DL4H_Team_137

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1 Reproduction of Paper `Learning the Graphical Structure of Electronic Health Records with Graph Convolutional Transformer` by DL4H Team 137

1.1 Introduction

- Background of the problem
  - This study focuses on readmission/mortality prediction.
  - Unstructured data, particularly claims data, lacks a clear structure, making it challenging for models like MiME (Choi et al., 2018) to be utilized effectively.
  - The primary difficulties include discovering the hidden structure of the data while simultaneously making predictions.
  - The approach outlined in the paper is effective according to their test metrics.
- Paper explanation
  - The paper proposes a new method, the Graph Convolutional Transformer (GCT), to jointly learn the hidden structure and perform the prediction task. This method uses unstructured data as the initial input and achieves accurate predictions for general medical tasks.
  - It offers significant benefits for individuals without access to structured data. Additionally, the learned structure can be useful for others who wish to reuse the learned structure for future studies.

2

3 Scope of reproducibility (5)

The scope of this reproducibility study focuses on verifying the results claimed in the paper "Learning the Graphical Structure of Electronic Health Records with Graph Convolutional Transformer". The goal is to reproduce the model's ability to predict readmission/mortality using electronic health records as described in the original research.

4 Methodology (15)

4.1 Environment

4.1.1 Python version

- Python 3.10 ### Dependencies/packages needed

- torch==1.7.1
- numpy==1.19.5
- pandas==1.2.0
- scikit-learn==0.24.1
- matplotlib==3.3.3

4.2 Data

4.2.1 Data download instruction

- The eICU data comes from https://physionet.org/content/eicu-crd/2.0/.
- You are required to participate in the CITI training.
- Download the patient, admissionDx, diagnosis, treatment CSV files
- Decompress and upload to your environment. ### Data descriptions with helpful charts and visualizations
- Admission Diagnosis without Encounter ID: 450589
- Diagnosis without Encounter ID: 2483092
- Treatment without Encounter ID: 3372000
- Accepted treatments: 316745
- Total eicu as input: 40410 ### Preprocessing code
- shown below

load data

[2]:
```
from google.colab import drive
drive.mount('/content/drive')
```

```
Mounted at /content/drive
```

[3]:
```
#load data
import pandas as pd
import numpy as np
import gc
import matplotlib.pyplot as plt
filenames = ['patient', 'admissionDx', 'diagnosis', 'treatment']
#raw_data_dir='./'
print("change 'raw_data_dir' if you are using different environment")
raw_data_dir = '/content/drive/My Drive/Colab_Notebooks/'
SUBSET_RATIO=1

def load_raw_data(raw_data_dir, filenames, subset_ratio=SUBSET_RATIO):

    data_frames = {}
    for filename in filenames:
        file_path = raw_data_dir + filename +'.csv'
        df = pd.read_csv(file_path)

        if subset_ratio < 1.0:
            df = df.sample(frac=subset_ratio)
```

```
        data_frames[filename]=df
    return data_frames
data_frames = load_raw_data(raw_data_dir, filenames)
```

change 'raw_data_dir' if you are using different environment

Preprocess data and generate the eicu record

[4]:
```
import sys
# preprocess patient data
def process_patient(df, hour_threshold=24):
    # Calculate encounter_timestamp and create a temporary DataFrame for sorting
    if df['patientunitstayid'].duplicated().any():
        print('Duplicate encounter ID!!')
        sys.exit(0)
    df['encounter_timestamp'] = -df['hospitaladmitoffset'].astype(int)

    # Sorting patients by their IDs and then by the encounter timestamp
    df_sorted = df.sort_values(['patienthealthsystemstayid',␣
↪'encounter_timestamp'])

    # Detect readmissions by checking if the next stay is within the same␣
↪patient ID

    df_sorted['readmission'] = True  # Initially mark all as True
    df_sorted.loc[df_sorted.
↪groupby('patienthealthsystemstayid')['patientunitstayid'].tail(1).index,␣
↪'readmission'] = False
    df_sorted['unitdischargestatus'] =␣
↪df_sorted['unitdischargestatus']=='Expired'

    duration_threshold = hour_threshold * 60.0
    mask = df_sorted['unitdischargeoffset'] <= duration_threshold

    df_sorted = df_sorted[mask]
    rename_dict = {'patienthealthsystemstayid':'patient_id',
                   'patientunitstayid':'encounter_id',
                   'encounter_timestamp':'encounter_timestamp',
                   'unitdischargestatus':'expired',
                  }
    df_selected = df_sorted[ list(rename_dict.keys())+['readmission'] ]
    df_renamed = df_selected.rename(columns=rename_dict)
    return df_renamed
```

[5]:
```
#
patient_dataframe = process_patient(data_frames['patient'])
```

[6]:
```
patient_dataframe[:5]
```

[6]:

	patient_id	encounter_id	encounter_timestamp	expired	readmission
1	128927	141178	14	False	True
5	128943	141197	25	False	True
7	128952	141208	1	False	False
9	128970	141229	4	False	False
12	128995	141260	18	False	False

[7]:
```
# test correctness

# patient_dataframe[patient_dataframe['readmission']==True][:5]
# pdf = data_frames['patient']
# pdf[ pdf['patienthealthsystemstayid']==133737]
# patient_dataframe[pdf['patientunitstayid']==147378]['readmission']
```

[8]:
```
# process admission
def process_admission_dx(df,patient_df):
    # Check and report the number of missing encounter IDs

    df['admitdxpath'] = df['admitdxpath'].str.lower()

    patient_encounter_ids = set(patient_df['encounter_id'])

    mask = df['patientunitstayid'].isin(patient_encounter_ids)

    missing_eid = df[~mask]

    print('admission without Encounter ID:', len(missing_eid))

    df = df[mask]
    rename_dict = {'patientunitstayid':'encounter_id',
                   'admitdxpath':'dx_id'
                  }
    df_selected = df[list(rename_dict.keys()) ]
    df_renamed = df_selected.rename(columns=rename_dict)

    return df_renamed

admission_dataframe =␣
 ↪process_admission_dx(data_frames['admissionDx'],patient_dataframe)
```

admission without Encounter ID: 450589

[9]:
```
admission_dataframe[:5]
```

[9]:
```
    encounter_id                                              dx_id
26       2900366  admission diagnosis|was the patient admitted f…
27       2900366  admission diagnosis|all diagnosis|non-operativ…
28       2900366  admission diagnosis|non-operative organ system…
36       2900423  admission diagnosis|non-operative organ system…
37       2900423  admission diagnosis|was the patient admitted f…
```

[10]:
```python
def process_diagnosis(df,patient_df):
    # Check and report the number of missing encounter IDs

    df['diagnosisstring'] = df['diagnosisstring'].str.lower()

    patient_encounter_ids = set(patient_df['encounter_id'])

    mask = df['patientunitstayid'].isin(patient_encounter_ids)

    missing_eid = df[~mask]

    print('Admission Diagnosis without Encounter ID:', len(missing_eid))

    df = df[mask]
    rename_dict = {'patientunitstayid':'encounter_id',
                   'diagnosisstring':'dx_id'
                  }
    df_selected = df[list(rename_dict.keys()) ]
    df_renamed = df_selected.rename(columns=rename_dict)

    return df_renamed
diagnosis_dataframe =␣
 ↪process_diagnosis(data_frames['diagnosis'],patient_dataframe)
```

```
Admission Diagnosis without Encounter ID: 2483092
```

[11]:
```python
diagnosis_dataframe[:5]
```

[11]:
```
    encounter_id                                              dx_id
30        141229     cardiovascular|arrhythmias|atrial fibrillation
31        141229  cardiovascular|ventricular disorders|acute pul…
32        141229  cardiovascular|ventricular disorders|congestiv…
33        141229  neurologic|altered mental status / pain|change…
34        141229  cardiovascular|ventricular disorders|acute pul…
```

[12]:
```python
def process_treatment(df, patient_df):

    df['treatmentstring'] = df['treatmentstring'].str.lower()

    patient_encounter_ids = set(patient_df['encounter_id'])
```

```
    mask = df['patientunitstayid'].isin(patient_encounter_ids)

    missing_eid = df[~mask]

    print('treatment without Encounter ID:', len(missing_eid))

    df = df[mask]
    rename_dict = {'patientunitstayid':'encounter_id',
                   'treatmentstring':'treatment'
                  }

    df_selected = df[list(rename_dict.keys()) ]
    df_renamed = df_selected.rename(columns=rename_dict)

    return df_renamed

treatment_dataframe = process_treatment(data_frames['treatment'],␣
↪patient_dataframe)
```

```
treatment without Encounter ID: 3372000
```

[13]:
```
treatment_dataframe[:5]
```

[13]:

	encounter_id	treatment
224	242203	gastrointestinal|medications|stress ulcer prop…
225	242203	pulmonary|ventilation and oxygenation|oxygen t…
226	242203	renal|urinary catheters|foley catheter
227	242203	renal|electrolyte correction|treatment of hype…
228	242203	gastrointestinal|medications|antiemetic|seroto…

4.3

[14]:
```
"""double check ok"""
# output from python 2.7 environment
# Processing patient.csv
# Processing admission diagnosis.csv
# Admission Diagnosis without Encounter ID: 450589
# Processing diagnosis.csv
# Diagnosis without Encounter ID: 2483092
# Processing treatment.csv
# Treatment without Encounter ID: 3372000
# Accepted treatments: 316745

# This is the same as above log output
```

[14]: 'double check ok'

[15]:
```
print(len(patient_dataframe),len(admission_dataframe),len(diagnosis_dataframe),len(treatment_d
```

68076 176269 227580 316745

[16]:
```
'The content in sequence seqex_list'
# Context Features:
# key: label.expired value: int64_list {
#   value: 0
# }

# key: label.readmission value: int64_list {
#   value: 0
# }

# key: patientId value: bytes_list {
#   value: "2630449:3229400"
# }

# Feature Lists:
# key: proc_ids
# feature: bytes_list {
#   value: "pulmonary|ventilation and oxygenation|oxygen therapy (< 40%)|nasal␣
↪cannula"
#   value: "cardiovascular|intravenous fluid|normal saline administration"
#   value: "endocrine|glucose metabolism|insulin|continuous infusion"
#   value: "gastrointestinal|medications|stress ulcer prophylaxis|famotidine"
#   value: "cardiovascular|arrhythmias|anticoagulant administration|low␣
↪molecular weight heparin|enoxaparin"
# }

# key: dx_ints
# feature: int64_list {
#   value: 202
#   value: 0
#   value: 201
#   value: 164
# }

# key: dx_ids
# feature: bytes_list {
#   value: "endocrine|glucose metabolism|dka"
#   value: "admission diagnosis|was the patient admitted from the o.r. or went␣
↪to the o.r. within 4 hours of admission?|no"
#   value: "admission diagnosis|all diagnosis|non-operative|diagnosis|metabolic/
↪endocrine|diabetic ketoacidosis"
#   value: "admission diagnosis|non-operative organ systems|organ␣
↪system|metabolic/endocrine"
```

```
# }

# key: proc_ints
# feature: int64_list {
#   value: 68
#   value: 27
#   value: 273
#   value: 80
#   value: 417
# }

# first key: 1392393:1774519
# content of dx_str2int:
# key: surgery|respiratory failure|ventilatory failure|suspected value: 2762
# key: burns/trauma|trauma-other injuries|traumatic amputation|arm/hand value:␣
↪3196
# key: endocrine|fluids and electrolytes|hypernatremia|moderate (146 - 155 meq/
↪dl) value: 1284
# key: admission diagnosis|all␣
↪diagnosis|operative|diagnosis|cardiovascular|thrombectomy (with general␣
↪anesthesia) value: 975
# key: endocrine|fluids and electrolytes|hyponatremia|severe (< 125 meq/dl)␣
↪value: 709
# content of treat_str2int:
# key: pulmonary|surgery / incision and drainage of thorax|pulmonary␣
↪resection|lobectomy value: 1083
# key: neurologic|ich/ cerebral infarct|anticonvulsants|phenytoin value: 603
# key: cardiovascular|arrhythmias|digoxin value: 284
# key: toxicology|drug overdose|agent specific therapy|beta blockers␣
↪overdose|atropine value: 1489
# key: oncology|medications|analgesics|oral analgesics value: 17
```

[16]: 'The content in sequence seqex_list'

[17]:
```
del data_frames
gc.collect()
```

[17]: 31

[18]:
```
def build_dataframe(patient_dataframe,␣
↪treatment_dataframe,diagnosis_dataframe,admission_dataframe, min_num_codes=1,
                max_num_codes=50):

    '''
    This function is to bulid the dataframe for training,
    it is equals to build_seqex in process_eicu.py
```

```
    '''
    filter = lambda x: len(x)>=min_num_codes and len(x)<=max_num_codes

    # merge admission and diagnosis
    merged_admission_diagnosis = pd.concat([admission_dataframe,␣
↪diagnosis_dataframe], axis=0)

    dx_list = list(set(merged_admission_diagnosis['dx_id']))

    dx_str2int = {s:i for i,s in enumerate(dx_list)}

    merged_admission_diagnosis['dx_ints'] = merged_admission_diagnosis['dx_id'].
↪map(dx_str2int)

    merged_admission_diagnosis = merged_admission_diagnosis.
↪groupby('encounter_id')['dx_ints'].agg(list).reset_index()

    merged_admission_diagnosis␣
↪=merged_admission_diagnosis[merged_admission_diagnosis['dx_ints'].
↪apply(filter)]

    # aggrigate treatment_dataframe

    treat_list = list(set(treatment_dataframe['treatment']))

    treat_str2int = {s:i for i,s in enumerate(treat_list)}

    treatment_dataframe['proc_ints'] =  treatment_dataframe['treatment'].
↪map(treat_str2int)

    treatment_dataframe = treatment_dataframe.
↪groupby('encounter_id')['proc_ints'].agg(list).reset_index()

    treatment_dataframe =treatment_dataframe[treatment_dataframe['proc_ints'].
↪apply(filter)]

    #print(len(merged_admission_diagnosis),len(treatment_dataframe))

    # merge patient, admission and diagnosis
    merged_patient_proc_ints = pd.merge(merged_admission_diagnosis,␣
↪patient_dataframe, on='encounter_id', how='inner')

    # merge patient, all

    merged_df= pd.merge(merged_patient_proc_ints, treatment_dataframe,␣
↪on='encounter_id', how='inner')
```

```
    merged_df['patientId'] = merged_df.apply(lambda row: (row['patient_id'],␣
↪row['encounter_id']), axis=1)

    merged_df.drop(['patient_id','encounter_timestamp'], axis=1, inplace=True)

    merged_df.set_index('encounter_id', inplace=True)

    return  merged_df, dx_str2int, treat_str2int,dx_list,treat_list

df, dx_str2int, treat_str2int,dx_list,treat_list =␣
↪build_dataframe(patient_dataframe,␣
↪treatment_dataframe,diagnosis_dataframe,admission_dataframe)
```

[19]:
```
#TODO
# Need to check the difference,
# data process_eicu.py gives 41026
# It may comes from the joining method and datatype
print(len(df))
```

```
40410
```

