# МГТУ им. Н. Э. Баумана, кафедра ИУ5 курс "Методы машинного обучения"

# Лабораторная работа №6

«Создание рекомендательной модели»

ВЫПОЛНИЛ:

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Группа: ИУ5-24М

ПРОВЕРИЛ:

Гапанюк Ю.Е.

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

## Задание:

- 1. Подготовить датасет графовых данных
- 2. Подобрать модель и гиперпараметры обучения для получения качества AUC > 0.65
- 3. Сформировать отчет и разместить его в своем репозитории на github.

# Выполнение работы:

# 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

### 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

Looking in links: https://pytorch-geometric.com/whl/torch-1.11.0%2Bcu113.html

Looking in links: https://pytorch-geometric.com/whl/torch-1.11.0%2Bcu113.html

```
In [5]:
         # 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 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 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)
```

Requirement already satisfied: torch-spline-conv in /usr/local/lib/python3.7/dist-packages (1.2.1)

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: pyparsing in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (3.0.9)

Requirement already satisfied: torch-geometric in /usr/local/lib/python3.7/dist-packages (2.0.4)

```
Requirement already satisfied: jinja2 in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (2.11.3)
Requirement already satisfied: tqdm in /usr/local/lib/python3.7/dist-packages (from torch-geometric) (4.64.0)
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-geometric) (1.0
Requirement already satisfied: MarkupSafe>=0.23 in /usr/local/lib/python3.7/dist-packages (from jinja2->torch-geo
metric) (2.0.1)
Requirement already satisfied: pytz>=2017.3 in /usr/local/lib/python3.7/dist-packages (from pandas->torch-geometr
ic) (2022.1)
Requirement already satisfied: python-dateutil>=2.7.3 in /usr/local/lib/python3.7/dist-packages (from pandas->tor
ch-geometric) (2.8.2)
Requirement already satisfied: six>=1.5 in /usr/local/lib/python3.7/dist-packages (from python-dateutil>=2.7.3->p
andas->torch-geometric) (1.15.0)
Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3.7/dist-packages (from requests->torch
-geometric) (2021.10.8)
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: 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-geome
tric) (2.10)
Requirement already satisfied: joblib>=0.11 in /usr/local/lib/python3.7/dist-packages (from scikit-learn->torch-g
eometric) (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)
Looking in links: https://data.pyg.org/whl/torch-1.11.0%2Bcu113.html
Requirement already satisfied: torch-scatter==2.0.9 in /usr/local/lib/python3.7/dist-packages (2.0.9)
```

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

```
In [7]: # Check if CUDA is available for colab
torch.cuda.is_available
```

Out[7]: <function torch.cuda.is\_available>

```
In [8]:
# 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

```
# 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 mixe d types.Specify dtype option on import or set low\_memory=False. exec(code\_obj, self.user\_global\_ns, self.user\_ns)

Out[9]:		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

```
In [10]:
           # 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()
                                                        price quantity
Out[10]:
          session_id
                                   timestamp
                                                item id
                420374 2014-04-06T18:44:58.314Z 214537888
                                                        12462
                420374 2014-04-06T18:44:58.325Z 214537850
                                                        10471
                489758 2014-04-06T09:59:52.422Z 214826955
                                                                    2
          2
                                                         1360
          3
                489758 2014-04-06T09:59:52.476Z 214826715
                                                          732
                                                                    2
                489758 2014-04-06T09:59:52.578Z 214827026
In [11]:
           # 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[11]: session_id
                          1000000
          timestamp
                         5557758
                            37644
          item id
          category
                              275
          dtype: int64
In [12]:
           # 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()
Out[12]: session_id
                           60000
                          334990
          timestamp
          item id
                           20043
                             103
          category
          dtype: int64
In [13]:
           # Average length of session
           df.groupby('session id')['item id'].size().mean()
          5.583416666666665
Out[13]:
In [14]:
           \# 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
Out[14]:
           91
                     131 2014-04-03T04:46:08.891Z
                                                 13649
                                                             0
           92
                     131 2014-04-03T04:46:53.499Z
                                                 13445
                                                             0
           93
                     131 2014-04-03T04:47:32.085Z
                                                 13585
                                                             0
          177
                     309 2014-04-06T07:59:23.727Z
                                                 14064
                                                             0
          178
                     309 2014-04-06T08:02:02.034Z
                                                 15547
                                                             0
```

19 2014-04-01T20:52:12.357Z 214561790
19 2014-04-01T20:52:13.758Z 214561790

In [15]:

# 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
```

```
        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
```

```
In [16]:
           # Get item dictionary with grouping by session
           buy_item_dict = dict(buy_df.groupby('session_id')['item_id'].apply(list))
           buy_item_dict
Out[16]: {714: [16129, 16324, 16326, 3323],
            3517: [11939, 13381],
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            7173: [13549],
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...}
```

#### Сборка выборки для обучения

```
In [17]:
          # 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
                  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
                      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):
                  __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 [18]:
          # Prepare dataset
          dataset = YooChooseDataset('./')
         Processing...
           0%|
                        | 0/60000 [00:00<?, ?it/s]/usr/local/lib/python3.7/dist-packages/ipykernel_launcher.py:21: UserWar
         ning: Creating a tensor from a list of numpy.ndarrays is extremely slow. Please consider converting the list to a
         single numpy.ndarray with numpy.array() before converting to a tensor. (Triggered internally at ../torch/csrc/ut
         ils/tensor new.cpp:210.)
         100%|
                       | 60000/60000 [05:05<00:00, 196.46it/s]
         Done!
```

#### Разделение выборки

```
In [19]:
          # 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[19]: (48000, 6000, 6000)
In [20]:
          # 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 depre
         cated, use 'loader.DataLoader' instead
         warnings.warn(out)
In [21]:
          # Load dataset into PyG loaders
          num items = df.item id.max() +1
          num_categories = df.category.max()+1
          num_items , num_categories
```

#### Настройка модели для обучения

Out[21]: (20043, 102)

```
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)
                        _, batch, _, _ = self.pool1(x, edge_index, None, batch)
       x, edge index,
       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 [23]: # 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()

In [24]: # Train function
    def train():
        model.train()
```

```
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 [25]:
         # 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 [26]:
         # 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 [01:23<12:35, 83.94s/it]
         Epoch: 000, Loss: 0.64618, Train Auc: 0.54206, Val Auc: 0.54058, Test Auc: 0.53312
         20%|
                | 2/10 [02:41<10:39, 79.99s/it]
         Epoch: 001, Loss: 0.45930, Train Auc: 0.58907, Val Auc: 0.55887, Test Auc: 0.55532
        30%| | 3/10 [03:57<09:08, 78.35s/it]
         Epoch: 002, Loss: 0.40134, Train Auc: 0.63227, Val Auc: 0.57910, Test Auc: 0.57072
                      | 4/10 [05:13<07:45, 77.51s/it]
         Epoch: 003, Loss: 0.36662, Train Auc: 0.67441, Val Auc: 0.59295, Test Auc: 0.59049
                       | 5/10 [06:28<06:23, 76.66s/it]
         Epoch: 004, Loss: 0.34265, Train Auc: 0.71249, Val Auc: 0.61112, Test Auc: 0.61277
         60%|
                  | 6/10 [07:44<05:04, 76.17s/it]
         Epoch: 005, Loss: 0.33223, Train Auc: 0.74366, Val Auc: 0.62061, Test Auc: 0.62761
                   | 7/10 [09:00<03:48, 76.07s/it]
         Epoch: 006, Loss: 0.30576, Train Auc: 0.78091, Val Auc: 0.63387, Test Auc: 0.63352
         80%|
                  | 8/10 [10:15<02:31, 75.91s/it]
         Epoch: 007, Loss: 0.28174, Train Auc: 0.81766, Val Auc: 0.64153, Test Auc: 0.64433
                      | 9/10 [11:30<01:15, 75.63s/it]
         Epoch: 008, Loss: 0.26621, Train Auc: 0.85218, Val Auc: 0.65124, Test Auc: 0.65225
                       | 10/10 [12:45<00:00, 76.55s/it]
         Epoch: 009, Loss: 0.24922, Train Auc: 0.88251, Val Auc: 0.65665, Test Auc: 0.66046
```

loss all = 0

#### Проверка результата с помощью примеров

```
In [46]:
         # 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 depre
         cated, use 'loader.DataLoader' instead
          warnings.warn(out)
Out[46]: 0.7247191011235956
In [28]:
         # 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)
                     | 3/3 [00:00<00:00, 183.19it/s]
         DataBatch(x=[4, 1, 2], edge index=[2, 3], y=[4], batch=[4], ptr=[2]) [4.1785872e-05 2.6933427e-04 1.6458357e-03 2
         .7660092e-03]
         /usr/local/lib/python 3.7/dist-packages/torch\_geometric/deprecation.py: 12: UserWarning: 'data.DataLoader' is deprecated, use 'loader.DataLoader' instead
          warnings.warn(out)
```

Как видно из результатов, значение метрики AUC = 72.5%

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