

pre__process

September 18, 2024

1 Preprocess Required for Generating Train Data:

```
[1]: import urllib.request
import time
import sys
import getopt
import pandas as pd
import numpy as np
import pickle
```

```
[11]: %run ../utils.ipynb
```

```
[2]: embSize = 200

ftrain='../data/EUADR_target_disease.csv'
# Replace with path of word embdding file
#wefile = "/mnt/admin/GDA_backup/Dataset/embeddings/PubMed-and-PMC-w2v.bin"
wefile = "../support/PubMed-and-PMC-w2v.bin"
random_seed=1331
```

```
[11]: import pandas as pd
from tabulate import tabulate
ftrain = '../data/EUADR_target_disease.csv'
with open(ftrain, 'r', encoding='latin1') as file:
    first_line = file.readline()
    print(first_line)
import pandas as pd

ftrain = '../data/EUADR_target_disease.csv'

# Specify the delimiter for tabs
df = pd.read_csv(ftrain, encoding='latin1', sep='\t')

# Display the first 10 rows of the DataFrame as a table
print(tabulate(df.head(4), headers='keys', tablefmt='grid'))
```

```
"ASSOCIATION_TYPE"      "PMID"  "NUM_SENTENCE"  "ENTITY1_TEXT"  "ENTITY1_INI"
```

```
"ENTITY1_END"    "ENTITY1_TYPE"  "ENTITY2_TEXT"  "ENTITY2_INI"   "ENTITY2_END"
"ENTITY2_TYPE"   "SENTENCE"
```

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|   | ASSOCIATION_TYPE |   PMID |   NUM_SENTENCE | ENTITY1_TEXT   |
ENTITY1_INI |   ENTITY1_END | ENTITY1_TYPE           | ENTITY2_TEXT   |
ENTITY2_INI |   ENTITY2_END | ENTITY2_TYPE           | SENTENCE
|
```

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```
| 0 | SA           | 17241106 |   16 | LRP5           |
19 |               23 | Genes & Molecular Sequences | osteoporosis   |
80 |               92 | Diseases & Disorders | Our work supported LRP5 genetic
variants as possible susceptibility factors for osteoporosis and fractures in
humans. |
```

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| 1 | SA           | 17241106 |   17 | rs491347       |
20 |               28 | SNP & Sequence variations | osteoporosis   |
108 |              120 | Diseases & Disorders | Especially, the SNP rs491347 and
its strongly associated SNPs (e.g., rs1784235) could be important to human
osteoporosis phenotypes. |
```

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| 2 | SA           | 17241106 |   17 | rs1784235      |
69 |               78 | SNP & Sequence variations | osteoporosis   |
108 |              120 | Diseases & Disorders | Especially, the SNP rs491347 and
its strongly associated SNPs (e.g., rs1784235) could be important to human
osteoporosis phenotypes. |
```

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```
-----+
| 3 | FA           | 18697826 |   0 | fetal haemoglobin |
```


-----+						
2 SA	17241106	17 rs1784235				
69	78 SNP & Sequence variations	osteoporosis				
108	120 Diseases & Disorders	Especially, the SNP				
rs491347 and its strongly associated SNPs (e.g., rs1784235) could be important to human osteoporosis phenotypes.						
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-----+						
3 FA	18697826	0 fetal haemoglobin				
93	110 Genes & Molecular Sequences	beta-				
thalassaemia	132	149 Diseases &				
Disorders The HBS1L-MYB intergenic region on chromosome 6q23 is a quantitative trait locus controlling fetal haemoglobin level in carriers of beta-						
thalassaemia.						
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4 PA	18697826	1 HbF				
19	22 Genes & Molecular Sequences	HBB disorders				
64	77 Diseases & Disorders	Fetal haemoglobin (HbF)				
level modifies the clinical severity of HBB disorders.						
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5 PA	18697826	1 Fetal haemoglobin				

unravel the biological significance of this region in regulating HbF production is clearly indicated, which may lead to new strategies to modify the disease course of severe HBB disorders.

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| 9 | PA | 18322311 | 0 | TNFalpha gene
polymorphisms | 16 | 43 | Genes & Molecular Sequences
| multiple sclerosis | 69 | 87 |
Diseases & Disorders | IL-1, IL-1R and TNFalpha gene polymorphisms in Iranian
patients with multiple sclerosis.