[20]:
```
# df.loc[3353254]
```

[21]:
```
print("""
Output of the process_eicu.py for encounter Id: 3353254
The number of the "dx_ints" and "proc_ints" is the same
The value is different,which is ok, the value is just an
index to dictionary
""")
# seqx for 3353254: context {
#   feature {
#     key: "label.expired"
#     value {
#       int64_list {
#         value: 0
#       }
#     }
#   }
#   feature {
#     key: "label.readmission"
#     value {
#       int64_list {
#         value: 0
#       }
#     }
#   }
```

```
#   feature {
#     key: "patientId"
#     value {
#       bytes_list {
#         value: "2743102:3353254"
#       }
#     }
#   }
# }
# feature_lists {
#   feature_list {
#     key: "dx_ids"
#     value {
#       feature {
#         bytes_list {
#           value: "admission diagnosis|non-operative organ systems|organ␣
↪system|gastrointestinal"
#           value: "admission diagnosis|was the patient admitted from the o.r.␣
↪or went to the o.r. within 4 hours of admission?|no"
#           value: "renal|disorder of kidney|acute renal failure|due to␣
↪hypovolemia/decreased circulating volume"
#           value: "admission diagnosis|all␣
↪diagnosis|non-operative|diagnosis|gastrointestinal|bleeding, lower gi"
#           value: "gastrointestinal|gi bleeding / pud|lower gi bleeding"
#         }
#       }
#     }
#   }
#   feature_list {
#     key: "dx_ints"
#     value {
#       feature {
#         int64_list {
#           value: 31
#           value: 0
#           value: 225
#           value: 323
#           value: 324
#         }
#       }
#     }
#   }
#   feature_list {
#     key: "proc_ids"
#     value {
#       feature {
#         bytes_list {
```

```
#           value: "cardiovascular|intravenous fluid|normal saline␣
↪administration|fluid bolus (250-1000mls)"
#           value: "cardiovascular|intravenous fluid|blood product␣
↪administration|packed red blood cells|transfusion of > 2 units prbc\'s"
#         }
#       }
#     }
#   }
#   feature_list {
#     key: "proc_ints"
#     value {
#       feature {
#         int64_list {
#           value: 105
#           value: 483
#         }
#       }
#     }
#   }
# }
```

```
Output of the process_eicu.py for encounter Id: 3353254
The number of the "dx_ints" and "proc_ints" is the same
The value is different,which is ok, the value is just an
index to dictionary
```

[22]:
```
print(len(dx_str2int),len(treat_str2int))
#TODO Check the difference. Code gives
```

```
3351 2212
```

[23]:
```
from sklearn.model_selection import train_test_split
```

[24]:
```
def select_train_valid_test(df, target ='readmission', random_seed=0):

    train_df, temp_df = train_test_split(df, test_size=0.2,␣
↪random_state=random_seed)
    valid_df, test_df = train_test_split(temp_df, test_size=0.5,␣
↪random_state=random_seed)

    return train_df,valid_df,test_df
train_df, validate_df, test_df = select_train_valid_test(df)
```

[25]:
```
from itertools import product
def generate_combinations(row):
```

```python
    return list(product(row['dx_ints'], row['proc_ints']))

total_visit = len(df)
def count_conditional_prob_dp(df,total_visit):
    """
    This is equals to the count_conditional_prob_dp in␣
↪graph_convolutional_transformer.py
    It is used for creating the prob_dp table

    """

    dx_explode = df['dx_ints'].explode()
    dx_freqs = dx_explode.value_counts().to_dict()
    proc_explode = df['proc_ints'].explode()
    proc_freqs = proc_explode.value_counts().to_dict()

    df['dp'] = df.apply(generate_combinations, axis=1)
    exploded_df = df.explode('dp')
    dp_freqs = exploded_df['dp'].value_counts().to_dict()

    # print(dp_freqs)

    dx_probs = dict([(k, v / float(total_visit)) for k, v in dx_freqs.items()])
    proc_probs = dict([(k, v / float(total_visit)) for k, v in proc_freqs.
↪items()])
    dp_probs = dict([(k, v / float(total_visit)) for k, v in dp_freqs.items()])

    dp_cond_probs = {}
    pd_cond_probs = {}
    for dx, dx_prob in dx_probs.items():
        for proc, proc_prob in proc_probs.items():
            dp = tuple([dx, proc])
            pd = tuple([proc, dx])
            if dp in dp_probs:
                dp_cond_probs[dp] = dp_probs[dp] / dx_prob
                pd_cond_probs[pd] = dp_probs[dp] / proc_prob
            else:
                dp_cond_probs[dp] = 0.0
                pd_cond_probs[pd] = 0.0

    return dx_probs, proc_probs, dp_probs, dp_cond_probs, pd_cond_probs


dx_probs, proc_probs, dp_probs, dp_cond_probs, pd_cond_probs =␣
↪count_conditional_prob_dp(train_df,total_visit)
```

[26]:
```python
len(dp_cond_probs),len(pd_cond_probs),len(dp_probs)
```

[26]: (6381180, 6381180, 259759)

[27]:
```
print(next(iter(pd_cond_probs.items())))
```

((2149, 1995), 0.7152446564211271)

[28]:
```
import numpy as np


def add_sparse_prior_guide_dp(df,dp_cond_probs,pd_cond_probs,max_num_codes=50):
    #simliar to funciton add_sparse_prior_guide_dp in code base
    # This is used for create the prior guide matrix
    # Prior guide is used for guiding the GCN to search the most possible␣
↪direction
    df['prior_indices'] = None
    df['prior_values'] = None

    # Iterate through DataFrame rows

    for idx, row in df.iterrows():
        dx_ids = row['dx_ints']
        proc_ids = row['proc_ints']

        dp_combinations = list(product(range(len(dx_ids)),␣
↪range(len(proc_ids))))
        pd_combinations = list(product(range(len(proc_ids)),␣
↪range(len(dx_ids))))

        # Adjust indices for procedures
        dp_combinations_adjusted = [(x[0], max_num_codes + x[1]) for x in␣
↪dp_combinations]
        pd_combinations_adjusted = [(max_num_codes + x[0], x[1]) for x in␣
↪pd_combinations]

        # Combine indices and calculate values
        all_indices = dp_combinations_adjusted + pd_combinations_adjusted

        # Fetch probabilities using dictionary get method with default of 0.0␣
↪for missing entries

        dp_values = [dp_cond_probs.get((dx_ids[i],proc_ids[j]), 0.0) for i, j␣
↪in dp_combinations]
        pd_values = [pd_cond_probs.get((proc_ids[i],dx_ids[j]), 0.0) for i, j␣
↪in pd_combinations]
        # Assign to DataFrame
        df.at[idx, 'prior_indices'] = all_indices
        df.at[idx, 'prior_values'] = dp_values + pd_values
```

```python
    return df
```

[29]:
```python
print(len(df),len(train_df))
```

40410 32328

[30]:
```python
# create the train/validate/test split of dataframe
train_df= add_sparse_prior_guide_dp(train_df,dp_cond_probs,pd_cond_probs)

validate_df = add_sparse_prior_guide_dp(validate_df,dp_cond_probs,pd_cond_probs)

test_df = add_sparse_prior_guide_dp(test_df,dp_cond_probs,pd_cond_probs)

del df
gc.collect()
# check the memory usage
# The size may not accurate in cloud
total_memory = train_df.memory_usage(deep=True).sum()
print(f"Total Memory Usage: {total_memory} bytes")
total_memory = validate_df.memory_usage(deep=True).sum()
print(f"Total Memory Usage: {total_memory} bytes")
total_memory = test_df.memory_usage(deep=True).sum()
print(f"Total Memory Usage: {total_memory} bytes")
```

Total Memory Usage: 122069640 bytes
Total Memory Usage: 11693282 bytes
Total Memory Usage: 11485490 bytes

[31]:
```python
# This is the content in the tf record.
# Used to verify the correctness of the dataframe
# seqex for key '2743102:3353254':
# context {
#   feature {
#     key: "label.expired"
#     value {
#       int64_list {
#         value: 0
#       }
#     }
#   }
#   feature {
#     key: "label.readmission"
#     value {
#       int64_list {
#         value: 0
#       }
```

```
#     }
#   }
#   feature {
#     key: "patientId"
#     value {
#       bytes_list {
#         value: "2743102:3353254"
#       }
#     }
#   }
# }
# feature_lists {
#   feature_list {
#     key: "dx_ids"
#     value {
#       feature {
#         bytes_list {
#           value: "admission diagnosis|non-operative organ systems|organ␣
↪system|gastrointestinal"
#           value: "admission diagnosis|was the patient admitted from the o.r.␣
↪or went to the o.r. within 4 hours of admission?|no"
#           value: "renal|disorder of kidney|acute renal failure|due to␣
↪hypovolemia/decreased circulating volume"
#           value: "admission diagnosis|all␣
↪diagnosis|non-operative|diagnosis|gastrointestinal|bleeding, lower gi"
#           value: "gastrointestinal|gi bleeding / pud|lower gi bleeding"
#         }
#       }
#     }
#   }
  # feature_list {
  #   key: "dx_ints"
  #   value {
  #     feature {
  #       int64_list {
  #         value: 31
  #         value: 0
  #         value: 225
  #         value: 323
  #         value: 324
  #       }
  #     }
  #   }
  # }
#   feature_list {
#     key: "prior_indices"
#     value {
```

```
#       feature {
#         int64_list {
#           value: 0
#           value: 50
#           value: 0
#           value: 51
#           value: 1
#           value: 50
#           value: 1
#           value: 51
#           value: 2
#           value: 50
#           value: 2
#           value: 51
#           value: 3
#           value: 50
#           value: 3
#           value: 51
#           value: 4
#           value: 50
#           value: 4
#           value: 51
#           value: 50
#           value: 0
#           value: 50
#           value: 1
#           value: 50
#           value: 2
#           value: 50
#           value: 3
#           value: 50
#           value: 4
#           value: 51
#           value: 0
#           value: 51
#           value: 1
#           value: 51
#           value: 2
#           value: 51
#           value: 3
#           value: 51
#           value: 4
#         }
#       }
#     }
#   }
  # feature_list {
```

```
  #   key: "prior_values"
  #   value {
  #     feature {
  #       float_list {
  #         value: 0.0373423844576
  #         value: 0.0242483019829
  #         value: 0.0424405224621
  #         value: 0.00441289320588
  #         value: 0.129310339689
  #         value: 0.00862068962306
  #         value: 0.0530973449349
  #         value: 0.030973451212
  #         value: 0.0440097786486
  #         value: 0.0366748161614
  #         value: 0.0655877366662
  #         value: 0.942078351974
  #         value: 0.012776831165
  #         value: 0.0204429309815
  #         value: 0.0153321977705
  #         value: 0.3355704844
  #         value: 0.771812081337
  #         value: 0.00671140942723
  #         value: 0.0939597338438
  #         value: 0.10067114234
  #       }
  #     }
  #   }
  # }
#   feature_list {
#     key: "proc_ids"
#     value {
#       feature {
#         bytes_list {
#           value: "cardiovascular|intravenous fluid|normal saline
administration|fluid bolus (250-1000mls)"
#           value: "cardiovascular|intravenous fluid|blood product
administration|packed red blood cells|transfusion of > 2 units prbc\'s"
#         }
#       }
#     }
#   }
#   feature_list {
#     key: "proc_ints"
#     value {
#       feature {
#         int64_list {
#           value: 105
```

```
#           value: 483
#         }
#       }
#     }
#   }
# }
```

[32]:
```
#print(list(train_df.loc[3353254]['prior_indices']))
```

[33]:
```
#print(list(train_df.loc[3353254]['prior_values']))
```

[34]:
```
train_df[:5]
```

[34]:
```
                                                       dx_ints  expired  \
encounter_id
2968542                                 [3245, 1995, 780, 2009]    False
1198112         [2509, 1995, 780, 2653, 1575, 1706, 2637, 2017]    False
990206                                         [752, 329, 2821]    False
2764033       [1995, 780, 1997, 2557, 2557, 2557, 2667, 2667…   False
1549215                [873, 1995, 3043, 2753, 329, 1029, 171]    False

              readmission                                          proc_ints  \
encounter_id
2968542              True                                             [1915]
1198112             False                         [267, 8, 1100, 487, 2101]
990206              False                                       [1512, 226]
2764033              True  [1929, 951, 226, 8, 2178, 2190, 1931, 2190, 95…
1549215             False                           [1512, 1782, 2149, 26]

                       patientId  \
encounter_id
2968542       (2406228, 2968542)
1198112        (895769, 1198112)
990206          (730623, 990206)
2764033       (2227126, 2764033)
1549215       (1193171, 1549215)


                                                          dp  \
encounter_id
2968542       [(3245, 1915), (1995, 1915), (780, 1915), (200…
1198112       [(2509, 267), (2509, 8), (2509, 1100), (2509, …
990206        [(752, 1512), (752, 226), (329, 1512), (329, 2…
2764033       [(1995, 1929), (1995, 951), (1995, 226), (1995…
1549215       [(873, 1512), (873, 1782), (873, 2149), (873, …

                                                prior_indices  \
encounter_id
```

```
2968542       [(0, 50), (1, 50), (2, 50), (3, 50), (50, 0), …
1198112       [(0, 50), (0, 51), (0, 52), (0, 53), (0, 54), …
990206        [(0, 50), (0, 51), (1, 50), (1, 51), (2, 50), …
2764033       [(0, 50), (0, 51), (0, 52), (0, 53), (0, 54), …
1549215       [(0, 50), (0, 51), (0, 52), (0, 53), (1, 50), …

                                                  prior_values
encounter_id
2968542       [0.2540106951871658, 0.07454792922418822, 0.08…
1198112       [0.030645161290322583, 0.3193548387096774, 0.0…
990206        [0.06666666666666667, 0.18333333333333335, 0.5…
2764033       [0.007427571456348435, 0.0006610927474236827, …
1549215       [0.054989816700611, 0.0622636019784696, 0.1844…
```

[ ]:
```
# create the data loader
```

create the data loader

[35]:
```
import torch
import numpy as np
import pandas as pd
from torch.utils.data import Dataset, DataLoader

# create the data loader
# Example DataFrame
print(len(dx_str2int),len(treat_str2int))
# 3351 2212

vcob_size={
    "dx_ints":len(dx_str2int),
    "proc_ints":len(treat_str2int)
}
selected_features = ['dx_ints','proc_ints']
# encounter_id is not in selected feature, because it is now a index of the␣
↪dataframe
# prior_indices and prior_values features are not selected to enter the model,
# they are only used to calculate the guide matrix and the prior matrix
# they have vary lenght and some of them too large to pad
# they will be selected by the encounter_id from the df when used
class CustomDataset(Dataset):
    def __init__(self, dataframe, max_num_code=50,␣
↪vcob_size=vcob_size,selected_features = selected_features, label_name =␣
↪'readmission'):
        self.dataframe = dataframe[selected_features +[label_name]]
        self.max_num_code = max_num_code
        self.vcob_size = vcob_size
        self.label_name = label_name
```

```
    def __len__(self):
        return len(self.dataframe)

    def __getitem__(self, idx):

        row = self.dataframe.iloc[idx]
        encounter_id = self.dataframe .index[idx]

        dict_row =row.to_dict()
        feature_dict = {}

        feature_dict['encounter_id']=encounter_id
        for name in selected_features:

            if name in self.vcob_size:
                n= len(dict_row[name])
                pad = self.vcob_size[name]
                feature_dict[name] = torch.tensor(dict_row[name] + [pad]*(self.
↪max_num_code-n),dtype=torch.int)
            else:
                feature_dict[name] = torch.tensor(dict_row[name],dtype=long)

        return feature_dict, torch.tensor(dict_row[self.label_name])

batch_size=32
train_dataset = CustomDataset(train_df)
train_dataloader = DataLoader(train_dataset, batch_size=batch_size,shuffle=True)

validate_dataset = CustomDataset(validate_df)
validate_dataloader = DataLoader(validate_dataset,␣
↪batch_size=batch_size,shuffle=False)

test_dataset = CustomDataset(test_df)
test_dataloader = DataLoader(test_dataset, batch_size=batch_size,shuffle=False)
# Iterate through the DataLoader in a training loop
# for dict_row,label in dataloader:
#     #print(dict_row,label)
#     for encounter_id in dict_row["encounter_id"]:
#         eid  = int(encounter_id)
#         print(example_df.loc[eid][["prior_indices","prior_values"]])
```

```
3351 2212
```

