Protein_Embedding

November 18, 2023

1 Protein Embedding

In this project we will focus on `protein_embedding` by using one of the two methods:

- `GAE` - Graph Auto Encoder
- `struc2vec`

Important references for that project :

- *BioNEV GitHub site* - that github site contains lot of inforamtion that required for that project(such as code, explanations and running examples):

https://github.com/xiangyue9607/BioNEV/tree/master

- *Graph embedding on biomedical network* - an article about graph embedding and methods (such as `GAE` and `struc2vec`) :

https://academic.oup.com/bioinformatics/article/36/4/1241/5581350?login=false

- *STRING PPI* - site that contains the data we are going to work with in that project:

https://version-11-0.string-db.org/cgi/input.pl?sessionId=8aVJal1k2wit&input_page_show_search=on

1.1 Import Libraries

The first step in the project is to import some libraries that important for the next steps leading to the final that, graph embedding.

[1]:
```
import pandas as pd
import networkx as nx
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
import matplotlib
import csv
import random
import warnings
import requests
import shutil
warnings.filterwarnings('ignore')
```

[2]:
```
def PRINT_():
    print('#' *80)
```

1.2 Downloading the data set from STRING PPI

Downloading the protein interaction data set versio `11.0` from *STRING PPI* as `.txt` file, and converting that into `.csv`

[3]:
```
# URL of the file to download
url = "https://stringdb-static.org/download/protein.links.v11.0/9606.protein.
 ↪links.v11.0.txt.gz"

# Define the local file name
local_file_name = "9606.protein.links.v11.0.txt.gz"

# Send an HTTP GET request to the URL
response = requests.get(url, stream=True)

# Check if the request was successful
if response.status_code == 200:
    # Open the local file in binary write mode
    with open(local_file_name, 'wb') as local_file:
        # Iterate through the response content and write it to the local file
        for chunk in response.iter_content(chunk_size=1024):
            if chunk:
                local_file.write(chunk)
else:
    print("Failed to download the file. HTTP status code:", response.
 ↪status_code)

# Close the response
response.close()
```

After downloading the dataset from STRING PPI, the next step will be to extract the `.txt` file from it and convert that file into `.csv` file

1.3 Data Exploring

Upon downloading the dataset, the initial phase involves data examination and preparation for subsequent analytical procedures:

- Normalize the values of 'combined_score' to be in the range of 0-1

Normalize the 'combined_score' values to a 0-1 range, enhancing comparability and mitigating scale-related biases in data analysis or machine learning models. This involves adjusting each value by subtracting the minimum 'combined_score' and dividing by the range (difference between maximum and minimum values)

- Data Cleaning:

The primary task involves the refinement of the dataset by retaining only those protein pairs whose combined score exceeds the threshold of 0.7. This criterion is employed to ensure that only interactions with a significant degree of confidence are considered for further analysis.

- Deduplication:

The dataset is subjected to a process of deduplication, where redundant or repeated values are systematically removed. This step is imperative to maintain the integrity of the dataset and prevent biases that may arise from duplicate entries.

- Protein ID Replacement with Numeric Encoding:

In order to facilitate subsequent analytical procedures, the original protein identifiers are substituted with encoded numeric values. This transformation is undertaken to enhance computational efficiency and to enable the application of numerical methods in subsequent stages of analysis

1.3.1 View the data

[4]:
```
import pandas as pd

# Load the data from the .txt file
df = pd.read_csv('9606.protein.links.v11.0.txt', sep=' ')

# Convert it to a .csv file
df.to_csv('9606.protein.links.v11.0.csv', index=False)
df
```

[4]:

	protein1	protein2	combined_score
0	9606.ENSP00000000233	9606.ENSP00000272298	490
1	9606.ENSP00000000233	9606.ENSP00000253401	198
2	9606.ENSP00000000233	9606.ENSP00000401445	159
3	9606.ENSP00000000233	9606.ENSP00000418915	606
4	9606.ENSP00000000233	9606.ENSP00000327801	167
…	…	…	…
11759449	9606.ENSP00000485678	9606.ENSP00000310488	167
11759450	9606.ENSP00000485678	9606.ENSP00000342448	175
11759451	9606.ENSP00000485678	9606.ENSP00000350222	195
11759452	9606.ENSP00000485678	9606.ENSP00000367590	900
11759453	9606.ENSP00000485678	9606.ENSP00000349930	213

[11759454 rows x 3 columns]

[5]:
```
len(df)
```

[5]: 11759454

The next step is createing a `.txt` file to see if there are duplicated pairs of `protein1` and `protein2` and `combined_score` in the dataset

[6]:
```
output_file = 'proteins_check.txt'
input_file = '9606.protein.links.v11.0.csv'
# Open the input CSV file and the output text file
with open(input_file, 'r') as csv_file, open(output_file, 'w') as txt_file:
    csv_reader = csv.DictReader(csv_file)
```

```
    # Write the header to the output text file
    txt_file.write(f"'protein1' 'protein2' 'combined_score\n")

    # Iterate through the rows in the CSV and write them to the text file
    for row in csv_reader:
        txt_file.write(f"{row['protein1']} {row['protein2']}␣
 ↪{row['combined_score']}\n")

PRINT_()
print("Conversion complete. The text file has been created.")
PRINT_()
```

```
################################################################################
Conversion complete. The text file has been created.
################################################################################
```

1.3.2 Normalize the values of 'combined_score' to be in the range of 0-1

[7]:
```
# View the min& max values of the column 'combined_score':

max_value = df['combined_score'].max()
min_value = df['combined_score'].min()

PRINT_()
print(f"The maximum value of the column 'combined_score' is -> {max_value}, or␣
 ↪{max_value/10}%")
print(f"The minimum value of the column 'combined_score is -> {min_value} or␣
 ↪{min_value/10}%")
PRINT_()
```

```
################################################################################
The maximum value of the column 'combined_score' is -> 999, or 99.9%
The minimum value of the column 'combined_score is -> 150 or 15.0%
################################################################################
```

[8]:
```
# Normalize the 'combined_score' column to the range 0-1
# Extract the 'combined_score' column
combined_score = df['combined_score']

df['combined_score'] = (combined_score - min_value) / (max_value - min_value)

print(len(df))
```

```
11759454
```

