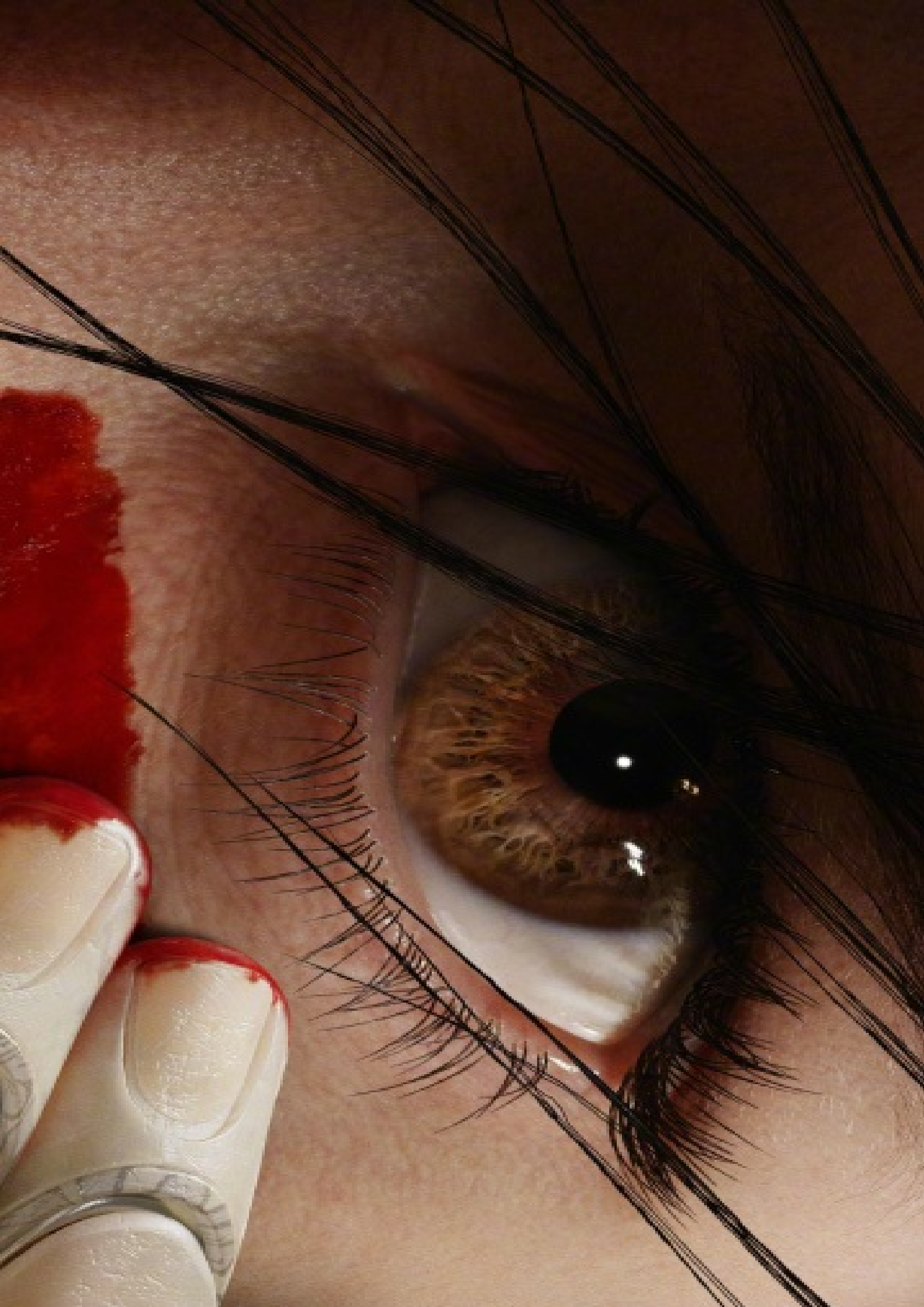

Table of Contents

Introduction

这是一本私人笔记

书籍：

1. The Art of Computer Programming
2. Programming Pearis
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4. Structure and Interpretation of Computer Program
5. The Art of Unix Programming
6. The Practice of Programming
7. The Productive Programmer
8. How to Solve it
9. Cosmos