[36]:
```
example_batch, example_label = next(iter(train_dataloader))
```

[37]:
```
print("One example input to the model, for testing function:\n", example_batch,␣
↪example_label)
```

```
One example input to the model, for testing function:
 {'encounter_id': tensor([1653601, 2707486,  753949, 2630727, 2419420,  944730,
1212301,  687445,
        1096928, 1091733, 3146147, 3330193, 1660870, 1153501,  972237, 1817805,
        2613884, 1752855, 1125819, 2896753, 1811032, 1244134, 3237268, 2965165,
         536727, 1994192,  733513, 3200331, 3046405,  684681, 1740503,
2970059]), 'dx_ints': tensor([[1995, 3290, 2491,  …, 3351, 3351, 3351],
        [1995,  780, 1600,  …, 3351, 3351, 3351],
        [1525, 1995,  913,  …, 3351, 3351, 3351],
        …,
        [ 560, 2495, 2009,  …, 3351, 3351, 3351],
        [2329,  780, 1995,  …, 3351, 3351, 3351],
        [2002, 1995,  780,  …, 3351, 3351, 3351]], dtype=torch.int32),
'proc_ints': tensor([[1272,  427, 2183,  …, 2212, 2212, 2212],
        [1292,  354, 1512,  …, 2212, 2212, 2212],
        [2149, 2212, 2212,  …, 2212, 2212, 2212],
        …,
        [1915, 2212, 2212,  …, 2212, 2212, 2212],
        [  55,  286, 1974,  …, 2212, 2212, 2212],
        [ 712,  548, 2212,  …, 2212, 2212, 2212]], dtype=torch.int32)}
tensor([False, False,  True, False, False,  True,  True,  True,  True,  True,
        False, False, False, False, False, False, False, False, False, False,
        False, False, False, False, False, False,  True, False, False, False,
        False,  True])
```

5 Model

5.0.1 Citation to the original paper

- Learning the Graphical Structure of Electronic Health Records with Graph Convolutional Transformer Edward Choi, Zhen Xu, Yujia Li, Michael W. Dusenberry, Gerardo Flores, Yuan Xue, Andrew M. Dai
  AAAI 2020 ### Link to the original paper's repo
- `[GitHub Repo](https://github.com/Google-Health/records-research/tree/master/graph-convolut`
  ### Model descriptions
- The GCT model uses graph convolution combined with a transformer architecture to process unstructured EHR data.

5.0.2 Implementation code

- code

[38]:
```
import torch
import torch.nn as nn
# create embedder
```

```python
class FeatureEmbedder(nn.Module):
    def __init__(self, embedding_size,
                 vocab_sizes=vcob_size,
                 feature_keys = ["dx_ints","proc_ints"]):

        super(FeatureEmbedder, self).__init__()
        self.embeddings = nn.ModuleDict()
        self.vocab_sizes = vocab_sizes
        self.embedding_size = embedding_size
        self.feature_keys=feature_keys
        # Adding one for the padding index
        for key in feature_keys:
            self.embeddings[key] = nn.Embedding(num_embeddings=vocab_sizes[key]␣
↪+ 1, embedding_dim=embedding_size, padding_idx=vocab_sizes[key])
            #print(self.embeddings[key].weight.size())
        # Special case for 'visit' embedding
        self.embeddings['visit'] = nn.Embedding(num_embeddings=1,␣
↪embedding_dim=embedding_size)


    def forward(self, feature_map):
        '''
        feature_map: key to  max_num_codes length code, one key "idx_ints" is␣
↪like: {"idx_ints":[[11,0,1,12,...],[[1,12,3,5...]]]}
        the shape of the tensor is (batch,max_num_codes)

        result:
            embeddings: embeddings' shape is␣
↪(batch_size,1+max_num_codes+max_num_codes,embedding_size)
                max_num_codes+max_num_codes+1 is for visit, idx embeddings,␣
↪proc embeddings
            masks: a mask for each embeddings, the shape is␣
↪(batch_size,1+max_num_codes+max_num_codes)
        '''
        embeddings = {}
        masks = {}
        batch_size, max_num_codes = feature_map['proc_ints'].shape
        #print(self.feature_keys)

        for key in self.feature_keys:
            # pad unused to vocab_size
            padding = self.vocab_sizes[key]
            ids = feature_map[key]
            #print(key,ids.shape)

            embeddings[key] = self.embeddings[key](ids)
```

```
            # Create mask
            mask = (ids != padding).int()
            masks[key] = mask

        # Handle the 'visit' embedding separately

        embeddings['visit'] = self.embeddings['visit'](torch.
↪zeros((batch_size,1),dtype=torch.int32))
        masks['visit'] = torch.ones(batch_size,1)

        # hardcode here to ensure the order of the embedings
        feature_names = ['visit','dx_ints','proc_ints']
        embeddings = [embeddings[name] for name in feature_names]
        embeddings = torch.cat(embeddings,axis=1)

        masks = [masks[name] for name in feature_names]
        masks = torch.cat(masks,axis=1)

        return embeddings, masks
```

[43]:
```
embedder = FeatureEmbedder(128)
embeddings, masks = embedder(example_batch)
```

[44]:
```
print("If you encoutered kernel dead here, please run it in cloud like colab")
```

```
If you encoutered kernel dead here, please run it in cloud like colab
```

[45]:
```
import torch
import torch.nn.functional as F

def create_matrix_vdp(df, features, mask, use_prior=True, use_inf_mask=True,␣
↪max_num_codes=50, prior_scalar=0.5):
    """
    Creates guide matrix and prior matrix when feature_set='vdp' in PyTorch.

    Args:
        features (dict): Dictionary of lists of integers for each feature.
        mask (Tensor): 3D tensor (batch_size, num_features) indicating padded␣
↪parts.
        use_prior (bool): Whether to create the prior matrix.
        use_inf_mask (bool): Whether to create the guide matrix.
        max_num_codes (int): Maximum number of codes per feature inside a␣
↪single visit.
        prior_scalar (float): Scalar to hard-code the diagonal elements of the␣
↪prior matrix.
```

```
    Returns:
        Tuple of Tensors: guide matrix and prior guide matrix.
    """
    #print(features)
    eids = features['encounter_id']

    batch_size = eids.size(0)
    num_dx_ids = max_num_codes
    num_proc_ids = max_num_codes
    num_codes = 1 + num_dx_ids + num_proc_ids  # 1 for 'visit'

    guide = None
    if use_inf_mask:
        row0 = torch.cat([torch.zeros(1, 1), torch.ones(1, num_dx_ids), torch.
↪zeros(1, num_proc_ids)], dim=1)
        row1 = torch.cat([torch.zeros(num_dx_ids, 1 + num_dx_ids), torch.
↪ones(num_dx_ids, num_proc_ids)], dim=1)
        row2 = torch.zeros(num_proc_ids, num_codes)

        guide = torch.cat([row0, row1, row2], dim=0)
        guide = guide + guide.T
        guide = guide.unsqueeze(0).repeat(batch_size, 1, 1)  # replicate for␣
↪each batch
        guide = guide * mask.unsqueeze(2) * mask.unsqueeze(1) + torch.
↪eye(num_codes).unsqueeze(0)

    prior_guide = None

    if use_prior:

        prior_guide = torch.zeros(batch_size, max_num_codes*2, max_num_codes*2)

        prior_indices = df.loc[eids][['prior_indices']]  #
        prior_values = df.loc[eids][['prior_values']]     #

        for i in range(batch_size):

            indices = torch.tensor(prior_indices.iloc[i]).view(-1, 2).t().long()
            values = torch.tensor(prior_values.iloc[i]).squeeze()
            #print(indices.shape,values.shape)=>torch.Size([2, 640]) torch.
↪Size([1, 640])
            sparse_matrix = torch.sparse.FloatTensor(indices, values, torch.
↪Size([max_num_codes*2, max_num_codes*2]))

            # Store the dense version in the batch matrices
            prior_guide[i] = sparse_matrix.to_dense()
```

```
        #add visit
        row_vector = torch.tensor([prior_scalar] * max_num_codes + [0.0] *␣
↪max_num_codes)
        top = row_vector.reshape((1,1,-1)).repeat(batch_size, 1, 1)

        prior_guide = torch.cat([top,prior_guide],axis=1)

        col_vector = torch.tensor([0.0]+[prior_scalar] * max_num_codes + [0.0]␣
↪* max_num_codes)
        left = col_vector.reshape((1,-1,1)).repeat(batch_size,1,1)
        prior_guide = torch.cat([left,prior_guide],axis=2)

        #apply mask
        prior_guide = prior_guide*mask.unsqueeze(2)*mask.unsqueeze(1)
        # add diag
        diag_mx = prior_scalar * torch.eye(num_codes).unsqueeze(0)
        prior_guide = prior_guide+diag_mx

        # normalize
        degrees = prior_guide.sum(dim=2, keepdim=True)
        prior_guide = prior_guide / degrees

    return guide, prior_guide
```

[46]:
```
guide, prior_guide = create_matrix_vdp(train_df,example_batch,masks)
print(guide.shape, prior_guide.shape)
```

```
torch.Size([32, 101, 101]) torch.Size([32, 101, 101])
```

```
<ipython-input-45-ec9fbb4a5dc4>:52: UserWarning:
torch.sparse.SparseTensor(indices, values, shape, *, device=) is deprecated.
Please use torch.sparse_coo_tensor(indices, values, shape, dtype=, device=).
(Triggered internally at ../torch/csrc/utils/tensor_new.cpp:618.)
  sparse_matrix = torch.sparse.FloatTensor(indices, values,
torch.Size([max_num_codes*2, max_num_codes*2]))
```

