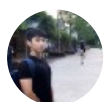


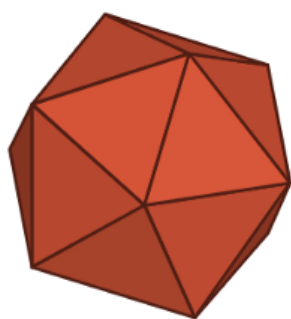
Hands-on Graph Neural Networks with PyTorch & PyTorch Geometric



黃功詳 Steeve Huang in Towards Data Science

Following

May 31 · 9 min read ★



PyTorch geometric

In my last article, I introduced the concept of Graph Neural Network (GNN) and some recent advancements of it. Since this topic is getting seriously hyped up, I decided to make this tutorial on how to easily implement your Graph Neural Network in your project. You will learn how to construct your own GNN with PyTorch Geometric, and how to use GNN to solve a real-world problem (Recsys Challenge 2015).

In this blog post, we will be using PyTorch and PyTorch Geometric (PyG), a Graph Neural Network framework built on top of PyTorch that runs blazingly fast. It is several times faster than the most well-known GNN framework, DGL.

Aside from its remarkable speed, PyG comes with a collection of well-implemented GNN models illustrated in various papers. Therefore, it would be very handy to reproduce the experiments with PyG.

- **SplineConv** from Fey et al.: [SplineCNN: Fast Geometric Deep Learning with Continuous B-Spline Kernels](#) (CVPR 2018)
- **GCNConv** from Kipf and Welling: [Semi-Supervised Classification with Graph Convolutional Networks](#) (ICLR 2017)
- **ChebConv** from Defferrard et al.: [Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering](#) (NIPS 2016)
- **NNConv** adapted from Gilmer et al.: [Neural Message Passing for Quantum Chemistry](#) (ICML 2017)
- **GATConv** from Veličković et al.: [Graph Attention Networks](#) (ICLR 2018)
- **SAGEConv** from Hamilton et al.: [Inductive Representation Learning on Large Graphs](#) (NIPS 2017)
- **GraphConv** from, e.g., Morris et al.: [Weisfeiler and Leman Go Neural: Higher-order Graph Neural Networks](#) (AAAI 2019)
- **GatedGraphConv** from Li et al.: [Gated Graph Sequence Neural Networks](#) (ICLR 2016)
- **GINConv** from Xu et al.: [How Powerful are Graph Neural Networks?](#) (ICLR 2019)