GNN(Graph Neural Network)

from: Graph Neural Networks: A Review of Methods and Applications

Why GNN from CNN

1. graphs are the most typical locally connected structure
2. share weights reduce the computational cost compared with traditional spectral graph theory, approximation
3. multilayer structure is the key to deal with hierarchical patterns, which captures the featuofres of various sizes
4. CNNs or RNNs need a specific order, but there is no natural order of nodes in graph, GNNs output is input order invarient
5. human intelligencce is most based on the graph, GNNs can do information propagation guided by the graph structure
6. GNNs explores to generate the graph from non-structural data

Drawback of traditional algorithm

1. no parameter-share cause computational inefficiency
2. lack of generalization

Origin GNN

target: learn a state embedding $\mathbf{h}_v \in \mathbb{R}^s$ for each node

procedure:

$$\mathbf{h}_v = f(\mathbf{x}_v, edge\_attr_v, \mathbf{h}_u, \mathbf{x}_u)$$

u means neighbors of v, f is local parameterized transition function

$$\mathbf{o}_v = g(\mathbf{h}_v, \mathbf{x}_v)$$

g is local output function

loss:

$$loss = \sum_{i=1}^{p}(target_i - output_i)$$

variants:

1. Directed Graphs
2. Heterogeneous Graphs
3. Graphs with edge information
4. Dynamics Graphs
5. Convolution
    i. spectral network
   ii. non-spectral metworks
        i. Neural FPs
       ii. DCNN (Diffusion-convolutional neural network)
      iii. DGCN (Dual graph convolutional network)
       iv. PATCHY-SAN
        v. LGCN
       vi. MoNet
      vii. GraphSAGE
     viii. Gate
            i. Child-sum Tree-LSTM
           ii. N-ary Tree-LSTM
          iii. Sentence LSTM
       ix. GAT (Graph Attention Network)
        x. Ship Connection
       xi. Hierarchical Pooling

General Framework

1. **Message Passing NN**

2. Non-Local NN
3. GN (Graph networks)

Applications

1. Structural Scenarios
    i. Physics: CommNet
    ii. Chemistry and Biology
        i. Molecular Fingerprints
        ii. Protein Interface Prediction
    iii. Knowledge Graph
2. Non-structural Scenarios
    i. Image Classification
    ii. Visual Reasoning
    iii. Semantic Segmentation
    iv. Machine translation
    v. Sequence labeling
    vi. Text Classification
    vii. Relation & Event extraction
3. Others
    i. Generative Model
    ii. Combinational Optimization

Open Problems

1. Hard to build Deep GNN: over-smoothing

2. Dynamic Graphs
3. Non-structral Scenarios
4. **Scalablity**

Datasets

Websites:

1. tu-dortmund
2. networkrepository

group by raw data size:

1. small graph ($\leq 300MB$)
2. big graph (500MB~5GB)
3. huge graph ($\geq 5GB$)

Message Passing Model

Message passing phase (T times propagation step)

M_t: message function

U_t: vertex update function

$\mathbf{m}_v^{t+1} = \sum_{w \in \mathcal{N}_v} M_t(\mathbf{h}_v^t, \mathbf{h}_w^t, \mathbf{e}_{vw})$

$$w \in \mathcal{N}$$

$$\mathbf{h}_v^{t+1} = U_t(\mathbf{h}_v^t, \mathbf{m}_v^{t+1})$$

Readout phase

R: readout function

$$\hat{\mathbf{y}} = R(\mathbf{h}_v^T | v \in G)$$

DFF: Deep Feature Flow for Video Recognition

Question: per-frame evaluation is too slow and unaffordable

Solution: run expensive convolutional sub-network only on sparse **key frames（关键帧）** and propagates their deep feature maps to other frames via a **flow field（流域）**.