[47]:
```
from torch.nn import LayerNorm
import torch.nn.functional as F
class GraphConvolutionalTransformer(nn.Module):
    """Graph Convolutional Transformer class.

    This is an implementation of Graph Convolutional Transformer. With a proper
    set of options, it can be used as a vanilla Transformer.
    """

    def __init__(self,
```

```
               num_codes = 50,
               embedding_size=128,
               num_transformer_stack=3,
               num_feedforward=2,
               num_attention_heads=1,
               ffn_dropout=0.1,
               attention_normalizer='softmax',
               multihead_attention_aggregation='concat',
               directed_attention=False,
               use_inf_mask=True,
               use_prior=True,
               num_classes=1,
               lr = 0.001,
               **kwargs):
        """Init function.

        Args:
          embedding_size: The size of the dimension for hidden layers.
          num_transformer_stack: The number of Transformer blocks.
          num_feedforward: The number of layers in the feedforward part of
            Transformer.
          num_attention_heads: The number of attention heads.
          ffn_dropout: Dropout rate used inside the feedforward part.
          attention_normalizer: Use either 'softmax' or 'sigmoid' to normalize␣
↪the
            attention values.
          multihead_attention_aggregation: Use either 'concat' or 'sum' to␣
↪handle
            the outputs from multiple attention heads.
          directed_attention: Decide whether you want to use the unidirectional
            attention, where information accumulates inside the dummy visit␣
↪node.
          use_inf_mask: Decide whether you want to use the guide matrix.␣
↪Currently
            unused.
          use_prior: Decide whether you want to use the conditional probablility
            information. Currently unused.
          **kwargs: Other arguments to tf.keras.layers.Layer init.
        """

        super(GraphConvolutionalTransformer, self).__init__(**kwargs)
        self._hidden_size = embedding_size
        self._num_stack = num_transformer_stack
        self._num_feedforward = num_feedforward
        self._num_heads = num_attention_heads
        self._ffn_dropout = ffn_dropout
        self._attention_normalizer = attention_normalizer
```

```
        self._multihead_aggregation = multihead_attention_aggregation
        self._directed_attention = directed_attention
        self._use_inf_mask = use_inf_mask
        self._use_prior = use_prior
        self.num_classes = num_classes


        self.embedder = FeatureEmbedder(embedding_size)
        self._layers_Q = nn.ModuleList()
        self._layers_K = nn.ModuleList()
        self._layers_V = nn.ModuleList()
        self._layers_ffn = nn.ModuleList()
        self._layers_head_agg = nn.ModuleList()
        self._layers_logit = nn.Linear(self._hidden_size, num_classes)



        hidden_size = self._hidden_size
        num_heads = self._num_heads

        for i in range(self._num_stack):
            self._layers_Q.append(nn.Linear(hidden_size * num_heads,␣
↪hidden_size * num_heads, bias=False))
            self._layers_K.append(nn.Linear(hidden_size * num_heads,␣
↪hidden_size * num_heads, bias=False))
            self._layers_V.append(nn.Linear(hidden_size * num_heads,␣
↪hidden_size * num_heads, bias=False))

            if self._multihead_aggregation == 'concat':
                self._layers_head_agg.append(nn.Linear(hidden_size * num_heads,␣
↪hidden_size, bias=False))

            # Feed-forward network per stack
            ffn = []
            for j in range(num_feedforward - 1):
                ffn.append(nn.Linear(hidden_size, hidden_size, bias=True))  #␣
↪Bias is True by default
                ffn.append(nn.ReLU())  # Adding ReLU activation
                ffn.append(nn.Dropout(self._ffn_dropout))
            ffn.append(nn.Linear(hidden_size, hidden_size, bias=False))  # Last␣
↪layer without activation
            self._layers_ffn.append(nn.Sequential(*ffn))

    def safe_softmax(self, matrix, dim=-1):
        # Check if any row (or column) is entirely -inf
        is_inf = torch.isinf(matrix)
```

```
        all_inf = is_inf.all(dim=dim, keepdim=True)  # True where all are -inf␣
↪along `dim`

        # Apply softmax normally
        softmax_output = F.softmax(matrix, dim=dim)

        # If a row (or column) was entirely -inf, replace it with zeros␣
↪explicitly
        softmax_output = torch.where(all_inf, torch.zeros_like(softmax_output),␣
↪softmax_output)

        return softmax_output

    def qk_op(self, features, stack_index, batch_size, num_codes,␣
↪attention_mask, inf_mask=None, directed_mask=None):
        """
        Generate the attention scores using query and key projections.
        """

        # Process queries
        #self.print_abnormal(features,"features")
        q = self._layers_Q[stack_index](features)

        q = q.view(batch_size, num_codes, self._hidden_size, self._num_heads)

        q = q.permute(0, 3, 1, 2)  # (batch_size, num_heads, num_codes,␣
↪hidden_size)

        # Process keys
        k = self._layers_K[stack_index](features)
        k = k.view(batch_size, num_codes, self._hidden_size, self._num_heads)
        k = k.permute(0, 3, 2, 1)  # (batch_size, num_heads, hidden_size,␣
↪num_codes)


        # Calculate the raw attention scores
        pre_softmax = torch.matmul(q, k) / (self._hidden_size ** 0.5)



        # Apply attention masks
        if attention_mask is not None:
            pre_softmax = pre_softmax - attention_mask.unsqueeze(1).unsqueeze(2)


        if inf_mask is not None:
```

```python
            #self.print_abnormal(pre_softmax, "before inf_max pre_softmax")
            pre_softmax = pre_softmax - inf_mask.unsqueeze(1)
            #self.print_abnormal(pre_softmax, "after inf_max pre_softmax")

        if directed_mask is not None:
            pre_softmax = pre_softmax - directed_mask

        # Normalize the attention scores


        if self._attention_normalizer == 'softmax':
            attention = F.softmax(pre_softmax, dim=-1) #self.
↪safe_softmax(pre_softmax) #
        else:
            attention = torch.sigmoid(pre_softmax)

        #self.print_abnormal(attention, "attention")

        return attention

    def feedforward(self, post_attention, i):

        for i in range(self._num_feedforward):
            post_attention = self._layers_ffn[i](post_attention)

        return post_attention

    def print_abnormal(self,attention, name):

        negative_inf_mask_torch = torch.isinf(attention) & (attention < 0)
        all_neg_inf_last_axis_torch = negative_inf_mask_torch.all(dim=-1)
        positive_inf_mask_torch = torch.isinf(attention) & (attention > 0)
        all_pos_inf_last_axis_torch = positive_inf_mask_torch.all(dim=-1)
        print(name,":", attention.numel(), "shape:", attention.shape ,"nan:
↪",torch.sum(torch.isnan(attention)).item())
        print(name," last axis -inf:",all_neg_inf_last_axis_torch )
        print(name," last axis inf:",all_pos_inf_last_axis_torch )

        print(name," -inf:",torch.sum(torch.isinf(attention) & (attention < 0)).
↪item() )
        print(name," inf:",torch.sum(torch.isinf(attention) & (attention > 0)).
↪item() )
        print(name," 0:",torch.sum(attention == 0).item())

    def forward(self, batch_data, df):

        features, masks = self.embedder(batch_data)
```

```python
        #print("features:", features.numel(), features.shape, "features nans:
↪",torch.sum(torch.isnan(features)).item() )

        batch_size, num_codes, hidden_dim = features.shape

        guide, prior_guide = create_matrix_vdp(df, batch_data, masks)

        num_heads = self._num_heads

        #set inf to mask value==0
        masks = masks.unsqueeze(-1)
        mask_idx = masks == 0

        attention_mask = torch.zeros_like(masks, dtype=torch.float32)
        attention_mask[mask_idx] = float('inf')
        attention_mask = attention_mask.squeeze(2)
        max_float32 = torch.finfo(torch.float32).max
        inf_mask = None
        if self._use_inf_mask:
            inf_mask = torch.zeros_like(guide, dtype=torch.float32)
            inf_mask[guide == 0] = max_float32
            #self.print_abnormal(inf_mask,"inf_mask")

        directed_mask = None
        if self._directed_attention:
            inf_matrix = torch.full((num_codes, num_codes), max_float32)
            inf_matrix.fill_diagonal_(0)
            directed_mask = torch.tril(inf_matrix).unsqueeze(0).unsqueeze(0)


        attentions = []
        for i in range(self._num_stack):

            features = masks * features

            attention=None

            if self._use_prior and i == 0:
                attention = prior_guide.unsqueeze(1).repeat(1, num_heads, 1, 1)
            else:

                attention = self.qk_op(features, i, batch_size, num_codes,␣
↪attention_mask, inf_mask, directed_mask)



            attentions.append(attention)
```

```
            v = self._layers_V[i](features).view(-1, num_codes, self.
↪_hidden_size, num_heads)
            v = v.permute(0, 3, 1, 2)  # Reorder dimensions

            post_attention = torch.matmul(attention, v)

            if num_heads == 1:
                post_attention = post_attention.squeeze(1)
            elif self._multihead_aggregation == 'concat':
                post_attention = post_attention.permute(0, 2, 1, 3).contiguous()
                post_attention = post_attention.view(-1, num_codes, self.
↪_num_heads * self._hidden_size)
                post_attention = self._layers_head_agg[i](post_attention)
            else:
                post_attention = post_attention.sum(dim=1)

            post_attention += features
            post_attention = LayerNorm(post_attention.size()[1:],␣
↪elementwise_affine=True)(post_attention)

            post_ffn = self.feedforward(post_attention, i)

            post_ffn += post_attention

            post_ffn = LayerNorm(post_ffn.size()[1:],␣
↪elementwise_affine=True)(post_ffn)

            features = post_ffn

        #print("features:", features.numel(), features.shape, "features nans:
↪",torch.sum(torch.isnan(features)).item())
        hidden = features * masks

        pre_logit = hidden[:, 0, :].reshape(-1,self._hidden_size)
        #print("pre_logits:", pre_logit.numel(), pre_logit.shape, "pre_logit␣
↪nans:",torch.sum(torch.isnan(pre_logit)).item() )
        logits = self._layers_logit(pre_logit)

        return logits.squeeze(1), attentions
```

[48]:
```
model = GraphConvolutionalTransformer()
#print(model)
# model.train()
logits,attentions = model(example_batch,train_df)
```

```
# fets.shape, len(attentions)
print(logits)
```

```
tensor([ 1.1810,  1.4235, -0.4063,  1.5866,  2.5392,  0.5198,  1.1685,  1.9874,
         0.7844,  1.5559,  1.4890,  1.4861,  2.5715,  2.3386,  0.4137,  1.5116,
         1.6837, -0.4172,  1.1561,  1.4136,  1.5535,  2.0391,  2.1318,  2.1787,
         1.2449,  2.7704,  1.6630,  1.8929,  1.2257, -0.5102,  2.6131,  3.2133],
       grad_fn=<SqueezeBackward1>)
```

[49]:

```
from sklearn.metrics import precision_recall_fscore_support, roc_auc_score
from sklearn.metrics import precision_recall_curve, auc
class EHRTransformer(object):
    """Transformer-based EHR encounter modeling train and envalue function
    """

    def __init__(self,
                 gct_params,
                 feature_keys=['dx_ints', 'proc_ints'],
                 label_key='label.readmission',
                 vocab_sizes={'dx_ints':3249, 'proc_ints':2210},
                 feature_set='vdp',
                 max_num_codes=50,
                 prior_scalar=0.5,
                 reg_coef=0.1,
                 num_classes=1,
                 learning_rate=1e-3,
                 batch_size=32):

        self._feature_keys = feature_keys
        self._label_key = label_key
        self._vocab_sizes = vocab_sizes
        self._feature_set = feature_set
        self._max_num_codes = max_num_codes
        self._prior_scalar = prior_scalar
        self._reg_coef = reg_coef
        self._num_classes = num_classes
        self._learning_rate = learning_rate
        self._batch_size = batch_size

        self._gct_params = gct_params
        self._embedding_size = gct_params['embedding_size']
        self._num_transformer_stack = gct_params['num_transformer_stack']
        self._use_inf_mask = gct_params['use_inf_mask']
        self._use_prior = gct_params['use_prior']
        self._lr = gct_params['lr']

    def get_loss(self, logits, labels, attentions):
```

```
        loss = F.binary_cross_entropy_with_logits(logits, labels.float(),␣
↪reduction='mean')

        # Attention regularization using KL divergence if prior is used
        if self._use_prior and len(attentions) > 1:
            kl_terms = []
            # Convert list of tensors to a tensor
            attention_tensor = torch.stack(attentions)

            # Calculate KL divergence between successive attention matrices
            for i in range(1, self._num_transformer_stack):
                log_p = torch.log(attention_tensor[i - 1] + 1e-12)
                log_q = torch.log(attention_tensor[i] + 1e-12)
                kl_term = attention_tensor[i - 1] * (log_p - log_q)
                kl_term = torch.sum(kl_term, dim=-1)
                kl_term = torch.mean(kl_term)
                kl_terms.append(kl_term)

            reg_term = torch.mean(torch.stack(kl_terms))
            loss += self._reg_coef * reg_term

        return loss

    def eval_model(self,model, val_loader, val_df):
        model.eval()  # Set the model to evaluation mode
        all_labels = []
        all_probs = []
        with torch.no_grad():
            for data, labels in val_loader:
                logits, attentions = model(data, val_df)
                probs = torch.sigmoid(logits)
                all_labels.extend(labels.numpy())
                all_probs.extend(probs.numpy())

        precision, recall, _ = precision_recall_curve(all_labels, all_probs)

        return auc(recall, precision)

    def check_for_nans(self, model):

        for name, param in model.named_parameters():
            if torch.isnan(param).any():
                print(f"NaN detected in {name}")
            else:
                print(f"No NaNs in {name}")
```

```
    def train_and_val(self, model, train_loader=train_dataloader,␣
↪val_loader=validate_dataloader,train_df=train_df,val_df=validate_df,␣
↪n_epochs=1):
        """
        train the model.

        Arguments:
            model:
            train_loader: training dataloder
            val_loader: validation dataloader
            n_epochs: total number of epochs
        """
        optimizer = torch.optim.Adam(model.parameters(), lr=self._lr)
        auc_pr_history = []
        for epoch in range(n_epochs):

            model.train()
            train_loss = 0
            count=1
            for data, labels in train_loader:
                optimizer.zero_grad()

                logits,attentions=model(data,train_df)
                #self.check_for_nans(model)

                labels = labels.float()
                loss = self.get_loss(logits, labels, attentions)
                loss.backward()
                optimizer.step()
                train_loss += loss.item()
                count+=1
                if count%100==0:
                    print('Epoch: {} \t Step: {} Training Loss: {:.6f}'.
↪format(epoch+1,count, train_loss / count))

            AUC_PR = self.eval_model(model, val_loader, val_df)
            auc_pr_history.append(AUC_PR)
            print('Epoch: {} \t Validation AUC_PR: {:.2f}'
                  .format(epoch+1, AUC_PR))

        return auc_pr_history
```

[50]:
```
gct_params = {
      "embedding_size": 128,
      "num_transformer_stack": 3,
      "num_feedforward": 2,
      "num_attention_heads": 1,
```

```
        "ffn_dropout": 0.08,
        "attention_normalizer": "softmax",
        "multihead_attention_aggregation": "concat",
        "directed_attention": False,
        "use_inf_mask": True,
        "use_prior": True,
        "lr":0.001
  }
model = GraphConvolutionalTransformer(**gct_params)
transformer = EHRTransformer(gct_params=gct_params)
print(model)
transformer.train_and_val(model,train_loader=train_dataloader,␣
 ↪val_loader=validate_dataloader)
```

```
Epoch: 1        Step: 100 Training Loss: 1.655594
Epoch: 1        Step: 200 Training Loss: 1.643562
Epoch: 1        Step: 300 Training Loss: 1.637234
Epoch: 1        Step: 400 Training Loss: 1.634386
Epoch: 1        Step: 500 Training Loss: 1.632227
```

```
---------------------------------------------------------------------------
KeyboardInterrupt                         Traceback (most recent call last)
<ipython-input-50-e80d053ce8d3> in <cell line: 17>()
     15 transformer = EHRTransformer(gct_params=gct_params)
     16
---> 17 transformer.train_and_val(model,train_loader=train_dataloader,␣
 ↪val_loader=validate_dataloader)

<ipython-input-49-c59ff86a74aa> in train_and_val(self, model, train_loader,␣
 ↪val_loader, train_df, val_df, n_epochs)
    107                 optimizer.zero_grad()
    108
--> 109                 logits,attentions=model(data,train_df)
    110                 #self.check_for_nans(model)
    111

/usr/local/lib/python3.10/dist-packages/torch/nn/modules/module.py in␣
 ↪_wrapped_call_impl(self, *args, **kwargs)
   1509             return self._compiled_call_impl(*args, **kwargs)  # type:␣
 ↪ignore[misc]
   1510         else:
-> 1511             return self._call_impl(*args, **kwargs)
   1512
   1513     def _call_impl(self, *args, **kwargs):

/usr/local/lib/python3.10/dist-packages/torch/nn/modules/module.py in␣
 ↪_call_impl(self, *args, **kwargs)
```

```
   1518                    or _global_backward_pre_hooks or _global_backward_hooks
   1519                    or _global_forward_hooks or _global_forward_pre_hooks):
-> 1520                return forward_call(*args, **kwargs)
   1521
   1522            try:

<ipython-input-47-b0dbf27ea5f8> in forward(self, batch_data, df)
    242                post_ffn += post_attention
    243
--> 244                post_ffn = LayerNorm(post_ffn.size()[1:],␣
 ↪elementwise_affine=True)(post_ffn)
    245
    246                features = post_ffn

/usr/local/lib/python3.10/dist-packages/torch/nn/modules/module.py in␣
 ↪_wrapped_call_impl(self, *args, **kwargs)
   1509                return self._compiled_call_impl(*args, **kwargs)  # type:␣
 ↪ignore[misc]
   1510            else:
-> 1511                return self._call_impl(*args, **kwargs)
   1512
   1513        def _call_impl(self, *args, **kwargs):

/usr/local/lib/python3.10/dist-packages/torch/nn/modules/module.py in␣
 ↪_call_impl(self, *args, **kwargs)
   1518                    or _global_backward_pre_hooks or _global_backward_hooks
   1519                    or _global_forward_hooks or _global_forward_pre_hooks):
-> 1520                return forward_call(*args, **kwargs)
   1521
   1522            try:

/usr/local/lib/python3.10/dist-packages/torch/nn/modules/normalization.py in␣
 ↪forward(self, input)
    199
    200        def forward(self, input: Tensor) -> Tensor:
--> 201            return F.layer_norm(
    202                input, self.normalized_shape, self.weight, self.bias, self.
 ↪eps)
    203

/usr/local/lib/python3.10/dist-packages/torch/nn/functional.py in␣
 ↪layer_norm(input, normalized_shape, weight, bias, eps)
   2544                layer_norm, (input, weight, bias), input, normalized_shape,␣
 ↪weight=weight, bias=bias, eps=eps
   2545            )
-> 2546        return torch.layer_norm(input, normalized_shape, weight, bias, eps,␣
 ↪torch.backends.cudnn.enabled)
```

```
2547
2548

KeyboardInterrupt:
```

[ ]:
```
# 4m50s for one epoch in CPU
```

5.1 Training

5.1.1 Hyperparams

Report at least 3 types of hyperparameters such as learning rate, batch size, hidden size, dropout

- Learning rate: 0.001
- hidden_size: 128
- Dropout rate: 0.5

[51]:
```
def plot_AUC_PR(auc_pr_history,title):
    plt.figure(figsize=(10, 6))

    # Loop through the dictionary to plot each dropout rate's AUC-PR over epochs
    for name, auc_prs in auc_pr_history.items():
        epochs = range(1, len(auc_prs) + 1)
        name = title+'_'+name
        plt.plot(epochs, auc_prs, label=f'{name}', marker='o')

    # Add some plot decorations
    plt.title('AUC-PR Across Epochs for Different {}'.format(title))
    plt.xlabel('Epoch')
    plt.ylabel('AUC-PR')
    plt.legend(title=title)
    plt.grid(True)

    # Show plot
    #plt.savefig('auc_pr_plot_{}.png'.format(title), format='png', dpi=300)
    plt.show()

# auc_pr_history = {
#     "dropout_0.1": [0.50, 0.52, 0.54, 0.56, 0.59],
#     "dropout_0.2": [0.48, 0.51, 0.53, 0.57, 0.60],
#     "dropout_0.3": [0.47, 0.49, 0.52, 0.54, 0.57],
#     "dropout_0.4": [0.45, 0.48, 0.50, 0.53, 0.55]
# }
# plot_AUC_PR(auc_pr_history)
```

