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Кафедра «Системы обработки информации и управления»



Лабораторная работа №5
«Создание рекомендательной модели»

ИСПОЛНИТЕЛЬ:

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"__" _____ 2022 г.

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

Требования к отчету:

Отчет по лабораторной работе должен содержать:

1. титульный лист;
2. описание задания;
3. текст программы;
4. экранные формы с примерами выполнения программы.

Задание:

1. Подготовить датасет графовых данных
2. 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. 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> (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

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

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

Looking in indexes: <https://pypi.org/simple>, <https://us-python.pkg.dev/colab-wheels>

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-cp

| 3.5 MB 4.9 MB/s

Requirement already satisfied: scipy in /usr/local/lib/python3.7/dist-packages (from

Requirement already satisfied: numpy>=1.13.3 in /usr/local/lib/python3.7/dist-packa

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>

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-cp

| 2.5 MB 5.1 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>

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

| 750 kB 4.6 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>

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 5.2 MB/s

Requirement already satisfied: tqdm in /usr/local/lib/python3.7/dist-packages (from

Requirement already satisfied: numpy in /usr/local/lib/python3.7/dist-packages (from

Requirement already satisfied: scipy in /usr/local/lib/python3.7/dist-packages (from

Requirement already satisfied: pandas in /usr/local/lib/python3.7/dist-packages (fr

Requirement already satisfied: jinja2 in /usr/local/lib/python3.7/dist-packages (fr

Requirement already satisfied: requests in /usr/local/lib/python3.7/dist-packages

Requirement already satisfied: pyparsing in /usr/local/lib/python3.7/dist-packages

Requirement already satisfied: scikit-learn in /usr/local/lib/python3.7/dist-packag

Requirement already satisfied: MarkupSafe>=0.23 in /usr/local/lib/python3.7/dist-pa

Requirement already satisfied: pytz>=2017.3 in /usr/local/lib/python3.7/dist-packag

Requirement already satisfied: python-dateutil>=2.7.3 in /usr/local/lib/python3.7/c

Requirement already satisfied: six>=1.5 in /usr/local/lib/python3.7/dist-packages

Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3.7/dist-

Requirement already satisfied: idna<3,>=2.5 in /usr/local/lib/python3.7/dist-packag

```

Requirement already satisfied: urllib3!=1.25.0,!1.25.1,<1.26,>=1.21.1 in /usr/local/lib/python3.7/dist-packages
Requirement already satisfied: chardet<4,>=3.0.2 in /usr/local/lib/python3.7/dist-packages
Requirement already satisfied: joblib>=0.11 in /usr/local/lib/python3.7/dist-packages
Requirement already satisfied: threadpoolctl>=2.0.0 in /usr/local/lib/python3.7/dist-packages
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
  Stored in directory: /root/.cache/pip/wheels/18/a6/a4/ca18c3051fced866fe7b85700e
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/simple
Looking in links: https://data.pyg.org/whl/torch-1.11.0%2Bcu113.html
Collecting torch-scatter==2.0.8
  Downloading torch_scatter-2.0.8.tar.gz (21 kB)

```

```

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

```

RANDOM_SEED: 71

```

from sklearn.preprocessing import LabelEncoder

```

```

import torch

```

```

# PyG - PyTorch Geometric

```

```

from torch_geometric.data import Data, DataLoader, InMemoryDataset

```

```

from tqdm import tqdm

```

```

RANDOM_SEED = 71 #@param { type: "integer" }
BASE_DIR = '/content/' #@param { type: "string" }
np.random.seed(RANDOM_SEED)

```

```

CUDA_LAUNCH_BLOCKING = "1"

```

```

# 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('/content/yoochoose-data-lite.zip', 'r') as zip_ref:
    zip_ref.extractall(BASE_DIR)

```

```

-----
BadZipFile                                Traceback (most recent call last)
<ipython-input-3-5b7ba636a1ee> in <module>()
      1 # Unpack files from zip-file
      2 import zipfile
----> 3 with zipfile.ZipFile('/content/yoochoose-data-lite.zip', 'r') as zip_ref:
      4     zip_ref.extractall(BASE_DIR)

```

```

----- 1 frames -----
/usr/lib/python3.7/zipfile.py in _RealGetContents(self)
    1323         raise BadZipFile("File is not a zip file")
    1324     if not endrec:
-> 1325         raise BadZipFile("File is not a zip file")
    1326     if self.debug > 1:
    1327         print(endrec)

```

```

import os
cwd = os.getcwd()
cwd

```

```

'/content'

```

▼ 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()

```

	session_id	timestamp	item_id	category
0	9	2014-04-06T11:26:24.127Z	214576500.0	0.0
1	9	2014-04-06T11:28:54.654Z	214576500.0	0.0
2	9	2014-04-06T11:29:13.479Z	214576500.0	0.0
3	19	2014-04-01T20:52:12.357Z	214561790.0	0.0
4	19	2014-04-01T20:52:13.758Z	214561790.0	0.0