```

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| 10 | FA | 18322311 | 7 | IL-1alpha TT -889
| 35 | 52 | SNP & Sequence variations | multiple
sclerosis | 406 | 424 | Diseases &
Disorders | On the other hand the frequency of IL-1alpha TT -889 genotype
(p=0.028), IL-1R C pst1 1970 allele (p=0.0001) and CC genotype (p=0.00006),
TNFalpha G -308 allele (p=0.0002) and GG genotype (p=0.000001) decreased
significantly in the patients versus normal subjects. These results suggest that
polymorphic variations of these pro-inflammatory cytokines may play an important
role in susceptibility of Iranian multiple sclerosis patients.

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| 11 | PA | 18322311 | 7 | TNFalpha G -308 allele
| 138 | 160 | Genes & Molecular Sequences | multiple

```


the GNAS1 | 127 | 158 | SNP & Sequence variations |
hypopharyngeal squamous cell carcinoma | 55 | 93 |
Diseases & Disorders | Overall and relapse-free survival in oropharyngeal and
hypopharyngeal squamous cell carcinoma are associated with genotypes of T393C
polymorphism of the GNAS1 gene.

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```

```
[16]: import pandas as pd
from tabulate import tabulate

# Load the CSV file
ftrain = '../data/EUADR_target_disease.csv'
df = pd.read_csv(ftrain, encoding='latin1', sep='\t')

# Display the first line to understand the structure
with open(ftrain, 'r', encoding='latin1') as file:
    first_line = file.readline()
    print("First line of the file:", first_line)

# Display the column names to identify the one that corresponds to the entity
↳ association type
print("Column names:", df.columns)

# Get unique association types and their counts
association_type_counts = df['ASSOCIATION_TYPE'].value_counts()
print("Association types and their counts:")
print(tabulate(association_type_counts.reset_index(), headers=['Association_
↳ Type', 'Count'], tablefmt='grid'))

# If you want to see a sample of rows for each association type
# Display the first 10 rows for each unique association type
for assoc_type in df['ASSOCIATION_TYPE'].unique():
    print(f"\nSample rows for association type '{assoc_type}':")
    sample_df = df[df['ASSOCIATION_TYPE'] == assoc_type].head(10)
    print(tabulate(sample_df, headers='keys', tablefmt='grid'))
```

```
First line of the file: "ASSOCIATION_TYPE"      "PMID"      "NUM_SENTENCE"
"ENTITY1_TEXT"  "ENTITY1_INI"      "ENTITY1_END"      "ENTITY1_TYPE"  "ENTITY2_TEXT"
"ENTITY2_INI"   "ENTITY2_END"      "ENTITY2_TYPE"      "SENTENCE"
```

```
Column names: Index(['ASSOCIATION_TYPE', 'PMID', 'NUM_SENTENCE', 'ENTITY1_TEXT',
                    'ENTITY1_INI', 'ENTITY1_END', 'ENTITY1_TYPE', 'ENTITY2_TEXT',
                    'ENTITY2_INI', 'ENTITY2_END', 'ENTITY2_TYPE', 'SENTENCE'],
                    dtype='object')
```

Association types and their counts:

```
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|  | Association Type | Count |
+====+=====+=====+
| 0 | PA                | 213   |
+-----+-----+-----+
| 1 | FA                | 93    |
+-----+-----+-----+
| 2 | SA                | 30    |
+-----+-----+-----+
```

Sample rows for association type 'SA':

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|  | ASSOCIATION_TYPE | PMID | NUM_SENTENCE | ENTITY1_TEXT |
ENTITY1_INI | ENTITY1_END | ENTITY1_TYPE | ENTITY2_TEXT
| ENTITY2_INI | ENTITY2_END | ENTITY2_TYPE | SENTENCE
|
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=====+
| 0 | SA                | 17241106 | 16 | LRP5          |
19 |                23 | Genes & Molecular Sequences | osteoporosis          |
80 |                92 | Diseases & Disorders | Our work supported LRP5 genetic
variants as possible susceptibility factors for osteoporosis and fractures in
humans.                |
+-----+-----+-----+-----+-----+-----+-----+
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---+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+
| 1 | SA                | 17241106 | 17 | rs491347      |
20 |                28 | SNP & Sequence variations | osteoporosis          |
108 |               120 | Diseases & Disorders | Especially, the SNP rs491347 and
its strongly associated SNPs (e.g., rs1784235) could be important to human
osteoporosis phenotypes.                |
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2	SA	17241106	17	rs1784235	
69	78	SNP & Sequence variations		osteoporosis	
108	120	Diseases & Disorders		Especially, the SNP rs491347 and its strongly associated SNPs (e.g., rs1784235) could be important to human osteoporosis phenotypes.	
23	SA	17593927	11	XRCC1	
0	5	Genes & Molecular Sequences		gastric cancer	
61	75	Diseases & Disorders		XRCC1 genotyping might make tailor chemotherapy possible for gastric cancer patients treated with oxaliplatin-based chemotherapy.	
32	SA	19035720	6	rs42524	
4	11	SNP & Sequence variations		IAs	
79	82	Diseases & Disorders		The rs42524 polymorphism of COL1A2 could be a genetic risk factor for sporadic IAs among individuals of Chinese Han ethnicity.	
43	SA	19110417	2	CYP1A1	
56	62	Genes & Molecular Sequences		HCC	
70	73	Diseases & Disorders		However, the contribution of common genetic variants in CYP1A1 to the HCC risk in Chinese populations has not been thoroughly investigated.	
50	SA	19110417	11	CYP1A1	
54	60	Genes & Molecular Sequences		HCC	
97	100	Diseases & Disorders		Our results suggested that common genetic variants in CYP1A1 may modulate the risk of developing HCC in the study population, particularly in non-smokers.	

[illegible][illegible]

ENTITY2_INI	ENTITY2_END	ENTITY2_TYPE	SENTENCE
3	18697826	0	fetal haemoglobin
93	110	Genes & Molecular Sequences	beta-thalassaemia
132	149	Diseases & Disorders	The HBS1L-MYB intergenic region on chromosome 6q23 is a quantitative trait locus controlling fetal haemoglobin level in carriers of beta-thalassaemia.
6	18697826	0	HBS1L-MYB
4	13	Genes & Molecular Sequences	beta-thalassaemia
132	149	Diseases & Disorders	The HBS1L-MYB intergenic region on chromosome 6q23 is a quantitative trait locus controlling fetal haemoglobin level in carriers of beta-thalassaemia.
7	18697826	0	6q23
46	50	Genes & Molecular Sequences	beta-thalassaemia
132	149	Diseases & Disorders	The HBS1L-MYB intergenic region on chromosome 6q23 is a quantitative trait locus controlling fetal haemoglobin level in carriers of beta-thalassaemia.

[illegible]

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| 17 | FA | 18347176 | 3 | T393C |
28 | 33 | SNP & Sequence variations | oropharyngeal |
121 | 134 | Diseases & Disorders | The prognostic value of the T393C
SNP was evaluated in an unselected series of patients treated with curative
intent for oropharyngeal and hypopharyngeal squamous cell carcinomas, including
all tumor stages with different therapeutic regimens.
|
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| 18 | FA | 17430902 | 3 | Wnt |
69 | 72 | Genes & Molecular Sequences | colon cancer |
25 | 37 | Diseases & Disorders | However, the majority of colon
cancer cells have deregulation of the Wnt/beta-catenin pathway.
|
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| 19 | FA | 17430902 | 0 | Krüppel-like factor 5 |
87 | 108 | Genes & Molecular Sequences | colon cancer |
51 | 63 | Diseases & Disorders | Lysophosphatidic acid facilitates
proliferation of colon cancer cells via induction of Krüppel-like factor 5.
|
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| 16 | PA | 18347176 | 9 | T393C
| 4 | 9 | SNP & Sequence variations | oropharyngeal
| 112 | 125 | Diseases & Disorders | The T393C SNP could be
considered as a genetic marker to predict the clinical course of patients
suffering from oropharyngeal and hypopharyngeal cancer.
|
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| 20 | PA | 17430902 | 2 | beta-catenin
| 99 | 111 | Genes & Molecular Sequences | colon cancer
| 57 | 69 | Diseases & Disorders | A recent study showed
that LPA-mediated proliferation of colon cancer cells requires activation of
beta-catenin.
|
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| 21 | PA | 18930278 | 6 | CYP3A5 A6986G genotype
*3/*3 | 29 | 57 | Genes & Molecular Sequences |
leukocytopenia | 211 | 225 |
Diseases & Disorders | On multivariate analysis the CYP3A5 A6986G genotype *3/*3
(OR 8.205, 95% CI 1.616-41.667, p = 0.011) and smaller number of treatment
cycles (OR 0.156, 95% CI 0.037-0.659, p = 0.011) were independent factors for
leukocytopenia (grade 3 or greater) throughout the period of chemotherapy.
|

```

Sample rows for association type 'nan':

```
[18]: import pandas as pd

# Load the CSV file
ftrain = '../data/EUADR_target_disease.csv'
df = pd.read_csv(ftrain, encoding='latin1', sep='\t')

# Display the column names to identify the one that corresponds to the entity_↵
↵association type
print("Column names:", df.columns)

# Check if 'SA' exists in the 'ASSOCIATION_TYPE' column
association_types = df['ASSOCIATION_TYPE'].unique()
if 'NA' in association_types:
    print("Association type 'SA' is present in the data.")
else:
    print("Association type 'SA' is not present in the data.")
```

Association type 'SA' is not present in the data.