[9]:
```
df
```

[9]:

	protein1	protein2	combined_score
0	9606.ENSP00000000233	9606.ENSP00000272298	0.400471
1	9606.ENSP00000000233	9606.ENSP00000253401	0.056537
2	9606.ENSP00000000233	9606.ENSP00000401445	0.010601
3	9606.ENSP00000000233	9606.ENSP00000418915	0.537102
4	9606.ENSP00000000233	9606.ENSP00000327801	0.020024
…	…	…	…
11759449	9606.ENSP00000485678	9606.ENSP00000310488	0.020024
11759450	9606.ENSP00000485678	9606.ENSP00000342448	0.029446
11759451	9606.ENSP00000485678	9606.ENSP00000350222	0.053004
11759452	9606.ENSP00000485678	9606.ENSP00000367590	0.883392
11759453	9606.ENSP00000485678	9606.ENSP00000349930	0.074205

[11759454 rows x 3 columns]

[10]:
```
# Create a set of unique proteins by combining both columns
unique_proteins = set(df['protein1']).union(df['protein2'])

# Count the unique proteins
unique_protein_count = len(unique_proteins)

PRINT_()
print(f"The number of unique proteins in the data set of version 11.0 is ->␣
 ↪{unique_protein_count}")
print(f"The number of unique proteins if the data set of version 10.5 is ->␣
 ↪15131")
print(f"There are {unique_protein_count - 15131} new unique proteins in the 11.
 ↪0 version of STRING PPI")
PRINT_()
```

```
################################################################################
The number of unique proteins in the data set of version 11.0 is -> 19354
The number of unique proteins if the data set of version 10.5 is -> 15131
There are 4223 new unique proteins in the 11.0 version of STRING PPI
################################################################################
```

[11]:
```
PRINT_()
print(f"Nex maximum of the column 'combined_score' is -> {df['combined_score'].
 ↪max()}")
print(f"New minimum of the column 'combied_score' is -> {df['combined_score'].
 ↪min()}")
PRINT_()
```

```
################################################################################
Nex maximum of the column 'combined_score' is -> 1.0
New minimum of the column 'combied_score' is -> 0.0
################################################################################
```

1.3.3 Drop all the values that their 'combined_score' is under 0.7

Before we move on, we will want to work only with sets of proteins that their `combined_socore` in the range of `0.7-1.0`. Therefore, we will need to drop all the values that their `combined_score < 0.7`

[12]:
```
number_of_rows_before_dropping = len(df)
# Drop rows where 'combined_score' is less than 0.7
df = df[df['combined_score'] >= 0.7]

# Reset the index if you want to keep it continuous
df.reset_index(drop=True, inplace=True)

unique_proteins_after_dropping = len(set(df['protein1']).union(df['protein2']))
```

[13]:
```
PRINT_()
print(f"The number of rows before dropping the rows with `combined_values` < 0.
 ↪7 -> [{number_of_rows_before_dropping}]")
print(f"The number of rows after dropping the rows with 'combined_score` < 0.7␣
 ↪are -> [{len(df)}]")
print(f"Got rid of -> [{number_of_rows_before_dropping - len(df)}] values in␣
 ↪total, that is {((((number_of_rows_before_dropping - len(df))/
 ↪number_of_rows_before_dropping))*100):.2f}% of the total data")
PRINT_()
print(f"The number of unique proteins before dropping is ->␣
 ↪{len(unique_proteins)}")
print(f"The number of unique proteins after dropping is ->␣
 ↪{unique_proteins_after_dropping}")
print(f"Dropped {len(unique_proteins) - unique_proteins_after_dropping} unique␣
 ↪proteins")
PRINT_()
```

```
################################################################################
The number of rows before dropping the rows with `combined_values` < 0.7 ->
[11759454]
The number of rows after dropping the rows with 'combined_score` < 0.7 are ->
[779364]
Got rid of -> [10980090] values in total, that is 93.37% of the total data
################################################################################
The number of unique proteins before dropping is -> 19354
The number of unique proteins after dropping is -> 16063
Dropped 3291 unique proteins
################################################################################
```

[14]:
```
df
```

[14]:

	protein1	protein2	combined_score
0	9606.ENSP00000000233	9606.ENSP00000432568	0.893993

```
1         9606.ENSP00000000233  9606.ENSP00000427900         0.895171
2         9606.ENSP00000000233  9606.ENSP00000350199         0.707892
3         9606.ENSP00000000233  9606.ENSP00000354878         0.895171
4         9606.ENSP00000000233  9606.ENSP00000405926         0.890459
…                          …                     …              …
779359    9606.ENSP00000485678  9606.ENSP00000438346         0.883392
779360    9606.ENSP00000485678  9606.ENSP00000303482         0.883392
779361    9606.ENSP00000485678  9606.ENSP00000481878         0.883392
779362    9606.ENSP00000485678  9606.ENSP00000296142         0.883392
779363    9606.ENSP00000485678  9606.ENSP00000367590         0.883392

[779364 rows x 3 columns]
```

1.3.4 Remove duplicated rows from the data

The next step is remove duplicated rows in our data set. The idea is if `protein1` and `protein2` appear in our data which means that there are edge between them, and *also* there is a row with the same values of `protein1` and `protein2` but in different order, remove that duplicated row to reduce data.

