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ФАКУЛЬТЕТ ____Информатика, искусственный интеллект и системы управления ___

КАФЕДРА _____Системы обработки информации и управления_____

ОТЧЁТ
К ЛАБОРАТОРНОЙ РАБОТЕ №6

НА ТЕМУ:
Разработка системы предсказания поведения на основании графовых моделей

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Группа: ИУ5-23М

Преподаватель: Гапанюк Ю.Е.

2022 г.

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

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

Лабораторная работа №6:

"Разработка системы предсказания поведения на основании графовых моделей"

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

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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-c0RwVOKreMrZ3bfSmCwl2y-?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 [5]:
```
import torch
print(torch.__version__)
```

```
1.11.0+cu113
```

In [7]:
```
# Install pytorch geometric
!pip install gdown
!pip install torch
!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
```

```
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/public/simple/
Requirement already satisfied: gdown in /usr/local/lib/python3.7/dist-packages (4.4.0)
Requirement already satisfied: six in /usr/local/lib/python3.7/dist-packages (from gdown) (1.15.0)
Requirement already satisfied: requests[socks] in /usr/local/lib/python3.7/dist-packages (from gdown) (2.23.0)
Requirement already satisfied: tqdm in /usr/local/lib/python3.7/dist-packages (from gdown) (4.64.0)
Requirement already satisfied: filelock in /usr/local/lib/python3.7/dist-packages (from gdown) (3.7.0)
Requirement already satisfied: beautifulsoup4 in /usr/local/lib/python3.7/dist-packages (from gdown) (4.6.3)
Requirement already satisfied: idna<3,>=2.5 in /usr/local/lib/python3.7/dist-packages (from requests[socks]->gdown) (2.10)
Requirement already satisfied: chardet<4,>=3.0.2 in /usr/local/lib/python3.7/dist-packages (from requests[socks]->gdown) (3.0.4)
Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3.7/dist-packages (from requests[socks]->gdown) (2022.5.18.1)
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[socks]->gdown) (1.24.3)
Requirement already satisfied: PySocks!=1.5.7,>=1.5.6 in /usr/local/lib/python3.7/dist-packages (from requests[socks]->gdown) (1.7.1)
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/public/simple/
Requirement already satisfied: torch in /usr/local/lib/python3.7/dist-packages (1.11.0+cu113)
Requirement already satisfied: typing-extensions in /usr/local/lib/python3.7/dist-packages (from torch) (4.2.0)
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-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) (1.4.1)
Requirement already satisfied: numpy>=1.13.3 in /usr/local/lib/python3.7/dist-packages (from scipy->torch-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: pyparsing in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (3.0.9)
Requirement already satisfied: pandas in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (1.3.5)
Requirement already satisfied: requests in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (2.23.0)
Requirement already satisfied: tqdm in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (4.64.0)
Requirement already satisfied: scipy in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (1.4.1)
Requirement already satisfied: scikit-learn in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (1.0.2)
Requirement already satisfied: jinja2 in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (2.11.3)
Requirement already satisfied: numpy in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (1.21.6)
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 pandas->torch-geometric) (2.8.2)
Requirement already satisfied: pytz>=2017.3 in /usr/local/lib/python3.7/dist-packages (from pandas->torch-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: chardet<4,>=3.0.2 in /usr/local/lib/python3.7/dist-packages (from requests->torch-geometric) (3.0.4)
Requirement already satisfied: idna<3,>=2.5 in /usr/local/lib/python3.7/dist-packages (from requests->torch-geometric) (2.10)
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)
Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3.7/dist-packages (from requests->torch-geometric) (2022.5.18.1)
Requirement already satisfied: joblib>=0.11 in /usr/local/lib/python3.7/dist-packages (from scikit-learn->torch-geometric) (1.1.0)
Requirement already satisfied: threadpoolctl>=2.0.0 in /usr/local/lib/python3.7/dist-packages (from scikit-learn->torch-geometric) (3.1.0)
```

In [8]:
```
!pip install torch-scatter -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://data.pyg.org/whl/torch-1.11.0%2Bcu113.html
Collecting torch-scatter
  Downloading https://data.pyg.org/whl/torch-1.11.0%2Bcu113/torch_scatter-2.0.9-cp37-cp37m-linux_x86_64.whl (7.9 MB)
     |████████████████████████████████████████| 7.9 MB 53.1 MB/s
Installing collected packages: torch-scatter
Successfully installed torch-scatter-2.0.9
```

