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Отчет по лабораторной работе №6

«Разработка системы предсказаний поведения на основании графовых моделей»

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Описание задания

Цель лабораторной работы: обучение работе с предварительной обработкой графовых типов данных и обучением нейронных сетей на графовых данных.

- 1. Подготовить датасет графовых данных
- 2. Подобрать модель и гиперпараметры обучения для получения качества AUC > 0.65

```
1 # Slow method of installing pytorch geometric
            2 # !pip install torch_geometric
3 # !pip install torch_sparse
            4 # !pip install torch_scatter
            6 # Install pytorch geometric
             7 !pip install torch-sparse -f https://pytorch-geometric.com/whl/torch-1.11.0%2Bcu113.html
            8 !pip install torch-cluster -f https://pytorch-geometric.com/whl/torch-1.11.0%2Bcu113.html
           9 |pip install torch-spline-conv -f https://pytorch-geometric.com/whl/torch-1.11.0%2Bcu113.html 10 |pip install torch-geometric -f https://pytorch-geometric.com/whl/torch-1.11.0%2Bcu113.html
           11 !pip install torch-scatter==2.0.8 -f https://data.pyg.org/whl/torch-1.11.0%2Bcu113.html
1 import numpy as np
2 import pandas as pd
3 import pickle
4 import csv
5 import os
                                                                                                                                                     RANDOM_SEED: 42
                                                                                                                                                     BASE_DIR: "/content/
           7 from sklearn.preprocessing import LabelEncoder
          11 # PyG - PyTorch Geometric
12 from torch_geometric.data import Data, DataLoader, InMemoryDataset
          13
14 from tqdm import tqdm
         10
17 RANDOM_SEED = 42 #@param { type: "integer" }
18 BASE_DIR = '/content/' #@param { type: "string" }
19 np.random.seed(RANDOM_SEED)
[5] 1 # Check if CUDA is available for colab
2 torch.cuda.is_available()
[6] 1 # Unpack files from zip-file
2 import zipfile
3 with zipfile/Zipfile(BASE_DIR + 'yoochoose-data-lite.zip', 'r') as zip_ref:
4 zip_ref.extractall(BASE_DIR)
```

Анализ исходных данных

```
1 # Read dataset of items in store
         2 df = pd.read_csv(BASE_DIR + 'yoochoose-clicks-lite.dat')
3 # df.columns = ['session_id', 'timestamp', 'item_id', 'category']
         4 df.head()
   _______/usr/local/lib/python3.7/dist-packages/IPython/core/interactiveshell.py:2882: DtypeWarning: Columns (3) have mixed types.Specify
          exec(code_obj, self.user_global_ns, self.user_ns)
                                         timestamp item_id category 🎢
              9 2014-04-06T11:26:24.127Z 214576500
                      9 2014-04-06T11:28:54.654Z 214576500
                   9 2014-04-06T11:29:13.479Z 214576500
                                                                           0
                      19 2014-04-01T20:52:12.357Z 214561790
                     19 2014-04-01T20:52:13.758Z 214561790
                                                                           0
[8] 1 # Read dataset of purchases
         2 buy_df = pd.read_csv(BASE_DIR + 'yoochoose-buys-lite.dat')
         3 # buy_df.columns = ['session_id', 'timestamp', 'item_id', 'price', 'quantity']
         4 buy_df.head()
                                         timestamp item_id price quantity 🤾
           session_id
         0 420374 2014-04-06T18:44:58.314Z 214537888 12462
                 420374 2014-04-06T18:44:58.325Z 214537850 10471
                489758 2014-04-06T09:59:52.422Z 214826955 1360
                 489758 2014-04-06T09:59:52.476Z 214826715
                                                                                    2
                489758 2014-04-06T09:59:52.578Z 214827026 1046
[9] 1 # Filter out item session with length < 2
2 df['valid_session'] = df.session_id.map(df.groupby('session_id')['item_id'].size() > 2)
3 df = df.loc[df.valid_session].drop('valid_session',axis=1)
   session_id 1000000
       timestamp
                     5557758
       item_id
                      37644
       category
                         275
       dtype: int64
[ 1 # Randomly sample a couple of them
                                                                                                                                 NUM_SESSIONS: 50000
        2 NUM_SESSIONS = 50000 #@param { type: "integer" }
3 sampled_session_id = np.random.choice(df.session_id.unique(), NUM_SESSIONS, replace=False)
4 df = df.loc[df.session_id.isin(sampled_session_id)]
        5 df.nunique()

    session_id

       timestamp
item_id
                     278442
                      18461
       category
                        110
       dtype: int64
[11] 1 # Average length of session
       2 df.groupby('session_id')['item_id'].size().mean()
      5.56902
```

```
1 # Encode item and category id in item dataset so that ids will be in range (0,len(df.item.unique()))
2 item_encoder = LabelEncoder()
3 category_encoder = LabelEncoder()
4 df['item_id'] = item_encoder.fit_transform(df.item_id)
5 df['category'] = category_encoder.fit_transform(df.category.apply(str))
6 df.head()
```