[15]:
```
num_of_rows_before_drop = len(df)

# Create a new DataFrame with sorted tuples of 'protein1' and 'protein2'
df['sorted_nodes'] = df.apply(lambda row: tuple(sorted([row['protein1'],␣
 ↪row['protein2']])), axis=1)

# Use .loc to drop duplicates while preserving the first occurrence
df = df.loc[df.duplicated(subset=['sorted_nodes'], keep='first')]

# Drop the 'sorted_nodes' column if you no longer need it
df = df.drop(columns='sorted_nodes')

# Reset the index to maintain the order
df.reset_index(drop=True, inplace=True)

# Save the cleaned DataFrame back to a CSV file
#df.to_csv('cleaned_file.csv', index=False)

num_of_rows_after_drop = len(df)
unique_proteins_after_dropping = len(set(df['protein1']).union(df['protein2']))

PRINT_()
print(f"Number of rows before removing duplicated values ->␣
 ↪{num_of_rows_before_drop}")
print(f"Number of rows after removing duplicated values ->␣
 ↪{num_of_rows_after_drop}")
```

```
print(f"Total number of duplicated values -> {num_of_rows_before_drop -␣
 ↪num_of_rows_after_drop}")
PRINT_()
print(f"The number of unique proteins after dropping is ->␣
 ↪{unique_proteins_after_dropping}")
PRINT_()
```

```
################################################################################
Number of rows before removing duplicated values -> 779364
Number of rows after removing duplicated values -> 389682
Total number of duplicated values -> 389682
################################################################################
The number of unique proteins after dropping is -> 16063
################################################################################
```

1.3.5 Creating text file that mapps index to unique protein

Before moving forward, we need to create `.txt` file that mapps unique `index` for each unique `protein`. The reason behind that step -> prepare for creating `.edgelist` file for the graph embedding input.

[20]:
```
# Helper function to make .txt that contains of 'index protein_id' rows
def write_graph_to_txt(graph, filename):
    with open(filename, 'w') as file:
        for index, node in enumerate(graph.nodes):
            file.write(f"{index} {node}\n")
```

[21]:
```
output_file_ = "indx_to_protein.txt"

write_graph_to_txt(G_, output_file_)
```

1.4 Building a graph with NetworkX

The next step is beuild a graph data structure s.t. edge exsist between `protein1` and `protein2` that in the same row in `df` with `combined_score` as attribute on the edge between them.

For that, we need to install `networkx` library.

[16]:
```
G_ = nx.Graph()

# Iterate through the DataFrame and add edges with 'combined_score' as edge␣
 ↪attribute
for index, row in df.iterrows():
    protein1 = row['protein1']
    protein2 = row['protein2']
    combined_score = row['combined_score']
    G_.add_edge(protein1, protein2, combined_score=combined_score)
```

[17]:
```
PRINT_()
print(f"Number of nodes in G_ -> {G_.number_of_nodes()}")
print(f"Number of edges in G_ -> {G_.number_of_edges()}")
PRINT_()
```

```
################################################################################
Number of nodes in G_ -> 16063
Number of edges in G_ -> 389682
################################################################################
```

Visualize subsampled graph of the original graph in order in reduce run time.

[18]:
```
# Assuming you have your original graph 'G'
nodes = list(G_.nodes())
subsampled_nodes = random.sample(nodes, int(len(G_) * 0.05))
subsampled_graph = G_.subgraph(subsampled_nodes)
```

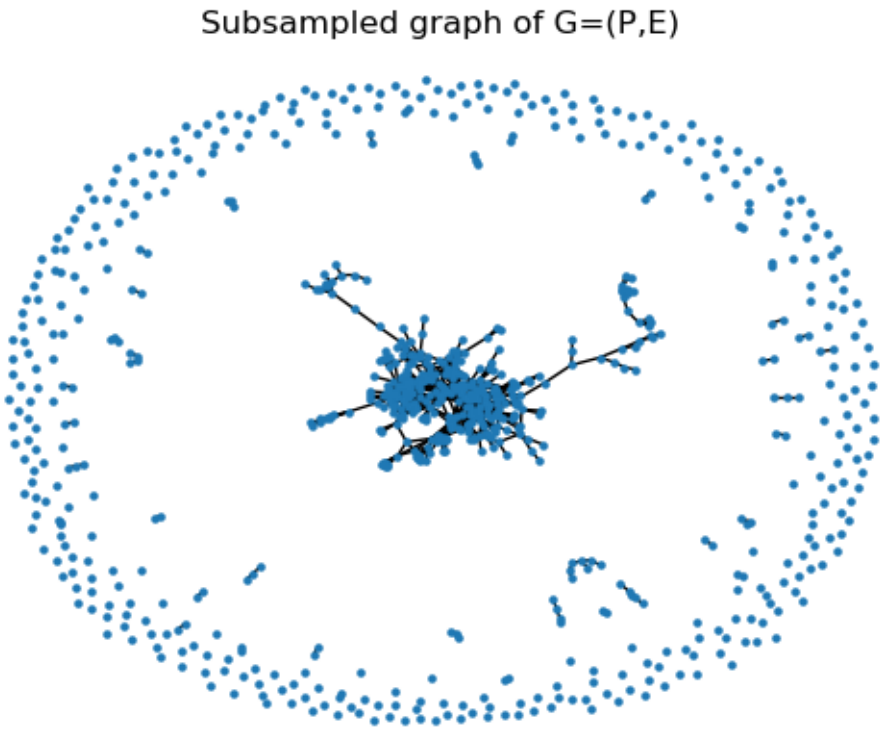
[19]:
```
import matplotlib.pyplot as plt

# Assuming you have your subsampled graph 'subsampled_graph'
layout = nx.spring_layout(subsampled_graph)

# Draw the nodes
nx.draw_networkx_nodes(subsampled_graph, layout, node_size=5)

# Draw the edges (if needed)
nx.draw_networkx_edges(subsampled_graph, layout)

# Show the graph
plt.title("Subsampled graph of G=(P,E)") # 'P' stands for proteins, 'E' stand␣
 ↪for edges
plt.axis('off')
plt.show()
```



As we can see in the graph above, there are some nodes (i.e. proteins) which are not connected to any other node. One of the reasons for that can be our divided data in graph G, that graph does not contain all of the edges in our data set. Therefore, there can be some edges that does not exist in graph G. Another reason can be the cause of our `subsampled` graph of G that we generated for faster graph plotting time.