- Decompose neutral network $\mathcal{N}$ into **feature network** and **task network**
- Run $\mathcal{N}_{feat}$ only on key-frame and propagate featuremap to following non-key frame

Deep Feature Flow

- feature propagation function（特征传播函数）

$$f_i = \mathcal{W}(f_k, M_{i\to k}, S_{i\to k})$$

- where $M_{i\to k}$ is a two dimensional flow field
-

learn-pytorch-geometric

Installation

```
pip3 install --verbose --no-cache-dir torch-scat
ter
pip3 install --verbose --no-cache-dir torch-spar
se
pip3 install --verbose --no-cache-dir torch-clus
ter
pip3 install --verbose --no-cache-dir torch-spli
ne-conv
pip3 install torch-geometric
```

Data Representation:

For Graph $\mathcal{G} = (X, (I, E))$

where:

1. node feature matrix: $X \in \mathbb{R}^{N \times F}$
2. sparse adjacency tuple (I, E), $I \in \mathbb{N}^{2 \times E}$ encodes edges in Coordinate format (COO: the first list contains the index of the source nodes, while the index of target nodes is specified in the second

list.) , $E \in \mathbb{R}^{E \times D}$ holds D-dimensional edge features

Neighborhood Aggregation

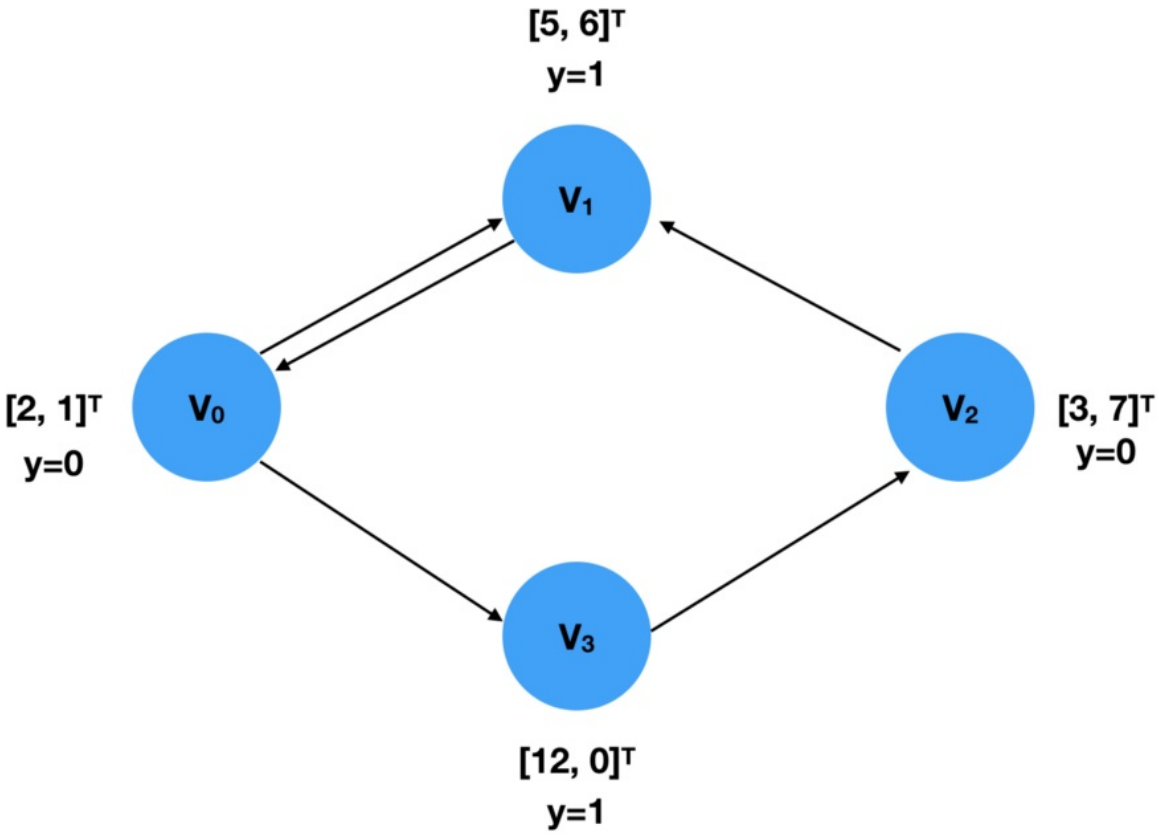
$$x_i' = \gamma \left(x_i, \underset{j \in \mathcal{N}(i)}{AS} \phi(x_i, x_j, e_{i,j}) \right)$$

