os.environ["PYSPARK_DRIVER_PYTHON"]="/usr/bin/python3"
```

Setup cluster

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

spark = SparkSession \
    .builder \
    .appName("Python Knowledge Graph Project") \
    .config("spark.driver.memory", "55g") \
    .master("local[*]") \
    .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.

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

In [5]:
```
df_keywords = df_keywords.repartition(16)
df_arxiv = df_arxiv.repartition(16)
```

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

Out[6]:
```
16
```

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,

# 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 o

    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[
abstracts = abstracts.select("id","normalized")
```

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

```
+---------+--------------------+
|       id|          normalized|
+---------+--------------------+
|0705.2030|  the group eso s...|
|0801.0970|  this paper is c...|
|0709.3236|  we present a ge...|
|0809.3030|  the tragedy of ...|
|0712.0290|  the ability to ...|
|0805.2349|  this article pr...|
|0805.1292|  we turn the chu...|
|0712.3567|  the random sequ...|
|0705.1654|  a smallscale tr...|
|0803.3867|  we present a ch...|
|0709.0351|  for precision s...|
|0711.4659|  in a newly intr...|
|0705.1358|  we propose two ...|
|0710.2002|  we present prec...|
|0801.1957|  we calculate th...|
|0707.0756|  many topologica...|
|0808.0066|  the reasonablen...|
|0801.3027|  in this paper w...|
|0707.0344|  in this paper w...|
|0807.4946|  we establish lo...|
+---------+--------------------+
only showing top 20 rows
```

Keyword List for Query

- `keywords_dict` : Hash table is used to find whether documents contain keywords
- My frist 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()['normalized
keyword_dict = {word:0 for word in keywords_list}
```

Extract Keyword from the keyword list

In [13]:

```
import re, nltk

# Define the function you want to return
def extract(s):
    all_matches = set()

    ngrams = list()
    ngrams.append(s.split(" "))
    for i in range(1,12): # all ngrams in keyword list
        ngrams.append(nltk.ngrams(ngrams[0], i))

    for ngram in ngrams:
        for token in ngram:
            token = ' '.join(token)
            if keyword_dict.get(token, -1) >=0:
                keyword_dict[token] += 1
                all_matches.add(token)
    return ','.join(all_matches)

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

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

In [14]:

```
df.show()
```

```
+---------+--------------------+--------------------+
|       id|          normalized|           extracted|
+---------+--------------------+--------------------+
|0705.2030|  the group eso s...|power,momentum,ro...|
|0801.0970|  this paper is c...|selection,minimax...|
|0709.3236|  we present a ge...|perturbation theo...|
|0809.3030|  the tragedy of ...|set,crowdsourcing...|
|0712.0290|  the ability to ...|mechanism,morphol...|
|0805.2349|  this article pr...|liquid helium,pha...|
|0805.1292|  we turn the chu...|physics,computati...|
|0712.3567|  the random sequ...|deposition,initia...|
|0705.1654|  a smallscale tr...|thermal,temperatu...|
|0803.3867|  we present a ch...|        product,term|
|0709.0351|  for precision s...|field,perturbatio...|
|0711.4659|  in a newly intr...|square,phase,posi...|
|0705.1358|  we propose two ...|phase,phase trans...|
|0710.2002|  we present prec...|pair production,d...|
|0801.1957|  we calculate th...|quantum,phase,fie...|
|0707.0756|  many topologica...|generalization,se...|
|0808.0066|  the reasonablen...|perturbation theo...|
|0801.3027|  in this paper w...|brownian motion,p...|
|0707.0344|  in this paper w...|bridge,is a,devia...|
|0807.4946|  we establish lo...|inflow,outflow,la...|
+---------+--------------------+--------------------+
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 keywords

In [15]:
```
corpus_temp = df.select("extracted").rdd.repartition(16).flatMap(lambda x: (x
corpus = corpus_temp.countByValue()
```

In [53]:
```
len(corpus)
```

Out[53]:
```
70342
```

2. Get Cooccurence Count

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

In [16]:
```
rdds = df.select("extracted").rdd.repartition(16).map(lambda x: x['extracted'
```

In [17]:
```
from itertools import combinations
corpus2_temp = rdds.flatMap(lambda x: combinations(x,2))
corpus2 = corpus2_temp.countByValue()
```

In [54]:
```
len(corpus2)
```

Out[54]:
```
15617821
```

3. How to avoid bottleneck?

- Use clusters! (Amazon EMR, S3)

4. Save Result Here

- Uncomment to save to text file

In [18]:
```
# corpus_temp.repartition(16).saveAsTextFile("./corpus_ngram.txt")
# corpus2_temp.repartition(16).saveAsTextFile("./corpus2_ngram.txt")
```

5. Load From File

- Uncomment to load from file

In [ ]:
```
# corpus = spark.sparkContext.textFile("./corpus_ngram.txt").countByValue()
# corpus2 = spark.sparkContext.textFile("./corpus2_ngram.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
```

Part 2. Graph Visualization

Draw Graph

In [19]:
```
freq_threshold = 0
PMI_threshold = 10
```

In [20]:
```
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), cooccurence in corpus2.items():
    if corpus[n1] > freq_threshold and corpus[n2] > freq_threshold and cooccu
        pa = corpus[n1] / total_word_freq
        pb = corpus[n2] / total_word_freq
        pab = cooccurence / total_pair_freq