1.5 Write the graph G=(P,E) as `edgelist`

The next step is to convert (i.e. write) the graph `G=(P,E)` to name `edgelist`, that is simply going to convert the graph into `.txt` file with the next format:

`protein1 protein2`

`protein3 protein4`

`protein5 protein6 . . .`

Note - we dont want to include the `combined_score` data in our `proteint_edgelist.txt`. Therefore, turn `data=Flase`

[22]:
```
p_edgelist_ = nx.write_edgelist(G_, "STRING_PPI_11_0.edgelist", data=False)
```

[23]:
```
# Load the node index mapping from "node_list.txt"
index_to_protein = {}
with open("indx_to_protein.txt", 'r') as node_list_file:
```

```
    for line in node_list_file:
        parts = line.strip().split(' ')
        if len(parts) == 2:
            index, protein = parts
            index_to_protein[protein] = index

# Create a new file to write the updated edge list for the data:
with open("STRING_PPI_11_0_.edgelist", 'w') as updated_file:
    with open("STRING_PPI_11_0.edgelist", 'r') as proteins_file:
        for line in proteins_file:
            source_protein, target_protein = line.strip().split(' ')
            source_index = index_to_protein.get(source_protein)
            target_index = index_to_protein.get(target_protein)
            if source_index is not None and target_index is not None:
                updated_file.write(f"{source_index} {target_index}\n")
```

1.6 Graph Embedding

The next steps, will include downloading BioNEV repository from GitHub and making graph embeddings using our proteins edgelist data structure we created above.

1.6.1 Downloading BioNEV repository

The BioNEV repository is taken from GitHun linked:

https://github.com/xiangyue9607/BioNEV/tree/master

[24]:
```
!git clone https://github.com/xiangyue9607/BioNEV.git
```

```
fatal: destination path 'BioNEV' already exists and is not an empty directory.
```

Next, move the STRING PPI edgelist to the `data` dir that located in `BioNEV` repository in order to execute the graph embedding later on.

[25]:
```
import shutil

source_file = "STRING_PPI_11_0_.edgelist"
destination_directory = "C:/Users/gavvi/Desktop/Programming/Python/DeepLearning␣
 ↪Research/BioNEV/data"

shutil.copy(source_file, destination_directory)
```

[25]:
```
'C:/Users/gavvi/Desktop/Programming/Python/DeepLearning
Research/BioNEV/data\\STRING_PPI_11_0_.edgelist'
```

[26]:
```
cd BioNEV
```

```
C:\Users\gavvi\Desktop\Programming\Python\DeepLearning Research\BioNEV
```

The next step will be downloading the BioNEV repository and then downloading the `code` from it.