PyTorch Geometric Basics

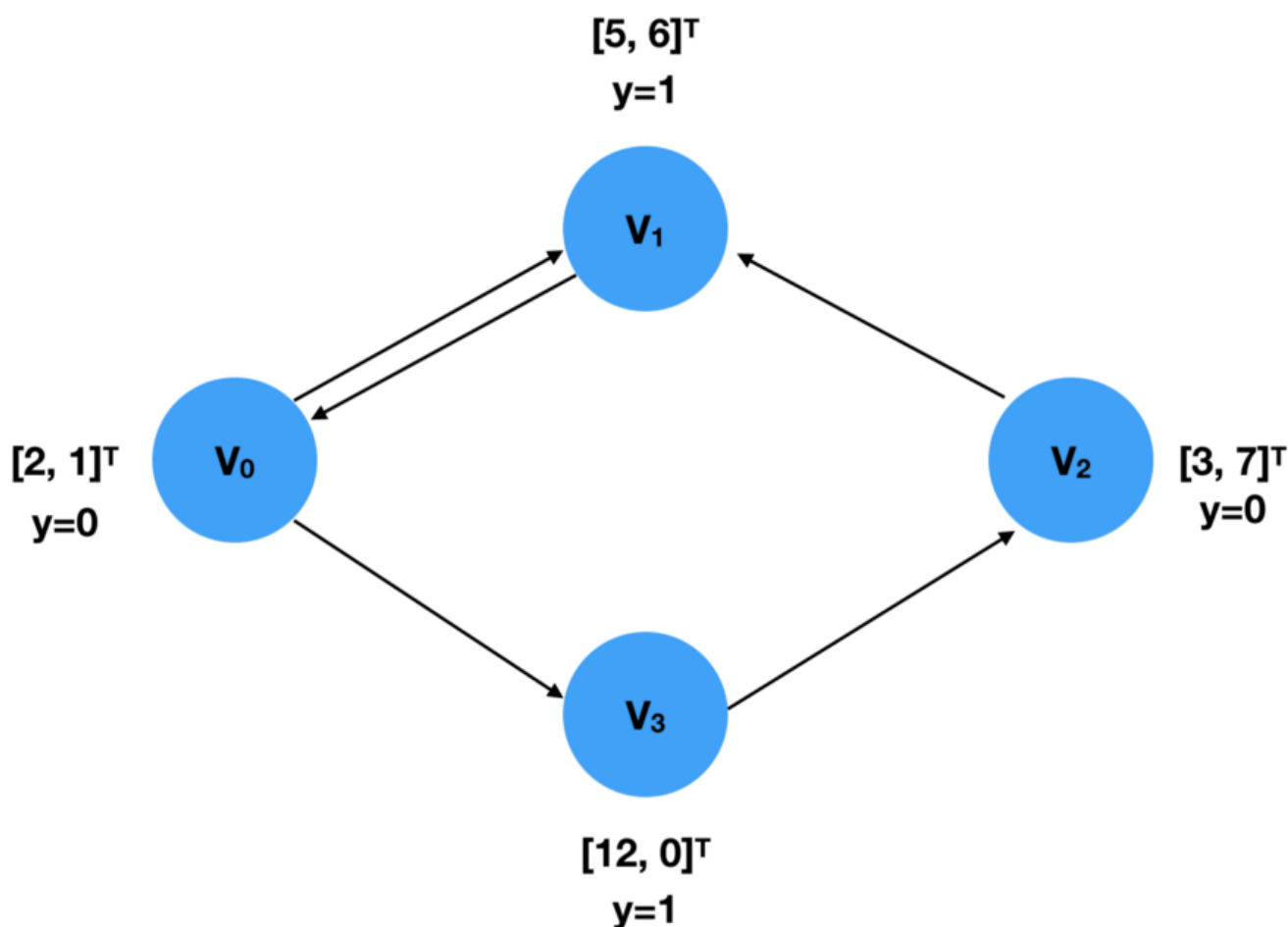
This section will walk you through the basics of PyG. Essentially, it will cover *torch_geometric.data* and *torch_geometric.nn*. You will learn how to pass geometric data into your GNN, and how to design a custom MessagePassing layer, the core of GNN.

Data

The *torch_geometric.data* module contains a Data class that allows you to create graphs from your data very easily. You only need to specify:

1. the attributes/ features associated with each node
2. the connectivity/adjacency of each node (edge index)

Let's use the following graph to demonstrate how to create a Data object



Example Graph

So there are 4 nodes in the graph, $v_1 \dots v_4$, each of which is associated with a 2-dimensional feature vector and a label y indicating its class. These two can be represented as FloatTensors:

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

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The graph connectivity (edge index) should be confined with the COO format, i.e. the first list contains the index of the source nodes, while the index of target nodes is specified in the second list.

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

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Putting them together, we can create a Data object as shown below:

```

1  import torch
2  from torch_geometric.data import Data
3
4
5  x = torch.tensor([[2,1], [5,6], [3,7], [12,0]], dtype=torch.float)
6  y = torch.tensor([0, 1, 0, 1], dtype=torch.float)
7
8  edge_index = torch.tensor([[0, 2, 1, 0, 3],
9                             [3, 1, 0, 1, 2]], dtype=torch.long)
10
11
12  data = Data(x=x, y=y, edge_index=edge_index)
13  >>> Data(edge_index=[2, 5], x=[4, 2], y=[4])

```

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Dataset

The dataset creation procedure is not very straightforward, but it may seem familiar to those who've used *torchvision*, as PyG is following its convention. PyG provides two different types of dataset classes, *InMemoryDataset* and *Dataset*. As they indicate literally, the former one is for data that fit in your RAM, while the second one is for much larger data. Since their implementations are quite similar, I will only cover *InMemoryDataset*.