where:

1. $\underset{i \in \mathcal{N}(i)}{AS}$: **aggregation function**, differentiable, permutation invarient
2. γ: **update function**, differentiable
3. ϕ: **message function**, differentiable

How to load data set?

PyG Graph Data Structure: `torch_geometric.data.Data`



- `data.x` : node feature matrix

```
x = torch.tensor([[2,1], [5,6], [3,7], [12,0]],
dtype=torch.float)
```

- `data.edge_index` : I

```
edge_index = torch.tensor([[0, 1, 2, 0, 3],
                           [1, 0, 1, 3, 2]], dty
pe=torch.long)
```

- `data.edge_attr` : edge feature matrix
- `data.y` : train target

```
y = torch.tensor([0, 1, 0, 1], dtype=torch.float)
```

- `data.pos` : data position matrix

How to build a graph?

```
import torch
from torch_geometric.data import Data

x = torch.tensor([[2,1], [5,6], [3,7], [12,0]],
dtype=torch.float)
y = torch.tensor([0, 1, 0, 1], dtype=torch.float)


edge_index = torch.tensor([[0, 2, 1, 0, 3],
                           [3, 1, 0, 1, 2]], dty
pe=torch.long)

data = Data(x=x, y=y, edge_index=edge_index)
```

How to build Graph DataSet

Example: PPI DataSet

```
from itertools import product
import os
import os.path as osp
import json

import torch
import numpy as np
import networkx as nx
from networkx.readwrite import json_graph
from torch_geometric.data import (InMemoryDataset
, Data, download_url, extract_zip)
from torch_geometric.utils import remove_self_lo
ops

class PPI(InMemoryDataset):
    r"""The protein-protein interaction networks
 from the `"Predicting
    Multicellular Function through Multi-layer T
issue Networks"
    <https://arxiv.org/abs/1707.04638>`_ paper,
containing positional gene
    sets, motif gene sets and immunological sign
atures as features (50 in
    total) and gene ontology sets as labels (121
 in total).

    Args:
        数据集根文件夹
        root (string): Root directory where the
```

```
dataset should be saved.
        数据集参数
        split (string):
            If :obj:`"train"`, loads the trainin
g dataset.
            If :obj:`"val"`, loads the validatio
n dataset.
            If :obj:`"test"`, loads the test dat
aset. (default: :obj:`"train"`)
        转换函数
        transform (callable, optional): A functi
on/transform that takes in an
            :obj:`torch_geometric.data.Data` obj
ect and returns a transformed
            version. The data object will be tra
nsformed before every access.
            (default: :obj:`None`)
        保存格式
        pre_transform (callable, optional): A fu
nction/transform that takes in
            an :obj:`torch_geometric.data.Data`
object and returns a
            transformed version. The data object
 will be transformed before
            being saved to disk. (default: :obj:
`None`)
        判断是否要保留到最后使用
        pre_filter (callable, optional): A funct
ion that takes in an
            :obj:`torch_geometric.data.Data` obj
```

```
ect and returns a boolean
            value, indicating whether the data o
bject should be included in the
            final dataset. (default: :obj:`None`
)
    """

    url = 'https://s3.us-east-2.amazonaws.com/dg
l.ai/dataset/ppi.zip'

    def __init__(self,
                 root,
                 split='train',
                 transform=None,
                 pre_transform=None,
                 pre_filter=None):

        assert split in ['train', 'val', 'test']

        super(PPI, self).__init__(root, transform
, pre_transform, pre_filter)

        if split == 'train':
            self.data, self.slices = torch.load(
self.processed_paths[0])
        elif split == 'val':
            self.data, self.slices = torch.load(
self.processed_paths[1])
        elif split == 'test':
            self.data, self.slices = torch.load(
```

```
self.processed_paths[2])

    @property
    def raw_file_names(self):
        '''
                    It returns a list that shows
 a list of raw, unprocessed file names.
        '''