In [9]:
```
import numpy as np
import pandas as pd
import pickle
import csv
import os

from sklearn.preprocessing import LabelEncoder

import torch

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

from tqdm import tqdm


RANDOM_SEED = 42 #@param { type: "integer" }
BASE_DIR = '/content/' #@param { type: "string" }
np.random.seed(RANDOM_SEED)
```

In [11]:
```
# Check if CUDA is available for colab
torch.cuda.is_available
```

```
Out[11]:<function torch.cuda.is_available>
```

In [12]:
```
!gdown --id 1ebYsQlb6PRQMOE7Cnx1CwWVFDNJkYuzR
```

```
/usr/local/lib/python3.7/dist-packages/gdown/cli.py:131: FutureWarning: Option `--id` was deprecated in version 4.3.1 and will be removed in 5.0. You don't ne
ed to pass it anymore to use a file ID.
  category=FutureWarning,
Downloading...
From: https://drive.google.com/uc?id=1ebYsQlb6PRQMOE7Cnx1CwWVFDNJkYuzR
To: /content/yoochoose-data-lite.zip
100% 49.8M/49.8M [00:01<00:00, 35.2MB/s]
```

In [13]:
```
# Unpack files from zip-file
import zipfile
with zipfile.ZipFile(BASE_DIR + 'yoochoose-data-lite.zip', 'r') as zip_ref:
    zip_ref.extractall(BASE_DIR)
```

Анализ исходных данных

In [14]:
```
# Read dataset of items in store
df = pd.read_csv(BASE_DIR + 'yoochoose-clicks-lite.dat')
# df.columns = ['session_id', 'timestamp', 'item_id', 'category']
df.head()
```

```
/usr/local/lib/python3.7/dist-packages/IPython/core/interactiveshell.py:2882: DtypeWarning: Columns (3) have mixed types.Specify dtype option on import or s
et low_memory=False.
  exec(code_obj, self.user_global_ns, self.user_ns)
```

Out[14]:

	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 [15]:
```
# 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[15]:

	session_id	timestamp	item_id	price	quantity
0	420374	2014-04-06T18:44:58.314Z	214537888	12462	1
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 [16]:
```
# 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[16]:
```
session_id    1000000
timestamp     5557758
item_id         37644
category          275
dtype: int64
```

In [17]:
```
# 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[17]:
```
session_id     50000
timestamp     278442
item_id        18461
category         110
dtype: int64
```

In [18]:
```
# Average length of session
df.groupby('session_id')['item_id'].size().mean()
```

Out[18]:
```
5.56902
```

In [19]:
```
# 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[19]:

