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Факультет «Информатика и системы управления»
Кафедра «Системы обработки информации и управления»



Лабораторная работа №6
«Разработка системы предсказаний поведения на основании
графовых моделей»

по дисциплине
«Методы машинного обучения»

ИСПОЛНИТЕЛЬ:

Крюков Г.М.
Группа ИУ5-21М

"__" 2022 г.

Москва, 2022

Цель: 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

Набор данных:

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>).

Текст программы

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ЛР6_Крюков_Г_М_ИУ5_21M.ipynb - Colaboratory

▼ 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 применением 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

https://colab.research.google.com/drive/1vnZ9_Emweps8yUlyP9R4fbOHbL5Q7PNR

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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 импортировать его в колаб

▼ Установка библиотек, выгрузка исходных датасетов

```
# 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==2.0.9 -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
Collecting torch-sparse
  Downloading https://data.pyg.org/whl/torch-1.11.0%2Bcu113/torch\_sparse-0.6.13-cp37m-linux\_x86\_64.whl (3.5 MB)
[██████████] | 3.5 MB 1.3 MB/s
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
Installing collected packages: torch-sparse
Successfully installed torch-sparse-0.6.13
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
Collecting torch-cluster
  Downloading https://data.pyg.org/whl/torch-1.11.0%2Bcu113/torch\_cluster-1.6.0-cp37m-linux\_x86\_64.whl (2.5 MB)
[██████████] | 2.5 MB 26.3 MB/s
Installing collected packages: torch-cluster
```

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```

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Successfully installed torch-cluster-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
Collecting torch-spline-conv
  Downloading https://data.pyg.org/whl/torch-1.11.0%2Bcu113/torch\_spline\_conv-1.2.1-cp37-cp37m-linux\_x86\_64.whl (750 kB)
    [██████████] 750 kB 23.7 MB/s
Installing collected packages: torch-spline-conv
Successfully installed torch-spline-conv-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
Collecting torch-geometric
  Downloading torch_geometric-2.0.4.tar.gz (407 kB)
    [██████████] 407 kB 25.7 MB/s
Requirement already satisfied: tqdm in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (4.64.0)
Requirement already satisfied: numpy in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (1.21.6)
Requirement already satisfied: scipy in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (1.4.1)
Requirement already satisfied: pandas in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (1.3.5)
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: pyparsing in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (3.0.9)
Requirement already satisfied: scikit-learn in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (1.0.2)
Requirement already satisfied: MarkupSafe==0.23 in /usr/local/lib/python3.7/dist-packages (from jinja2->torch-geometric)
Requirement already satisfied: pytz==2017.3 in /usr/local/lib/python3.7/dist-packages (from pandas->torch-geometric)
Requirement already satisfied: python-dateutil>=2.7.3 in /usr/local/lib/python3.7/dist-packages (from pandas->torch-geometric)
Requirement already satisfied: six>1.5 in /usr/local/lib/python3.7/dist-packages (from python-dateutil)>=2.7.3->pand
Requirement already satisfied: urllib3!=1.25.0,>1.25.1 in /usr/local/lib/python3.7/dist-packages (from certifi->2017.4.17 in /usr/local/lib/python3.7/dist-packages (from requests->torch-geometric))
Requirement already satisfied: chardet<4,>=3.0.2 in /usr/local/lib/python3.7/dist-packages (from requests->torch-geometric)
Requirement already satisfied: idna>3,>=2.5 in /usr/local/lib/python3.7/dist-packages (from requests->torch-geometric)
Requirement already satisfied: joblib=>0.11 in /usr/local/lib/python3.7/dist-packages (from scikit-learn->torch-geometric)
Requirement already satisfied: threadpoolctl>=2.0.0 in /usr/local/lib/python3.7/dist-packages (from scikit-learn->torch-geometric)
Building wheels for collected packages: torch-geometric
  Building wheel for torch-geometric (setup.py) ... done
  Created wheel for torch-geometric: filename=torch_geometric-2.0.4-py3-none-any.whl size=616603 sha256=0eaf2157f99f
  Stored in directory: /root/.cache/pip/wheels/18/a6/a4/ca18c3051fcead866fe7b85700ee2240d883562a1bc70ce421
Successfully built torch-geometric
Installing collected packages: torch-geometric
Successfully installed torch-geometric-2.0.4
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==2.0.9

```

https://colab.research.google.com/drive/1vnZ9_Emweps8yUlyP9R4fbOHbL5Q7PNR 3/17

```

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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 = 17 #@param { type: "integer" }
BASE_DIR = '/content' #@param { type: "string" }
np.random.seed(RANDOM_SEED)