[53]:
```
def test_ffn_dropout_rates():
    auc_pr_history={}
```

```
    dropout_rates = [0.01, 0.1, 0.2,0.5]

    for rate in dropout_rates:
        gct_params = {
            "embedding_size": 128,
            "num_transformer_stack": 3,
            "num_feedforward": 2,
            "num_attention_heads": 1,
            "ffn_dropout": rate,
            "attention_normalizer": "softmax",
            "multihead_attention_aggregation": "concat",
            "directed_attention": False,
            "use_inf_mask": True,
            "use_prior": True,
            "lr":0.001
        }
        model = GraphConvolutionalTransformer(**gct_params)
        transformer = EHRTransformer(gct_params=gct_params)

        values = transformer.train_and_val(model,train_loader=train_dataloader,␣
↪val_loader=validate_dataloader,train_df=train_df,val_df=validate_df,␣
↪n_epochs=5)
        auc_pr_history[str(rate)]=values

    return auc_pr_history

auc_pr_history = test_ffn_dropout_rates()

plot_AUC_PR(auc_pr_history,"ffn_dropout")
```

```
Epoch: 1         Step: 100 Training Loss: 1.669270
Epoch: 1         Step: 200 Training Loss: 1.644789
Epoch: 1         Step: 300 Training Loss: 1.639042
Epoch: 1         Step: 400 Training Loss: 1.633531
Epoch: 1         Step: 500 Training Loss: 1.633055
Epoch: 1         Step: 600 Training Loss: 1.628148
Epoch: 1         Step: 700 Training Loss: 1.625847
Epoch: 1         Step: 800 Training Loss: 1.624646
Epoch: 1         Step: 900 Training Loss: 1.625692
Epoch: 1         Step: 1000 Training Loss: 1.622812
Epoch: 1         Validation AUC_PR: 0.37
Epoch: 2         Step: 100 Training Loss: 1.588730
Epoch: 2         Step: 200 Training Loss: 1.595431
Epoch: 2         Step: 300 Training Loss: 1.590345
Epoch: 2         Step: 400 Training Loss: 1.590347
Epoch: 2         Step: 500 Training Loss: 1.592052
Epoch: 2         Step: 600 Training Loss: 1.590197
```

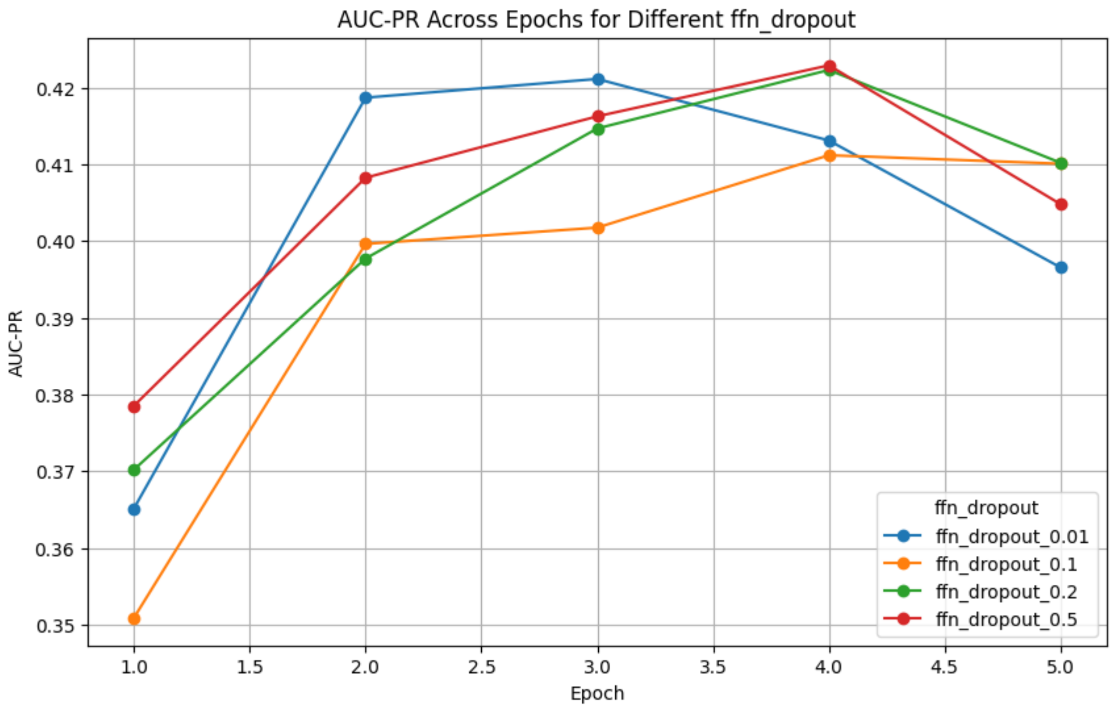
```
Epoch: 2        Step: 700 Training Loss: 1.590111
Epoch: 2        Step: 800 Training Loss: 1.589017
Epoch: 2        Step: 900 Training Loss: 1.589506
Epoch: 2        Step: 1000 Training Loss: 1.590003
Epoch: 2        Validation AUC_PR: 0.42
Epoch: 3        Step: 100 Training Loss: 1.565830
Epoch: 3        Step: 200 Training Loss: 1.568290
Epoch: 3        Step: 300 Training Loss: 1.567084
Epoch: 3        Step: 400 Training Loss: 1.570261
Epoch: 3        Step: 500 Training Loss: 1.569076
Epoch: 3        Step: 600 Training Loss: 1.568194
Epoch: 3        Step: 700 Training Loss: 1.569927
Epoch: 3        Step: 800 Training Loss: 1.571482
Epoch: 3        Step: 900 Training Loss: 1.573041
Epoch: 3        Step: 1000 Training Loss: 1.571889
Epoch: 3        Validation AUC_PR: 0.42
Epoch: 4        Step: 100 Training Loss: 1.559182
Epoch: 4        Step: 200 Training Loss: 1.558678
Epoch: 4        Step: 300 Training Loss: 1.559383
Epoch: 4        Step: 400 Training Loss: 1.555513
Epoch: 4        Step: 500 Training Loss: 1.554061
Epoch: 4        Step: 600 Training Loss: 1.553132
Epoch: 4        Step: 700 Training Loss: 1.554966
Epoch: 4        Step: 800 Training Loss: 1.555365
Epoch: 4        Step: 900 Training Loss: 1.557743
Epoch: 4        Step: 1000 Training Loss: 1.558472
Epoch: 4        Validation AUC_PR: 0.41
Epoch: 5        Step: 100 Training Loss: 1.525188
Epoch: 5        Step: 200 Training Loss: 1.535227
Epoch: 5        Step: 300 Training Loss: 1.546377
Epoch: 5        Step: 400 Training Loss: 1.545826
Epoch: 5        Step: 500 Training Loss: 1.542588
Epoch: 5        Step: 600 Training Loss: 1.544015
Epoch: 5        Step: 700 Training Loss: 1.547219
Epoch: 5        Step: 800 Training Loss: 1.543701
Epoch: 5        Step: 900 Training Loss: 1.545078
Epoch: 5        Step: 1000 Training Loss: 1.544610
Epoch: 5        Validation AUC_PR: 0.40
Epoch: 1        Step: 100 Training Loss: 1.660384
Epoch: 1        Step: 200 Training Loss: 1.645656
Epoch: 1        Step: 300 Training Loss: 1.638313
Epoch: 1        Step: 400 Training Loss: 1.636514
Epoch: 1        Step: 500 Training Loss: 1.636012
Epoch: 1        Step: 600 Training Loss: 1.630388
Epoch: 1        Step: 700 Training Loss: 1.628238
Epoch: 1        Step: 800 Training Loss: 1.629135
Epoch: 1        Step: 900 Training Loss: 1.627329
Epoch: 1        Step: 1000 Training Loss: 1.624698
```

```
Epoch: 1        Validation AUC_PR: 0.35
Epoch: 2        Step: 100 Training Loss: 1.576431
Epoch: 2        Step: 200 Training Loss: 1.580080
Epoch: 2        Step: 300 Training Loss: 1.591677
Epoch: 2        Step: 400 Training Loss: 1.591879
Epoch: 2        Step: 500 Training Loss: 1.591345
Epoch: 2        Step: 600 Training Loss: 1.590030
Epoch: 2        Step: 700 Training Loss: 1.590781
Epoch: 2        Step: 800 Training Loss: 1.587044
Epoch: 2        Step: 900 Training Loss: 1.586948
Epoch: 2        Step: 1000 Training Loss: 1.587573
Epoch: 2        Validation AUC_PR: 0.40
Epoch: 3        Step: 100 Training Loss: 1.567983
Epoch: 3        Step: 200 Training Loss: 1.568407
Epoch: 3        Step: 300 Training Loss: 1.575001
Epoch: 3        Step: 400 Training Loss: 1.573488
Epoch: 3        Step: 500 Training Loss: 1.574057
Epoch: 3        Step: 600 Training Loss: 1.576012
Epoch: 3        Step: 700 Training Loss: 1.574513
Epoch: 3        Step: 800 Training Loss: 1.573851
Epoch: 3        Step: 900 Training Loss: 1.572227
Epoch: 3        Step: 1000 Training Loss: 1.572123
Epoch: 3        Validation AUC_PR: 0.40
Epoch: 4        Step: 100 Training Loss: 1.543805
Epoch: 4        Step: 200 Training Loss: 1.549901
Epoch: 4        Step: 300 Training Loss: 1.552503
Epoch: 4        Step: 400 Training Loss: 1.558025
Epoch: 4        Step: 500 Training Loss: 1.562766
Epoch: 4        Step: 600 Training Loss: 1.561032
Epoch: 4        Step: 700 Training Loss: 1.559065
Epoch: 4        Step: 800 Training Loss: 1.558970
Epoch: 4        Step: 900 Training Loss: 1.560266
Epoch: 4        Step: 1000 Training Loss: 1.560904
Epoch: 4        Validation AUC_PR: 0.41
Epoch: 5        Step: 100 Training Loss: 1.521012
Epoch: 5        Step: 200 Training Loss: 1.529771
Epoch: 5        Step: 300 Training Loss: 1.538186
Epoch: 5        Step: 400 Training Loss: 1.540660
Epoch: 5        Step: 500 Training Loss: 1.546045
Epoch: 5        Step: 600 Training Loss: 1.545851
Epoch: 5        Step: 700 Training Loss: 1.545210
Epoch: 5        Step: 800 Training Loss: 1.547893
Epoch: 5        Step: 900 Training Loss: 1.550329
Epoch: 5        Step: 1000 Training Loss: 1.547404
Epoch: 5        Validation AUC_PR: 0.41
Epoch: 1        Step: 100 Training Loss: 1.663238
Epoch: 1        Step: 200 Training Loss: 1.653143
Epoch: 1        Step: 300 Training Loss: 1.647065
```

```
Epoch: 1        Step: 400 Training Loss: 1.637518
Epoch: 1        Step: 500 Training Loss: 1.633722
Epoch: 1        Step: 600 Training Loss: 1.631990
Epoch: 1        Step: 700 Training Loss: 1.625945
Epoch: 1        Step: 800 Training Loss: 1.625697
Epoch: 1        Step: 900 Training Loss: 1.625252
Epoch: 1        Step: 1000 Training Loss: 1.625853
Epoch: 1        Validation AUC_PR: 0.37
Epoch: 2        Step: 100 Training Loss: 1.579774
Epoch: 2        Step: 200 Training Loss: 1.603447
Epoch: 2        Step: 300 Training Loss: 1.598863
Epoch: 2        Step: 400 Training Loss: 1.602349
Epoch: 2        Step: 500 Training Loss: 1.602969
Epoch: 2        Step: 600 Training Loss: 1.599827
Epoch: 2        Step: 700 Training Loss: 1.603315
Epoch: 2        Step: 800 Training Loss: 1.599963
Epoch: 2        Step: 900 Training Loss: 1.597789
Epoch: 2        Step: 1000 Training Loss: 1.595446
Epoch: 2        Validation AUC_PR: 0.40
Epoch: 3        Step: 100 Training Loss: 1.552678
Epoch: 3        Step: 200 Training Loss: 1.561666
Epoch: 3        Step: 300 Training Loss: 1.565279
Epoch: 3        Step: 400 Training Loss: 1.571967
Epoch: 3        Step: 500 Training Loss: 1.572263
Epoch: 3        Step: 600 Training Loss: 1.574751
Epoch: 3        Step: 700 Training Loss: 1.575180
Epoch: 3        Step: 800 Training Loss: 1.574112
Epoch: 3        Step: 900 Training Loss: 1.574321
Epoch: 3        Step: 1000 Training Loss: 1.574339
Epoch: 3        Validation AUC_PR: 0.41
Epoch: 4        Step: 100 Training Loss: 1.564830
Epoch: 4        Step: 200 Training Loss: 1.562889
Epoch: 4        Step: 300 Training Loss: 1.562551
Epoch: 4        Step: 400 Training Loss: 1.558879
Epoch: 4        Step: 500 Training Loss: 1.559415
Epoch: 4        Step: 600 Training Loss: 1.556921
Epoch: 4        Step: 700 Training Loss: 1.556373
Epoch: 4        Step: 800 Training Loss: 1.558437
Epoch: 4        Step: 900 Training Loss: 1.560363
Epoch: 4        Step: 1000 Training Loss: 1.562121
Epoch: 4        Validation AUC_PR: 0.42
Epoch: 5        Step: 100 Training Loss: 1.523478
Epoch: 5        Step: 200 Training Loss: 1.532758
Epoch: 5        Step: 300 Training Loss: 1.539231
Epoch: 5        Step: 400 Training Loss: 1.546907
Epoch: 5        Step: 500 Training Loss: 1.548554
Epoch: 5        Step: 600 Training Loss: 1.551953
Epoch: 5        Step: 700 Training Loss: 1.551831
```

```
Epoch: 5         Step: 800 Training Loss: 1.552637
Epoch: 5         Step: 900 Training Loss: 1.553616
Epoch: 5         Step: 1000 Training Loss: 1.552041
Epoch: 5         Validation AUC_PR: 0.41
Epoch: 1         Step: 100 Training Loss: 1.666096
Epoch: 1         Step: 200 Training Loss: 1.648577
Epoch: 1         Step: 300 Training Loss: 1.642438
Epoch: 1         Step: 400 Training Loss: 1.639149
Epoch: 1         Step: 500 Training Loss: 1.635472
Epoch: 1         Step: 600 Training Loss: 1.631777
Epoch: 1         Step: 700 Training Loss: 1.631244
Epoch: 1         Step: 800 Training Loss: 1.629601
Epoch: 1         Step: 900 Training Loss: 1.627455
Epoch: 1         Step: 1000 Training Loss: 1.627028
Epoch: 1         Validation AUC_PR: 0.38
Epoch: 2         Step: 100 Training Loss: 1.580001
Epoch: 2         Step: 200 Training Loss: 1.591597
Epoch: 2         Step: 300 Training Loss: 1.598423
Epoch: 2         Step: 400 Training Loss: 1.596294
Epoch: 2         Step: 500 Training Loss: 1.592846
Epoch: 2         Step: 600 Training Loss: 1.594376
Epoch: 2         Step: 700 Training Loss: 1.592243
Epoch: 2         Step: 800 Training Loss: 1.590350
Epoch: 2         Step: 900 Training Loss: 1.590714
Epoch: 2         Step: 1000 Training Loss: 1.589898
Epoch: 2         Validation AUC_PR: 0.41
Epoch: 3         Step: 100 Training Loss: 1.556642
Epoch: 3         Step: 200 Training Loss: 1.566889
Epoch: 3         Step: 300 Training Loss: 1.565889
Epoch: 3         Step: 400 Training Loss: 1.566416
Epoch: 3         Step: 500 Training Loss: 1.569338
Epoch: 3         Step: 600 Training Loss: 1.568852
Epoch: 3         Step: 700 Training Loss: 1.571356
Epoch: 3         Step: 800 Training Loss: 1.572293
Epoch: 3         Step: 900 Training Loss: 1.570284
Epoch: 3         Step: 1000 Training Loss: 1.571755
Epoch: 3         Validation AUC_PR: 0.42
Epoch: 4         Step: 100 Training Loss: 1.534033
Epoch: 4         Step: 200 Training Loss: 1.540415
Epoch: 4         Step: 300 Training Loss: 1.544539
Epoch: 4         Step: 400 Training Loss: 1.547344
Epoch: 4         Step: 500 Training Loss: 1.551000
Epoch: 4         Step: 600 Training Loss: 1.552538
Epoch: 4         Step: 700 Training Loss: 1.554854
Epoch: 4         Step: 800 Training Loss: 1.557614
Epoch: 4         Step: 900 Training Loss: 1.558731
Epoch: 4         Step: 1000 Training Loss: 1.561587
Epoch: 4         Validation AUC_PR: 0.42
```

```
Epoch: 5        Step: 100 Training Loss: 1.524788
Epoch: 5        Step: 200 Training Loss: 1.537000
Epoch: 5        Step: 300 Training Loss: 1.549173
Epoch: 5        Step: 400 Training Loss: 1.552074
Epoch: 5        Step: 500 Training Loss: 1.551549
Epoch: 5        Step: 600 Training Loss: 1.554073
Epoch: 5        Step: 700 Training Loss: 1.555630
Epoch: 5        Step: 800 Training Loss: 1.554135
Epoch: 5        Step: 900 Training Loss: 1.553942
Epoch: 5        Step: 1000 Training Loss: 1.554857
Epoch: 5        Validation AUC_PR: 0.40
```



[56]:
```
def test_embedding_size():
    auc_pr_history={}
    embedding_size = [16, 32, 64,128]

    for size in embedding_size:
        gct_params = {
            "embedding_size": size,
            "num_transformer_stack": 3,
            "num_feedforward": 2,
            "num_attention_heads": 1,
            "ffn_dropout": 0.01,
            "attention_normalizer": "softmax",
```

```
            "multihead_attention_aggregation": "concat",
            "directed_attention": False,
            "use_inf_mask": True,
            "use_prior": True,
            "lr":0.001
        }
        model = GraphConvolutionalTransformer(**gct_params)
        transformer = EHRTransformer(gct_params=gct_params)

        values = transformer.train_and_val(model,train_loader=train_dataloader,␣
↪val_loader=validate_dataloader,train_df=train_df,val_df=validate_df,␣
↪n_epochs=5)
        auc_pr_history[str(size)]=values

    return auc_pr_history

auc_pr_history = test_embedding_size()

plot_AUC_PR(auc_pr_history,"embedding")
```

```
Epoch: 1         Step: 100 Training Loss: 1.647264
Epoch: 1         Step: 200 Training Loss: 1.647760
Epoch: 1         Step: 300 Training Loss: 1.639206
Epoch: 1         Step: 400 Training Loss: 1.639019
Epoch: 1         Step: 500 Training Loss: 1.636149
Epoch: 1         Step: 600 Training Loss: 1.633240
Epoch: 1         Step: 700 Training Loss: 1.629728
Epoch: 1         Step: 800 Training Loss: 1.626776
Epoch: 1         Step: 900 Training Loss: 1.624601
Epoch: 1         Step: 1000 Training Loss: 1.622506
Epoch: 1         Validation AUC_PR: 0.34
Epoch: 2         Step: 100 Training Loss: 1.577381
Epoch: 2         Step: 200 Training Loss: 1.594691
Epoch: 2         Step: 300 Training Loss: 1.597283
Epoch: 2         Step: 400 Training Loss: 1.599286
Epoch: 2         Step: 500 Training Loss: 1.598441
Epoch: 2         Step: 600 Training Loss: 1.596848
Epoch: 2         Step: 700 Training Loss: 1.597274
Epoch: 2         Step: 800 Training Loss: 1.596483
Epoch: 2         Step: 900 Training Loss: 1.598012
Epoch: 2         Step: 1000 Training Loss: 1.598507
Epoch: 2         Validation AUC_PR: 0.37
Epoch: 3         Step: 100 Training Loss: 1.582697
Epoch: 3         Step: 200 Training Loss: 1.576443
Epoch: 3         Step: 300 Training Loss: 1.579531
Epoch: 3         Step: 400 Training Loss: 1.581142
Epoch: 3         Step: 500 Training Loss: 1.582140
```

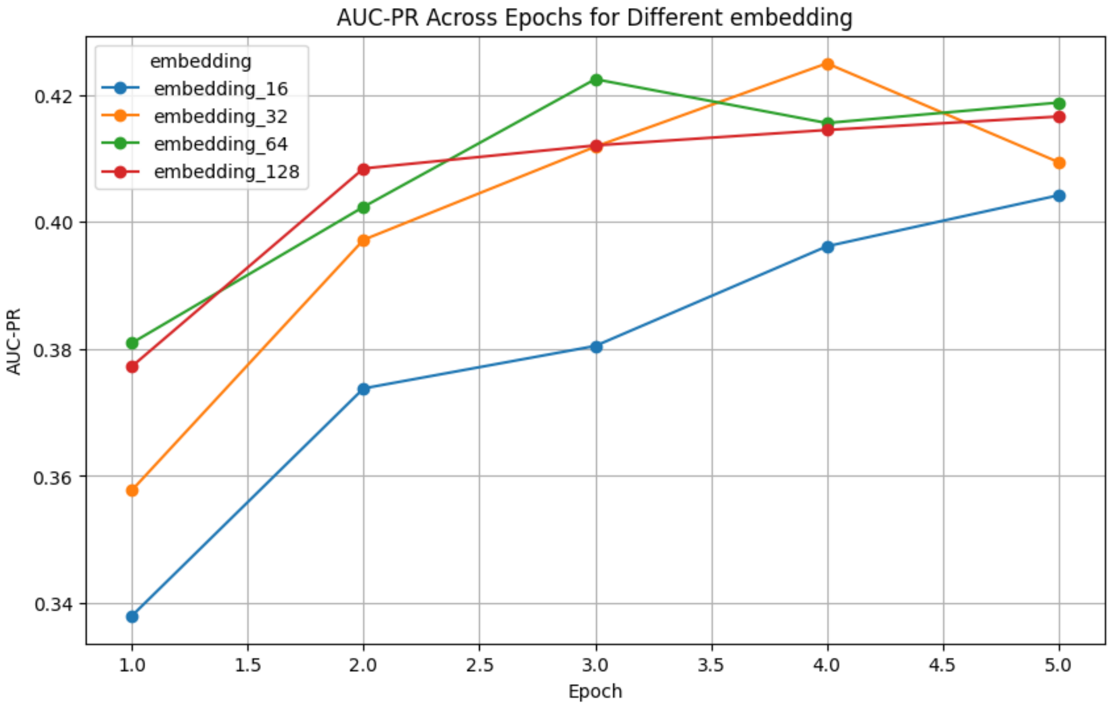
```
Epoch: 3         Step: 600 Training Loss: 1.584084
Epoch: 3         Step: 700 Training Loss: 1.585029
Epoch: 3         Step: 800 Training Loss: 1.585361
Epoch: 3         Step: 900 Training Loss: 1.586787
Epoch: 3         Step: 1000 Training Loss: 1.585816
Epoch: 3         Validation AUC_PR: 0.38
Epoch: 4         Step: 100 Training Loss: 1.561572
Epoch: 4         Step: 200 Training Loss: 1.572724
Epoch: 4         Step: 300 Training Loss: 1.575243
Epoch: 4         Step: 400 Training Loss: 1.576378
Epoch: 4         Step: 500 Training Loss: 1.576633
Epoch: 4         Step: 600 Training Loss: 1.576191
Epoch: 4         Step: 700 Training Loss: 1.578109
Epoch: 4         Step: 800 Training Loss: 1.576836
Epoch: 4         Step: 900 Training Loss: 1.576092
Epoch: 4         Step: 1000 Training Loss: 1.576716
Epoch: 4         Validation AUC_PR: 0.40
Epoch: 5         Step: 100 Training Loss: 1.561471
Epoch: 5         Step: 200 Training Loss: 1.563554
Epoch: 5         Step: 300 Training Loss: 1.562737
Epoch: 5         Step: 400 Training Loss: 1.565286
Epoch: 5         Step: 500 Training Loss: 1.567025
Epoch: 5         Step: 600 Training Loss: 1.567812
Epoch: 5         Step: 700 Training Loss: 1.567668
Epoch: 5         Step: 800 Training Loss: 1.566436
Epoch: 5         Step: 900 Training Loss: 1.567548
Epoch: 5         Step: 1000 Training Loss: 1.568719
Epoch: 5         Validation AUC_PR: 0.40
Epoch: 1         Step: 100 Training Loss: 1.671757
Epoch: 1         Step: 200 Training Loss: 1.660899
Epoch: 1         Step: 300 Training Loss: 1.647851
Epoch: 1         Step: 400 Training Loss: 1.638852
Epoch: 1         Step: 500 Training Loss: 1.636023
Epoch: 1         Step: 600 Training Loss: 1.633137
Epoch: 1         Step: 700 Training Loss: 1.629404
Epoch: 1         Step: 800 Training Loss: 1.626881
Epoch: 1         Step: 900 Training Loss: 1.625504
Epoch: 1         Step: 1000 Training Loss: 1.621600
Epoch: 1         Validation AUC_PR: 0.36
Epoch: 2         Step: 100 Training Loss: 1.580968
Epoch: 2         Step: 200 Training Loss: 1.585482
Epoch: 2         Step: 300 Training Loss: 1.598169
Epoch: 2         Step: 400 Training Loss: 1.594397
Epoch: 2         Step: 500 Training Loss: 1.593703
Epoch: 2         Step: 600 Training Loss: 1.594531
Epoch: 2         Step: 700 Training Loss: 1.592672
Epoch: 2         Step: 800 Training Loss: 1.594225
Epoch: 2         Step: 900 Training Loss: 1.593795
```

```
Epoch: 2        Step: 1000 Training Loss: 1.592873
Epoch: 2        Validation AUC_PR: 0.40
Epoch: 3        Step: 100 Training Loss: 1.585563
Epoch: 3        Step: 200 Training Loss: 1.579652
Epoch: 3        Step: 300 Training Loss: 1.581181
Epoch: 3        Step: 400 Training Loss: 1.583841
Epoch: 3        Step: 500 Training Loss: 1.581100
Epoch: 3        Step: 600 Training Loss: 1.579384
Epoch: 3        Step: 700 Training Loss: 1.580814
Epoch: 3        Step: 800 Training Loss: 1.580090
Epoch: 3        Step: 900 Training Loss: 1.581580
Epoch: 3        Step: 1000 Training Loss: 1.580279
Epoch: 3        Validation AUC_PR: 0.41
Epoch: 4        Step: 100 Training Loss: 1.565154
Epoch: 4        Step: 200 Training Loss: 1.564483
Epoch: 4        Step: 300 Training Loss: 1.563409
Epoch: 4        Step: 400 Training Loss: 1.564002
Epoch: 4        Step: 500 Training Loss: 1.561595
Epoch: 4        Step: 600 Training Loss: 1.566010
Epoch: 4        Step: 700 Training Loss: 1.568384
Epoch: 4        Step: 800 Training Loss: 1.569228
Epoch: 4        Step: 900 Training Loss: 1.568400
Epoch: 4        Step: 1000 Training Loss: 1.568654
Epoch: 4        Validation AUC_PR: 0.42
Epoch: 5        Step: 100 Training Loss: 1.544692
Epoch: 5        Step: 200 Training Loss: 1.549763
Epoch: 5        Step: 300 Training Loss: 1.552960
Epoch: 5        Step: 400 Training Loss: 1.556836
Epoch: 5        Step: 500 Training Loss: 1.555514
Epoch: 5        Step: 600 Training Loss: 1.557835
Epoch: 5        Step: 700 Training Loss: 1.557853
Epoch: 5        Step: 800 Training Loss: 1.560175
Epoch: 5        Step: 900 Training Loss: 1.558664
Epoch: 5        Step: 1000 Training Loss: 1.560663
Epoch: 5        Validation AUC_PR: 0.41
Epoch: 1        Step: 100 Training Loss: 1.641590
Epoch: 1        Step: 200 Training Loss: 1.633341
Epoch: 1        Step: 300 Training Loss: 1.628320
Epoch: 1        Step: 400 Training Loss: 1.626825
Epoch: 1        Step: 500 Training Loss: 1.620891
Epoch: 1        Step: 600 Training Loss: 1.621981
Epoch: 1        Step: 700 Training Loss: 1.622573
Epoch: 1        Step: 800 Training Loss: 1.621236
Epoch: 1        Step: 900 Training Loss: 1.618940
Epoch: 1        Step: 1000 Training Loss: 1.615674
Epoch: 1        Validation AUC_PR: 0.38
Epoch: 2        Step: 100 Training Loss: 1.565716
Epoch: 2        Step: 200 Training Loss: 1.580355
```

```
Epoch: 2         Step: 300 Training Loss: 1.587909
Epoch: 2         Step: 400 Training Loss: 1.591453
Epoch: 2         Step: 500 Training Loss: 1.591661
Epoch: 2         Step: 600 Training Loss: 1.589346
Epoch: 2         Step: 700 Training Loss: 1.588337
Epoch: 2         Step: 800 Training Loss: 1.588126
Epoch: 2         Step: 900 Training Loss: 1.588806
Epoch: 2         Step: 1000 Training Loss: 1.588971
Epoch: 2         Validation AUC_PR: 0.40
Epoch: 3         Step: 100 Training Loss: 1.553193
Epoch: 3         Step: 200 Training Loss: 1.566156
Epoch: 3         Step: 300 Training Loss: 1.579122
Epoch: 3         Step: 400 Training Loss: 1.579951
Epoch: 3         Step: 500 Training Loss: 1.579332
Epoch: 3         Step: 600 Training Loss: 1.578254
Epoch: 3         Step: 700 Training Loss: 1.581352
Epoch: 3         Step: 800 Training Loss: 1.578853
Epoch: 3         Step: 900 Training Loss: 1.578552
Epoch: 3         Step: 1000 Training Loss: 1.577658
Epoch: 3         Validation AUC_PR: 0.42
Epoch: 4         Step: 100 Training Loss: 1.554743
Epoch: 4         Step: 200 Training Loss: 1.568982
Epoch: 4         Step: 300 Training Loss: 1.570028
Epoch: 4         Step: 400 Training Loss: 1.563501
Epoch: 4         Step: 500 Training Loss: 1.561483
Epoch: 4         Step: 600 Training Loss: 1.566577
Epoch: 4         Step: 700 Training Loss: 1.568762
Epoch: 4         Step: 800 Training Loss: 1.566615
Epoch: 4         Step: 900 Training Loss: 1.568455
Epoch: 4         Step: 1000 Training Loss: 1.568430
Epoch: 4         Validation AUC_PR: 0.42
Epoch: 5         Step: 100 Training Loss: 1.538370
Epoch: 5         Step: 200 Training Loss: 1.551563
Epoch: 5         Step: 300 Training Loss: 1.547628
Epoch: 5         Step: 400 Training Loss: 1.546277
Epoch: 5         Step: 500 Training Loss: 1.550079
Epoch: 5         Step: 600 Training Loss: 1.551543
Epoch: 5         Step: 700 Training Loss: 1.553873
Epoch: 5         Step: 800 Training Loss: 1.556133
Epoch: 5         Step: 900 Training Loss: 1.555999
Epoch: 5         Step: 1000 Training Loss: 1.556710
Epoch: 5         Validation AUC_PR: 0.42
Epoch: 1         Step: 100 Training Loss: 1.678045
Epoch: 1         Step: 200 Training Loss: 1.658799
Epoch: 1         Step: 300 Training Loss: 1.650451
Epoch: 1         Step: 400 Training Loss: 1.645422
Epoch: 1         Step: 500 Training Loss: 1.638851
Epoch: 1         Step: 600 Training Loss: 1.636738
```

```
Epoch: 1        Step: 700 Training Loss: 1.634879
Epoch: 1        Step: 800 Training Loss: 1.629913
Epoch: 1        Step: 900 Training Loss: 1.629113
Epoch: 1        Step: 1000 Training Loss: 1.626347
Epoch: 1        Validation AUC_PR: 0.38
Epoch: 2        Step: 100 Training Loss: 1.559836
Epoch: 2        Step: 200 Training Loss: 1.587505
Epoch: 2        Step: 300 Training Loss: 1.585207
Epoch: 2        Step: 400 Training Loss: 1.583833
Epoch: 2        Step: 500 Training Loss: 1.582196
Epoch: 2        Step: 600 Training Loss: 1.582554
Epoch: 2        Step: 700 Training Loss: 1.585247
Epoch: 2        Step: 800 Training Loss: 1.587200
Epoch: 2        Step: 900 Training Loss: 1.588164
Epoch: 2        Step: 1000 Training Loss: 1.587836
Epoch: 2        Validation AUC_PR: 0.41
Epoch: 3        Step: 100 Training Loss: 1.562207
Epoch: 3        Step: 200 Training Loss: 1.567411
Epoch: 3        Step: 300 Training Loss: 1.573631
Epoch: 3        Step: 400 Training Loss: 1.574537
Epoch: 3        Step: 500 Training Loss: 1.576958
Epoch: 3        Step: 600 Training Loss: 1.574865
Epoch: 3        Step: 700 Training Loss: 1.573888
Epoch: 3        Step: 800 Training Loss: 1.572526
Epoch: 3        Step: 900 Training Loss: 1.570965
Epoch: 3        Step: 1000 Training Loss: 1.572092
Epoch: 3        Validation AUC_PR: 0.41
Epoch: 4        Step: 100 Training Loss: 1.545224
Epoch: 4        Step: 200 Training Loss: 1.549752
Epoch: 4        Step: 300 Training Loss: 1.552412
Epoch: 4        Step: 400 Training Loss: 1.551445
Epoch: 4        Step: 500 Training Loss: 1.557274
Epoch: 4        Step: 600 Training Loss: 1.557418
Epoch: 4        Step: 700 Training Loss: 1.560322
Epoch: 4        Step: 800 Training Loss: 1.561072
Epoch: 4        Step: 900 Training Loss: 1.560369
Epoch: 4        Step: 1000 Training Loss: 1.558743
Epoch: 4        Validation AUC_PR: 0.41
Epoch: 5        Step: 100 Training Loss: 1.528304
Epoch: 5        Step: 200 Training Loss: 1.549534
Epoch: 5        Step: 300 Training Loss: 1.544825
Epoch: 5        Step: 400 Training Loss: 1.547486
Epoch: 5        Step: 500 Training Loss: 1.543274
Epoch: 5        Step: 600 Training Loss: 1.547247
Epoch: 5        Step: 700 Training Loss: 1.545211
Epoch: 5        Step: 800 Training Loss: 1.547220
Epoch: 5        Step: 900 Training Loss: 1.548171
Epoch: 5        Step: 1000 Training Loss: 1.548092
```

```
Epoch: 5         Validation AUC_PR: 0.42
```



[57]:

```
def test_learning_rate():
    auc_pr_history={}
    lrs = [0.0001,0.001,0.01,0.1]

    for lr in lrs:
        gct_params = {
            "embedding_size": 128,
            "num_transformer_stack": 3,
            "num_feedforward": 2,
            "num_attention_heads": 1,
            "ffn_dropout": 0.01,
            "attention_normalizer": "softmax",
            "multihead_attention_aggregation": "concat",
            "directed_attention": False,
            "use_inf_mask": True,
            "use_prior": True,
            "lr":lr
        }
        model = GraphConvolutionalTransformer(**gct_params)
        transformer = EHRTransformer(gct_params=gct_params)
```

```
        values = transformer.train_and_val(model,train_loader=train_dataloader,␣
↪val_loader=validate_dataloader,train_df=train_df,val_df=validate_df,␣
↪n_epochs=5)
        auc_pr_history[str(lr)]=values

    return auc_pr_history

auc_pr_history = test_learning_rate()

plot_AUC_PR(auc_pr_history,"lr")
```

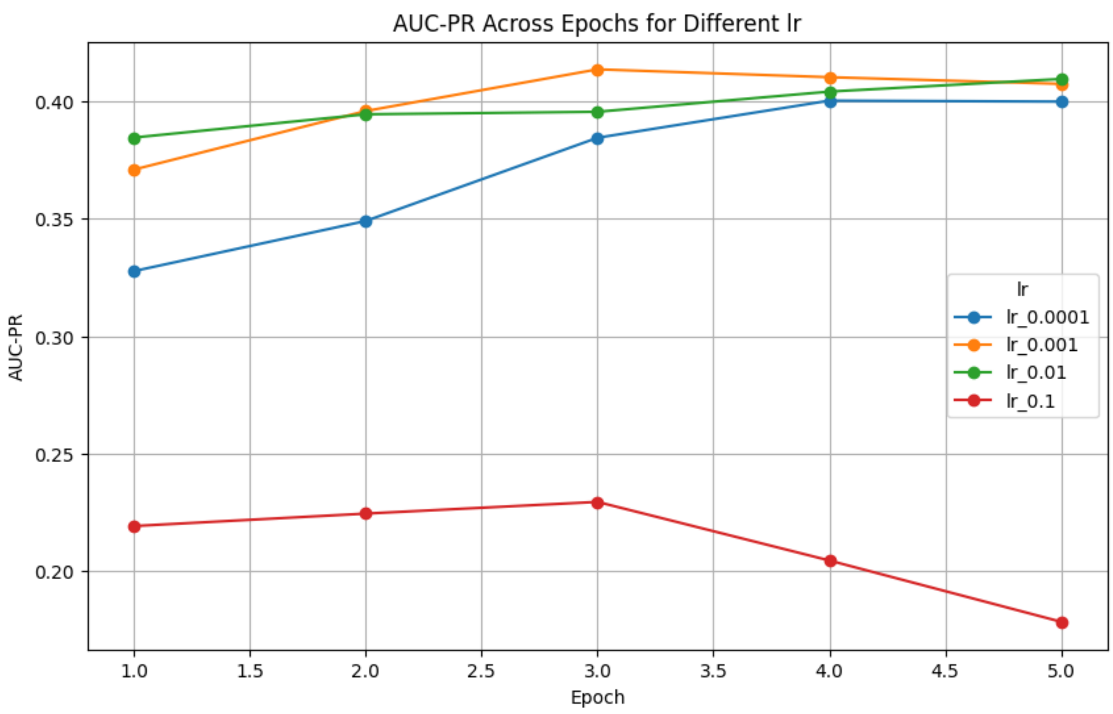
```
Epoch: 1         Step: 100 Training Loss: 1.721334
Epoch: 1         Step: 200 Training Loss: 1.685307
Epoch: 1         Step: 300 Training Loss: 1.672036
Epoch: 1         Step: 400 Training Loss: 1.663872
Epoch: 1         Step: 500 Training Loss: 1.656829
Epoch: 1         Step: 600 Training Loss: 1.654970
Epoch: 1         Step: 700 Training Loss: 1.652667
Epoch: 1         Step: 800 Training Loss: 1.649471
Epoch: 1         Step: 900 Training Loss: 1.646809
Epoch: 1         Step: 1000 Training Loss: 1.641557
Epoch: 1         Validation AUC_PR: 0.33
Epoch: 2         Step: 100 Training Loss: 1.592819
Epoch: 2         Step: 200 Training Loss: 1.598757
Epoch: 2         Step: 300 Training Loss: 1.600225
Epoch: 2         Step: 400 Training Loss: 1.602157
Epoch: 2         Step: 500 Training Loss: 1.604401
Epoch: 2         Step: 600 Training Loss: 1.606220
Epoch: 2         Step: 700 Training Loss: 1.606705
Epoch: 2         Step: 800 Training Loss: 1.609506
Epoch: 2         Step: 900 Training Loss: 1.610863
Epoch: 2         Step: 1000 Training Loss: 1.610094
Epoch: 2         Validation AUC_PR: 0.35
Epoch: 3         Step: 100 Training Loss: 1.568391
Epoch: 3         Step: 200 Training Loss: 1.587058
Epoch: 3         Step: 300 Training Loss: 1.593917
Epoch: 3         Step: 400 Training Loss: 1.596564
Epoch: 3         Step: 500 Training Loss: 1.597877
Epoch: 3         Step: 600 Training Loss: 1.595466
Epoch: 3         Step: 700 Training Loss: 1.597214
Epoch: 3         Step: 800 Training Loss: 1.597394
Epoch: 3         Step: 900 Training Loss: 1.595043
Epoch: 3         Step: 1000 Training Loss: 1.594879
Epoch: 3         Validation AUC_PR: 0.38
Epoch: 4         Step: 100 Training Loss: 1.576749
Epoch: 4         Step: 200 Training Loss: 1.586617
Epoch: 4         Step: 300 Training Loss: 1.584782
```

```
Epoch: 4        Step: 400 Training Loss: 1.585937
Epoch: 4        Step: 500 Training Loss: 1.580353
Epoch: 4        Step: 600 Training Loss: 1.580423
Epoch: 4        Step: 700 Training Loss: 1.580471
Epoch: 4        Step: 800 Training Loss: 1.583540
Epoch: 4        Step: 900 Training Loss: 1.583337
Epoch: 4        Step: 1000 Training Loss: 1.582335
Epoch: 4        Validation AUC_PR: 0.40
Epoch: 5        Step: 100 Training Loss: 1.551215
Epoch: 5        Step: 200 Training Loss: 1.564142
Epoch: 5        Step: 300 Training Loss: 1.566963
Epoch: 5        Step: 400 Training Loss: 1.570060
Epoch: 5        Step: 500 Training Loss: 1.569041
Epoch: 5        Step: 600 Training Loss: 1.567734
Epoch: 5        Step: 700 Training Loss: 1.570395
Epoch: 5        Step: 800 Training Loss: 1.571481
Epoch: 5        Step: 900 Training Loss: 1.571022
Epoch: 5        Step: 1000 Training Loss: 1.571154
Epoch: 5        Validation AUC_PR: 0.40
Epoch: 1        Step: 100 Training Loss: 1.636091
Epoch: 1        Step: 200 Training Loss: 1.640878
Epoch: 1        Step: 300 Training Loss: 1.637072
Epoch: 1        Step: 400 Training Loss: 1.638742
Epoch: 1        Step: 500 Training Loss: 1.635118
Epoch: 1        Step: 600 Training Loss: 1.634162
Epoch: 1        Step: 700 Training Loss: 1.630290
Epoch: 1        Step: 800 Training Loss: 1.626206
Epoch: 1        Step: 900 Training Loss: 1.623069
Epoch: 1        Step: 1000 Training Loss: 1.620771
Epoch: 1        Validation AUC_PR: 0.37
Epoch: 2        Step: 100 Training Loss: 1.591889
Epoch: 2        Step: 200 Training Loss: 1.592642
Epoch: 2        Step: 300 Training Loss: 1.595257
Epoch: 2        Step: 400 Training Loss: 1.598229
Epoch: 2        Step: 500 Training Loss: 1.597895
Epoch: 2        Step: 600 Training Loss: 1.593920
Epoch: 2        Step: 700 Training Loss: 1.596254
Epoch: 2        Step: 800 Training Loss: 1.595667
Epoch: 2        Step: 900 Training Loss: 1.593853
Epoch: 2        Step: 1000 Training Loss: 1.593384
Epoch: 2        Validation AUC_PR: 0.40
Epoch: 3        Step: 100 Training Loss: 1.557456
Epoch: 3        Step: 200 Training Loss: 1.567202
Epoch: 3        Step: 300 Training Loss: 1.569244
Epoch: 3        Step: 400 Training Loss: 1.572747
Epoch: 3        Step: 500 Training Loss: 1.572913
Epoch: 3        Step: 600 Training Loss: 1.576984
Epoch: 3        Step: 700 Training Loss: 1.576761
```

```
Epoch: 3        Step: 800 Training Loss: 1.577279
Epoch: 3        Step: 900 Training Loss: 1.575257
Epoch: 3        Step: 1000 Training Loss: 1.575071
Epoch: 3        Validation AUC_PR: 0.41
Epoch: 4        Step: 100 Training Loss: 1.549568
Epoch: 4        Step: 200 Training Loss: 1.553205
Epoch: 4        Step: 300 Training Loss: 1.556362
Epoch: 4        Step: 400 Training Loss: 1.561247
Epoch: 4        Step: 500 Training Loss: 1.558467
Epoch: 4        Step: 600 Training Loss: 1.560994
Epoch: 4        Step: 700 Training Loss: 1.560675
Epoch: 4        Step: 800 Training Loss: 1.563451
Epoch: 4        Step: 900 Training Loss: 1.563357
Epoch: 4        Step: 1000 Training Loss: 1.563557
Epoch: 4        Validation AUC_PR: 0.41
Epoch: 5        Step: 100 Training Loss: 1.520088
Epoch: 5        Step: 200 Training Loss: 1.542206
Epoch: 5        Step: 300 Training Loss: 1.548808
Epoch: 5        Step: 400 Training Loss: 1.547965
Epoch: 5        Step: 500 Training Loss: 1.550153
Epoch: 5        Step: 600 Training Loss: 1.551867
Epoch: 5        Step: 700 Training Loss: 1.552264
Epoch: 5        Step: 800 Training Loss: 1.552417
Epoch: 5        Step: 900 Training Loss: 1.550858
Epoch: 5        Step: 1000 Training Loss: 1.550327
Epoch: 5        Validation AUC_PR: 0.41
Epoch: 1        Step: 100 Training Loss: 1.735480
Epoch: 1        Step: 200 Training Loss: 1.690022
Epoch: 1        Step: 300 Training Loss: 1.675840
Epoch: 1        Step: 400 Training Loss: 1.672216
Epoch: 1        Step: 500 Training Loss: 1.662080
Epoch: 1        Step: 600 Training Loss: 1.651347
Epoch: 1        Step: 700 Training Loss: 1.645374
Epoch: 1        Step: 800 Training Loss: 1.641383
Epoch: 1        Step: 900 Training Loss: 1.637022
Epoch: 1        Step: 1000 Training Loss: 1.635357
Epoch: 1        Validation AUC_PR: 0.38
Epoch: 2        Step: 100 Training Loss: 1.568137
Epoch: 2        Step: 200 Training Loss: 1.593055
Epoch: 2        Step: 300 Training Loss: 1.601122
Epoch: 2        Step: 400 Training Loss: 1.594997
Epoch: 2        Step: 500 Training Loss: 1.592027
Epoch: 2        Step: 600 Training Loss: 1.591399
Epoch: 2        Step: 700 Training Loss: 1.588729
Epoch: 2        Step: 800 Training Loss: 1.591099
Epoch: 2        Step: 900 Training Loss: 1.588950
Epoch: 2        Step: 1000 Training Loss: 1.589319
Epoch: 2        Validation AUC_PR: 0.39
```

```
Epoch: 3        Step: 100 Training Loss: 1.559410
Epoch: 3        Step: 200 Training Loss: 1.562815
Epoch: 3        Step: 300 Training Loss: 1.569205
Epoch: 3        Step: 400 Training Loss: 1.576238
Epoch: 3        Step: 500 Training Loss: 1.578033
Epoch: 3        Step: 600 Training Loss: 1.576948
Epoch: 3        Step: 700 Training Loss: 1.573985
Epoch: 3        Step: 800 Training Loss: 1.573433
Epoch: 3        Step: 900 Training Loss: 1.573773
Epoch: 3        Step: 1000 Training Loss: 1.573389
Epoch: 3        Validation AUC_PR: 0.40
Epoch: 4        Step: 100 Training Loss: 1.535862
Epoch: 4        Step: 200 Training Loss: 1.546961
Epoch: 4        Step: 300 Training Loss: 1.551839
Epoch: 4        Step: 400 Training Loss: 1.550159
Epoch: 4        Step: 500 Training Loss: 1.551838
Epoch: 4        Step: 600 Training Loss: 1.554684
Epoch: 4        Step: 700 Training Loss: 1.558434
Epoch: 4        Step: 800 Training Loss: 1.559544
Epoch: 4        Step: 900 Training Loss: 1.560501
Epoch: 4        Step: 1000 Training Loss: 1.564218
Epoch: 4        Validation AUC_PR: 0.40
Epoch: 5        Step: 100 Training Loss: 1.549291
Epoch: 5        Step: 200 Training Loss: 1.555940
Epoch: 5        Step: 300 Training Loss: 1.561983
Epoch: 5        Step: 400 Training Loss: 1.556100
Epoch: 5        Step: 500 Training Loss: 1.555522
Epoch: 5        Step: 600 Training Loss: 1.553924
Epoch: 5        Step: 700 Training Loss: 1.553312
Epoch: 5        Step: 800 Training Loss: 1.553349
Epoch: 5        Step: 900 Training Loss: 1.554818
Epoch: 5        Step: 1000 Training Loss: 1.555358
Epoch: 5        Validation AUC_PR: 0.41
Epoch: 1        Step: 100 Training Loss: 2.110180
Epoch: 1        Step: 200 Training Loss: 2.016670
Epoch: 1        Step: 300 Training Loss: 2.000307
Epoch: 1        Step: 400 Training Loss: 1.983979
Epoch: 1        Step: 500 Training Loss: 2.051789
Epoch: 1        Step: 600 Training Loss: 2.060351
Epoch: 1        Step: 700 Training Loss: 2.052472
Epoch: 1        Step: 800 Training Loss: 2.033120
Epoch: 1        Step: 900 Training Loss: 2.014546
Epoch: 1        Step: 1000 Training Loss: 2.001593
Epoch: 1        Validation AUC_PR: 0.22
Epoch: 2        Step: 100 Training Loss: 1.829078
Epoch: 2        Step: 200 Training Loss: 1.870830
Epoch: 2        Step: 300 Training Loss: 1.885571
Epoch: 2        Step: 400 Training Loss: 1.966146
```

```
Epoch: 2        Step: 500 Training Loss: 1.970297
Epoch: 2        Step: 600 Training Loss: 1.972502
Epoch: 2        Step: 700 Training Loss: 1.980128
Epoch: 2        Step: 800 Training Loss: 1.982610
Epoch: 2        Step: 900 Training Loss: 1.986214
Epoch: 2        Step: 1000 Training Loss: 1.983775
Epoch: 2        Validation AUC_PR: 0.22
Epoch: 3        Step: 100 Training Loss: 1.924599
Epoch: 3        Step: 200 Training Loss: 1.929065
Epoch: 3        Step: 300 Training Loss: 1.945169
Epoch: 3        Step: 400 Training Loss: 1.947213
Epoch: 3        Step: 500 Training Loss: 1.949155
Epoch: 3        Step: 600 Training Loss: 1.946860
Epoch: 3        Step: 700 Training Loss: 1.946238
Epoch: 3        Step: 800 Training Loss: 1.935722
Epoch: 3        Step: 900 Training Loss: 1.971950
Epoch: 3        Step: 1000 Training Loss: 1.965438
Epoch: 3        Validation AUC_PR: 0.23
Epoch: 4        Step: 100 Training Loss: 1.866997
Epoch: 4        Step: 200 Training Loss: 1.902765
Epoch: 4        Step: 300 Training Loss: 2.573709
Epoch: 4        Step: 400 Training Loss: 2.433573
Epoch: 4        Step: 500 Training Loss: 2.344769
Epoch: 4        Step: 600 Training Loss: 2.287086
Epoch: 4        Step: 700 Training Loss: 2.242218
Epoch: 4        Step: 800 Training Loss: 2.211637
Epoch: 4        Step: 900 Training Loss: 2.187340
Epoch: 4        Step: 1000 Training Loss: 2.165577
Epoch: 4        Validation AUC_PR: 0.20
Epoch: 5        Step: 100 Training Loss: 2.006616
Epoch: 5        Step: 200 Training Loss: 2.005214
Epoch: 5        Step: 300 Training Loss: 1.983702
Epoch: 5        Step: 400 Training Loss: 2.043437
Epoch: 5        Step: 500 Training Loss: 2.042086
Epoch: 5        Step: 600 Training Loss: 2.041785
Epoch: 5        Step: 700 Training Loss: 2.037645
Epoch: 5        Step: 800 Training Loss: 2.032162
Epoch: 5        Step: 900 Training Loss: 2.034512
Epoch: 5        Step: 1000 Training Loss: 2.031491
Epoch: 5        Validation AUC_PR: 0.18
```