        splits = ['train', 'valid', 'test']
        files  = ['feats.npy', 'graph_id.npy', '
graph.json', 'labels.npy']
        return ['{}_{}'.format(s, f) for s, f in
 product(splits, files)]

    @property
    def processed_file_names(self):
        '''
                returns a list containing the f
ile names of all the processed data.
                After process() is called, Usua
lly, the returned list should only have one elem
ent,
                storing the only processed data
 file name.
        '''
        return ['train.pt', 'val.pt', 'test.pt']

    def download(self):
        '''
                    This function should downloa
```

```
d the data you are working on to
                    the directory as specified i
n self.raw_dir.
        '''
        path = download_url(self.url, self.root)
        extract_zip(path, self.raw_dir)
        os.unlink(path)

    def process(self):
        '''
                    You need to gather your data
 into a list of Data objects.
                    Then, call self.collate() to
 compute the slices that will be used by the Dat
aLoader object.
        '''
        for s, split in enumerate(['train', 'val
id', 'test']):
            path = osp.join(self.raw_dir, '{}_gr
aph.json').format(split)
            with open(path, 'r') as f:
                G = nx.DiGraph(json_graph.node_l
ink_graph(json.load(f)))

            x = np.load(osp.join(self.raw_dir, '
{}_feats.npy' ).format(split))
            x = torch.from_numpy(x).to(torch.flo
at)

            y = np.load(osp.join(self.raw_dir, '
```

```
{}_labels.npy').format(split))
            y = torch.from_numpy(y).to(torch.flo
at)

            data_list = []
            path = osp.join(self.raw_dir, '{}_gr
aph_id.npy').format(split)
            idx = torch.from_numpy(np.load(path))
.to(torch.long)
            idx = idx - idx.min()

            for i in range(idx.max().item() + 1):

                mask = idx == i

                G_s = G.subgraph(mask.nonzero().
view(-1).tolist())
                edge_index = torch.tensor(list(G
_s.edges)).t().contiguous()
                edge_index = edge_index - edge_i
ndex.min()
                edge_index, _ = remove_self_loops
(edge_index)

                data = Data(edge_index=edge_index
, x=x[mask], y=y[mask])

                if self.pre_filter is not None a
nd not self.pre_filter(data):
                    continue
```

```
                if self.pre_transform is not None
:
                    data = self.pre_transform(da
ta)

                data_list.append(data)
            torch.save(self.collate(data_list),
self.processed_paths[s])
```

DataLoader

The DataLoader class allows you to feed data by batch into the model effortlessly. To create a DataLoader object, you simply specify the Dataset and the batch size you want.

```
loader = DataLoader(dataset, batch_size=512, shu
ffle=True)
```

Every iteration of a DataLoader object yields a Batch object, which is very much like a Data object but with an attribute, “batch”. It indicates which graph each node is associated with. Since a DataLoader aggregates `x`, `y`, and `edge_index` from different samples/ graphs

into Batches, the GNN model needs this “batch” information to know which nodes belong to the same graph within a batch to perform computation.

```
for batch in loader:
    batch
    >>> Batch(x=[1024, 21], edge_index=[2, 1568],
 y=[512], batch=[1024])
```

MessagePassing / Neighborhood Aggregation

propagate(edge_index, size=None, **kwargs):

It takes in edge index and other optional information, such as node features (embedding). Calling this function will consequently call message and update.

message(**kwargs):

construct “message” for each of the node pair (x_i, x_j)

update(aggr_out,**kwargs):

It takes in the aggregated message and other arguments passed into propagate, assigning a new embedding value for each node.