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

RUN QUERY HERE

- Type `your query` here
- Sample queries include
  `gene, entitiy relationship model, business concept, data mining`

In [40]:
```
query = 'entity relationship model'
sorted(G.adj[query].items(), key=lambda x: x[1]['weight'], reverse=True)[:5]
```

Out[40]:
```
[('requirement document', {'weight': 21.543808138427178}),
 ('data entity', {'weight': 21.543808138427178}),
 ('database design', {'weight': 16.589611828040304}),
 ('business process', {'weight': 13.857307611243959}),
 ('business', {'weight': 10.290551558646024})]
```

In [41]:
```
query = 'second language acquisition'
sorted(G.adj[query].items(), key=lambda x: x[1]['weight'], reverse=True)[:5]
```

Out[41]:
```
[('second language writing', {'weight': 18.958845637706023}),
 ('contrastive analysis', {'weight': 18.958845637706023}),
 ('english as second language', {'weight': 17.37388313698487}),
 ('question analysis', {'weight': 16.958845637706023}),
 ('english as a second language', {'weight': 16.958845637706023})]
```

In [42]:
```
query = 'bernoulli distribution'
sorted(G.adj[query].items(), key=lambda x: x[1]['weight'], reverse=True)[:5]
```

Out[42]:
```
[('multiple outcome', {'weight': 13.698318087482804}),
 ('dynamic decision making', {'weight': 13.698318087482804}),
 ('multivariate gaussian model', {'weight': 13.43528368164901}),
 ('disorder problem', {'weight': 13.212891260312562}),
 ('simultaneous perturbation stochastic approximation',
  {'weight': 13.020246182370165})]
```

In [43]:
```
query = 'business concept'
sorted(G.adj[query].items(), key=lambda x: x[1]['weight'], reverse=True)[:5]
```

Out[43]:
```
[('customer segment', {'weight': 21.543808138427178}),
 ('strategic change', {'weight': 21.543808138427178}),
 ('research knowledge', {'weight': 18.736453216369576}),
 ('secondary data', {'weight': 16.685827143299605}),
 ('business model', {'weight': 15.168768707080254})]
```

In [52]:
```
query = 'algorithm'
sorted(G.adj[query].items(), key=lambda x: x[1]['weight'], reverse=True)[:5]
```

Out[52]:
```
[('attribute oriented induction', {'weight': 5.063633283582013}),
 ('coding algorithm', {'weight': 5.063633283582013}),
 ('resource allocation algorithm', {'weight': 5.063633283582013}),
 ('power control algorithm', {'weight': 5.063633283582013}),
 ('extraction algorithm', {'weight': 5.063633283582013})]
```

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

word 1	word 2	count word 1	count word2	co-occurence	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