[27]:
```
pip install -e.
```

```
Obtaining
file:///C:/Users/gavvi/Desktop/Programming/Python/DeepLearning%20Research/BioNEV
  Preparing metadata (setup.py): started
  Preparing metadata (setup.py): finished with status 'done'
Requirement already satisfied: numpy in c:\users\gavvi\anaconda3\lib\site-
packages (from bionev==0.1.0.dev0) (1.24.3)
Requirement already satisfied: networkx in c:\users\gavvi\anaconda3\lib\site-
packages (from bionev==0.1.0.dev0) (3.1)
Requirement already satisfied: scipy in c:\users\gavvi\anaconda3\lib\site-
packages (from bionev==0.1.0.dev0) (1.11.1)
Requirement already satisfied: tensorflow in c:\users\gavvi\anaconda3\lib\site-
packages (from bionev==0.1.0.dev0) (2.14.0)
Requirement already satisfied: gensim in c:\users\gavvi\anaconda3\lib\site-
packages (from bionev==0.1.0.dev0) (4.3.0)
Requirement already satisfied: scikit-learn in
c:\users\gavvi\anaconda3\lib\site-packages (from bionev==0.1.0.dev0) (1.3.0)
Requirement already satisfied: tqdm in c:\users\gavvi\anaconda3\lib\site-
packages (from bionev==0.1.0.dev0) (4.65.0)
Requirement already satisfied: fastdtw in c:\users\gavvi\anaconda3\lib\site-
packages (from bionev==0.1.0.dev0) (0.3.4)
Requirement already satisfied: smart-open>=1.8.1 in
c:\users\gavvi\anaconda3\lib\site-packages (from gensim->bionev==0.1.0.dev0)
(5.2.1)
Requirement already satisfied: FuzzyTM>=0.4.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from gensim->bionev==0.1.0.dev0)
(2.0.5)
Requirement already satisfied: joblib>=1.1.1 in
c:\users\gavvi\anaconda3\lib\site-packages (from scikit-
learn->bionev==0.1.0.dev0) (1.2.0)
Requirement already satisfied: threadpoolctl>=2.0.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from scikit-
learn->bionev==0.1.0.dev0) (2.2.0)
Requirement already satisfied: tensorflow-intel==2.14.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow->bionev==0.1.0.dev0)
(2.14.0)
Requirement already satisfied: absl-py>=1.0.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (2.0.0)
Requirement already satisfied: astunparse>=1.6.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (1.6.3)
Requirement already satisfied: flatbuffers>=23.5.26 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (23.5.26)
Requirement already satisfied: gast!=0.5.0,!=0.5.1,!=0.5.2,>=0.2.1 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
```

```
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (0.5.4)
Requirement already satisfied: google-pasta>=0.1.1 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (0.2.0)
Requirement already satisfied: h5py>=2.9.0 in c:\users\gavvi\anaconda3\lib\site-
packages (from tensorflow-intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (3.9.0)
Requirement already satisfied: libclang>=13.0.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (16.0.6)
Requirement already satisfied: ml-dtypes==0.2.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (0.2.0)
Requirement already satisfied: opt-einsum>=2.3.2 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (3.3.0)
Requirement already satisfied: packaging in c:\users\gavvi\anaconda3\lib\site-
packages (from tensorflow-intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (23.1)
Requirement already satisfied:
protobuf!=4.21.0,!=4.21.1,!=4.21.2,!=4.21.3,!=4.21.4,!=4.21.5,<5.0.0dev,>=3.20.3
in c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (4.24.4)
Requirement already satisfied: setuptools in c:\users\gavvi\anaconda3\lib\site-
packages (from tensorflow-intel==2.14.0->tensorflow->bionev==0.1.0.dev0)
(68.0.0)
Requirement already satisfied: six>=1.12.0 in c:\users\gavvi\anaconda3\lib\site-
packages (from tensorflow-intel==2.14.0->tensorflow->bionev==0.1.0.dev0)
(1.16.0)
Requirement already satisfied: termcolor>=1.1.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (2.3.0)
Requirement already satisfied: typing-extensions>=3.6.6 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (4.7.1)
Requirement already satisfied: wrapt<1.15,>=1.11.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (1.14.1)
Requirement already satisfied: tensorflow-io-gcs-filesystem>=0.23.1 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (0.31.0)
Requirement already satisfied: grpcio<2.0,>=1.24.3 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (1.59.0)
Requirement already satisfied: tensorboard<2.15,>=2.14 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (2.14.1)
Requirement already satisfied: tensorflow-estimator<2.15,>=2.14.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (2.14.0)
```

```
Requirement already satisfied: keras<2.15,>=2.14.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (2.14.0)
Requirement already satisfied: colorama in c:\users\gavvi\anaconda3\lib\site-
packages (from tqdm->bionev==0.1.0.dev0) (0.4.6)
Requirement already satisfied: pandas in c:\users\gavvi\anaconda3\lib\site-
packages (from FuzzyTM>=0.4.0->gensim->bionev==0.1.0.dev0) (2.0.3)
Requirement already satisfied: pyfume in c:\users\gavvi\anaconda3\lib\site-
packages (from FuzzyTM>=0.4.0->gensim->bionev==0.1.0.dev0) (0.2.25)
Requirement already satisfied: wheel<1.0,>=0.23.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from astunparse>=1.6.0->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (0.38.4)
Requirement already satisfied: google-auth<3,>=1.6.3 in
c:\users\gavvi\anaconda3\lib\site-packages (from
tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (2.23.3)
Requirement already satisfied: google-auth-oauthlib<1.1,>=0.5 in
c:\users\gavvi\anaconda3\lib\site-packages (from
tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (1.0.0)
Requirement already satisfied: markdown>=2.6.8 in
c:\users\gavvi\anaconda3\lib\site-packages (from
tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (3.4.1)
Requirement already satisfied: requests<3,>=2.21.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from
tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (2.31.0)
Requirement already satisfied: tensorboard-data-server<0.8.0,>=0.7.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from
tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (0.7.2)
Requirement already satisfied: werkzeug>=1.0.1 in
c:\users\gavvi\anaconda3\lib\site-packages (from
tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (2.2.3)
Requirement already satisfied: python-dateutil>=2.8.2 in
c:\users\gavvi\anaconda3\lib\site-packages (from
pandas->FuzzyTM>=0.4.0->gensim->bionev==0.1.0.dev0) (2.8.2)
Requirement already satisfied: pytz>=2020.1 in
c:\users\gavvi\anaconda3\lib\site-packages (from
pandas->FuzzyTM>=0.4.0->gensim->bionev==0.1.0.dev0) (2023.3.post1)
Requirement already satisfied: tzdata>=2022.1 in
c:\users\gavvi\anaconda3\lib\site-packages (from
pandas->FuzzyTM>=0.4.0->gensim->bionev==0.1.0.dev0) (2023.3)
Requirement already satisfied: simpful in c:\users\gavvi\anaconda3\lib\site-
packages (from pyfume->FuzzyTM>=0.4.0->gensim->bionev==0.1.0.dev0) (2.11.0)
Requirement already satisfied: fst-pso in c:\users\gavvi\anaconda3\lib\site-
```

```
packages (from pyfume->FuzzyTM>=0.4.0->gensim->bionev==0.1.0.dev0) (1.8.1)
Requirement already satisfied: cachetools<6.0,>=2.0.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from google-
auth<3,>=1.6.3->tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (5.3.2)
Requirement already satisfied: pyasn1-modules>=0.2.1 in
c:\users\gavvi\anaconda3\lib\site-packages (from google-
auth<3,>=1.6.3->tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (0.2.8)
Requirement already satisfied: rsa<5,>=3.1.4 in
c:\users\gavvi\anaconda3\lib\site-packages (from google-
auth<3,>=1.6.3->tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (4.9)
Requirement already satisfied: requests-oauthlib>=0.7.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from google-auth-
oauthlib<1.1,>=0.5->tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (1.3.1)
Requirement already satisfied: charset-normalizer<4,>=2 in
c:\users\gavvi\anaconda3\lib\site-packages (from
requests<3,>=2.21.0->tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (2.0.4)
Requirement already satisfied: idna<4,>=2.5 in
c:\users\gavvi\anaconda3\lib\site-packages (from
requests<3,>=2.21.0->tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (3.4)
Requirement already satisfied: urllib3<3,>=1.21.1 in
c:\users\gavvi\anaconda3\lib\site-packages (from
requests<3,>=2.21.0->tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (1.26.16)
Requirement already satisfied: certifi>=2017.4.17 in
c:\users\gavvi\anaconda3\lib\site-packages (from
requests<3,>=2.21.0->tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (2023.7.22)
Requirement already satisfied: MarkupSafe>=2.1.1 in
c:\users\gavvi\anaconda3\lib\site-packages (from
werkzeug>=1.0.1->tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (2.1.1)
Requirement already satisfied: miniful in c:\users\gavvi\anaconda3\lib\site-
packages (from fst-pso->pyfume->FuzzyTM>=0.4.0->gensim->bionev==0.1.0.dev0)
(0.0.6)
Requirement already satisfied: pyasn1<0.5.0,>=0.4.6 in
c:\users\gavvi\anaconda3\lib\site-packages (from pyasn1-modules>=0.2.1->google-
auth<3,>=1.6.3->tensorboard<2.15,>=2.14->tensorflow-
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (0.4.8)
Requirement already satisfied: oauthlib>=3.0.0 in
c:\users\gavvi\anaconda3\lib\site-packages (from requests-
oauthlib>=0.7.0->google-auth-
oauthlib<1.1,>=0.5->tensorboard<2.15,>=2.14->tensorflow-
```

```
intel==2.14.0->tensorflow->bionev==0.1.0.dev0) (3.2.2)
Installing collected packages: bionev
  Attempting uninstall: bionev
    Found existing installation: bionev 0.1.0.dev0
    Uninstalling bionev-0.1.0.dev0:
      Successfully uninstalled bionev-0.1.0.dev0
  Running setup.py develop for bionev
Successfully installed bionev-0.1.0.dev0
Note: you may need to restart the kernel to use updated packages.
```

1.6.2 Graph Embedding using GAE

Finally, we can generate the embedding for our PPI data set.