To create an *InMemoryDataset* object, there are 4 functions you need to implement:

- *raw_file_names()*

It returns a list that shows a list of raw, unprocessed file names. If you only have a file then the returned list should only contain 1 element. In fact, you can simply return an empty list and specify your file later in *process()*.

- *processed_file_names()*

Similar to the last function, it also returns a list containing the file names of all the processed data. After *process()* is called, Usually, the returned list should only have one element, storing the only processed data file name.

- *download()*

This function should download the data you are working on to the directory as specified in *self.raw_dir*. If you don't need to download data, simply drop in

pass

in the function.

- *process()*

This is the most important method of *Dataset*. 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 *DataLoader* object. The following shows an example of the custom dataset from PvG official website.

```

1  import torch
2  from torch_geometric.data import InMemoryDataset
3
4

```

```
10 @property
11 def raw_file_names(self):
12     return ['some_file_1', 'some_file_2', ...]
13
14 @property
15 def processed_file_names(self):
16     return ['data.pt']
17
18 def download(self):
19     # Download to `self.raw_dir`.
20
21 def process(self):
22     # Read data into huge `Data` list.
23     data_list = [...]
24
25     if self.pre_filter is not None:
26         data_list = [data for data in data_list if self.pre_filter(data)]
27
28     if self.pre_transform is not None:
29         data_list = [self.pre_transform(data) for data in data_list]
30
31     data, slices = self.collate(data_list)
32     torch.save((data, slices), self.processed_paths[0])
```

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I will show you how I create a custom dataset from the data provided in Kéecy's Challenge 2019 later in this article.

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, shuffle=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

Message passing is the essence of GNN which describes how node embeddings are learned. I have talked about in my last post, so I will just briefly run through this with terms that conform to the PyG documentation.

denotes the **aggregation** function, γ denotes the **update** function. If the edges in the graph have no feature other than connectivity, e is essentially the edge index of the graph. The superscript represents the index of the layer. When $k=1$, x represents the input feature of each node. Below I will illustrate how each function works:

- `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)`:

You specify how you construct “message” for each of the node pair (x_i, x_j). Since it follows the calls of `propagate`, it can take any argument passing to `propagate`. One thing to note is that you can define the mapping from arguments to the specific nodes with “ $_i$ ” and “ $_j$ ”. Therefore, you must be very careful when naming the argument of this function.

- `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

Let’s see how we can implement a **SageConv** layer from the paper “Inductive Representation Learning on Large Graphs”. The message passing formula of SageConv is defined as:

$$\mathbf{h}_{\mathcal{N}(v)}^k \leftarrow \text{AGGREGATE}_k(\{\mathbf{h}_u^{k-1}, \forall u \in \mathcal{N}(v)\});$$

$$\mathbf{h}_v^k \leftarrow \sigma \left(\mathbf{W}^k \cdot \text{CONCAT}(\mathbf{h}_v^{k-1}, \mathbf{h}_{\mathcal{N}(v)}^k) \right)$$

<https://arxiv.org/abs/1706.02216>

Here, we use max pooling as the aggregation method. Therefore, the right-hand side of the first line can be written as:

$$\max(\{\sigma(\mathbf{W}_{\text{pool}} \mathbf{h}_{u_i}^k + \mathbf{b}), \forall u_i \in \mathcal{N}(v)\})$$