```

# 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

```
# 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    24709
timestamp     141212
item_id       11476
category       1
dtype: int64
```

```
# Randomly sample a couple of them
NUM_SESSIONS = 10000 #@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()
```

```
session_id    10000
timestamp     57081
item_id       7827
category       1
dtype: int64
```

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

```
5.7085
```

```
# Encode item and category id in item dataset so that ids will be in range (0,len(df.item_id.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	1717	0
1	9	2014-04-06T11:28:54.654Z	1717	0
2	9	2014-04-06T11:29:13.479Z	1717	0
3	19	2014-04-01T20:52:12.357Z	1496	0
4	19	2014-04-01T20:52:13.758Z	1496	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/using_indexers.html
This is separate from the ipykernel package so we can avoid doing imports until

	session_id	timestamp	item_id	price	quantity
23	70529	2014-04-03T11:07:51.984Z	5714	2617	2
26	140973	2014-04-02T20:24:15.190Z	3619	15603	1
45	209936	2014-04-03T18:28:30.862Z	352	837	2
53	210076	2014-04-07T05:50:20.837Z	1636	313	12
54	210076	2014-04-07T05:50:20.879Z	7366	627	6

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

```
{396: [6451],
 432: [5250],
 484: [4457, 4457],
 737: [6754],
 873: [6302],
1167: [7448],
1311: [394],
1372: [6425, 6428, 6426, 6427],
1426: [1977],
1877: [6326],
1896: [6502],
2071: [6451, 6422, 6489, 6429],
2168: [6375],
3687: [6462, 6460, 192, 6435, 7425, 1788, 191, 68],
4036: [1770, 2461],
4761: [6188, 6188],
4868: [144, 4718],
4988: [7306],
5296: [7419, 6040],
5492: [2320],
5761: [5921, 5994],
5802: [4306, 6264],
6016: [7522],
6528: [6041, 6055, 1382],
7054: [6422],
7173: [6188],
7176: [4189, 4189],
7189: [7306],
7742: [2319],
7798: [5363],
7866: [7419, 5181, 5123],
8427: [353, 353],
```



```

8793: [6434, 5846],
9272: [1939],
9787: [5709],
10648: [6375, 6379],
11311: [1314, 6331],
11524: [6029],
11527: [5779],
11718: [6485, 6487, 6039],
12017: [2497],
12031: [129],
12101: [6281, 6506],
12184: [6434],
12282: [6377,
6379,
6375,
4475,
6379,
6377,
6375,
4475,
6379,
6377,
6375,
4475],
12356: [641],
13073: [5709, 5709],

```

▼ 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')
        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('./')

```

▼ 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)

(8000, 1000, 1000)

```

```

# 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
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
```

```
(7827, 1)
```

▼ 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=0.01)
# optimizer = torch.optim.Adagrad(model.parameters(), lr=0.01)
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)
```

```
# model.to(device)
```

```
# 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))
```

NUM_EPOCHS: 10



0%| | 0/10 [00:00<?, ?it/s]

RuntimeError Traceback (most recent call last)

```
<ipython-input-28-194a343510ba> in <module>()
      2 NUM_EPOCHS = 10#@param { type: "integer" }
      3 for epoch in tqdm(range(NUM_EPOCHS)):
----> 4     loss = train()
      5     train_acc = evaluate(train_loader)
      6     val_acc = evaluate(val_loader)
```

----- 5 frames -----
/usr/local/lib/python3.7/dist-packages/torch_geometric/data/data.py in <lambda>(x)
 215 only the ones given in :obj:`*args`."""
 216 return self.apply(
--> 217 lambda x: x.to(device=device, non_blocking=non_blocking), *args)
 218
 219 def cpu(self, *args: List[str]):

RuntimeError: CUDA error: device-side assert triggered
CUDA kernel errors might be asynchronously reported at some other API call,so the
stacktrace below might be incorrect.
For debugging consider passing CUDA_LAUNCH_BLOCKING=1.

▼ 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  
    warnings.warn(out)  
0.4639639639639639
```

```
# 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, 216.61it/s]
/usr/local/lib/python3.7/dist-packages/torch_geometric/deprecation.py:12: UserWarning
  warnings.warn(out)
```

RuntimeError Traceback (most recent call last)

```
<ipython-input-32-d0e950e4242f> in <module>()
    17     model.eval()
    18     for data in test_data:
--> 19         data = data.to(device)
    20         pred = model(data).detach().cpu().numpy()
    21
```

⌵ 4 frames

```
/usr/local/lib/python3.7/dist-packages/torch_geometric/data/data.py in <lambda>(x)
    215     only the ones given in :obj:`*args`."""
    216     return self.apply(
--> 217         lambda x: x.to(device=device, non_blocking=non_blocking), *args)
    218
    219     def cpu(self, *args: List[str]):
```

RuntimeError: CUDA error: device-side assert triggered
CUDA kernel errors might be asynchronously reported at some other API call,so the
stacktrace below might be incorrect.
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