

▼ Лабораторная работа №6:

Щипицина К.В.

ИУ5-22М

"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. Типичными 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-c0RwVOKreMrZ3bfSmCwl2y-?usp=sharing> (литература 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

```
# 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

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)
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-cp37-cp37m-linux_x86_64.whl (2.5 MB)
    |████████████████████████████████████████| 2.5 MB 26.1 MB/s
Installing collected packages: torch-cluster
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
```


▼ Анализ исходных данных

```
# 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.Spec
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()
```

```
session_id    1000000
timestamp     5557758
item_id       37644
category      275
dtype: int64
```

```
# Randomly sample a couple of them
NUM_SESSIONS = 60000 #@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()
```

NUM_SESSIONS: 60000

```
session_id    60000
timestamp     334117
item_id       19486
category      118
dtype: int64
```

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

5.568833333333333

```
# 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()
```

| | session_id | timestamp | item_id | category | |
|--|------------|-----------|--------------------------|----------|---|
| | 0 | 9 | 2014-04-06T11:26:24.127Z | 3695 | 0 |
| | 1 | 9 | 2014-04-06T11:28:54.654Z | 3695 | 0 |
| | 2 | 9 | 2014-04-06T11:29:13.479Z | 3695 | 0 |
| | 102 | 171 | 2014-04-03T17:45:25.575Z | 10635 | 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/user_guide/indexing.html#returning-a-view.
This is separate from the ipykernel package so we can avoid doing imports until

| | session_id | timestamp | item_id | price | quantity | |
|--|------------|-----------|--------------------------|-------|----------|---|
| | 33 | 189 | 2014-04-04T07:23:10.719Z | 5576 | 4711 | 1 |
| | 46 | 489491 | 2014-04-06T12:41:34.047Z | 13388 | 1046 | 4 |
| | 47 | 489491 | 2014-04-06T12:41:34.091Z | 13389 | 627 | 2 |
| | 57 | 396 | 2014-04-06T17:53:45.147Z | 13579 | 523 | 1 |
| | 61 | 70353 | 2014-04-06T10:55:06.086Z | 15174 | 41783 | 1 |

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

```
{10968: [10968, 11081],
11081: [11081, 10968],
1213: [1213, 8930],
14448: [14448, 1442774],
1442774: [1442774, 14448],
13390: [13390, 1445273],
1445273: [1445273, 13390],
15865: [15865, 1449601],
14036: [14036, 1450532],
1165: [1165, 1450532],
4359: [4359, 1452693],
13408: [13408, 1452693],
14451: [14451, 1452693],
13523: [13523, 1452693],
6082: [6082, 1454342],
4374: [4374, 1456618],
11776: [11776, 1456618],
13438: [13438, 1459927],
15622: [15622, 1459927],
14450: [14450, 1460198],
14451: [14451, 1460198],
14451: [14451, 1460198],
14450: [14450, 1460198],
5544: [5544, 1460323],
12326: [12326, 1460323],
13216: [13216, 1460323],
13592: [13592, 1460323],
13633: [13633, 1460323],
7163: [7163, 1460323],
8761: [8761, 1460323],
11650: [11650, 1460323],
6974: [6974, 1460323],
13144: [13144, 1460323],
6973: [6973, 1460323],
11649: [11649, 1460323],
11648: [11648, 1460323],
181: [181, 1460323],
13766: [13766, 1463706],
13766: [13766, 1463706],
13766: [13766, 1463706],
13766: [13766, 1463706],
9795: [9795, 1464933],
14450: [14450, 1468993],
13535: [13535, 1468993],
14451: [14451, 1468993],
13848: [13848, 1473907],
13439: [13439, 1473907],
9275: [9275, 1473907],
13848: [13848, 1473907],
15793: [15793, 1475487],
15791: [15791, 1475487],
13840: [13840, 1477591],
14425: [14425, 1477591],
13529: [13529, 1477591],
14451: [14451, 1477591],
13840: [13840, 1477591],
14425: [14425, 1477591],
13529: [13529, 1477591],
14451: [14451, 1477591],
13394: [13394, 1479551],
655: [655, 1481656],
13846: [13846, 1482626],
14450: [14450, 1482626],
13438: [13438, 1482626],
2094: [2094, 1482757],
13535: [13535, 1489531],
14451: [14451, 1489531],
13037: [13037, 1489998],
12507: [12507, 1492547],
11213: [11213, 1492547],
14451: [14451, 1495173],
13401: [13401, 1495173],
13035: [13035, 1495173],
14451: [14451, 1498052],
11081: [11081, 1498052],
13764: [13764, 1506466],
13655: [13655, 1506563],
8943: [8943, 1506563],
3598: [3598, 1506563],
14278: [14278, 1510023],
14448: [14448, 1519191],
14450: [14450, 1519934],
14425: [14425, 1519934],
14451: [14451, 1519934],
13438: [13438, 1519934],
14450: [14450, 1521264],
14451: [14451, 1521264],
12926: [12926, 1521999],
```

```

15760,
2800,
11139,
1747,
10619,
14554,
13109,
3067,
11608,
2215],
1526834: [5404, 5146, 5404, 5146],