# Check if CUDA is available for colab
torch.cuda.is_available()

<function torch.cuda.is_available>

# Unpack files from zip-file
import zipfile
with zipfile.ZipFile(BASE_DIR + 'yochoose-data-lite.zip', 'r') as zip_ref:
    zip_ref.extractall(BASE_DIR)

```

▼ Анализ исходных данных

```

# Read dataset of items in store
df = pd.read_csv(BASE_DIR + 'yochoose-clicks-lite.dat')
https://colab.research.google.com/drive/1vnZ9_Emweps8yUlyP9R4fbOHbL5Q7PNR 4/17

```

```

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# 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 type
exec(code_obj, self.user_global_ns, self.user_ns)



|   | 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        |


```

```

# 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()



|   | 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        |


```

```

# 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()

```

https://colab.research.google.com/drive/1vnZ9_Emweps8yUlyP9R4fbOHbL5Q7PNR

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```

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session_id      1000000
timestamp       5557758
item_id         37644
category        275
dtype: int64

# Randomly sample a couple of them
NUM_SESSIONS = 60000 #@param { type: "integer" }                               NUM_SESSIONS: 60000
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()



| session_id | timestamp | item_id | category |
|------------|-----------|---------|----------|
| 60000      | 334990    | 20043   | 103      |


```

```

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

5.5834166666666665

# 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()

```

https://colab.research.google.com/drive/1vnZ9_Emweps8yUlyP9R4fbOHbL5Q7PNR

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```
session_id      timestamp item_id category
91            131 2014-04-03T04:46:08.891Z    13649      0

# 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
This is separate from the ipykernel package so we can avoid doing imports until

session_id      timestamp item_id price quantity
5            70427 2014-04-02T15:54:07.144Z   13729    3769      1
25           140964 2014-04-04T07:02:02.655Z   10268    2408      1
62           489671 2014-04-03T15:48:37.392Z   13710    4188      1
63           489671 2014-04-03T15:59:35.495Z   13710    4188      1
64           489671 2014-04-03T16:00:06.917Z   13710    4188      1

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

{714: [16129, 16324, 16326, 3323],
 3517: [11939, 13381],
 4832: [12191, 12191, 12191],
 5002: [12217],
 5942: [16913, 14322, 14040, 14040, 14040, 14040, 14322, 16913],
 7054: [14021],
 7173: [13549],
 8628: [280, 281],
 9292: [13783, 4280],
```

https://colab.research.google.com/drive/1vnZ9_Emweps8yUlyP9R4fbOHbL5Q7PNR

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```
9782: [15763, 15756, 14250, 3096, 9004, 13708, 11207, 14092],
10879: [2311, 2362],
12017: [5219],
12282: [13864,
 13866,
 13862,
 9463,
 13866,
 13864,
 13862,
 9463,
 13866,
 13864,
 13862,
 13862,
 9463,
 13073: [12213, 12213],
 14227: [11645, 11646],
 14314: [12227, 13658, 13585, 13773],
 16053: [4365, 13874, 13872],
 16946: [8864],
 19576: [13862, 13862],
 21812: [1049],
 23934: [14142],
 24703: [14079, 14079],
 28668: [14065],
 35699: [1758],
 38117: [8306,
 12079,
 13907,
 13907,
 13618,
 13775,
 13775,
 13625,
 13625,
 12959,
 12960,
 14764],
 39247: [13862, 13866],
 40176: [4277],
 40209: [15763, 15762, 15756, 10293],
 40717: [15058],
```

https://colab.research.google.com/drive/1vnZ9_Emweps8yUlyP9R4fbOHbL5Q7PNR

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```
40827: [16129, 16129],
42536: [14840, 14322],
44097: [13520],
44714: [1468, 13523, 14321, 13523],
45836: [10705],
46132: [14021, 2584],  
.....
```

▼ Сборка выборки для обучения

```
# 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']]
        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
```

https://colab.research.google.com/drive/1vnZ9_Emweps8yUlyP9R4fbOHbL5Q7PNR 9/17

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```
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])

    # Prepare dataset
dataset = YooChooseDataset('./')
```

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Processing...
0%|██████████| 0/60000 [00:00<?, ?it/s]/usr/local/lib/python3.7/dist-packages/ipykernel_launcher.py:21: UserWarning:
100%|██████████| 60000/60000 [03:23<00:00, 294.14it/s]
Done!