Example:

```
import torch
from torch.nn import Sequential as Seq, Linear,
ReLU
from torch_geometric.nn import MessagePassing
from torch_geometric.utils import remove_self_lo
ops, add_self_loops
class SAGEConv(MessagePassing):
    def __init__(self, in_channels, out_channels)
:
        super(SAGEConv, self).__init__(aggr='max'
) #  "Max" aggregation.
        self.lin = torch.nn.Linear(in_channels,
out_channels)
        self.act = torch.nn.ReLU()
        self.update_lin = torch.nn.Linear(in_cha
nnels + out_channels, in_channels, bias=False)
        self.update_act = torch.nn.ReLU()

    def forward(self, x, edge_index):
        # x has shape [N, in_channels]
        # edge_index has shape [2, E]


        edge_index, _ = remove_self_loops(edge_i
```

```
ndex)
        edge_index, _ = add_self_loops(edge_index
, num_nodes=x.size(0))


        return self.propagate(edge_index, size=(x
.size(0), x.size(0)), x=x)

    def message(self, x_j):
        # x_j has shape [E, in_channels]

        x_j = self.lin(x_j)
        x_j = self.act(x_j)

        return x_j

    def update(self, aggr_out, x):
        # aggr_out has shape [N, out_channels]


        new_embedding = torch.cat([aggr_out, x],
 dim=1)

        new_embedding = self.update_lin(new_embe
dding)
        new_embedding = self.update_act(new_embe
dding)

        return new_embedding
```

Build a Graph Neural Network

```
embed_dim = 128
from torch_geometric.nn import TopKPooling
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__()

        self.conv1 = SAGEConv(embed_dim, 128)
        self.pool1 = TopKPooling(128, ratio=0.8)
        self.conv2 = SAGEConv(128, 128)
        self.pool2 = TopKPooling(128, ratio=0.8)
        self.conv3 = SAGEConv(128, 128)
        self.pool3 = TopKPooling(128, ratio=0.8)
        self.item_embedding = torch.nn.Embedding(
num_embeddings=df.item_id.max() +1, embedding_dim
=embed_dim)
        self.lin1 = torch.nn.Linear(256, 128)
        self.lin2 = torch.nn.Linear(128, 64)
        self.lin3 = torch.nn.Linear(64, 1)
        self.bn1 = torch.nn.BatchNorm1d(128)
        self.bn2 = torch.nn.BatchNorm1d(64)
        self.act1 = torch.nn.ReLU()
        self.act2 = torch.nn.ReLU()
    def forward(self, data):
        x, edge_index, batch = data.x, data.edge
```

```
_index, data.batch
        x = self.item_embedding(x)
        x = x.squeeze(1)

        x = F.relu(self.conv1(x, edge_index))

        x, edge_index, _, batch, _ = self.pool1(x
, edge_index, None, batch)
        x1 = torch.cat([gmp(x, batch), gap(x, ba
tch)], 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, ba
tch)], 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, ba
tch)], dim=1)

        x = x1 + x2 + x3

        x = self.lin1(x)
        x = self.act1(x)
        x = self.lin2(x)
```

```
        x = self.act2(x)
        x = F.dropout(x, p=0.5, training=self.tr
aining)

        x = torch.sigmoid(self.lin3(x)).squeeze(1
)

        return x
```

Train

```
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)

device = torch.device('cuda')
```

```
model = Net().to(device)
optimizer = torch.optim.Adam(model.parameters(),
 lr=0.005)
crit = torch.nn.BCELoss()
train_loader = DataLoader(train_dataset, batch_s
ize=batch_size)
for epoch in range(num_epochs):
    train()
```

Validation

```
def evaluate(loader):
    model.eval()

    predictions = []
    labels = []

    with torch.no_grad():
        for data in loader:

            data = data.to(device)
            pred = model(data).detach().cpu().nu
mpy()

            label = data.y.detach().cpu().numpy()

            predictions.append(pred)
            labels.append(label)
```