2 Read Data

```
[13]: from tabulate import tabulate
Tr_sent_contents, Tr_entity1_list, Tr_entity2_list, Tr_sent_labels = utils.
↳dataRead_befree_EUADR(ftrain)
# Convert the lists to a DataFrame
df = pd.DataFrame({
    'Sent Contents': Tr_sent_contents,
    'Entity 1': Tr_entity1_list,
    'Entity 2': Tr_entity2_list,
    'Sent Labels': Tr_sent_labels
})

# Display the first 10 rows of the DataFrame as a table
print(tabulate(df.head(4), headers='keys', tablefmt='grid'))

Tr_word_list, Tr_d1_list, Tr_d2_list = utils.
↳get_wordList_and_distances_befree(Tr_sent_contents)

df = pd.DataFrame({
    'word list': Tr_word_list,
    'd1 list': Tr_d1_list,
    'd2 list': Tr_d2_list,
})

# Display the first 10 rows of the DataFrame as a table
print(tabulate(df.head(4), headers='keys', tablefmt='grid'))

print ("train_size", len(Tr_word_list))
```

Input File Reading
train_size 355

2.1 Prepare Label Matrix

```
[17]: # Y : is positive association
# N: is negative association
label_dict = {'FA':0, 'NA':0, 'PA':1, 'SA':1}

Y_t = mapLabelToId_befree_EUADR(Tr_sent_labels, label_dict)
Y_train = np.zeros((len(Y_t), 2))
for i in range(len(Y_t)):
    Y_train[i][Y_t[i]] = 1.0
```

3 Generate Word and Position Embedding Vectors

3.0.1 Word Embedding

```
[18]: word_dict, word_to_id, id_to_word = word_mapping(Tr_word_list)

print( "word dictionary length", len(word_dict))

# Word Embedding
word_vectors = readWordEmb(word_dict,id_to_word,word_to_id, wefile,
    ↪embSize,limit=1356)
W_train = mapWordToId(Tr_word_list, word_to_id)
print("W_train",len(W_train))
print("word_vectors",len(word_vectors))
```

```
Found 1355 unique words (10062 in total)
word dictionary length 1355
Reading word vectors
Loaded 1356 pretrained embeddings.
number of unknown word in word embedding 814
W_train 355
word_vectors 1355
```

3.0.2 Position Embedding

```
[19]: d1_dict = makeDistanceList([Tr_d1_list])
d2_dict = makeDistanceList([Tr_d2_list])
d1_train = mapWordToId_list(Tr_d1_list, d1_dict)
d2_train = mapWordToId_list(Tr_d2_list, d2_dict)
```

3.0.3 Pad Embdding Vectors

```
[20]: train_sent_lengths= findSentLengths([Tr_word_list])

sentMax =max(max(train_sent_lengths[:]))

W_train, d1_train, d2_train = paddData([W_train, d1_train, d2_train ],
    ↪sentMax,padd_num=1354)
print("sentMax",sentMax)
print("W_train",len(W_train))
print("d1_train",len(d1_train))
print("d2_train",len(d2_train))
```

```
sentMax 102
W_train 355
d1_train 355
d2_train 355
```

4 Save Prepared Data as Pickle File

```
[21]: with open('../data/pickles/befree_EUADR_2class_PubMed-and-PMC-w2v.pickle',  
↪ 'wb') as handle:  
    pickle.dump(W_train, handle)  
    pickle.dump(d1_train, handle)  
    pickle.dump(d2_train, handle)  
    pickle.dump(Y_train, handle)  
    pickle.dump(Tr_word_list, handle)  
    pickle.dump(word_vectors, handle)  
    pickle.dump(word_dict, handle)  
    pickle.dump(d1_dict, handle)  
    pickle.dump(d2_dict, handle)  
    pickle.dump(label_dict, handle)  
    pickle.dump(sentMax, handle)
```

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