▼ Разделение выборки

```
# 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)

(48000, 6000, 6000)

# 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,
warnings.warn(out)

# Load dataset into PyG loaders
num_items = df.item_id.max() +1
num_categories = df.category.max()+1
num_items , num_categories

(20043, 102)
```

https://colab.research.google.com/drive/1vnZ9_Emweps8yUlyP9R4fbOHbL5Q7PNR

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▼ Настройка модели для обучения

```
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)
```

https://colab.research.google.com/drive/1vnZ9_Emweps8yUlyP9R4fbOHbL5Q7PNR

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```
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
```

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▼ Обучение нейронной сверточной сети

```
# Enable CUDA computing
device = torch.device('cuda')
model = Net().to(device)
# Choose optimizer and criterion for learning
optimizer = torch.optim.Adam(model.parameters(), lr=0.002)
crit = torch.nn.BCELoss()

# 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)

# 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:
```

https://colab.research.google.com/drive/1vnZ9_Emweps8yUlyP9R4fbOHbL5Q7PNR

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```

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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)

# Train a model
NUM_EPOCHS = 12 #@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: {:.3d}, Loss: {:.5f}, Train Auc: {:.5f}, Val Auc: {:.5f}, Test Auc: {:.5f}'.format(epoch, loss, train_acc, val_acc, test_acc))

    8% [██████████| 1/12 [00:48<08:50, 48.23s/it]Epoch: 000, Loss: 0.66438, Train Auc: 0.53963, Val Auc: 0.54502, Test Au
17% [███████████| 2/12 [01:32<07:41, 46.10s/it]Epoch: 001, Loss: 0.49811, Train Auc: 0.58664, Val Auc: 0.57268, Test Au
25% [███████████| 3/12 [02:17<06:48, 45.42s/it]Epoch: 002, Loss: 0.44270, Train Auc: 0.61824, Val Auc: 0.58817, Test Au
33% [███████████| 4/12 [03:02<06:00, 45.08s/it]Epoch: 003, Loss: 0.40889, Train Auc: 0.65620, Val Auc: 0.60315, Test Au
42% [███████████| 5/12 [03:46<05:14, 45.00s/it]Epoch: 004, Loss: 0.38101, Train Auc: 0.69724, Val Auc: 0.62240, Test Au
50% [███████████| 6/12 [04:30<04:28, 44.70s/it]Epoch: 005, Loss: 0.35971, Train Auc: 0.71789, Val Auc: 0.62465, Test Au
58% [███████████| 7/12 [05:15<03:43, 44.64s/it]Epoch: 006, Loss: 0.33764, Train Auc: 0.76569, Val Auc: 0.64367, Test Au
67% [███████████| 8/12 [05:59<02:58, 44.53s/it]Epoch: 007, Loss: 0.32084, Train Auc: 0.79539, Val Auc: 0.64680, Test Au
75% [███████████| 9/12 [06:44<02:13, 44.47s/it]Epoch: 008, Loss: 0.30261, Train Auc: 0.82702, Val Auc: 0.65226, Test Au
83% [███████████| 10/12 [07:28<01:28, 44.37s/it]Epoch: 009, Loss: 0.28681, Train Auc: 0.85143, Val Auc: 0.65794, Test A
92% [███████████| 11/12 [08:12<00:44, 44.46s/it]Epoch: 010, Loss: 0.26965, Train Auc: 0.87717, Val Auc: 0.65435, Test A
100% [███████████| 12/12 [08:56<00:00, 44.75s/it]Epoch: 011, Loss: 0.26058, Train Auc: 0.89207, Val Auc: 0.65470, Test Au

    ↪ ↩
https://colab.research.google.com/drive/1vnZ9_Ermweps8yUlyP9R4fbOHbL5Q7PNR                                         15/17

```

```

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▼ Проверка результата с помощью примеров

# Подход №1 - из датасета
evaluate(DataLoader(test_dataset[25:45], batch_size=10))

/usr/local/lib/python3.7/dist-packages/torch_geometric/deprecation.py:12: UserWarning: 'data.DataLoader' is deprecated,
warnings.warn(out)
0.8218390804597702

    ↪ ↩
# 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, 144.95t/s]DataBatch(x=[1, 1, 2], edge_index=[2, 0], y=[1], batch=[1], ptr=[2]) [0.6
DataBatch(x=[3, 1, 2], edge_index=[2, 2], y=[3], batch=[3], ptr=[2]) [0.05040454 0.01688893 0.01116091]
DataBatch(x=[4, 1, 2], edge_index=[2, 3], y=[4], batch=[4], ptr=[2]) [0.00638917 0.01556076 0.09219604 0.27488992]
https://colab.research.google.com/drive/1vnZ9_Ermweps8yUlyP9R4fbOHbL5Q7PNR                                         16/17

```

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



Как видно из результатов, значение метрики $AUC = 72.5\%$

В ходе работы были изменены следующие гиперпараметры: количество эпох (5->10), скорость обучения (0.001->0.002), количество сессий (50000->60000)

Вывод:

При выполнении работы был подготовлен датасет графовых данных и подобрана модель и гиперпараметры обучения для получения качества $AUC > 0.65$. Удалось добиться значения метрики $AUC = 0.725$.