Extracting the proteins embeddings after executing GAE method Due to the intricacy of the methodology employed, we opted to utilize the Google Colab environment with a T4 Graphics Processing Unit (GPU) to execute struc2vec. This decision was motivated by the desire to achieve expedited runtime during the generation of protein embeddings.

The model's performance was as follows:

Link Prediction Performance

`AUC-ROC: 0.874, AUC-PR: 0.863, Accuracy: 0.800, F1: 0.801`

Prediction Task Time: `1888.33` s (~ `31` min)

Restore the genuine identifiers of proteins to the embedding text file The subsequent phase involves accessing the `.txt` file containing protein embeddings generated through the `GAE` method on the `GPU`. Subsequently, it necessitates the conversion of all numeric identifiers of the proteins to their original identifiers, as they were present in the initial *STRING* dataset.

For example: for the protein with the id number `7539` will turn into -> `9606.ENSP00000350012`

[42]:
```
cd embeddings
```

```
C:\Users\gavvi\Desktop\Programming\Python\DeepLearning
Research\BioNEV\embeddings
```

[43]:
```
import shutil

source_file = "STRING_PPI_11_0_GAE_embeddings.txt"
destination_directory = "C:/Users/gavvi/Desktop/Programming/Python/DeepLearning␣
 ↪Research"

shutil.copy(source_file, destination_directory)
```

[43]:
```
'C:/Users/gavvi/Desktop/Programming/Python/DeepLearning
Research\\STRING_PPI_11_0_GAE_embeddings.txt'
```

[44]:
```
import os

os.chdir(destination_directory)
current_directory = os.getcwd()
print("Current directory:", current_directory)
```

```
Current directory: C:\Users\gavvi\Desktop\Programming\Python\DeepLearning
Research
```

[45]:
```
def replace_mapped_ids(embeddings_file, node_list_file):
    """
    The function takes the embedding file and return the proteins integer id to␣
 ↪their original
    id as originated from STRING PPI dataset
    """

    # Create a dictionary to map mapped IDs to real protein IDs
    id_mapping = {}

    with open(node_list_file, 'r') as node_list:
        for line in node_list:
            mapped_id, real_id = line.strip().split()
            id_mapping[mapped_id] = real_id

    # Read the embeddings file, replace mapped IDs with real IDs, and write to␣
 ↪a new file
    with open(embeddings_file, 'r') as embeddings:
        lines = embeddings.readlines()

    with open(embeddings_file, 'w') as embeddings:
        for line in lines:
            if not line.strip():  # Skip empty lines
                continue
            tokens = line.strip().split()
            mapped_id = tokens[0]
            if mapped_id in id_mapping:
                real_id = id_mapping[mapped_id]
                tokens[0] = real_id
                new_line = ' '.join(tokens)
                embeddings.write(new_line + '\n')
            else:
                embeddings.write(line)
```

[46]:
```
embeddings_file = "STRING_PPI_11_0_GAE_embeddings.txt"
node_list_file = "indx_to_protein.txt"
replace_mapped_ids(embeddings_file, node_list_file)
```

The next step is to convert the `.txt` file into `.csv` file, so we can visualize our embedding `.txt` file

in more informative way with the format:

protein1_id _ protein1_embedding_vector

protein2_id _ protein2_embedding_vector

protein3_id _ protein3_embedding_vector

....

Generate a CSV file to enhance the visualization of the embedding data

[47]:
```
import csv

def create_csv_from_embeddings(embeddings_file, csv_output_file):
    """
    The function takes '.txt' file of proteins and their corresponding
    embeddings vectors, and turns that into '.csv' file
    """
    data = []

    # Read the modified embeddings file and extract the data
    with open(embeddings_file, 'r') as embeddings:
        for line in embeddings:
            line = line.strip()
            if line:
                values = line.split()
                data.append(values)

    # Write the data to a CSV file
    with open(csv_output_file, 'w', newline='') as csvfile:
        csvwriter = csv.writer(csvfile)

        # Write the header (column names)
        header = ["Protein"] + [f"Embedding_{i}" for i in range(1,␣
 ↪len(data[0]))]
        csvwriter.writerow(header)

        # Write the data rows
        for values in data:
            protein_id, embeddings = values[0], values[1:]
            csvwriter.writerow([protein_id] + embeddings)
```

[48]:
```
embeddings_file = "STRING_PPI_11_0_GAE_embeddings.txt"
csv_output_file = "output_embeddings_GAE.csv"
create_csv_from_embeddings(embeddings_file, csv_output_file)
```

Creating a text file to examine zero vectors We observed a prevalence of zero vector embeddings for certain proteins. Various factors may contribute to this phenomenon, with one potential explanation being the utilization of outdated code sourced from the BioNEV repository for the gen-

eration of protein vector embeddings. The necessity to adapt numerous sections of the code to align with our dataset and the updated versions of libraries, no longer readily available for installation, constituted a crucial step in addressing this issue.

In preparation for the subsequent application of the struc2vec method to generate protein vector embeddings, we will compile a text file encompassing the identifiers of all such proteins. Additionally, this file will provide an enumeration of the quantity of proteins exhibiting zero vector embeddings.

[49]:
```
import pandas as pd

def write_zero_vector_proteins(csv_file_path, output_file_path):
    # Load the CSV file into a DataFrame, skipping the first two rows
    df = pd.read_csv(csv_file_path, skiprows=2)

    # Identify rows where all columns have values equal to 0
    zero_rows = df[df.iloc[:, 1:].eq(0).all(axis=1)]

    # Extract all protein IDs from the rows with all-zero vector embeddings
    zero_protein_ids = zero_rows.iloc[:, 0].unique()

    # Count the number of rows with all zeros
    num_zero_rows = len(zero_rows)

    print(f"Number of rows with all zero vector embeddings: {num_zero_rows}")

    # Write the count information to the first row of the output file
    with open(output_file_path, 'w') as file:
        file.write(f"Number of rows with all zero vector embeddings:␣
 ↪{num_zero_rows}\n")

        # Write all unique protein IDs to the file
        for protein_id in zero_protein_ids:
            file.write(f"{protein_id}\n")

    print(f"All unique protein IDs with all zero vector embeddings written to␣
 ↪{output_file_path}")
```