	session_id	timestamp	item_id	category
0	9	2014-04-06T11:26:24.127Z	3496	0
1	9	2014-04-06T11:28:54.654Z	3496	0
2	9	2014-04-06T11:29:13.479Z	3496	0
102	171	2014-04-03T17:45:25.575Z	10049	0
103	171	2014-04-03T17:45:33.177Z	10137	0

₽

```
[13] 1 # Encode item and category id in purchase dataset
2 buy_df = buy_df.loc[buy_df.session_id.isin(df.session_id)]
3 buy_df['item_id'] = item_encoder.transform(buy_df.item_id)
4 buy_df.head()
```

/usr/local/lib/python3.7/dist-packages/ipykernel_launcher.py:3: SettingWithCopyWarning: A value is trying to be set on a copy of a slice from a DataFrame.

Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#
This is separate from the ipykernel package so we can avoid doing imports until

```
session id
                             timestamp item id price quantity
46
        489491 2014-04-06T12:41:34.047Z
                                                  1046
                                                               4
                                          12633
47
        489491 2014-04-06T12:41:34.091Z
                                          12634
                                                   627
                                                               2
        70353 2014-04-06T10:55:06.086Z
                                          14345 41783
61
62
        489671 2014-04-03T15:48:37.392Z
                                          12489
                                                  4188
        489671 2014-04-03T15:59:35.495Z
                                          12489
                                                  4188
```

```
[14] \, 1 # Get item dictionary with grouping by session
        2 buy_item_dict = dict(buy_df.groupby('session_id')['item_id'].apply(list))
        3 buy item dict
        2204/09. [320, 1412, 13203, 1320/],
2289552: [13164, 13168],
        2290431: [13498],
2290698: [11827, 11824],
        2291707
                     [15758, 15758],
        2292108: [18460],
        2292426:
                    [11208],
                    [13156, 13108],
[7964, 7965],
        2292499:
        2293224:
                    [13494],
[13110],
        2294903:
        2295932:
        2300511:
                    [13167, 13164, 9691, 13286],
        2300966: [14062, 1121],
2301182: [12974, 10465, 1819],
        2301826:
                    [13164, 13167, 13286, 13166],
        2302889: [2125],
        2303773: [13166, 13164, 13290, 13288, 15921],
2305544: [13164, 13168],
        2306951:
                    [13164, 13164, 13286, 13168, 13166, 13167, 13285],
        2307524: [13164, 13286, 13167],
2310501: [13168, 8393, 13168],
                    [13285, 13165, 13168],
[13164, 13286, 9699],
        2311333:
        2312773:
        2316132: [7877],
2317759: [14951, 7439, 7439, 14951],
        2318429:
                    [18460],
                    [11221, 12355],
[13279, 13285, 13164],
        2318877:
        2319826:
        2320679:
                    [13108],
                    [12869, 13510],
[3718, 8278, 10962],
        2322056:
        2322739:
        2323802:
                    [18460],
[13279, 10606, 10607],
        2324881:
        2325937: [18460],
2326769: [12826, 13832],
2330123: [13603, 8531],
        2330138: [13286, 13164],
        2331598: [13165, 13285, 13066],
2332823: [12701 11662 12362 11830 13712]
```