	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

In [20]:
```
# 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[20]:

	session_id	timestamp	item_id	price	quantity
46	489491	2014-04-06T12:41:34.047Z	12633	1046	4
47	489491	2014-04-06T12:41:34.091Z	12634	627	2
61	70353	2014-04-06T10:55:06.086Z	14345	41783	1
62	489671	2014-04-03T15:48:37.392Z	12489	4188	1
63	489671	2014-04-03T15:59:35.495Z	12489	4188	1

In [21]:
```
# Get item dictionary with grouping by session
buy_item_dict = dict(buy_df.groupby('session_id')['item_id'].apply(list))
buy_item_dict
```

Out[21]:
```
{714: [14720, 14915, 14917, 3089],
 6016: [15154],
 9797: [12459, 11831],
 9862: [13621],
 10457: [10079, 2951],
 10587: [11764],
 10678: [6310, 3914],
 13476: [13631, 12881, 12878, 12880, 12852],
 16953: [2883, 7739],
 19029: [8276, 2171, 10385, 11419],
 19958: [10059, 10059],
 23548: [11236],
 24439: [12506, 12497],
 28709: [4037],
 29647: [12830, 12827],
 33907: [2480, 6012],
 34541: [627, 12827],
 36548: [14720, 14916],
 38019: [11222, 11227],
 38261: [3447],
 41333: [11839, 12826, 11839],
 41598: [10712, 10711, 2034, 10713],
 43834: [11203, 11203],
 44153: [15075, 15088],
 44813: [12819, 12634],
 48974: [7428, 12774],
 49886: [2373, 11207, 11221, 10625],
 54961: [1965, 11360, 12812, 7803],
 55877: [4804],
 62553: [12793],
 64802: [11317],
 69277: [7933],
 70353: [14345],
 71832: [11839, 12362],
 73271: [11236, 11236, 11237],
 74083: [12864],
 79937: [11884, 11825, 11825, 11884],
 87673: [12608],
 88198: [11201, 11201],
 88723: [11236, 11236],
 89393: [11236],
 91903: [11200],
 92224: [255],
 93282: [14842,
  5737,
  5733,
  421,
  4275,
```

4489,
7043,
7047,
5739,
4498,
7048,
4508,
7140,
2065,
2071,
2066],
100952: [9849, 9849],
103133: [11228],
104659: [11424, 4839, 8471],
108344: [13479, 11221, 11208],
110788: [1187],
114461: [2376, 12826],
116004: [9730],
116373: [9868],
122179: [316],
125163: [3548, 5766],
126769: [3318, 12770, 12769],
127311: [12831, 12552, 12846, 12342, 12772, 12773],
128359: [4483],
128562: [11476, 12787, 12812, 12552],
132646: [5654],
136192: [12880, 12852, 12878],
138344: [4827],
142132: [627, 12767],
142902: [11226, 11226],
143246: [4791],
144241: [12632],
150664: [12825, 11333, 13046, 12839, 10484],
150723: [12621, 13444, 12619, 4145],
150926: [12812, 12787, 12813],
152571: [3943],
157247: [8285],
160843: [11792],
164104: [12839, 12825, 12616, 9932],
169179: [10715, 10714],
171209: [12789],
171554: [15058],
172101: [11469, 8711, 8721, 12629],
172324: [14720, 14915, 14917, 14916],
175289: [12634],
175897: [11223],
177247: [12634, 12632],
177641: [2248],
182148: [13793, 12367],
185409: [11200],
187838: [3409],
188339: [12630, 12788],
188726: [11605],
189138: [12812, 12787],
192869: [12766],
193483: [6333],
197056: [13481, 13481, 13481],
197889: [12557],
198147: [11221],
198939: [12557],
201316: [12360],
202037: [13479, 11227, 11202],
203623: [8253],
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214007: [12632],
218862: [15058],
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221904: [6044, 7972, 12619],
222178: [9269],
222293: [12881, 12852, 12880, 13631, 11658, 12878],
223497: [12571, 12549, 7670, 12674, 7697, 12548, 12550, 8303, 12625, 8306],
224769: [3914],
224788: [4483],
227657: [11226, 10534, 11249],
229858: [14618, 576],
232349: [179, 4804],
232521: [12321, 12321],
239123: [12677, 12632],
239224: [4901, 4901],
241053: [12813, 15582, 15554, 15560, 15249, 15446],
242477: [12789, 12634, 1032, 12632],

242477: [12789, 12554, 1052, 12552],
242636: [390],
243838: [14989, 13981],
245392: [7934, 10052, 12793],
245427: [4484],
245733: [12417, 12770, 12630],
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248291: [11203, 11222],
249438: [15015],
251596: [12374],
251777: [1835],
256753: [11206],
257992: [446, 11372, 12489, 9358],
259584: [15304, 15303, 15064],
260656: [16],
270696: [7436, 1105, 7436, 1105],
272839: [10292],
276266: [9791],
277534: [11521, 12832, 337],
283099: [15058],
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287659: [8278],
291433: [13666, 12620, 12618, 2971],
294559: [8190],
295229: [8293, 7924, 7908, 6489, 12548, 11740, 12550, 12832, 7919],
295338: [12601],
295684: [12766, 10480, 12443, 627, 12830],
297264: [12789, 12811, 12788],
298599: [12793, 7576],
299953: [8681, 8820, 8785, 8791, 15101, 8820, 8681, 8785, 8791, 15101],
300253: [1187],
301426: [191, 12788],
302057: [11202, 11202],
304968: [3702, 1158, 231],
305804: [11222],
308539: [12619, 12388, 12677, 12393],
314311: [9716, 1746, 11236, 11236],
318261: [15058],
319517: [12500, 12825, 12986, 8303],
320068: [14174],
321967: [12888, 10038],
333733: [12864, 12776, 10998],
336051: [14946, 14944],
337309: [12864, 12766],
341142: [2373, 12767, 12819],
345242: [10049, 10059],
349007: [12497, 12506],
350491: [12633, 11839],
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...}
```

Сборка выборки для обучения

In [22]:
```
# Transform df 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])

        @property
        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 [23]:
```
# Prepare dataset
dataset = YooChooseDataset('./')
```