```

▼ 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']].dro
        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])

```

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

```
Processing...
0%|          | 0/60000 [00:00<?, ?it/s]/usr/local/lib/python3.7/dist-packages/ipykernel_launcher.py:21: UserWarning: Creati
100%|██████████| 60000/60000 [03:22<00:00, 296.26it/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, use
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
```

```
(19486, 117)
```

▼ 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)

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

```

# Enable CUDA computing
device = torch.device('cuda')
model = Net().to(device)
# Choose optimizer and criterion for learning
optimizer = torch.optim.Adam(model.parameters(), lr=0.0015)
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:

    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: {:03d}, Loss: {:.5f}, Train Auc: {:.5f}, Val Auc: {:.5f}, Test Auc: {:.5f}'.
          format(epoch, loss, train_acc, val_acc, test_acc))

```

NUM_EPOCHS: 12



```

8%|██████| 1/12 [00:47<08:45, 47.75s/it]Epoch: 000, Loss: 0.69025, Train Auc: 0.52159, Val Auc: 0.52578, Test Auc: 0.5
17%|██████| 2/12 [01:31<07:33, 45.38s/it]Epoch: 001, Loss: 0.49150, Train Auc: 0.57037, Val Auc: 0.56462, Test Auc: 0.5
25%|██████| 3/12 [02:14<06:40, 44.53s/it]Epoch: 002, Loss: 0.41170, Train Auc: 0.60795, Val Auc: 0.57826, Test Auc: 0.5
33%|██████| 4/12 [02:58<05:51, 43.98s/it]Epoch: 003, Loss: 0.37954, Train Auc: 0.63892, Val Auc: 0.59589, Test Auc: 0.5
42%|██████| 5/12 [03:41<05:05, 43.61s/it]Epoch: 004, Loss: 0.35453, Train Auc: 0.66910, Val Auc: 0.60876, Test Auc: 0.5
50%|██████| 6/12 [04:23<04:19, 43.28s/it]Epoch: 005, Loss: 0.33685, Train Auc: 0.70074, Val Auc: 0.62465, Test Auc: 0.6
58%|██████| 7/12 [05:06<03:35, 43.17s/it]Epoch: 006, Loss: 0.31992, Train Auc: 0.73408, Val Auc: 0.63180, Test Auc: 0.6
67%|██████| 8/12 [05:49<02:52, 43.05s/it]Epoch: 007, Loss: 0.30017, Train Auc: 0.76687, Val Auc: 0.64112, Test Auc: 0.6
75%|██████| 9/12 [06:32<02:08, 42.96s/it]Epoch: 008, Loss: 0.28806, Train Auc: 0.79602, Val Auc: 0.64866, Test Auc: 0.6
83%|██████| 10/12 [07:15<01:25, 42.98s/it]Epoch: 009, Loss: 0.27429, Train Auc: 0.82846, Val Auc: 0.65896, Test Auc: 0.
92%|██████| 11/12 [07:58<00:43, 43.14s/it]Epoch: 010, Loss: 0.25916, Train Auc: 0.85200, Val Auc: 0.66123, Test Auc: 0.
100%|██████| 12/12 [08:41<00:00, 43.50s/it]Epoch: 011, Loss: 0.25032, Train Auc: 0.86827, Val Auc: 0.66505, Test Auc: 0.6

```

▼ Проверка результата с помощью примеров

```

# 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
warnings.warn(out)
0.8325581395348838

```

```

# Подход №2 - через создание сессии покупки
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, 218.42it/s]DataBatch(x=[1, 1, 2], edge_index=[2, 0], y=[1], batch=[1], ptr=[2]) [0.000860:
DataBatch(x=[3, 1, 2], edge_index=[2, 2], y=[3], batch=[3], ptr=[2]) [0.04850192 0.02720772 0.0045843 ]
DataBatch(x=[4, 1, 2], edge_index=[2, 3], y=[4], batch=[4], ptr=[2]) [0.01518223 0.00499504 0.37376937 0.02905548]

```

```

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

```


Результаты

Значение метрики AUC = 0.83

В ходе работы были изменены следующие гиперпараметры: количество сессий (50000->60000), количество эпох (5->12), скорость обучения (0.001->0.0015)

✓ 0 сек. выполнено в 13:05