5.1.2 Computational requirements

Report at least 3 types of requirements such as type of hardware, average runtime for each epoch, total number of trials, GPU hrs used,

- Hardware: colab CPU
- Average runtime per epoch: 4m50s
- trials:30 epochs

5.1.3 Training code

- best parameters are {'droprate':0.1, 'lr':0.001,'embedding_dim':128}

[60]:
```
# hepler funtion to test and split

gct_params = {
      "embedding_size": 128,
      "num_transformer_stack": 3,
      "num_feedforward": 2,
      "num_attention_heads": 1,
      "ffn_dropout": 0.1,
      "attention_normalizer": "softmax",
      "multihead_attention_aggregation": "concat",
      "directed_attention": False,
      "use_inf_mask": True,
```

```
      "use_prior": True,
      "lr":0.0001
  }
model = GraphConvolutionalTransformer(**gct_params)
transformer = EHRTransformer(gct_params=gct_params)

transformer.train_and_val(model,train_loader=train_dataloader,␣
 ↪val_loader=validate_dataloader,train_df=train_df,val_df=validate_df,␣
 ↪n_epochs=5)
```

```
Epoch: 1         Step: 100 Training Loss: 1.627589
Epoch: 1         Step: 200 Training Loss: 1.639133
Epoch: 1         Step: 300 Training Loss: 1.632226
Epoch: 1         Step: 400 Training Loss: 1.627298
Epoch: 1         Step: 500 Training Loss: 1.630651
Epoch: 1         Step: 600 Training Loss: 1.630009
Epoch: 1         Step: 700 Training Loss: 1.631293
Epoch: 1         Step: 800 Training Loss: 1.630656
Epoch: 1         Step: 900 Training Loss: 1.629003
Epoch: 1         Step: 1000 Training Loss: 1.628991
Epoch: 1         Validation AUC_PR: 0.36
Epoch: 2         Step: 100 Training Loss: 1.598355
Epoch: 2         Step: 200 Training Loss: 1.604076
Epoch: 2         Step: 300 Training Loss: 1.605354
Epoch: 2         Step: 400 Training Loss: 1.602199
Epoch: 2         Step: 500 Training Loss: 1.604844
Epoch: 2         Step: 600 Training Loss: 1.606469
Epoch: 2         Step: 700 Training Loss: 1.605503
Epoch: 2         Step: 800 Training Loss: 1.604027
Epoch: 2         Step: 900 Training Loss: 1.602975
Epoch: 2         Step: 1000 Training Loss: 1.602953
Epoch: 2         Validation AUC_PR: 0.37
Epoch: 3         Step: 100 Training Loss: 1.586465
Epoch: 3         Step: 200 Training Loss: 1.590312
Epoch: 3         Step: 300 Training Loss: 1.595662
Epoch: 3         Step: 400 Training Loss: 1.595720
Epoch: 3         Step: 500 Training Loss: 1.594694
Epoch: 3         Step: 600 Training Loss: 1.591997
Epoch: 3         Step: 700 Training Loss: 1.592206
Epoch: 3         Step: 800 Training Loss: 1.591438
Epoch: 3         Step: 900 Training Loss: 1.593143
Epoch: 3         Step: 1000 Training Loss: 1.592122
Epoch: 3         Validation AUC_PR: 0.39
Epoch: 4         Step: 100 Training Loss: 1.564588
Epoch: 4         Step: 200 Training Loss: 1.581907
Epoch: 4         Step: 300 Training Loss: 1.584299
Epoch: 4         Step: 400 Training Loss: 1.587000
```

```
Epoch: 4         Step: 500 Training Loss: 1.586494
Epoch: 4         Step: 600 Training Loss: 1.585219
Epoch: 4         Step: 700 Training Loss: 1.584288
Epoch: 4         Step: 800 Training Loss: 1.583043
Epoch: 4         Step: 900 Training Loss: 1.583034
Epoch: 4         Step: 1000 Training Loss: 1.582976
Epoch: 4         Validation AUC_PR: 0.39
Epoch: 5         Step: 100 Training Loss: 1.541478
Epoch: 5         Step: 200 Training Loss: 1.568955
Epoch: 5         Step: 300 Training Loss: 1.566150
Epoch: 5         Step: 400 Training Loss: 1.566009
Epoch: 5         Step: 500 Training Loss: 1.568595
Epoch: 5         Step: 600 Training Loss: 1.570347
Epoch: 5         Step: 700 Training Loss: 1.571463
Epoch: 5         Step: 800 Training Loss: 1.574434
Epoch: 5         Step: 900 Training Loss: 1.572187
Epoch: 5         Step: 1000 Training Loss: 1.573847
Epoch: 5         Validation AUC_PR: 0.39
```

[60]:
```
[0.3592529275372732,
 0.37411525877802115,
 0.38802388591875653,
 0.38937967695142806,
 0.3947565923202996]
```

5.2 Evaluation

5.2.1 Metrics descriptions

- AUC-ROC ### Evaluation code
- transformer.eval_model(model, test_loader, test_df)

[61]:
```
gct_params = {
      "embedding_size": 128,
      "num_transformer_stack": 3,
      "num_feedforward": 2,
      "num_attention_heads": 1,
      "ffn_dropout": 0.1,
      "attention_normalizer": "softmax",
      "multihead_attention_aggregation": "concat",
      "directed_attention": False,
      "use_inf_mask": True,
      "use_prior": True,
      "lr":0.001
  }
transformer = EHRTransformer(gct_params=gct_params)
transformer.eval_model(model, test_dataloader, test_df)
```

[61]: 0.38539847488326173

6 Results (15)

6.1 Table of results

- Readdmission tasks

Metric	Original Paper	Reproduced Results(test)	Reproduced Results(val)
AUC-ROC	0.5244	0.3854	0.3947

6.1.1 All claims should be supported by experiment results

- The result is not very closely align with those reported in the original paper.

6.1.2 Discuss with respect to the hypothesis and results from the original paper

- The hypothesis that GCT can learn the hidden structure of EHR data was uncertain.

6.1.3 Experiments beyond the original paper

Each experiment should include results and a discussion * Runing time experiment - The code in the original code base takes 153 second for 100 steps, which is equals to 12hr for each epoch in my cpu. However, the colab cup only needs 5 mins for each epoch. - The time saving comes from the panda dataframe. Input as dataframes are saved in memory, while the original code needs to get the tfrecord input from the disk each batch.

6.1.4 Ablation Study.

- Impact of varying dropout rates,learning rate, hidden dims on model performance.

7 Discussion (10)

7.1 Implications of the experimental results, whether the original paper was reproducible, and if it wasn't, what factors made it irreproducible

- The original paper demonstrates high reproducibility, with the final AUC-PR in some degree matching that of the original findings for the task of readmission. ## What was easy
- Transitioning from TensorFlow records to pytorch dataframes streamlined the workflow and enhanced accessibility.

7.2 What was difficult

- Bug detection proved time-consuming, exemplified by the discovery that tf.float32.max does not equate to float('inf'), but rather to torch.finfo(torch.float32).max. This discrepancy required extensive debugging and the development of numerous helper functions.
- The default value of `float('inf')` in `inf_mask` led to the generation of numerous `NaNs` and compromised the `pre_softmax` within `qk_op` function.

7.3 Recommendations to the original authors or others who work in this area for improving reproducibility

- The orignial paper gives 41026 piece of eicu data as input, while in the dataframe, it only gives 40410. The missing piece of data is because of the joining method. It will be better to write code to detect them for future student to reporduce this paper
- Other tasks, such as the synthesis of data and other prediction tasks like motility, were not reproduced within this study due to time constraints. Encouraging others to replicate these aspects using the provided codebase could enrich the scientific discourse and validate the findings further
- The code is not supporting GPU yet. The difficulties comes from the pandas dataframe column `prior_value`. This is a a list type and comes with variable length. Because of the time limit and easy to train in a CPU, I haven't spend time on that.

8 Public GitHub Repo (5)

8.1 Publish your code in a public repository on GitHub and attach the URL in the notebook.

- `[GitHub Repo URL](https://github.com/Alexuiuc/paperReplicateForDHL` ## Make sure your code is documented properly. ## A README.md file describing the exact steps to run your code is required.
- Include comprehensive instructions on setting up the environment, running preprocessing, training, and evaluation scripts.

8.1.1 video link : https://youtu.be/wIKq0NiEgLE

```
[ ]:
```