Лабораторная работа №6:

"Разработка системы предсказания поведения на основании графовых моделей"

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Цель: обучение работе с графовым типом данных и графовыми нейронными сетями.

Задача: подготовить графовый датасет из базы данных о покупках и построить модель предсказания совершения покупки.

Графовые нейронные сети

Графовые нейронные сети - тип нейронной сети, которая напрямую работает со структурой графа. Типичным применениями GNN являются:

- Классификация узлов;
- Предсказание связей;
- Графовая классификация;
- Распознавание движений;
- Рекомендательные системы.

В данной лабораторной работе будет происходить работа над **графовыми сверточными сетями**. Отличаются они от сверточных нейронных сетей нефиксированной структурой, функция свертки не является .

Подробнее можно прочитать тут: https://towardsdatascience.com/understanding-graph-convolutional-networks-for-node-classification-a2bfdb7aba7b

Тут можно почитать современные подходы к использованию графовых сверточных сетей https://paperswithcode.com/method/gcn

Датасет

В качестве базы данных предлагаем использовать датасет о покупках пользователей в одном магазине товаров RecSys Challenge 2015 (https://www.kaggle.com/datasets/chadgostopp/recsys-challenge-2015).

Скачать датасет можно отсюда: https://drive.google.com/drive/folders/1gtAeXPTj-c0RwVOKreMrZ3bfSmCw2y-?usp=sharing (lite-версия является облегченной версией исходного датасета, рекомендуем использовать её)

Также рекомендуем загружать данные в виде архива и распаковывать через пакет zipfile или/и скачивать датасет в собственный Google Drive и примонтировать его в колаб.

Установка библиотек, выгрузка исходных датасетов

```
In [1]:
```

```
# Slow method of installing pytorch geometric
# !pip install torch_geometric
# !pip install torch_sparse
# !pip install torch_scatter

# Install pytorch geometric
!pip install torch-sparse -f https://pytorch-geometric.com/whl/torch-1.11.0%2Bcu113.html
!pip install torch-cluster -f https://pytorch-geometric.com/whl/torch-1.11.0%2Bcu113.html
!pip install torch-spline-conv -f https://pytorch-geometric.com/whl/torch-1.11.0%2Bcu113.html
!pip install torch-geometric -f https://pytorch-geometric.com/whl/torch-1.11.0%2Bcu113.html
!pip install torch-scatter==2.0.8 -f https://data.pyg.org/whl/torch-1.11.0%2Bcu113.html
```

```
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/public/simple/
Looking in links: https://pytorch-geometric.com/whl/torch-1.11.0%2Bcu113.html
Requirement already satisfied: torch-sparse in /usr/local/lib/python3.7/dist-packages (0.6.13)
Requirement already satisfied: scipy in /usr/local/lib/python3.7/dist-packages (from torch-sparse) (1.4
Requirement already satisfied: numpy>=1.13.3 in /usr/local/lib/python3.7/dist-packages (from scipy->tor
ch-sparse) (1.21.6)
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/public/simple/
Looking in links: https://pytorch-geometric.com/whl/torch-1.11.0%2Bcu113.html
Requirement already satisfied: torch-cluster in /usr/local/lib/python3.7/dist-packages (1.6.0)
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/public/simple/
Looking in links: https://pytorch-geometric.com/whl/torch-1.11.0%2Bcu113.html
Requirement already satisfied: torch-spline-conv in /usr/local/lib/python3.7/dist-packages (1.2.1)
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/public/simple/
Looking in links: https://pytorch-geometric.com/whl/torch-1.11.0%2Bcu113.html
Requirement already satisfied: torch-geometric in /usr/local/lib/python3.7/dist-packages (2.0.4)
Requirement already satisfied: numpy in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (
1.21.6)
Requirement already satisfied: jinja2 in /usr/local/lib/python3.7/dist-packages (from torch-geometric)
(2.11.3)
Requirement already satisfied: requests in /usr/local/lib/python3.7/dist-packages (from torch-geometric
) (2.23.0)
Requirement already satisfied: pandas in /usr/local/lib/python3.7/dist-packages (from torch-geometric)
(1.3.5)
Requirement already satisfied: scikit-learn in /usr/local/lib/python3.7/dist-packages (from torch-geome
tric) (1.0.2)
Requirement already satisfied: scipy in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (
1.4.1)
Requirement already satisfied: pyparsing in /usr/local/lib/python3.7/dist-packages (from torch-geometri
c) (3.0.9)
Requirement already satisfied: tqdm in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (4
Requirement already satisfied: MarkupSafe>=0.23 in /usr/local/lib/python3.7/dist-packages (from jinja2-
>torch-geometric) (2.0.1)
Requirement already satisfied: python-dateutil>=2.7.3 in /usr/local/lib/python3.7/dist-packages (from p
andas->torch-geometric) (2.8.2)
ch-geometric) (2022.1)
Requirement already satisfied: six>=1.5 in /usr/local/lib/python3.7/dist-packages (from python-dateutil
>=2.7.3->pandas->torch-geometric) (1.15.0)
Requirement already satisfied: urllib3!=1.25.0,!=1.25.1,<1.26,>=1.21.1 in /usr/local/lib/python3.7/dist
-packages (from requests->torch-geometric) (1.24.3)
orch-geometric) (2.10)
Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3.7/dist-packages (from reque
sts->torch-geometric) (2022.5.18.1)
Requirement already satisfied: chardet<4,>=3.0.2 in /usr/local/lib/python3.7/dist-packages (from reques
ts->torch-geometric) (3.0.4)
Requirement already satisfied: threadpoolctl>=2.0.0 in /usr/local/lib/python3.7/dist-packages (from sci
kit-learn->torch-geometric) (3.1.0)
Requirement already satisfied: joblib>=0.11 in /usr/local/lib/python3.7/dist-packages (from scikit-lear
n->torch-geometric) (1.1.0)
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/public/simple/
Looking in links: https://data.pyg.org/whl/torch-1.11.0%2Bcu113.html
Collecting torch-scatter == 2.0.8
 Using cached torch scatter-2.0.8.tar.gz (21 kB)
Building wheels for collected packages: torch-scatter
 Building wheel for torch-scatter (setup.py) ... done
 Created wheel for torch-scatter: filename=torch scatter-2.0.8-cp37-cp37m-linux x86 64.whl size=322201
6 sha256=fd219fb4f6d94ae12055c88de126b1423740ab32400e1ff75ed5b63ca96d6135
 Stored in directory: /root/.cache/pip/wheels/96/e4/4e/2bcc6de6a801960aedbca43f7106d268f766c3f9f8ab49b
3a5
Successfully built torch-scatter
Installing collected packages: torch-scatter
Successfully installed torch-scatter-2.0.8
```