[50]:
```
write_zero_vector_proteins("output_embeddings_GAE.csv" ,␣
 ↪"zero_vector_proteins_GAE.txt")
```

```
Number of rows with all zero vector embeddings: 467
All unique protein IDs with all zero vector embeddings written to
zero_vector_proteins_GAE.txt
```

1.6.3 Graph Embedding using Struc2vev

After generating graph embeddingd for STRING PPI version 11.0 with GAE method, we will try also generating graph embeddings with `struc2vec` method. The reason is due to the most accurate

results of those two methods that shown in the article :

https://academic.oup.com/bioinformatics/article/36/4/1241/5581350?login=false

[1]:
```
import os

current_directory = os.getcwd()
print("Current directory:", current_directory)
```

```
Current directory: C:\Users\gavvi\Desktop\Programming\Python\DeepLearning
Research
```

Extracting the proteins embeddings after executing struc2vec method Due to the intricacy of the methodology employed, we opted to utilize the Google Colab environment with a T4 Graphics Processing Unit (GPU) to execute struc2vec. This decision was motivated by the desire to achieve expedited runtime during the generation of protein embeddings.

The model's performance was as follows:

Link Prediction Performance

`AUC-ROC: 0.915, AUC-PR: 0.911, Accuracy: 0.844, F1: 0.847`

Prediction Task Time: `675.44` s (~ `11.25` min)

Restore the genuine identifiers of proteins to the embedding text file The subsequent phase involves accessing the `.txt` file containing protein embeddings generated through the `struc2vec` method on the `GPU`. Subsequently, it necessitates the conversion of all numeric identifiers of the proteins to their original identifiers, as they were present in the initial *STRING* dataset.

For example: for the protein with the id number `7539` will turn into -> `9606.ENSP00000350012`

[15]:
```
cd "BioNEV/embeddings"
```

```
C:\Users\gavvi\Desktop\Programming\Python\DeepLearning
Research\BioNEV\embeddings
```

[16]:
```
import shutil

source_file = "STRING_PPI_11_0_s2vec_embeddings.txt"
destination_directory = "C:/Users/gavvi/Desktop/Programming/Python/DeepLearning␣
 ↪Research"

shutil.copy(source_file, destination_directory)
```

[16]:
```
'C:/Users/gavvi/Desktop/Programming/Python/DeepLearning
Research\\STRING_PPI_11_0_s2vec_embeddings.txt'
```

[17]:
```
import os
```

```
os.chdir(destination_directory)
current_directory = os.getcwd()
print("Current directory:", current_directory)
```

```
Current directory: C:\Users\gavvi\Desktop\Programming\Python\DeepLearning
Research
```

The function utilized for the conversion of protein identifiers subsequent to the implementation of the Graph Autoencoder (GAE) method can be employed once again for the purpose of reverting protein identifiers to their initial form.

[20]:
```
embeddings_file = source_file
node_list_file = "indx_to_protein.txt"
replace_mapped_ids(embeddings_file, node_list_file)
```

The next step is to convert the `.txt` file into `.csv` file, so we can visualize our embedding `.txt` file in more informative way with the format:

`protein1_id _ protein1_embedding_vector`

`protein2_id _ protein2_embedding_vector`

`protein3_id _ protein3_embedding_vector`

....

Generate a CSV file to enhance the visualization of the embedding data

[23]:
```
csv_output_file = "output_embeddings_st2vec.csv"
create_csv_from_embeddings(embeddings_file, csv_output_file)
```

Creating a text file to examine zero vectors

[51]:
```
write_zero_vector_proteins("output_embeddings_st2vec.csv" ,␣
↪"zero_vector_proteins_st2vec.txt")
```

```
Number of rows with all zero vector embeddings: 0
All unique protein IDs with all zero vector embeddings written to
zero_vector_proteins_st2vec.txt
```