Сборка выборки для обучения

[15] 1 # Transform df into tensor data

2 def transform_dataset(df, buy_item_dict):
3 data_list = []

```
# Group by session
                 grouped = df.groupby('session_id')
for session_id, group in tqdm(grouped):
                     le = LabelEncoder()
sess_item_id = le.fit_transform(group.item_id)
                   group = group.reset_index(drop=True)
group['sess_item_id'] = sess_item_id
         10
         11
         12
                     #get input features
                   14
         16
                    target_nodes = group.sess_item_id.values[1:]
source_nodes = group.sess_item_id.values[:-1]
         18
                   edge_index = torch.tensor([source_nodes,
target_nodes], dtype=torch.long)
         20
21
                     x = node_features
         22
         24
                   #get result
         25
                     if session_id in buy_item_dict:
                         positive_indices = le.transform(buy_item_dict[session_id])
label = np.zeros(len(node_features))
         26
27
         28
                           label[positive indices] = 1
         29
30
                   else:
label = [0] * len(node_features)
         31
                   y = torch.FloatTensor(label)
         32
33
                   data = Data(x=x, edge_index=edge_index, y=y)
         35
36
                   data_list.append(data)
         37
                return data_list
         40 # Pytorch class for creating datasets
         41 class YooChooseDataset(InMemoryDataset):
42    def __init__(self, root, transform=None, pre_transform=None):
43    super(YooChooseDataset, self).__init__(root, transform, pre_transform)
44    self.data, self.slices = torch.load(self.processed_paths[8])
         45
                @property
         47
48
                 def raw_file_names(self):
    return []
         49
                 @property
         51
                  def processed_file_names(self):
         52
                    return [BASE_DIR+'yoochoose_click_binary_100000_sess.dataset']
         53
54
                 def download(self):
         55
         56
57
                def process(self):
                     data_list = transform_dataset(df, buy_item_dict)
         59
                data, slices = self.collate(data_list)
torch.save((data, slices), self.processed_paths[0])
         61
1 s Fragary dataset.
| dataset = YuoChocoadataset('./')
 (4000), 5000, 5000)
```

```
[47] 1 embed_dim = 128
        2 from torch_geometric.nn import GraphConv, TopKPooling, GatedGraphConv, SAGEConv, SGConv
        3 from torch_geometric.nn import global_mean_pool as gap, global_max_pool as gmp
        4 import torch.nn.functional as F
        6 class Net(torch.nn.Module):
              def __init__(self):
                   super(Net, self).__init__()
                   # Model Structure
       10
                  self.conv1 = GraphConv(embed_dim * 2, 128)
                  self.pool1 = TopKPooling(128, ratio=0.9)
self.conv2 = GraphConv(128, 128)
       11
       12
                  self.pool2 = TopKPooling(128, ratio=0.9)
       13
                 self.conv3 = GraphConv(128, 128)
self.pool3 = TopKPooling(128, ratio=0.9)
self.item_embedding = torch.nn.Embedding(num_embeddings=num_items, embedding_dim=embed_dim)
       14
       15
       16
                 self.category_embedding = torch.nn.Embedding(num_embeddings=num_categories, embedding_dim=embed_dim)
self.lin1 = torch.nn.Linear(256, 256)
self.lin2 = torch.nn.Linear(256, 128)
self.bn1 = torch.nn.BatchNorm1d(128)
self.bn2 = torch.nn.BatchNorm1d(64)
       17
       18
       19
       20
       21
                  self.act1 = torch.nn.ReLU()
self.act2 = torch.nn.ReLU()
        22
       23
        24
             # Forward step of a model
       25
       26
             def forward(self, data):
       27
                   x, edge_index, batch = data.x, data.edge_index, data.batch
       28
                  item_id = x[:,:,0]
                 category = x[:,:,1]
        30
        32
                   emb_item = self.item_embedding(item_id).squeeze(1)
        33
                   emb_category = self.category_embedding(category).squeeze(1)
       34
       35
                  x = torch.cat([emb_item, emb_category], dim=1)
       36
       37
                   # print(x.shape)
       3.8
                   x = F.relu(self.conv1(x, edge_index))
       39
                   # print(x.shape)
       40
                   r = self.pool1(x, edge_index, None, batch)
                   x, edge_index, _, batch, _, _ = self.pool1(x, edge_index, None, batch)
                   x1 = torch.cat([gmp(x, batch), gap(x, batch)], dim=1)
       43
       44
                   x = F.relu(self.conv2(x, edge_index))
       45
       46
                   x, edge_index, _, batch, _, _ = self.pool2(x, edge_index, None, batch) x2 = torch.cat([gmp(x, batch), gap(x, batch)], dim=1)
       47
       48
       49
                   x = F.relu(self.conv3(x, edge_index))
       51
                   x, edge_index, _, batch, _, _ = self.pool3(x, edge_index, None, batch)
                   x3 = torch.cat([gmp(x, batch), gap(x, batch)], dim=1)
       55
                   x = x1 + x2 + x3
       56
                   x = self.lin1(x)
       58
                   x = self.act1(x)
                   x = self.lin2(x)
       59
       68 x = F.dronout(x, n=0.5, training=self.training)
```

```
62
  63
          outputs = []
  64
         for i in range(x.size(0)):
  65
              output = torch.matmul(emb_item[data.batch == i], x[i,:])
  66
  67
              outputs.append(output)
  68
  69
           x = torch.cat(outputs, dim=0)
  70
           x = torch.sigmoid(x)
  71
  72
           return x
```

```
1 # Train a model
2 NUM_EPOCHS = 50#8param { type: "integer" }
3 for epoch in tqom(range(NUM_EPOCHS)):
4 loss = train()
5 train_acc = evaluate(train_loader)
6 val_acc = evaluate(train_loader)
7 test_acc = evaluate(test_loader)
8 print('Epoch: (:03d), loss: (:.5f), Train Auc: {:.5f}, Val Auc: {:.5f}, Test_Auc: {:.5f}'.
9 format(epoch, loss, train_acc, val_acc, test_acc)

[] 2X| | 1/50 [00:37<30:45, 37.67s/it]Epoch: 000, loss: 0.71581, Train Auc: 0.51631, Val Auc: 0.51478, Test Auc: 0.51530
6X| 3/50 [01:14(20:56, 37.43s/it]Epoch: 001, loss: 0.66807, Train Auc: 0.5283), Val Auc: 0.51480, Test Auc: 0.51697
6X| 3/50 [01:14(20:56, 37.43s/it]Epoch: 001, loss: 0.66807, Train Auc: 0.5283), Val Auc: 0.51480, Test Auc: 0.51697
```