```
Processing...
  0%|          | 0/50000 [00:00<?, ?it/s]/usr/local/lib/python3.7/dist-packages/ipykernel_launcher.py:21: UserWarning: Creating a tensor from a list of numpy.nda
rrays is extremely slow. Please consider converting the list to a single numpy.ndarray with numpy.array() before converting to a tensor. (Triggered internally a
t  ../torch/csrc/utils/tensor_new.cpp:210.)
100%|██████████████████| 50000/50000 [02:51<00:00, 292.20it/s]
Done!
```

Разделение выборки

In [24]:
```
# 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[24]:(40000, 5000, 5000)

In [25]:
```
# 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 [26]:
```
# Load dataset into PyG loaders
num_items = df.item_id.max() +1
num_categories = df.category.max()+1
num_items , num_categories
```

Out[26]:(18461, 109)

Настройка модели для обучения

In [27]:
```
embed_dim = 128
from torch_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.conv1(x, edge_index))
        # print(x.shape)
        r = self.pool1(x, edge_index, None, batch)
        # print(r)
        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
```

Обучение нейронной сверточной сети

In [28]:
```
# 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 [29]:
```
# 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 [30]:
```
# 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 [35]:
```
# Train a model
NUM_EPOCHS =  10#@param { type: "integer" }
for epoch in tqdm(range(NUM_EPOCHS)):
    loss = train()
    train_acc = evaluate(train_loader)
    val_acc = evaluate(val_loader)
    test_acc = evaluate(test_loader)
    print('Epoch: {:03d}, Loss: {:.5f}, Train Auc: {:.5f}, Val Auc: {:.5f}, Test Auc: {:.5f}'.
          format(epoch, loss, train_acc, val_acc, test_acc))
```

```
 10%|         | 1/10 [00:35<05:23, 35.93s/it]
Epoch: 000, Loss: 0.24028, Train Auc: 0.84039, Val Auc: 0.62623, Test Auc: 0.59887
 20%|         | 2/10 [01:11<04:47, 35.98s/it]
Epoch: 001, Loss: 0.22922, Train Auc: 0.86706, Val Auc: 0.63198, Test Auc: 0.60424
 30%|         | 3/10 [01:47<04:10, 35.80s/it]
Epoch: 002, Loss: 0.21912, Train Auc: 0.88446, Val Auc: 0.63376, Test Auc: 0.60278
 40%|         | 4/10 [02:23<03:34, 35.78s/it]
Epoch: 003, Loss: 0.21538, Train Auc: 0.87072, Val Auc: 0.63450, Test Auc: 0.60192
 50%|         | 5/10 [02:58<02:58, 35.71s/it]
Epoch: 004, Loss: 0.21220, Train Auc: 0.88758, Val Auc: 0.63205, Test Auc: 0.60194
 60%|         | 6/10 [03:34<02:22, 35.71s/it]
Epoch: 005, Loss: 0.20281, Train Auc: 0.92588, Val Auc: 0.63424, Test Auc: 0.60568
 70%|         | 7/10 [04:10<01:47, 35.70s/it]
Epoch: 006, Loss: 0.19073, Train Auc: 0.94636, Val Auc: 0.63971, Test Auc: 0.61654
 80%|         | 8/10 [04:45<01:11, 35.67s/it]
Epoch: 007, Loss: 0.18077, Train Auc: 0.94925, Val Auc: 0.64910, Test Auc: 0.62152
 90%|         | 9/10 [05:21<00:35, 35.78s/it]
Epoch: 008, Loss: 0.17200, Train Auc: 0.95785, Val Auc: 0.64362, Test Auc: 0.61380
100%|         | 10/10 [05:57<00:00, 35.75s/it]
Epoch: 009, Loss: 0.16390, Train Auc: 0.96162, Val Auc: 0.64302, Test Auc: 0.61275
```

Проверка результата с помощью примеров

In [32]:
```
# 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[32]:0.4247311827956989

In [33]:
```
# 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, 179.58it/s]
DataBatch(x=[1, 1, 2], edge_index=[2, 0], y=[1], batch=[1], ptr=[2]) [0.00837703]
DataBatch(x=[3, 1, 2], edge_index=[2, 2], y=[3], batch=[3], ptr=[2]) [0.15967393 0.04956234 0.3698206 ]
DataBatch(x=[4, 1, 2], edge_index=[2, 3], y=[4], batch=[4], ptr=[2]) [0.04389836 0.04406342 0.19375472 0.03810767]
/usr/local/lib/python3.7/dist-packages/torch_geometric/deprecation.py:12: UserWarning: 'data.DataLoader' is deprecated, use 'loader.DataLoader' instead
  warnings.warn(out)
```