In [2]:

```
import numpy as np
import pandas as pd
import pickle
import csv
import os
```

```
import torch
# PyG - PyTorch Geometric
from torch_geometric.data import Data, DataLoader, InMemoryDataset
from tqdm import tqdm

RANDDM SEED = 125 #@param { type: "integer" }
BASE_DIR = '/content/' #@param { type: "string" }
np.random.seed(RANDOM_SEED)

In [3]:
# Check if CUDA is available for colab
torch.cuda.is_available

Out[3]:
<function torch.cuda.is_available>

In [5]:
# Unpack files from zip-file
```

Анализ исходных данных

zip ref.extractall(BASE DIR)

```
In [6]:
```

import zipfile

with zipfile.ZipFile(BASE DIR + 'yoochoose-data-lite.zip', 'r') as zip ref:

Out[6]:

	session_id	timestamp	item_id	category
0	9	2014-04-06T11:26:24.127Z	214576500	0
1	9	2014-04-06T11:28:54.654Z	214576500	0
2	9	2014-04-06T11:29:13.479Z	214576500	0
3	19	2014-04-01T20:52:12.357Z	214561790	0
4	19	2014-04-01T20:52:13.758Z	214561790	0

In [7]:

```
# Read dataset of purchases
buy_df = pd.read_csv(BASE_DIR + 'yoochoose-buys-lite.dat')
# buy_df.columns = ['session_id', 'timestamp', 'item_id', 'price', 'quantity']
buy_df.head()
```

Out[7]:

session_id timestamp item_id price quantity

```
        0
        ses$20376
        2014-04-06T18:##:58:###
        214#:67686
        1646
        quantity

        1
        420374
        2014-04-06T18:44:58.325Z
        214537850
        10471
        1

        2
        489758
        2014-04-06T09:59:52.422Z
        214826955
        1360
        2

        3
        489758
        2014-04-06T09:59:52.476Z
        214826715
        732
        2

        4
        489758
        2014-04-06T09:59:52.578Z
        214827026
        1046
        1
```

In [8]:

```
# Filter out item session with length < 2
df['valid_session'] = df.session_id.map(df.groupby('session_id')['item_id'].size() > 2)
df = df.loc[df.valid_session].drop('valid_session',axis=1)
df.nunique()
```

Out[8]:

session_id 1000000 timestamp 5557758 item_id 37644 category 275 dtype: int64

In [9]:

```
# Randomly sample a couple of them
NUM_SESSIONS = 50000 #@param { type: "integer" }
sampled_session_id = np.random.choice(df.session_id.unique(), NUM_SESSIONS, replace=False)
df = df.loc[df.session_id.isin(sampled_session_id)]
df.nunique()
```

Out[9]:

session_id 50000 timestamp 279522 item_id 18732 category 103 dtype: int64

In [10]:

```
# Average length of session
df.groupby('session_id')['item_id'].size().mean()
```

Out[10]:

5.5907

In [11]:

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

Out[11]:

	session_id	timestamp	item_id	category
27	26	2014-04-06T16:42:55.741Z	3639	0
28	26	2014-04-06T16:44:58.482Z	11053	0
29	26	2014-04-06T16:45:11.344Z	7533	0
30	26	2014-04-06T16:46:19.569Z	4866	0
105	187	2014-04-02T18:05:22.418Z	2395	0

In [12]:

```
# Encode item and category id in purchase dataset
buy_df = buy_df.loc[buy_df.session_id.isin(df.session_id)]
buy_df['item_id'] = item_encoder.transform(buy_df.item_id)
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#returning-a-view-versus-a-copy
This is separate from the ipykernel package so we can avoid doing imports until
```

Out[12]:

		session_id	timestamp	item_id	price	quantity
	0	420374	2014-04-06T18:44:58.314Z	1193	12462	1
	1	420374	2014-04-06T18:44:58.325Z	1186	10471	1
	57	396	2014-04-06T17:53:45.147Z	13004	523	1
	105	351689	2014-04-03T07:29:02.313Z	12598	2092	1
	141	420229	2014-04-02T18:51:54.172Z	14742	1883	2

In [13]:

```
# Get item dictionary with grouping by session
buy_item_dict = dict(buy_df.groupby('session_id')['item_id'].apply(list))
buy_item_dict
```

Out[13]:

```
{396: [13004],
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2432049: [15984, 11763],
2433002: [14351, 18731, 3930],
...}
```

Сборка выборки для обучения

In [14]:

```
# Transform of into tensor data
def transform_dataset(df, buy_item_dict):
   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
       #get input features
       node_features = group.loc[group.session_id==session_id,
                                    ['sess item id','item id','category']].sort values('sess item id')[
['item id', 'category']].drop duplicates().values
       node_features = torch.LongTensor(node_features).unsqueeze(1)
       target nodes = group.sess item id.values[1:]
       source_nodes = group.sess_item_id.values[:-1]
       edge index = torch.tensor([source nodes,
                                target_nodes], dtype=torch.long)
       x = node features
        #get result
       if session_id in buy_item_dict:
            positive indices = le.transform(buy item dict[session id])
            label = np.zeros(len(node features))
           label[positive indices] = 1
       else:
           label = [0] * len(node_features)
       y = torch.FloatTensor(label)
       data = Data(x=x, edge_index=edge_index, y=y)
       data list.append(data)
   return data list
# Pytorch class for creating datasets
class YooChooseDataset(InMemoryDataset):
   def init (self, root, transform=None, pre transform=None):
       super(YooChooseDataset, self). init (root, transform, pre transform)
       self.data, self.slices = torch.load(self.processed_paths[0])
   def raw file names(self):
       return []
   @property
   def processed file names(self):
        return [BASE DIR+'yoochoose click binary 100000 sess.dataset']
   def download(self):
       pass
```

```
def process(self):
    data list = transform dataset(df, buy item dict)
    data, slices = self.collate(data_list)
    torch.save((data, slices), self.processed paths[0])
```

In [15]:

```
# Prepare dataset
dataset = YooChooseDataset('./')
Processing...
               | 0/50000 [00:00<?, ?it/s]/usr/local/lib/python3.7/dist-packages/ipykernel launcher.py:2
 0% [
1: UserWarning: Creating a tensor from a list of numpy.ndarrays is extremely slow. Please consider conv
erting the list to a single numpy.ndarray with numpy.array() before converting to a tensor. (Triggered
internally at _../torch/csrc/utils/tensor_new.cpp:210.)
100%|
              | 50000/50000 [02:56<00:00, 283.83it/s]
Done!
```

Разделение выборки

In [16]:

```
# train_test_split
dataset = dataset.shuffle()
one tenth length = int(len(dataset) * 0.1)
train_dataset = dataset[:one_tenth_length * 8]
val dataset = dataset[one tenth length*8:one tenth length * 9]
test dataset = dataset[one tenth length*9:]
len(train_dataset), len(val_dataset), len(test_dataset)
```

Out[16]:

(40000, 5000, 5000)

In [17]:

```
# Load dataset into PyG loaders
batch size= 512
train loader = DataLoader(train dataset, batch size=batch size)
val loader = DataLoader(val dataset, batch size=batch size)
test loader = DataLoader(test dataset, batch size=batch size)
/usr/local/lib/python3.7/dist-packages/torch geometric/deprecation.py:12: UserWarning: 'data.DataLoader
' is deprecated, use 'loader.DataLoader' instead
 warnings.warn(out)
```

In [18]:

```
# Load dataset into PyG loaders
num items = df.item id.max() +1
num_categories = df.category.max()+1
num items , num categories
```

Out[18]:

(18732, 102)

Настройка модели для обучения

In [19]:

```
embed dim = 128
```

```
trom torcn_geometric.nn import GraphConv, TopkPooling, GatedGraphConv, SAGECOnv, SGCOnv
from torch geometric.nn import global mean pool as gap, global max pool as gmp
import torch.nn.functional as F
class Net(torch.nn.Module):
   def init (self):
       super(Net, self). init ()
       # Model Structure
       self.conv1 = GraphConv(embed dim * 2, 128)
       self.pool1 = TopKPooling(128, ratio=0.9)
       self.conv2 = GraphConv(128, 128)
       self.pool2 = TopKPooling(128, ratio=0.9)
       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)
       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)
       self.act1 = torch.nn.ReLU()
       self.act2 = torch.nn.ReLU()
    # Forward step of a model
   def forward(self, data):
       x, edge_index, batch = data.x, data.edge_index, data.batch
       item id = x[:,:,0]
       category = x[:,:,1]
       emb item = self.item embedding(item id).squeeze(1)
       emb category = self.category embedding(category).squeeze(1)
       x = torch.cat([emb item, emb category], dim=1)
       # print(x.shape)
       x = F.relu(self.convl(x, edge index))
       # print(x.shape)
       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)
       x = F.relu(self.conv2(x, edge_index))
       x, edge_index, _, batch, _, _ = self.pool2(x, edge_index, None, batch)
       x2 = torch.cat([gmp(x, batch), gap(x, batch)], dim=1)
       x = F.relu(self.conv3(x, edge index))
       x, edge_index, _, batch, _, _ = self.pool3(x, edge_index, None, batch)
       x3 = torch.cat([gmp(x, batch), gap(x, batch)], dim=1)
       x = x1 + x2 + x3
       x = self.lin1(x)
       x = self.act1(x)
       x = self.lin2(x)
       x = F.dropout(x, p=0.5, training=self.training)
       x = self.act2(x)
       outputs = []
       for i in range(x.size(0)):
            output = torch.matmul(emb item[data.batch == i], x[i,:])
           outputs.append(output)
       x = torch.cat(outputs, dim=0)
       x = torch.sigmoid(x)
       return x
```

In [20]:

```
# Enable CUDA computing
device = torch.device('cuda')
model = Net().to(device)
# Choose optimizer and criterion for learning
optimizer = torch.optim.Adam(model.parameters(), lr=0.001)
crit = torch.nn.BCELoss()
```

In [21]:

```
# Train function
def train():
    model.train()

loss_all = 0
    for data in train_loader:
        data = data.to(device)
        optimizer.zero_grad()
        output = model(data)

label = data.y.to(device)
    loss = crit(output, label)
    loss.backward()
    loss_all += data.num_graphs * loss.item()
        optimizer.step()

return loss_all / len(train_dataset)
```

In [22]:

```
# Evaluate result of a model
from sklearn.metrics import roc auc score
def evaluate(loader):
   model.eval()
    predictions = []
    labels = []
    with torch.no_grad():
       for data in loader:
            data = data.to(device)
            pred = model(data).detach().cpu().numpy()
            label = data.y.detach().cpu().numpy()
            predictions.append(pred)
            labels.append(label)
    predictions = np.hstack(predictions)
    labels = np.hstack(labels)
    return roc auc score (labels, predictions)
```

In [23]:

Epoch: 000, Loss: 0.67669, Train Auc: 0.52441, Val Auc: 0.53001, Test Auc: 0.52498

```
13%| | 2/15 [01:17<08:19, 38.46s/it]
Epoch: 001, Loss: 0.48399, Train Auc: 0.56859, Val Auc: 0.55746, Test Auc: 0.55136
20%| | 3/15 [01:54<07:34, 37.86s/it]
Epoch: 002, Loss: 0.40272, Train Auc: 0.60059, Val Auc: 0.56321, Test Auc: 0.56091
27%| | 4/15 [02:31<06:54, 37.64s/it]
Epoch: 003, Loss: 0.36485, Train Auc: 0.62781, Val Auc: 0.57539, Test Auc: 0.57249
33%| | 5/15 [03:08<06:12, 37.27s/it]
Epoch: 004, Loss: 0.34037, Train Auc: 0.65900, Val Auc: 0.58490, Test Auc: 0.59073
40%| | 6/15 [03:44<05:32, 36.99s/it]
Epoch: 005, Loss: 0.32349, Train Auc: 0.68062, Val Auc: 0.58279, Test Auc: 0.58951
47%| | 7/15 [04:21<04:54, 36.75s/it]
Epoch: 006, Loss: 0.31069, Train Auc: 0.71464, Val Auc: 0.59796, Test Auc: 0.59507
53%| | 8/15 [04:57<04:15, 36.54s/it]
Epoch: 007, Loss: 0.29609, Train Auc: 0.73714, Val Auc: 0.60001, Test Auc: 0.60194
60%| 9/15 [05:33<03:37, 36.32s/it]
Epoch: 008, Loss: 0.28586, Train Auc: 0.77141, Val Auc: 0.60433, Test Auc: 0.61670
67%| | 10/15 [06:09<03:01, 36.22s/it]
Epoch: 009, Loss: 0.27251, Train Auc: 0.78842, Val Auc: 0.61848, Test Auc: 0.62342
73%| | 11/15 [06:45<02:24, 36.18s/it]
Epoch: 010, Loss: 0.26538, Train Auc: 0.82290, Val Auc: 0.61437, Test Auc: 0.61963
80%| | 12/15 [07:21<01:48, 36.14s/it]
Epoch: 011, Loss: 0.24979, Train Auc: 0.85696, Val Auc: 0.61783, Test Auc: 0.62906
87%| | 13/15 [07:57<01:12, 36.06s/it]
Epoch: 012, Loss: 0.23585, Train Auc: 0.87090, Val Auc: 0.61519, Test Auc: 0.63079
93%| | 14/15 [08:33<00:35, 36.00s/it]
Epoch: 013, Loss: 0.22456, Train Auc: 0.89360, Val Auc: 0.61035, Test Auc: 0.62640
```

```
| 15/15 [09:09<00:00, 36.63s/it]
```

```
Epoch: 014, Loss: 0.20975, Train Auc: 0.91882, Val Auc: 0.61920, Test Auc: 0.63559
```

Проверка результата с помощью примеров

```
In [24]:
```

```
# Подход №1 - из датасета
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)
```

Out[24]:

0.5656565656565656

```
In [25]:
# Подход №2 - через создание сессии покупок
test_df = pd.DataFrame([
      [-1, 15219, 0],
      [-1, 15431, 0],
      [-1, 14371, 0],
      [-1, 15745, 0],
      [-2, 14594, 0],
      [-2, 16972, 11],
      [-2, 16943, 0],
      [-3, 17284, 0]
], columns=['session id', 'item id', 'category'])
test data = transform dataset(test df, buy item dict)
test_data = DataLoader(test_data, batch_size=1)
with torch.no grad():
   model.eval()
    for data in test_data:
        data = data.to(device)
        pred = model(data).detach().cpu().numpy()
        print (data, pred)
100%| 3/3 [00:00<00:00, 199.34it/s]
DataBatch(x=[3, 1, 2], edge_index=[2, 2], y=[3], batch=[3], ptr=[2]) [0.000564  0.01551606 0.07247568] DataBatch(x=[4, 1, 2], edge_index=[2, 3], y=[4], batch=[4], ptr=[2]) [2.5984054e-05 1.0836762e-06 1.749
2797e-06 3.5187886e-06]
```

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