[1]:
```
!jupyter nbconvert --to pdf Protein_Embedding.ipynb
```

```
This application is used to convert notebook files (*.ipynb)
[NbConvertApp] WARNING | pattern 'Protein_Embedding.ipynb' matched no files


        to various other formats.

        WARNING: THE COMMANDLINE INTERFACE MAY CHANGE IN FUTURE RELEASES.

Options
=======
The options below are convenience aliases to configurable class-options,
```

```
as listed in the "Equivalent to" description-line of the aliases.
To see all configurable class-options for some <cmd>, use:
    <cmd> --help-all

--debug
    set log level to logging.DEBUG (maximize logging output)
    Equivalent to: [--Application.log_level=10]
--show-config
    Show the application's configuration (human-readable format)
    Equivalent to: [--Application.show_config=True]
--show-config-json
    Show the application's configuration (json format)
    Equivalent to: [--Application.show_config_json=True]
--generate-config
    generate default config file
    Equivalent to: [--JupyterApp.generate_config=True]
-y
    Answer yes to any questions instead of prompting.
    Equivalent to: [--JupyterApp.answer_yes=True]
--execute
    Execute the notebook prior to export.
    Equivalent to: [--ExecutePreprocessor.enabled=True]
--allow-errors
    Continue notebook execution even if one of the cells throws an error and
include the error message in the cell output (the default behaviour is to abort
conversion). This flag is only relevant if '--execute' was specified, too.
    Equivalent to: [--ExecutePreprocessor.allow_errors=True]
--stdin
    read a single notebook file from stdin. Write the resulting notebook with
default basename 'notebook.*'
    Equivalent to: [--NbConvertApp.from_stdin=True]
--stdout
    Write notebook output to stdout instead of files.
    Equivalent to: [--NbConvertApp.writer_class=StdoutWriter]
--inplace
    Run nbconvert in place, overwriting the existing notebook (only
            relevant when converting to notebook format)
    Equivalent to: [--NbConvertApp.use_output_suffix=False
--NbConvertApp.export_format=notebook --FilesWriter.build_directory=]
--clear-output
    Clear output of current file and save in place,
            overwriting the existing notebook.
    Equivalent to: [--NbConvertApp.use_output_suffix=False
--NbConvertApp.export_format=notebook --FilesWriter.build_directory=
--ClearOutputPreprocessor.enabled=True]
--no-prompt
    Exclude input and output prompts from converted document.
    Equivalent to: [--TemplateExporter.exclude_input_prompt=True
```

```
--TemplateExporter.exclude_output_prompt=True]
--no-input
    Exclude input cells and output prompts from converted document.
            This mode is ideal for generating code-free reports.
    Equivalent to: [--TemplateExporter.exclude_output_prompt=True
--TemplateExporter.exclude_input=True
--TemplateExporter.exclude_input_prompt=True]
--allow-chromium-download
    Whether to allow downloading chromium if no suitable version is found on the
system.
    Equivalent to: [--WebPDFExporter.allow_chromium_download=True]
--disable-chromium-sandbox
    Disable chromium security sandbox when converting to PDF..
    Equivalent to: [--WebPDFExporter.disable_sandbox=True]
--show-input
    Shows code input. This flag is only useful for dejavu users.
    Equivalent to: [--TemplateExporter.exclude_input=False]
--embed-images
    Embed the images as base64 dataurls in the output. This flag is only useful
for the HTML/WebPDF/Slides exports.
    Equivalent to: [--HTMLExporter.embed_images=True]
--sanitize-html
    Whether the HTML in Markdown cells and cell outputs should be sanitized..
    Equivalent to: [--HTMLExporter.sanitize_html=True]
--log-level=<Enum>
    Set the log level by value or name.
    Choices: any of [0, 10, 20, 30, 40, 50, 'DEBUG', 'INFO', 'WARN', 'ERROR',
'CRITICAL']
    Default: 30
    Equivalent to: [--Application.log_level]
--config=<Unicode>
    Full path of a config file.
    Default: ''
    Equivalent to: [--JupyterApp.config_file]
--to=<Unicode>
    The export format to be used, either one of the built-in formats
            ['PDFviaHTML', 'asciidoc', 'custom', 'html', 'latex', 'markdown',
'notebook', 'pdf', 'pdfviahtml', 'python', 'qtpdf', 'qtpng', 'rst', 'script',
'slides', 'webpdf']
            or a dotted object name that represents the import path for an
            ``Exporter`` class
    Default: ''
    Equivalent to: [--NbConvertApp.export_format]
--template=<Unicode>
    Name of the template to use
    Default: ''
    Equivalent to: [--TemplateExporter.template_name]
--template-file=<Unicode>
```

```
    Name of the template file to use
    Default: None
    Equivalent to: [--TemplateExporter.template_file]
--theme=<Unicode>
    Template specific theme(e.g. the name of a JupyterLab CSS theme distributed
    as prebuilt extension for the lab template)
    Default: 'light'
    Equivalent to: [--HTMLExporter.theme]
--sanitize_html=<Bool>
    Whether the HTML in Markdown cells and cell outputs should be sanitized.This
    should be set to True by nbviewer or similar tools.
    Default: False
    Equivalent to: [--HTMLExporter.sanitize_html]
--writer=<DottedObjectName>
    Writer class used to write the
                                        results of the conversion
    Default: 'FilesWriter'
    Equivalent to: [--NbConvertApp.writer_class]
--post=<DottedOrNone>
    PostProcessor class used to write the
                                        results of the conversion
    Default: ''
    Equivalent to: [--NbConvertApp.postprocessor_class]
--output=<Unicode>
    Overwrite base name use for output files.
                Supports pattern replacements '{notebook_name}'.
    Default: '{notebook_name}'
    Equivalent to: [--NbConvertApp.output_base]
--output-dir=<Unicode>
    Directory to write output(s) to. Defaults
                                    to output to the directory of each notebook.
To recover
                                    previous default behaviour (outputting to the
current
                                    working directory) use . as the flag value.
    Default: ''
    Equivalent to: [--FilesWriter.build_directory]
--reveal-prefix=<Unicode>
    The URL prefix for reveal.js (version 3.x).
            This defaults to the reveal CDN, but can be any url pointing to a
copy
            of reveal.js.
            For speaker notes to work, this must be a relative path to a local
            copy of reveal.js: e.g., "reveal.js".
            If a relative path is given, it must be a subdirectory of the
            current directory (from which the server is run).
            See the usage documentation
            (https://nbconvert.readthedocs.io/en/latest/usage.html#reveal-js-
```

```
html-slideshow)
            for more details.
    Default: ''
    Equivalent to: [--SlidesExporter.reveal_url_prefix]
--nbformat=<Enum>
    The nbformat version to write.
            Use this to downgrade notebooks.
    Choices: any of [1, 2, 3, 4]
    Default: 4
    Equivalent to: [--NotebookExporter.nbformat_version]

Examples
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    The simplest way to use nbconvert is

            > jupyter nbconvert mynotebook.ipynb --to html

            Options include ['PDFviaHTML', 'asciidoc', 'custom', 'html',
'latex', 'markdown', 'notebook', 'pdf', 'pdfviahtml', 'python', 'qtpdf',
'qtpng', 'rst', 'script', 'slides', 'webpdf'].

            > jupyter nbconvert --to latex mynotebook.ipynb

            Both HTML and LaTeX support multiple output templates. LaTeX
includes
            'base', 'article' and 'report'.  HTML includes 'basic', 'lab' and
            'classic'. You can specify the flavor of the format used.

            > jupyter nbconvert --to html --template lab mynotebook.ipynb

            You can also pipe the output to stdout, rather than a file

            > jupyter nbconvert mynotebook.ipynb --stdout

            PDF is generated via latex

            > jupyter nbconvert mynotebook.ipynb --to pdf

            You can get (and serve) a Reveal.js-powered slideshow

            > jupyter nbconvert myslides.ipynb --to slides --post serve

            Multiple notebooks can be given at the command line in a couple of
            different ways:

            > jupyter nbconvert notebook*.ipynb
            > jupyter nbconvert notebook1.ipynb notebook2.ipynb
```

```
            or you can specify the notebooks list in a config file, containing::

                c.NbConvertApp.notebooks = ["my_notebook.ipynb"]

            > jupyter nbconvert --config mycfg.py

To see all available configurables, use `--help-all`.
```

[ ]: