# Multi-label Disease Classification from Medline Articles

A huge number of journal articles are published each year focusing on various kinds of diseases. The number of articles is further increased due to the overlapping of scope of various subjects; for instance, articles on medicine and journals on chemistry may both focus on autoimmune diseases.

We'll use this notebook to develop a model which will take in MEDLINE articles and will classify it into one or more disease categories (or even none of the categories) based on the abstract of the article.

#### Import basic packages & set seed for reproducibility

```
In [1]: import numpy as np
import pandas as pd
import os
import sys
import datetime
import matplotlib.pyplot as plt

np.random.seed(7)
```

# Load packages specific to MEDLINE

Use "Medline" package from "biopython" to parse the MEDLINE file(s)

Details of the package are found in:

- http://biopython.org/ (http://biopython.org/)
- <a href="http://biopython.org/DIST/docs/api/Bio-module.html">http://biopython.org/DIST/docs/api/Bio-module.html</a> (http://biopython.org/DIST/docs/api/Bio-module.html)
- http://biopython.org/DIST/docs/api/Bio.Medline-module.html (http://biopython.org/DIST/docs/api/Bio.Medline-module.html)

```
In [2]: from collections import defaultdict
from Bio import Medline
```

# Vectorization of Words (Word Embedding)

Natural language processing (NLP) systems traditionally treat words as discrete atomic symbols. For example, 'tiger' may be represented as "W1" and 'cat' as "W2". These encodings are arbitrary and provide no useful information regarding the relationships that may exist between the individual symbols. Representing words as unique, discrete symbols furthermore leads to data sparsity, and usually means that we may need more data in order to successfully train statistical models. Using vector representations can overcome some of these obstacles.

We want these vectors to be created in such a way that they somehow represent the word and its context, meaning, and semantics. For example, we'd like the vectors for the words 'tiger' and 'cat' to reside in relatively the same area in the vector space when compared to 'car' since they're both animals of the same family of species (viz., 'Felidae'). The vector representation of a word is also known as a word embedding.

To create these "word embedding" (i.e. vector representation of words), we will use the famous "Word2Vec" model instead of reinventing the wheel. The Word2Vec model is created by Google – one of the biggest players in the ML game and was trained on a massive Google News dataset that contained over 100 billion different words.

```
In [3]: import gensim

# Load pre-trained Word2Vec model
modelWord2Vec = gensim.models.KeyedVectors.load_word2vec_format('../utils/Pu
bMed-and-PMC-w2v.bin', binary=True)
vocab_size = len(modelWord2Vec.wv.vocab)

print('Loaded the word vectors!')
print('Total number of words:', vocab_size)
print('Most common words:', modelWord2Vec.wv.index2word[0], modelWord2Vec.wv
.index2word[1], modelWord2Vec.wv.index2word[2])
print('Least common words:', modelWord2Vec.wv.index2word[vocab_size-1], mode
lWord2Vec.wv.index2word[vocab_size-2], modelWord2Vec.wv.index2word[vocab_size-3])
```

```
Loaded the word vectors!
Total number of words: 4087446
Most common words: </s> the ,
Least common words: Fl-NC(11-55) MAA-mediated balsalazide-treated
/home/sxd24/anaconda3/lib/python3.6/site-packages/ipykernel_launcher.py:5: De
precationWarning: Call to deprecated `wv` (Attribute will be removed in 4.0.
0, use self instead).
/home/sxd24/anaconda3/lib/python3.6/site-packages/ipykernel_launcher.py:9: De
precationWarning: Call to deprecated `wv` (Attribute will be removed in 4.0.
0, use self instead).
 if __name__ == '_
                   main
/home/sxd24/anaconda3/lib/python3.6/site-packages/ipykernel_launcher.py:10: D
eprecationWarning: Call to deprecated `wv` (Attribute will be removed in 4.0.
0, use self instead).
  # Remove the CWD from sys.path while we load stuff.
```

# Demonstration - Word Embedding

Let us demonstrate the word embedding by searching our word list for a word like "malignancy" and then access its corresponding vector through the embedding matrix and find out the terms which are close by.

```
In [4]: print('Most similar word to \"malignancy\":')
print(modelWord2Vec.most_similar(positive="malignancy", topn=3))

Most similar word to "malignancy":
   [('neoplasm', 0.7846177816390991), ('neoplasms', 0.7320481538772583), ('malignancies', 0.7179752588272095)]
```

# **Vectorize our Vocabulary**

Set maximum size of the Vocabulary: In an ideal scenario, we would like to use the entire list of words. But due to limited memory availability we'll limit our vocabulary

```
In [5]: maxVocab = 100000
wordsList = list(modelWord2Vec.vocab.keys())[:maxVocab]
```

Create an array to hold the vector representation of all our vocabulary

Note: In case a given word is not present in our vocabulary, assign a random value

```
In [6]: wordVectors = np.zeros((maxVocab, modelWord2Vec.vector_size), dtype='float32')
idx = 0
for word in wordsList:
   if word in modelWord2Vec:
        wordVectors[idx] = modelWord2Vec[word]
   else:
        wordVectors[idx] = np.random.uniform(low=-1, high=1, size=(200, ))
   idx = idx+1
```

# Import a "test record"

Import a test record to test the functions until the main dataset is loaded. Being a single record, it'll also save time & memory during the sanity checks

```
In [7]: with open("../data/medline_abstracts/medline_27253005.txt") as handle:
    testRecord = Medline.read(handle)
    print("PubMed ID:", testRecord['PMID'])
    print("Title of the article:", testRecord['TI'])
    print("Abstract:", testRecord['AB'])
```

PubMed ID: 27253005

Title of the article: Childhood Vascular Tumors Treatment (PDQ(R)): Patient V ersion

Abstract: This PDQ cancer information summary has current information about the treatment of childhood vascular tumors. It is meant to inform and help patients, families, and caregivers. It does not give formal guidelines or recommendations for making decisions about health care. Editorial Boards write the PDQ cancer information summaries and keep them up to date. These Boards are made up of experts in cancer treatment and other specialties related to cancer. The summaries are reviewed regularly and changes are made when there is new information. The date on each summary ("Date Last Modified") is the date of the most recent change. The information in this patient summary was taken from the health professional version, which is reviewed regularly and updated as needed, by the PDQ Pediatric Treatment Editorial Board.

# **Define Utility Functions & Values**

Define the functions and set the values which will be used throughout the script

# Import packages required for data cleansing

```
In [8]: import re
         import nltk
         nltk.download('stopwords')
         nltk.download('punkt')
nltk.download('wordnet')
         from nltk.corpus import stopwords
         from nltk.util import ngrams
         from nltk.tokenize import word_tokenize
         from nltk.stem.wordnet import WordNetLemmatizer
         from string import punctuation
         [nltk_data] Downloading package stopwords to /home/sxd24/nltk_data...
                       Package stopwords is already up-to-date!
         [nltk_data] Downloading package punkt to /home/sxd24/nltk_data...
         [nltk_data] Package punkt is already up-to-date!
         [nltk_data] Downloading package wordnet to /home/sxd24/nltk_data...
                       Package wordnet is already up-to-date!
         [nltk_data]
```

#### **Define the Disease Category List**

Define a list with the category of diseases which we're trying to classify

```
In [9]: categoryList = defaultdict(list)
    categoryLabel = ["hemic-and-lymphatic-diseases", "immune-system-diseases", "mu
    sculoskeletal-diseases", "neoplasms", "other"]
```

# fnGetLabels - Function to return an array corresponding to a label

Define a function which will convert a given category of disease into a corresponding encoded array

```
In [10]: def fnGetLabels(recIdx):
    encodedLabel = np.zeros(len(categoryLabel), dtype='int32')
    idx = 0
    rec = whitelistedArticles[recIdx]
    for label in categoryLabel:
        if rec['diseaseCategory'] in label:
            encodedLabel[idx] = 1
        else:
            encodedLabel[idx] = 0
        idx = idx + 1
    return encodedLabel
```

# Define text cleansing categories

Define and set values for the text cleansing categories

```
In [11]: blacklistStopWords = ['over', 'only', 'very', 'not', 'no']
    additionalStopWords = ['background', 'objective']
                  customStopWords = set(stopwords.words('english') + additionalStopWords) - set(
                  blacklistStopWords)
                  print("Custom StopWords:\n", customStopWords)
                  greekLetters = [
                          (r'α', 'alpha'),
(r'β', 'beta'),
(r'γ', 'gamma'),
(r'δ', 'delta')
                  ]
                  negContractions = [
                          (r'aren\'t', 'are not'),
(r'can\'t', 'can not'),
                         (r'can\'t', 'can not'),
(r'couldn\'t', 'could not'),
(r'daren\'t', 'dare not'),
(r'didn\'t', 'did not'),
(r'doesn\'t', 'does not'),
(r'don\'t', 'do not'),
(r'isn\'t', 'is not'),
(r'hasn\'t', 'has not'),
(r'haven\'t', 'have not'),
(r'mayn\'t', 'may not'),
(r'mightn\'t', 'might not'),
(r'mustn\'t', 'must not'),
(r'oughtn\'t', 'ought not'),
(r'shan\'t', 'shall not'),
(r'shouldn\'t', 'should not')
                           (r'shouldn\'t', 'should not'),
                          (r'wasn\'t', 'was not'),
(r'weren\'t', 'were not'),
(r'won\'t', 'will not'),
                           (r'wouldn\'t', 'would not'),
                           (r'ain\'t', 'am not')
                  otherContractions = {
                          "'m": 'am',
                          "'11": 'will',
                          "'s": 'has',
                          "'d": 'had'
                  }
                  stripSpecialChars = re.compile("[^A-Za-z0-9]+")
                  stripNA = re.compile("^ NA$")
                  lmtzr = WordNetLemmatizer()
```

```
Custom StopWords:
{'been', 'to', 'than', 'd', 'from', 'ma', 'why', 'then', 'again', "you'll",
  "won't", 'such', 'those', 'o', "couldn't", 'myself', 'same', 'being', 'when',
  'have', 'a', 'won', 'they', 'as', 'background', 'y', 'all', 'most', 'so', "ha
  ven't", 'll', "you've", 'of', "weren't", "shan't", 'by', "should've", 'aren',
  'wasn', 'with', 'were', 'ourselves', 'herself', "hasn't", 'couldn', 'i', 'jus
  t', "shouldn't", 'mightn', 'my', 'few', 'each', 'haven', "aren't", 'where',
  'on', 'isn', 'own', 'or', 'out', 'don', 'do', 'be', "that'll", 'that', 'now',
  'weren', 'her', 'mustn', 'these', 'during', 'some', 've', 'them', 'its', 'the
  mselves', 'she', 'shan', "you'd", 'the', 'while', 'yourselves', 're', 'm', 'h
  adn', 'if', 'this', 'objective', "you're", "isn't", 'into', 'himself', 'an',
  's', 'hasn', 'your', 'did', 'doesn', 'above', 'is', 'doing', 'was', 'more',
  'what', 'under', 'too', 'but', 'whom', 'once', 'about', 't', 'his', 'in', 'it
  self', 'here', 'yours', 'ours', 'it', 'me', 'for', 'after', 'yourself', 'he',
  'had', 'can', "didn't", 'down', 'their', 'you', "wasn't", 'will', 'which', 'a
  re', 'through', 'who', "don't", 'we', 'having', 'how', 'at', 'wouldn', "might
  n't", 'until', 'between', 'before', 'hers', 'needn', 'our', 'further', "need
  n't", 'am', 'has', "mustn't", "it's", "doesn't", 'because', 'against', 'belo
  w', 'does', 'theirs', "she's", 'any', 'other', 'shouldn', "hadn't", 'didn',
  'him', 'and', 'both', 'should', 'off', "wouldn't", 'up', 'nor', 'ain', 'ther
  e'}
```

# Define max word length

Even though we'd like to use the entire abstract for prediction, due to hardware limitations we'll set the max word we'll consider per abstract. Similarly, for each sentence we'll set the max word length as 30 words.

```
In [12]: maxFVWordLength = 300
maxSentenceWordLength = 30
```

# fnCleanSentence - Function to cleanse the input text

Define a function to clean a given sentence

```
In [13]: def fnCleanSentence(text):
    text = re.sub(stripNA, "", text)
    text = text.replace("<br />", " ")
    return text
```

# fnComputeNGrams - Function to pre-process a given text

Define a function to process a given text, like transformation, stemming, removing stop-words, etc.

```
In [14]: def fnComputeNGrams(text, n, removeStopwords=True, stemWords=True):
             text = text.strip()
             text = text.lower()
             text = re.sub(r"[^A-Za-z0-9^,!.\/'+-=]", " ", text)
             sents = nltk.sent_tokenize(text)
             allTokens = []
             for doc in sents:
                 #--- Transform Negative Contractions ---#
                 for t in negContractions:
                      doc = re.sub(t[0], t[1], doc)
                 #--- Transform Greek symbols ---#
                 for t in greekLetters:
                      doc = re.sub(t[0], t[1], doc)
                 #--- Convert to Lower case ---#
                 doc = doc.lower()
                 #--- Tokenize the words ---#
                 tokens = word_tokenize(doc)
                 #--- If removal of stop words is requested, do the needful ---#
                 if removeStopwords:
                      #--- Transform other contractions ---#
                      tokens = [otherContractions[token] if otherContractions.get(toke
         n) else token for token in tokens]
                     #--- Remove punctuations ---#
                      r = r'[a-zA-Z]+'
                      tokens = [word for word in tokens if re.search(r, word)]
                      #--- Remove irrelevant stopwords ---#
                      tokens = [token for token in tokens if token not in customStopWo
         rds]
                 #--- If stemmer is requested, perform stemming ---#
                 if stemWords:
                      #--- Lemmatize ---#
                      tokens = [lmtzr.lemmatize(token) for token in tokens]
                 allTokens.extend(tokens)
             #--- If n = 1, then return the list of words (as if n=1, then n-grams =
          tokens), else compute n-grams ---#
             if n == 1:
                 return allTokens
             else:
                 return ngrams(allTokens, n)
```

Check the data cleansing functions (as defined above) with a test record

```
In [15]: | print("Original Text:\n", testRecord['AB'])
         print("\nCleaned Text:\n", fnCleanSentence(testRecord['AB']))
         print("\nn-Gram computed from Text:\n", fnComputeNGrams(testRecord['AB'], 1, T
         rue, True))
```

# Original Text:

This PDQ cancer information summary has current information about the treatm ent of childhood vascular tumors. It is meant to inform and help patients, fa milies, and caregivers. It does not give formal guidelines or recommendations for making decisions about health care. Editorial Boards write the PDQ cancer information summaries and keep them up to date. These Boards are made up of e xperts in cancer treatment and other specialties related to cancer. The summa ries are reviewed regularly and changes are made when there is new informatio n. The date on each summary ("Date Last Modified") is the date of the most re cent change. The information in this patient summary was taken from the healt h professional version, which is reviewed regularly and updated as needed, by the PDQ Pediatric Treatment Editorial Board.

#### Cleaned Text:

This PDQ cancer information summary has current information about the treatm ent of childhood vascular tumors. It is meant to inform and help patients, fa milies, and caregivers. It does not give formal guidelines or recommendations for making decisions about health care. Editorial Boards write the PDQ cancer information summaries and keep them up to date. These Boards are made up of e xperts in cancer treatment and other specialties related to cancer. The summa ries are reviewed regularly and changes are made when there is new informatio n. The date on each summary ("Date Last Modified") is the date of the most re cent change. The information in this patient summary was taken from the healt h professional version, which is reviewed regularly and updated as needed, by the PDQ Pediatric Treatment Editorial Board.

#### n-Gram computed from Text:

n-Gram computed from Text:
 ['pdq', 'cancer', 'information', 'summary', 'current', 'information', 'treat
ment', 'childhood', 'vascular', 'tumor', 'meant', 'inform', 'help', 'patien
t', 'family', 'caregiver', 'not', 'give', 'formal', 'guideline', 'recommendat
ion', 'making', 'decision', 'health', 'care', 'editorial', 'board', 'write',
'pdq', 'cancer', 'information', 'summary', 'keep', 'date', 'board', 'made',
'expert', 'cancer', 'treatment', 'specialty', 'related', 'cancer', 'summary',
'reviewed', 'regularly', 'change', 'made', 'new', 'information', 'date', 'sum
mary', 'date', 'last', 'modified', 'date', 'recent', 'change', 'information',
'patient', 'summary', 'taken', 'health', 'professional', 'version', 'reviewe
d', 'regularly', 'updated', 'needed', 'pdq', 'pediatric', 'treatment', 'edito
rial', 'board'] rial', 'board']

### fnGetArray - Function to convert a text into numerical array

Define a function to convert a text into numerical array for feeding it into the LSTM model

```
In [16]: def fnGetArray(articleRec):
             #--- Define the empty array ---#
             equivArray = np.zeros((maxFVWordLength), dtype='int32')
             idxCnt = 0
             print("Abstracts:", articleRec['AB'])
             cleanedAbstract = fnCleanSentence(articleRec['AB'])
             split = fnComputeNGrams(cleanedAbstract, 1, True, True)
             for word in split:
                 if idxCnt >= maxFVWordLength:
                 try:
                     equivArray[idxCnt] = wordsList.index(word)
                 except ValueError:
                     equivArray[idxCnt] = maxVocab - 1 #conflate all unknown words to t
         his one
                 idxCnt = idxCnt + 1
             return equivArray
```

Check the function fnGetArray to check if the conversion of text to numeric array is working

In [17]: print("Original Text:\n", testRecord['AB'])
print("\nCorresponding Array:\n", fnGetArray(testRecord))

#### Original Text:

This PDQ cancer information summary has current information about the treatm ent of childhood vascular tumors. It is meant to inform and help patients, fa milies, and caregivers. It does not give formal guidelines or recommendations for making decisions about health care. Editorial Boards write the PDQ cancer information summaries and keep them up to date. These Boards are made up of experts in cancer treatment and other specialties related to cancer. The summa ries are reviewed regularly and changes are made when there is new information. The date on each summary ("Date Last Modified") is the date of the most recent change. The information in this patient summary was taken from the healt h professional version, which is reviewed regularly and updated as needed, by the PDQ Pediatric Treatment Editorial Board.

Abstracts: This PDQ cancer information summary has current information about the treatment of childhood vascular tumors. It is meant to inform and help pa tients, families, and caregivers. It does not give formal guidelines or recom mendations for making decisions about health care. Editorial Boards write the PDQ cancer information summaries and keep them up to date. These Boards are m ade up of experts in cancer treatment and other specialties related to cance r. The summaries are reviewed regularly and changes are made when there is ne w information. The date on each summary ("Date Last Modified") is the date of the most recent change. The information in this patient summary was taken from the health professional version, which is reviewed regularly and updated as needed, by the PDQ Pediatric Treatment Editorial Board.

Corresponding Array	<b>/</b> :
---------------------	------------

	Jonatha	-									
[99999	120	248	2456	382	248	58	2033		209	11781	7003
1142	145	405	9904	29	1978	5248	6885	7805	1768	2012	166
207	17560	7153	14280	99999	120	248	2450	5839	1747	7153	490
5186	120	58	8617	241	120	2450	1173	6165	316	490	183
248	1747	2450	1747	1030	1015	1747	555	316	248	145	2450
862	166	2929	1621	1173	6165	7165	905	99999	2071	58	17560
7153	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0]

#### Set the disease categories

Set the disease categories

```
In [18]: diseaseCategories = []
         diseaseCategoryRec = {'diseaseType': 'hemic-and-lymphatic-diseases', 'fileNa
         me': '../data/medline_abstracts/hemic-and-lymphatic-diseases.medline.txt'}
         diseaseCategories.append(diseaseCategoryRec)
         diseaseCategoryRec = {'diseaseType': 'immune-system-diseases', 'fileName':
          ../data/medline abstracts/immune-system-diseases.medline.txt'}
         diseaseCategories.append(diseaseCategoryRec)
         diseaseCategoryRec = {'diseaseType': 'musculoskeletal-diseases', 'fileName':
           '../data/medline_abstracts/musculoskeletal-diseases.medline.txt'}
         diseaseCategories.append(diseaseCategoryRec)
         diseaseCategoryRec = {'diseaseType': 'neoplasms', 'fileName': '../data/medli
         ne_abstracts/neoplasms.medline.txt'}
         diseaseCategories.append(diseaseCategoryRec)
         diseaseCategoryRec = {'diseaseType': 'other', 'fileName': '../data/medline_a
         bstracts/none-of-the-above.medline.txt'}
         diseaseCategories.append(diseaseCategoryRec)
         print("diseaseCategories:\n", diseaseCategories)
```

#### diseaseCategories:

```
[{'diseaseType': 'hemic-and-lymphatic-diseases', 'fileName': '../data/medlin e_abstracts/hemic-and-lymphatic-diseases.medline.txt'}, {'diseaseType': 'immu ne-system-diseases', 'fileName': '../data/medline_abstracts/immune-system-diseases.medline.txt'}, {'diseaseType': 'musculoskeletal-diseases', 'fileName': '../data/medline_abstracts/musculoskeletal-diseases.medline.txt'}, {'diseaseType': 'neoplasms', 'fileName': '../data/medline_abstracts/neoplasms.medline.txt'}, {'diseaseType': 'other', 'fileName': '../data/medline_abstracts/none-of-the-above.medline.txt'}]
```

# Load and Prepare the Data

# Define the datasets for holding the data

```
In [19]: quarantineArticles = []
whitelistedArticles = []
```

### **Load the MEDLINE data (MEDLINE format)**

Set the baseline for minumum number of words in each abstract for the abstract to be qualified for processing. If it does not meet the criteria, discard the article

```
In [20]: minAbstractLength = 25
         for medlineCategory in diseaseCategories:
             print("\nCategory:", medlineCategory['diseaseType'])
             print("File Name:", medlineCategory['fileName'])
             numQuarantinedRec = 0
             numWhitelistedRec = 0
             with open(medlineCategory['fileName'], "r", encoding='utf-8') as f:
                 recArticle = Medline.parse(f)
                 for rec in recArticle:
                     lenAbstract = len(rec['AB'])
                     lenFeatureVector = len(rec['TI']) + len(rec['AB'])
                     articleRec = {'PMID': rec['PMID'], 'diseaseCategory': medlineCateg
         ory['diseaseType'], 'FV': rec['TI']+rec['AB'], 'numWords': lenFeatureVector}
                     if lenAbstract < minAbstractLength:</pre>
                         quarantineArticles.append(articleRec)
                         numQuarantinedRec = numQuarantinedRec + 1
                     else:
                         whitelistedArticles.append(articleRec)
                         numWhitelistedRec = numWhitelistedRec + 1
             print("For category,", medlineCategory['diseaseType'], "number of discarde
         d articles = ", numQuarantinedRec)
             print("For category,", medlineCategory['diseaseType'], "number of white-li
         sted articles = ", numWhitelistedRec)
         #--- Print the final numbers ---#
         print("\nFor categories, total number of discarded articles = ", len(quarantin
         eArticles))
         print("For all categories, total number of white-listed articles = ", len(whit
         elistedArticles))
         Category: hemic-and-lymphatic-diseases
         File Name: ../data/medline_abstracts/hemic-and-lymphatic-diseases.medline.txt
         For category, hemic-and-lymphatic-diseases number of discarded articles = 1
         For category, hemic-and-lymphatic-diseases number of white-listed articles =
         12242
         Category: immune-system-diseases
         File Name: ../data/medline_abstracts/immune-system-diseases.medline.txt
         For category, immune-system-diseases number of discarded articles = 2
         For category, immune-system-diseases number of white-listed articles = 23963
         Category: musculoskeletal-diseases
         File Name: ../data/medline abstracts/musculoskeletal-diseases.medline.txt
         For category, musculoskeletal-diseases number of discarded articles = 4
         For category, musculoskeletal-diseases number of white-listed articles = 179
         23
         Category: neoplasms
         File Name: ../data/medline_abstracts/neoplasms.medline.txt
         For category, neoplasms number of discarded articles = 7
         For category, neoplasms number of white-listed articles = 30559
         Category: other
         File Name: ../data/medline_abstracts/none-of-the-above.medline.txt
         For category, other number of discarded articles = 2
         For category, other number of white-listed articles = 12247
         For categories, total number of discarded articles = 16
         For all categories, total number of white-listed articles = 96934
```

Check the discarded records for assurity

```
In [21]: print ("Discarded records:\n")
for rec in quarantineArticles:
    print(rec['PMID'], rec['numWords'], rec['diseaseCategory'], rec['FV'])
```

#### Discarded records:

29033247 113 hemic-and-lymphatic-diseases Progressive reticulate skin pigment ation and anonychia in a patient with bone marrow failure.KEY TEACHING POINT S.

28536734 102 immune-system-diseases Livedo Reticularis on the Lower Limbs in a Patient with Lupus Erythematosus: A Quiz.is missing (Quiz).

28251232 87 immune-system-diseases Oral diseases associated with fixed prosth odontic restorations.[No Abstract Available].

29076861 103 musculoskeletal-diseases Nondrug Interventions Reduce Pain and O pioid Use After Total Knee Arthroplasty.According to this study.

29033247 113 musculoskeletal-diseases Progressive reticulate skin pigmentatio n and anonychia in a patient with bone marrow failure.KEY TEACHING POINTS.

28440364 91 musculoskeletal-diseases Diagnosis of an actively bleeding rectus sheath hematoma by Contrast- Enhanced ultrasound..

28440363 97 musculoskeletal-diseases Ultrasound Imaging for Posterior Knee Pain: Tibial Nerve Schwannoma Not Popliteus Muscle Strain..

29076862 106 neoplasms Similar Mortality Rates After Surgery or Observation of Localized Prostate Cancer. According to this study.

28686217 93 neoplasms Meta-Analysis on Dietary Patterns and Pancreatic Cancer Risk: Methodological Limitations.n/a.

28686193 88 neoplasms Reply to Alizadeh's Letter to the Editor Re: Lu, P.Y. e t al., Nutrients 2017, 9, 38.n/a.

28629197 243 neoplasms Reply to the Letter to the Editor by C. Nicolazzo et a l.: "Circulating Cell-Free DNA and Circulating Tumor Cells as Prognostic and Predictive Biomarkers in Advanced Non-Small Cell Lung Cancer Patients Treated with First-Line Chemotherapy".n/a.

28629196 207 neoplasms Letter to the Editor: "Circulating Cell-Free DNA and C irculating Tumor Cells as Prognostic and Predictive Biomarkers in Advanced No n-Small Cell Lung Cancer Patients Treated with First-Line Chemotherapy".n/a. 28578450 150 neoplasms Serologic evidence of Toxoplasma gondii infection amon g cancer patients. A prospective study from Qassim region, Saudi Arabia.[No A

bstract Available]. 28561877 79 neoplasms Subcutaneous Nodule on the Right Palm of a Young Boy: A Quiz.is missing (Quiz).

28000494 42 other Twiddler's syndrome.No abstract available.

27444081 88 other Early-onset stroke, polyarteritis nodosa (PAN), and livedo racemosa.KEY TEACHING POINTS.

#### Shuffle the data to achieve randomness

Shuffle the "whitelist" dataset multiple times so that we get a random order and records are not ordered by disease

```
In [22]: np.random.shuffle(whitelistedArticles)
    np.random.shuffle(whitelistedArticles)
```

#### Persist the data for reloadability

Save the data onto disk as numpy arrays for easier reloads

```
In [23]: np.save('../data/medline_abstracts/npQuarantineArticles_CloselyAssociatedDisea
    ses', quarantineArticles)
    np.save('../data/medline_abstracts/npWhiteListArticles_CloselyAssociatedDiseas
    es', whitelistedArticles)
```

# **Data Profiling**

Perform data profiling and also re-confirm the validity of the hypothesis made before

```
In [24]: numQuarantined = len(quarantineArticles)
    numWhiteListArticles = len(whitelistedArticles)

print("Number of articles discarded due to smaller than threshold abstracts
    =", numQuarantined)
print("Number of articles that will be processed =", numWhiteListArticles)
```

Number of articles discarded due to smaller than threshold abstracts = 16 Number of articles that will be processed = 96934

#### **Calculate the Metrices**

Calculate the following metrices:

- Number of words per abstract
- · Number of sentences per abstract
- · Number of words per sentence per abstract

```
wordCntPerSentence = []
In [25]:
         wordCntPerFV = []
         sentenceCntPerFV = []
         print("Convert whitelistedArticles into dataframe")
         dfWhiteListArticles = pd.DataFrame(whitelistedArticles, columns=['PMID', 'dise
         aseCategory', 'FV', 'numWords'])
         print(dfWhiteListArticles.head(5))
         for fv in dfWhiteListArticles['FV']:
             words = fv.split(' ')
             wordCntPerFV.append(len(words))
             sentences = fv.split('.')
             sentenceCntPerFV.append(len(sentences))
             for sentence in sentences:
                 words = sentence.split(' ')
                 wordCntPerSentence.append(len(words))
```

```
Convert whitelistedArticles into dataframe
       PMID
                     diseaseCategory
 28363295 musculoskeletal-diseases
0
  28188909 musculoskeletal-diseases
1
  28636109 musculoskeletal-diseases
  28704329
                           neoplasms
3
4 28813639
                           neoplasms
                                                 FV numWords
0 Biological Principles of Scar and Contracture....
                                                          700
1 Extensive preclinical evaluation of an inflixi...
                                                         1255
2 Xq26.1-26.3 duplication including MOSPD1 and G...
                                                         1316
  Long-Term Oncological Outcome After Convention...
                                                         1996
3
4 Exploitation of Gene Expression and Cancer Bio...
                                                         1794
```

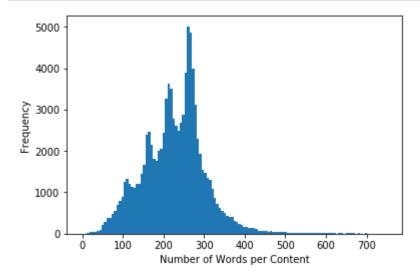
Print the number of words per content for 50 articles to eyeball the count

```
In [26]: print(wordCntPerFV[1:50])
      [160, 186, 271, 257, 214, 93, 272, 118, 180, 240, 51, 90, 165, 110, 369, 200, 148, 171, 284, 404, 132, 164, 159, 221, 218, 266, 278, 150, 224, 299, 266, 21 0, 164, 166, 268, 238, 392, 390, 711, 239, 331, 281, 139, 268, 184, 167, 98, 144, 165]
```

Plot the data to visualize the distribution of words by content

```
In [27]: %matplotlib inline
   plt.hist(wordCntPerFV, bins=125, range=(0, 750))
   plt.xlabel('Number of Words per Content')
   plt.ylabel('Frequency')
   plt.show()

   print("Median of the number of words per content =", np.median(wordCntPerFV))
```

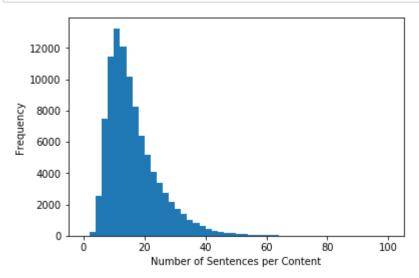


Median of the number of words per content = 231.0

Based on the above histogram we can say that our hypothesis of setting the maxFVWordLength to the value we've chosen earlier holds good!

```
In [28]: %matplotlib inline
   plt.hist(sentenceCntPerFV, bins=50, range=(0, 100))
   plt.xlabel('Number of Sentences per Content')
   plt.ylabel('Frequency')
   plt.show()

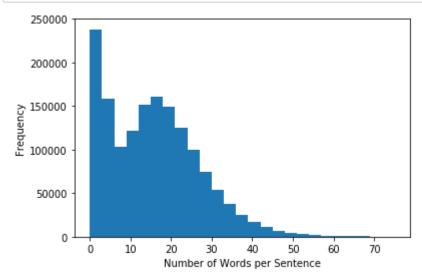
   print("Median of the number of sentences per content =", np.median(sentenceCnt PerFV))
```



Median of the number of sentences per content = 14.0

```
In [29]: %matplotlib inline
   plt.hist(wordCntPerSentence, bins=25, range=(0, 75))
   plt.xlabel('Number of Words per Sentence')
   plt.ylabel('Frequency')
   plt.show()

   print("Median of the number of words per sentences =", np.median(wordCntPerSen tence))
```



Median of the number of words per sentences = 15.0

Based on the above histogram we can say that our hypothesis of setting the maxSentenceWordLength to the value we've chosen earlier holds good!

```
In [30]: print("Total number of articles =", numWhiteListArticles)
    print("Median of the number of sentences per content =", np.median(sentenceCnt
    PerFV))
    print("Median of the number of words per content =", np.median(wordCntPerFV))
    print("Median of the number of words per sentences of articles =", np.median(w
    ordCntPerSentence))
```

```
Total number of articles = 96934

Median of the number of sentences per content = 14.0

Median of the number of words per content = 231.0

Median of the number of words per sentences of articles = 15.0
```

#### Vectorize the data - Encode all the Labels & Content

Convert all articles into categorized labels and all the contents into vectors

```
In [31]: print("Starting data encoding @", datetime.datetime.now().strftime("%Y-%m-%d _
          %H:%M:%S"))
         #--- Shuffle the dataset for one last time before encoding ---#
         np.random.shuffle(whitelistedArticles)
         articleIdx = 0
         articleToID = {}
         encodedLabels = np.zeros((numWhiteListArticles, len(categoryLabel)), dtype=
          'int32')
         encodedFV = np.zeros((numWhiteListArticles, maxFVWordLength), dtype='int32')
         articleToIDChkPoint = "../data/medline_abstracts/checkpoints/articleToID.che
         encodedLabelChkPoint = "../data/medline_abstracts/checkpoints/encodedLabel.c
         heckpoint-"
         encodedFVChkPoint = "../data/medline_abstracts/checkpoints/encodedFV.checkpo
         int-"
         #--- Loop through all white-listed articles in the dataset and convert them
          into vector ---#
         for articleRec in whitelistedArticles:
             #--- Convert the articles into IDs ---#
             articlePMID = articleRec['PMID']
             articleToID[articlePMID] = articleIdx
             #--- Encode the labels ---#
             encodedLabels[articleIdx] = fnGetLabels(articleIdx)
             #--- Encode the feature vectors ---#
             wordCounter = 0
             cleanedFV = fnCleanSentence(articleRec['FV'])
             split = fnComputeNGrams(cleanedFV, 1, True, True)
             for word in split:
                 try:
                      encodedFV[articleIdx][wordCounter] = wordsList.index(word)
                  except:
                      #--- Assign all unknown words to the maximum value possible ---#
                      encodedFV[articleIdx][wordCounter] = maxVocab - 1
                 #--- Increment the wordCounter ---#
                 wordCounter = wordCounter + 1
                  if wordCounter >= maxFVWordLength:
                      break
             #--- Increment the articleIdx ---#
             articleIdx = articleIdx + 1
             #--- Checkpoint ---#
             if articleIdx % 10000 == 0:
                 numChkPoint = int(articleIdx / 10000)
                 \label{lem:print("\nCheckpoint", numChkPoint, "@", datetime.datetime.now().strf} \\
         time("%Y-%m-%d %H:%M:%S"), "::", articleIdx, "articles processed")
                 np.save(articleToIDChkPoint+str(numChkPoint), articleToID)
                  np.save(encodedLabelChkPoint+str(numChkPoint), encodedLabels)
                 np.save(encodedFVChkPoint+str(numChkPoint), encodedFV)
         #--- Persist the final encoded dataset ---#
         np.save('.../data/medline_abstracts/articleToID', articleToID)
         np.save('../data/medline_abstracts/encodedLabels', encodedLabels)
         np.save('../data/medline_abstracts/encodedFV', encodedFV)
         print("Completed data encoding @", datetime.datetime.now().strftime("%Y-%m-%
         d %H:%M:%S"))
```

```
Starting data encoding @ 2018-04-08 20:34:14
```

```
Checkpoint 1 @ 2018-04-08 20:40:41 :: 10000 articles processed

Checkpoint 2 @ 2018-04-08 20:47:14 :: 20000 articles processed

Checkpoint 3 @ 2018-04-08 20:53:45 :: 30000 articles processed

Checkpoint 4 @ 2018-04-08 21:00:12 :: 40000 articles processed

Checkpoint 5 @ 2018-04-08 21:06:43 :: 50000 articles processed

Checkpoint 6 @ 2018-04-08 21:13:12 :: 60000 articles processed

Checkpoint 7 @ 2018-04-08 21:19:39 :: 70000 articles processed

Checkpoint 8 @ 2018-04-08 21:25:50 :: 80000 articles processed

Checkpoint 9 @ 2018-04-08 21:32:08 :: 90000 articles processed

Checkpoint 9 @ 2018-04-08 21:32:08 :: 90000 articles processed

Completed data encoding @ 2018-04-08 21:36:26
```

#### Remove the checkpoint files

```
In [32]: os.system('rm -f ../data/medline_abstracts/checkpoints/*.checkpoint-*.npy')
Out[32]: 0
```

# Eye ball the encoding, as done above

```
In [33]: print("articleToID for PMID = 29538200\n", articleToID['29538200'])
         print("Disease Label for PMID = 29538200\n", encodedLabels[articleToID['295382
         00'11)
         print("Encoded Abstract for PMID = 29538200\n", encodedFV[articleToID['2953820
         articleToID for PMID = 29538200
          41012
         Disease Label for PMID = 29538200
          [10000]
         Encoded Abstract for PMID = 29538200
                              516 429 603 4104 5125
                                                              925
                                                                    195
                                                                          327
                                                                                414
          [99999 7314 1010
          99999 50722
                        424 2467 1010
                                            87
                                                677 61403 16363 1680
                                                                         709
                                                                               566
           1065 1400 15560
                              505
                                    331 6484
                                               505 6756
                                                             314
                                                                   505 10691
                                                                               505
                                                      287 99999 7314
           3097 4279 9315
                               48
                                    416 27016 1906
                                                                         145 3062
                  195 29136 2075 1026 14671 9604 4824
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```

0]

#### fnLoadData - Function to split the dataset and make it ready for LSTM

Develop a function which will take the dataset and split it and return a LSTM ready dataset

```
In [34]: def fnLoadData(splitRatio):
    print("Starting the data wrangling @", datetime.datetime.now().strftime("%
    Y-%m-%d %H:%M:%S"))

    numTestSet = int(numWhiteListArticles*splitRatio)
    numTrainingSet = numWhiteListArticles - numTestSet
    print("Size of Test Set =", numTestSet)
    print("Size of Training Set =", numTrainingSet)

    x_train = encodedFV[0:numTrainingSet, ]
    y_train = encodedLabels[0:numTrainingSet, ]

    x_test = encodedFV[numTrainingSet:numWhiteListArticles, ]
    y_test = encodedLabels[numTrainingSet:numWhiteListArticles, ]

    return (x_train, y_train), (x_test, y_test)
```

# **Create Training and Validation Datasets**

#### Split the dataset into training & test data

Split the entire dataset into training data and test data. As of now, we'll keep 80% of the data for training and 20% for testing

```
In [35]: (x_train, y_train), (x_test, y_test) = fnLoadData(0.2)

Starting the data wrangling @ 2018-04-08 21:38:41
Size of Test Set = 19386
Size of Training Set = 77548
```

Check the dimensions of the training and test data sets

```
In [36]: [x_train.shape, y_train.shape, x_test.shape, y_test.shape]
Out[36]: [(77548, 300), (77548, 5), (19386, 300), (19386, 5)]
```

# ANN Architecture: Fully Connected Deep Learning Neural Network

# **Load Dependencies**

Load the packages that will be required

```
In [37]: import keras
    from keras import regularizers
    from keras.models import Sequential
    from keras.layers import Dense, Flatten, Dropout, Embedding
    from keras.layers.normalization import BatchNormalization
    from keras.optimizers import adam
```

/home/sxd24/anaconda3/lib/python3.6/site-packages/h5py/\_\_init\_\_.py:36: Future Warning: Conversion of the second argument of issubdtype from `float` to `np. floating` is deprecated. In future, it will be treated as `np.float64 == np.d type(float).type`.

from .\_conv import register\_converters as \_register\_converters Using TensorFlow backend.

#### Set the hyper parameters

Set the hyper-parameters which will be used in subsequent model generation

```
In [38]: #--- Training ---#
         epochs = 10
         batch_size = 128
         #--- Vector-Space Embedding ---#
         n_dim = modelWord2Vec.vector_size
         n_unique_words = maxVocab
         # n_words_to_skip = 5
         max_review_length = maxFVWordLength
         #--- Dense Layer Architecture ---#
         n dense = 128
         dropout_ratio = 0.35
         #--- Print the hyper-parameters which are set from other variables ---#
         print("n_dim =", n_dim)
         print("n_unique_words =", n_unique_words)
         print("max_review_length =", max_review_length)
         n_dim = 200
         n unique words = 100000
         max_review_length = 300
```

#### Design the ANN architecture

```
In [39]: modelFCDL = Sequential()
         \verb|modelFCDL.add| (Embedding (n\_unique\_words, n\_dim, input\_length=max\_review\_length)| \\
         ))
         # model.add(LSTM(units=200, activation='softsign'))
         modelFCDL.add(Dense(n_dense, activation='relu', input_dim=n_dim))
         modelFCDL.add(Dropout(dropout_ratio))
         modelFCDL.add(Dense(n_dense, activation='relu'))
         modelFCDL.add(Flatten())
         modelFCDL.add(Dense(5, activation='sigmoid')) # mathematically equivalent to s
         oftmax with 5 classes
         #--- Display the architecture of the generated model ---#
         modelFCDL.summary()
```

Layer (type)	Output Shape	Param #
embedding_1 (Embedding)	(None, 300, 200)	20000000
dense_1 (Dense)	(None, 300, 128)	25728
dropout_1 (Dropout)	(None, 300, 128)	0
dense_2 (Dense)	(None, 300, 128)	16512
dropout_2 (Dropout)	(None, 300, 128)	0
dense_3 (Dense)	(None, 300, 128)	16512
dropout_3 (Dropout)	(None, 300, 128)	0
dense_4 (Dense)	(None, 300, 128)	16512
dropout_4 (Dropout)	(None, 300, 128)	0
dense_5 (Dense)	(None, 300, 128)	16512
dropout_5 (Dropout)	(None, 300, 128)	0
dense_6 (Dense)	(None, 300, 128)	16512
flatten_1 (Flatten)	(None, 38400)	0
dense_7 (Dense)	(None, 5)	192005
Total params: 20,300,293 Trainable params: 20,300,2 Non-trainable params: 0	93	

# **Configure Model**

```
In [40]: modelFCDL.compile(loss='categorical_crossentropy', optimizer='adam', metrics=[
    'accuracy'])
# tensorboard = keras.callbacks.TensorBoard(log_dir="../logs", write_graph=Tru
    e, write_images=True, histogram_freq=1)
```

# **Train the Model**