Top 20 Related Words

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

In [22]:

```
result = list()
for i, q in enumerate(list(G.nodes)):
    weight = sorted(G.adj[q].items(), key=lambda x: x[1]['weight'], reverse=T

    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[:20]:
    print("query: {}".format(q))
    print("result: {0}, {1}, {2}\n".format(r1, r2, r3))
```

query: gibberellin
result: brassinosteroid, principal mechanism, signalling pathways

query: brassinosteroid
result: gibberellin, principal mechanism, signalling pathways

query: customer segment
result: strategic change, business concept, research knowledge

query: strategic change
result: customer segment, business concept, research knowledge

query: business concept
result: customer segment, strategic change, research knowledge

query: digital single market
result: language grid, single market, multilingualism

query: language grid
result: digital single market, single market, multilingualism

query: poor nutrition
result: mental development, chatbot, immunity

query: mental development
result: poor nutrition, chatbot, immunity

query: coronary ligation
result: isoprenaline, ligation, myocardial infarction

query: isoprenaline
result: coronary ligation, ligation, myocardial infarction

query: synthetic drugs
result: lipolysis, thermogenesis, high morbidity

query: lipolysis
result: synthetic drugs, thermogenesis, high morbidity

query: requirement document
result: data entity, entity relationship model, database design

query: data entity
result: requirement document, entity relationship model, database design

query: entity relationship model
result: requirement document, data entity, database design

query: genetic linkage map
result: superphylum, polyphemus, ecdysozoa

query: superphylum
result: genetic linkage map, polyphemus, ecdysozoa

query: polyphemus
result: genetic linkage map, superphylum, ecdysozoa

query: conductive hearing loss
result: sound stimulation, umbo, eardrum

Visualization

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

In [23]:
```
samples = ["spastic", "hypertonia", "reflex", "muscle", "endophyte", "jatroph
```

In [24]:
```
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("w
            row_temp.append(G.adj[w1][w2]["weight"])
        else:
            row_temp.append(0)
    matrix.append(row_temp)
```

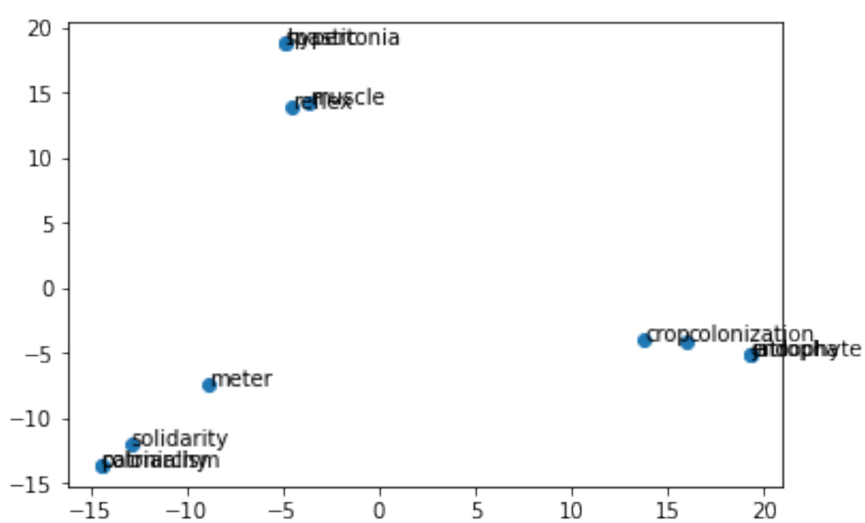
In [25]:
```
from sklearn.decomposition import PCA

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

In [26]:
```
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

- Term Frequency
  - Apply TF transformation when counting words. (`Sublinear tranformation`, `BM25`)
  - Apply smoothing

- Embedding
  - Use cooccurence matrix to train word embeddings (Glove)
  - Or, load word embedding from Glove or Word2Vec and proejct to 2D plot.
  - Evalutate the similarity of two words by using `l1 distance`, `l2 distance`, or `cosine similiarity`.

- Different Approach
  - Try `query expansion`
  - Try `information retrieval` methods to infinitely expand the knowledge graph

- Metric
  - We may investigate `NPMI`
  - `Entropy`

References

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- Useful tutorials
  - https://spark.apache.org/docs/1.6.3/ml-features.html
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  - https://web.stanford.edu/class/cs224n/assignments/a1_preview/exploring_word_vectors
  - https://machinelearningmastery.com/develop-word-embeddings-python-gensim/