Test

```
for epoch in range(1):
    loss = train()
    train_acc = evaluate(train_loader)
    val_acc = evaluate(val_loader)
    test_acc = evaluate(test_loader)
    print('Epoch: {:03d}, Loss: {:.5f}, Train Au
c: {:.5f}, Val Auc: {:.5f}, Test Auc: {:.5f}'.
          format(epoch, loss, train_acc, val_acc,
 test_acc))for epoch in range(1):
    loss = train()
    train_acc = evaluate(train_loader)
    val_acc = evaluate(val_loader)
    test_acc = evaluate(test_loader)
    print('Epoch: {:03d}, Loss: {:.5f}, Train Au
c: {:.5f}, Val Auc: {:.5f}, Test Auc: {:.5f}'.
          format(epoch, loss, train_acc, val_acc,
 test_acc))
```

Message Passing Networks

Generalizing the convolution operator to irregular domains is typically expressed as a neighborhood aggregation or message passing scheme.

$$\mathbf{x}_i^{(k)} = \gamma^{(k)} \left(\mathbf{x}_i^{(k-1)}, \square_{j \in \mathcal{N}(i)} \, \phi^{(k)} \left(\mathbf{x}_i^{(k-1)}, \mathbf{x}_j^{(k-1)}, \mathbf{e}_{i,j} \right) \right)$$

PyTorch Geometric provides the `torch_geometric.nn.MessagePassing` base class, which helps in creating such kinds of message passing graph neural networks by automatically taking care of message propagation. The user only has to define the functions ϕ , i.e. `message()` , and γ, .i.e. `update()` , as well as the aggregation scheme to use, .i.e. `aggr='add'` , `aggr='mean'` or `aggr='max'` .

- **torch_geometric.nn.MessagePassing(aggr="add", flow="source_to_target")**
- **torch_geometric.nn.MessagePassing.propagate(edge_index, size=None, \kwargs)**
  - In forward method
- **torch_geometric.nn.MessagePassing.message()**
- **torch_geometric.nn.MessagePassing.update()**

20190717note

meeting

summer intern requirements:

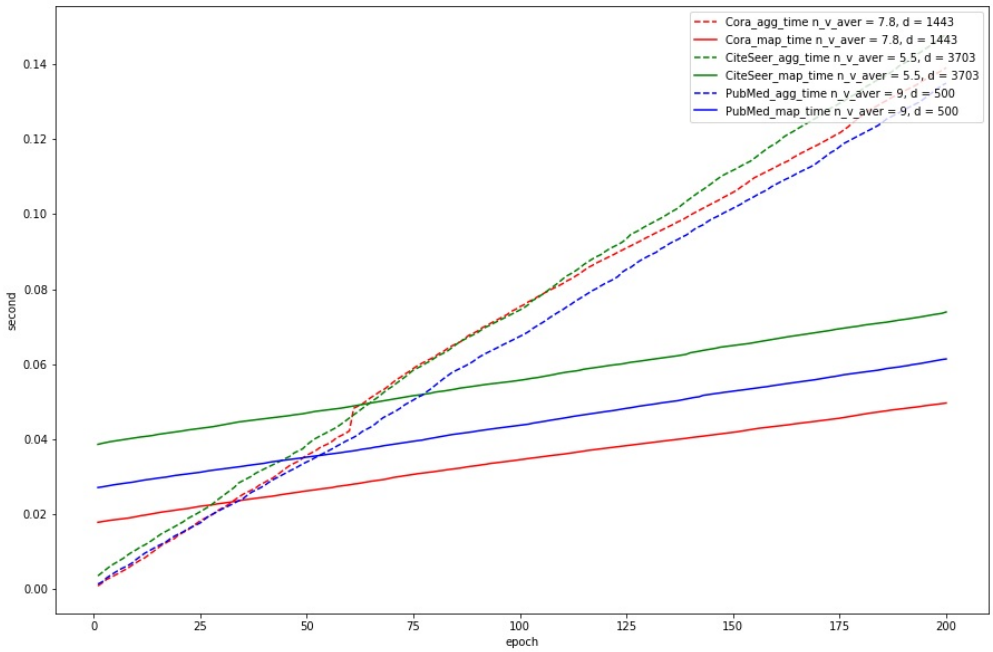
1. paper
2. technical report
3. weekly report

personal ability:

1. marhmatical understanding -> critical insight
2. implementation -> bug free
3. writing -> format, highlight key points
4. presentation

Profiling of GCN

1. polt insight



coding & basic knowledge

feature = attribute + its values

learn-tensorflow

define const

```
const = tf.constant(2.0, name='const')
```

define variable

```
c = tf.Variable(1.0, dtype=tf.float32, name='c')
```

define operation

```
e = tf.add(c, const, name='e')
```

init & creat session

```
# 1. 定义init operation
init_op = tf.global_variables_initializer()
# session
with tf.Session() as sess:
    # 2. 运行init operation
```

```
    sess.run(init_op)
    # 计算
    a_out = sess.run(a)
    print("Variable a is {}".format(a_out))
```

placeholder

```
# 创建placeholder
b = tf.placeholder(tf.float32, [None, 1], name='b')
a_out = sess.run(a, feed_dict={b: np.arange(0, 10)[:, np.newaxis]})
```

neural network

```
from tensorflow.examples.tutorials.mnist import input_data
mnist = input_data.read_data_sets("MNIST_data/", one_hot=True)
# 超参数
learning_rate = 0.5
epochs = 10
batch_size = 100

# placeholder
# 输入图片为28 x 28 像素 = 784
```

```
x = tf.placeholder(tf.float32, [None, 784])
# 输出为0-9的one-hot编码
y = tf.placeholder(tf.float32, [None, 10])

# hidden layer => w, b
W1 = tf.Variable(tf.random_normal([784, 300], st
ddev=0.03), name='W1')
b1 = tf.Variable(tf.random_normal([300]), name='
b1')
# output layer => w, b
W2 = tf.Variable(tf.random_normal([300, 10], std
dev=0.03), name='W2')
b2 = tf.Variable(tf.random_normal([10]), name='b
2')

# hidden layer
hidden_out = tf.add(tf.matmul(x, W1), b1)
hidden_out = tf.nn.relu(hidden_out)

# 计算输出
y_ = tf.nn.softmax(tf.add(tf.matmul(hidden_out,
W2), b2))

y_clipped = tf.clip_by_value(y_, 1e-10, 0.9999999
)
cross_entropy = -tf.reduce_mean(tf.reduce_sum(y *
 tf.log(y_clipped) + (1 - y) * tf.log(1 - y_clip
ped), axis=1))

# 创建优化器，确定优化目标
```

```
optimizer = tf.train.GradientDescentOptimizer(le
arning_rate=learning_rate).minimizer(cross_entro
py)

# init operator
init_op = tf.global_variables_initializer()

# 创建准确率节点
correct_prediction = tf.equal(tf.argmax(y, 1), tf
.argmax(y_, 1))
accuracy = tf.reduce_mean(tf.cast(correct_predic
tion, tf.float32))

# 创建session
with tf.Session() as sess:
    # 变量初始化
    sess.run(init_op)
    total_batch = int(len(mnist.train.labels) /
batch_size)
    for epoch in range(epochs):
        avg_cost = 0
        for i in range(total_batch):
            batch_x, batch_y = mnist.train.next_
batch(batch_size=batch_size)
            _, c = sess.run([optimizer, cross_en
tropy], feed_dict={x: batch_x, y: batch_y})
            avg_cost += c / total_batch
        print("Epoch:", (epoch + 1), "cost = ",
"{:.3f}".format(avg_cost))
    print(sess.run(accuracy, feed_dict={x: mnist.
```

```
  test.images, y: mnist.test.labels}))
```

Tigr