```
In [41]: print("Starting the model training @", datetime.datetime.now().strftime("%Y-_
      %m-%d %H:%M:%S"), "...")
      modelFCDL.fit(x train, y train,
            batch_size=batch_size,
            epochs=epochs,
            verbose=1,
            validation_data=(x_test, y_test),
            shuffle=False)
      print("Completed the model training @", datetime.datetime.now().strftime("%Y
      -%m-%d %H:%M:%S"))
      Starting the model training @ 2018-04-08 21:39:19 ...
      Train on 77548 samples, validate on 19386 samples
      Epoch 1/10
      acc: 0.5178 - val_loss: 1.0632 - val_acc: 0.5880
      Epoch 2/10
      acc: 0.6674 - val_loss: 0.9168 - val_acc: 0.6479
      Epoch 3/10
      acc: 0.7111 - val_loss: 0.8397 - val_acc: 0.6934
      Epoch 4/10
      acc: 0.7535 - val_loss: 0.7581 - val_acc: 0.7193
      Epoch 5/10
      acc: 0.7687 - val_loss: 0.7634 - val_acc: 0.7284
      Epoch 6/10
      acc: 0.7780 - val_loss: 0.7759 - val_acc: 0.7266
      Epoch 7/10
      77548/77548 [============ ] - 554s 7ms/step - loss: 0.5133 -
      acc: 0.7801 - val_loss: 0.8014 - val_acc: 0.7265
      acc: 0.7849 - val_loss: 0.7866 - val_acc: 0.7271
      Epoch 9/10
      77548/77548 [============== ] - 552s 7ms/step - loss: 0.4774 -
      acc: 0.7888 - val_loss: 0.8272 - val_acc: 0.7182
      Epoch 10/10
```

# Extra Code - Do not execute, but for reuse

acc: 0.7895 - val\_loss: 0.8288 - val\_acc: 0.7202 Completed the model training @ 2018-04-08 23:11:26

# ANN Architecture - Multi-ConvNet Deep Learning Neural Network

```
In [ ]: import keras
    from keras import regularizers
    from keras.models import Model
    from keras.layers import Dense, Dropout, Embedding, Input, concatenate, Spatia
    lDropout1D, Conv1D, GlobalMaxPooling1D
    from keras.layers.normalization import BatchNormalization
    from keras.optimizers import adam
```

#### Set the hyper parameters

Set the hyper-parameters which will be used in subsequent model generation

```
In [ ]: #--- Training ---#
        epochs = 6
         batch size = 128
         #--- Vector-Space Embedding ---#
        n_dim = modelWord2Vec.vector_size
         n_unique_words = maxVocab
         # n_words_to_skip = 5
         max_review_length = maxFVWordLength
         dropout_ratio_embed = 0.2
         #--- Convolutional Layer Architecture:
         n_{conv_1} = n_{conv_2} = n_{conv_3} = 128
         k_{\text{conv}} = 3
         k_{conv_2} = 2
         k_{conv_3} = 4
         #--- Dense Layer Architecture ---#
         n dense = 128
         dropout_ratio = 0.4
         #--- Print the hyper-parameters which are set from other variables ---#
         print("n_dim =", n_dim)
         print("n_unique_words =", n_unique_words)
         print("max_review_length =", max_review_length)
```

#### **Design the ConvNet Architecture**

ANN architecture with ConvNets

```
In [ ]: input_layer = Input(shape=(max_review_length,), dtype='int16', name='input') #
         supports integers +/- 32.7k
        embedding_layer = Embedding(n_unique_words, n_dim, input_length=max_review_len
        gth, name='embedding')(input_layer)
        drop_embed_layer = SpatialDropout1D(dropout_ratio_embed, name='drop_embed')(em
        bedding_layer)
        conv_1 = Conv1D(n_conv_1, k_conv_1, activation='relu', name='conv_1')(drop_emb
        ed_layer)
        maxp_1 = GlobalMaxPooling1D(name='maxp_1')(conv_1)
        conv_2 = Conv1D(n_conv_2, k_conv_2, activation='relu', name='conv_2')(drop_emb
        ed_layer)
        maxp_2 = GlobalMaxPooling1D(name='maxp_2')(conv_2)
        conv\_3 = Conv1D(n\_conv\_3, k\_conv\_3, activation='relu', name='conv\_3')(drop\_emb)
        ed layer)
        maxp_3 = GlobalMaxPooling1D(name='maxp_3')(conv_3)
        concat = concatenate([maxp_1, maxp_2, maxp_3])
        dense_layer = Dense(n_dense, activation='relu', name='dense')(concat)
        drop_dense_layer = Dropout(dropout_ratio, name='drop_dense_01')(dense_layer)
        dense_2 = Dense(128, activation='relu', name='dense_2')(drop_dense_layer)
        dropout_2 = Dropout(dropout_ratio, name='drop_dense_2')(dense_2)
        predictions = Dense(5, activation='sigmoid', name='output')(dropout_2)
        modelCNN = Model(input_layer, predictions)
        #--- Display the architecture of the generated model ---#
        modelCNN.summary()
```

#### **Configure Model**

```
In [ ]: modelCNN.compile(loss='categorical_crossentropy', optimizer='adam', metrics=[
    'accuracy'])
# tensorboard = keras.callbacks.TensorBoard(log_dir="../logs", write_graph=Tru
    e, write_images=True, histogram_freq=1)
```

#### **Train the Model**

```
In [ ]: print("Starting the model training @", datetime.datetime.now().strftime("%Y-%m
        -%d %H:%M:%S"), "...")
        modelCNN.fit(x_train, y_train,
                  batch_size=batch_size,
                  epochs=epochs,
                  verbose=1,
                  validation_data=(x_test, y_test),
                  shuffle=False)
        print("Completed the model training @", datetime.datetime.now().strftime("%Y-%
        m-%d %H:%M:%S"))
In [ ]: import psutil
        psutil.virtual_memory()
In [ ]: #--- Create model checkpoint ---#
        modelOutputDir = '../model-output/ann'
        modelcheckpoint = ModelCheckpoint(filepath=output_dir+"/weights.{epoch:02d}.hd
        f5")
        if not os.path.exists(output_dir):
            os.makedirs(output_dir)
```

Check the function fnGetLabels() with some test data

```
In [ ]: print("Encoded label for article with index = 0:\n", fnGetLabels(32000))
```

## Load the data if datasets are empty

Load data from the \*.npy if the datasets are empty

```
In [ ]: print(whitelistedArticles)
```