<https://arxiv.org/abs/1706.02216>

which illustrates how the “message” is constructed. Each neighboring node embedding is multiplied by a weight matrix, added a bias and passed through an activation function. This can be easily done with `torch.nn.Linear`.

```
class SAGEConv(MessagePassing):
    def __init__(self, in_channels, out_channels):
        super(SAGEConv, self).__init__(aggr='max')
        self.lin = torch.nn.Linear(in_channels, out_channels)
        self.act = torch.nn.ReLU()

    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
```

```
super(SAGEConv, self).__init__(aggr='max')
self.update_lin = torch.nn.Linear(in_channels + out_channels, in_channels, bias=False)
self.update_act = torch.nn.ReLU()
```

```
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_embedding)
    new_embedding = torch.update_act(new_embedding)

    return new_embedding
```

Putting it together, we have the following SageConv layer.

```
1 import torch
2 from torch.nn import Sequential as Seq, Linear, ReLU
3 from torch_geometric.nn import MessagePassing
4 from torch_geometric.utils import remove_self_loops, add_self_loops
5 class SAGEConv(MessagePassing):
6     def __init__(self, in_channels, out_channels):
7         super(SAGEConv, self).__init__(aggr='max') # "Max" aggregation.
8         self.lin = torch.nn.Linear(in_channels, out_channels)
9         self.act = torch.nn.ReLU()
10        self.update_lin = torch.nn.Linear(in_channels + out_channels, in_channels, bias=False)
11        self.update_act = torch.nn.ReLU()
12
13    def forward(self, x, edge_index):
14        # x has shape [N, in_channels]
15        # edge_index has shape [2, E]
16
17
18        edge_index, _ = remove_self_loops(edge_index)
19        edge_index, _ = add_self_loops(edge_index, num_nodes=x.size(0))
20
21
22        return self.propagate(edge_index, size=(x.size(0), x.size(0)), x=x)
23
24    def message(self, x_j):
25        # x_j has shape [E, in_channels]
26
27        x_j = self.lin(x_j)
28        x_j = self.act(x_j)
29
30        return x_j
31
32    def update(self, aggr_out, x):
33        # aggr_out has shape [N, out_channels]
34
```

41 return new_embedding

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The RecSys Challenge 2015 is challenging data scientists to build a session-based recommender system. Participants in this challenge are asked to solve two tasks:

1. Predict whether there will be a buy event followed by a sequence of clicks
2. Predict which item will be bought

First, we download the data from the official website of RecSys Challenge 2015 and construct a Dataset. We'll start with the first task as that one is easier.

The challenge provides two main sets of data, *yoochoose-clicks.dat*, and *yoochoose-buys.dat*, containing click events and buy events, respectively. Let's quickly glance through the data:

	session_id	timestamp	item_id	category
0	1	2014-04-07T10:51:09.277Z	214536502	0
1	1	2014-04-07T10:54:09.868Z	214536500	0
2	1	2014-04-07T10:54:46.998Z	214536506	0
3	1	2014-04-07T10:57:00.306Z	214577561	0
4	2	2014-04-07T13:56:37.614Z	214662742	0
5	2	2014-04-07T13:57:19.373Z	214662742	0
6	2	2014-04-07T13:58:37.446Z	214825110	0
7	2	2014-04-07T13:59:50.710Z	214757390	0
8	2	2014-04-07T14:00:38.247Z	214757407	0
9	2	2014-04-07T14:02:36.889Z	214551617	0
10	3	2014-04-02T13:17:46.940Z	214716935	0
11	3	2014-04-02T13:26:02.515Z	214774687	0
12	3	2014-04-02T13:30:12.318Z	214832672	0
13	4	2014-04-07T12:09:10.948Z	214836765	0
14	4	2014-04-07T12:26:25.416Z	214706482	0
15	6	2014-04-06T16:58:20.848Z	214701242	0
16	6	2014-04-06T17:02:26.976Z	214826623	0
17	7	2014-04-02T06:38:53.104Z	214826835	0
18	7	2014-04-02T06:39:05.854Z	214826715	0
19	8	2014-04-06T08:49:58.728Z	214838855	0

yoochoose-click.dat

	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	281626	2014-04-06T09:40:13.032Z	214535653	1883	1
3	420368	2014-04-04T06:13:28.848Z	214530572	6073	1
4	420368	2014-04-04T06:13:28.858Z	214835025	2617	1