print('Epoch: (-03d), Loss: (:.5f), Train Auc: (:.5f), Test Auc: (:.5f)'.
format(epoch, loss, train_acc, val_acc, test_acc))

2X| | 1/50 [00:17.09:45, 37.67/it|Epoch: 000, Loss: 0.7581, Train Auc: 0.51031, Val Auc: 0.51478, Test Auc: 0.51934

4X| | 2/50 [01:14.29:56, 37.42/it|Epoch: 001, Loss: 0.65067, Train Auc: 0.52203, Val Auc: 0.51489, Test Auc: 0.51867

8X| | 3/50 [01:52.29:16, 37.37/it|Epoch: 001, Loss: 0.65067, Train Auc: 0.52203, Val Auc: 0.51607, Test Auc: 0.51867

8X| | 4/50 [02:29.28:42, 37.45/it|Epoch: 003, Loss: 0.65087, Train Auc: 0.52417, Val Auc: 0.51609, Test Auc: 0.51867

12X| | 4/50 [03:44.27:22, 37.35/it|Epoch: 004, Loss: 0.65087, Train Auc: 0.52417, Val Auc: 0.51960, Test Auc: 0.51865

12X| | 6/50 [03:44.27:22, 37.35/it|Epoch: 007, Loss: 0.65719, Train Auc: 0.52417, Val Auc: 0.51560, Test Auc: 0.51865

12X| | 6/50 [03:44.27:22, 37.35/it|Epoch: 007, Loss: 0.65719, Train Auc: 0.52417, Val Auc: 0.51560, Test Auc: 0.51865

10X| | 8/50 [04:58.26:04, 37.36/it|Epoch: 007, Loss: 0.65718, Train Auc: 0.52417, Val Auc: 0.51560, Test Auc: 0.51865

10X| | 8/50 [06:12.224:43, 37.36/it|Epoch: 007, Loss: 0.65718, Train Auc: 0.52417, Val Auc: 0.51560, Test Auc: 0.51865

10X| | 1/50 [06:12.224:43, 37.36/it|Epoch: 007, Loss: 0.65718, Train Auc: 0.52417, Val Auc: 0.51560, Test Auc: 0.51862

20X| | 1/50 [06:12.224:43, 37.36/it|Epoch: 007, Loss: 0.65718, Train Auc: 0.52417, Val Auc: 0.51560, Test Auc: 0.51864

10/50 [06:12.224:43, 37.36/it|Epoch: 007, Loss: 0.65718, Train Auc: 0.52417, Val Auc: 0.51560, Test Auc: 0.51864

10/50 [07:222131, 37.15/it|Epoch: 007, Loss: 0.65718, Train Auc: 0.52417, Val Auc: 0.51560, Test Auc: 0.51864

10/50 [09:18.214.2], 37.15/it|Epoch: 007, Loss: 0.65718, Train Auc: 0.52417, Val Auc: 0.51560, Test Auc: 0.51864

10/50 [09:18.214.2], 37.15/it|Epoch: 007, Loss: 0.65718, Train Auc: 0.52417, Val Auc: 0.51560, Test Auc: 0.51864

10/50 [09:18.214.2], 37.15/it|Epoch: 007, Loss: 0.656918, Train Auc: 0.52417, Val Auc: 0.51560, Test Auc: 0.51864

10/50 [10:18.25.20.20.30.30.30.30.30.30.30.30

Проверка результата с помощью примеров

```
[53] 1 # Подход №1 - из датасета
2 evaluate(DataLoader(test_dataset[40:60], batch_size=10))
```

/usr/local/lib/python3.7/dist-packages/torch_geometric/deprecation.py:12: UserWarning: 'data.DataLoader' is deprecated, use 'loader.DataLoader' instead warnings.warn(out)