10	11	2014-04-03T11:04:11.417Z	214821371	1046	1
11	11	2014-04-03T11:04:18.097Z	214821371	1046	1
12	12	2014-04-02T10:42:17.227Z	214717867	1778	4
13	489758	2014-04-06T09:59:52.422Z	214826955	1360	2
14	489758	2014-04-06T09:59:52.476Z	214826715	732	2
15	489758	2014-04-06T09:59:52.578Z	214827026	1046	1
16	140802	2014-04-02T16:52:21.678Z	214716984	1883	1
17	489756	2014-04-05T16:51:59.947Z	214716932	6177	1
18	420378	2014-04-03T07:41:02.566Z	214821017	1046	1
19	420378	2014-04-03T07:41:02.616Z	214821020	732	1

yoochoose-buys.dat

Preprocessing

After downloading the data, we preprocess it so that it can be fed to our model. `item_ids` are categorically encoded to ensure the encoded `item_ids`, which will later be mapped to an embedding matrix, starts at 0.

```

1 from sklearn.preprocessing import LabelEncoder
2
3 df = pd.read_csv('../input/yoochoose-click.dat', header=None)
4 df.columns=['session_id','timestamp','item_id','category']
5
6 buy_df = pd.read_csv('../input/yoochoose-buys.dat', header=None)
7 buy_df.columns=['session_id','timestamp','item_id','price','quantity']
8
9 item_encoder = LabelEncoder()
10 df['item_id'] = item_encoder.fit_transform(df.item_id)
11 df.head()
```

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	session_id	timestamp	item_id	category
10	3	2014-04-02T13:17:46.940Z	21302	0
11	3	2014-04-02T13:26:02.515Z	25022	0
12	3	2014-04-02T13:30:12.318Z	29039	0
49	19	2014-04-01T20:52:12.357Z	5749	0
50	19	2014-04-01T20:52:13.758Z	5749	0

Since the data is quite large, we subsample it for easier demonstration.

```

1 #randomly sample a couple of them
2 sampled_session_id = np.random.choice(df.session_id.unique(), 1000000, replace=False)
3 df = df.loc[df.session_id.isin(sampled_session_id)]
4 df.nunique()
```

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dtype: int64

Number of unique elements in the subsampled data

To determine the ground truth, i.e. whether there is any buy event for a given session, we simply check if a `session_id` in `yoochoose-clicks.dat` presents in `yoochoose-buys.dat` as well.

```
1 df['label'] = df.session_id.isin(buy_df.session_id)
2 df.head()
```

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	session_id	timestamp	item_id	category	label
10	3	2014-04-02T13:17:46.940Z	21302	0	False
11	3	2014-04-02T13:26:02.515Z	25022	0	False
12	3	2014-04-02T13:30:12.318Z	29039	0	False
49	19	2014-04-01T20:52:12.357Z	5749	0	False
50	19	2014-04-01T20:52:13.758Z	5749	0	False

Dataset Construction

The data is ready to be transformed into a Dataset object after the preprocessing step. Here, we treat each item in a session as a node, and therefore all items in the same session form a graph. To build the dataset, we group the preprocessed data by `session_id` and iterate over these groups. In each iteration, the `item_id` in each group are categorically encoded again since for each graph, the node index should count from 0. Thus, we have the following:

```
1 import torch
2 from torch_geometric.data import InMemoryDataset
3 from tqdm import tqdm
4
5 class YooChooseBinaryDataset(InMemoryDataset):
6     def __init__(self, root, transform=None, pre_transform=None):
7         super(YooChooseBinaryDataset, self).__init__(root, transform, pre_transform)
8         self.data, self.slices = torch.load(self.processed_paths[0])
9
10    @property
11    def raw_file_names(self):
12        return []
13
14    @property
15    def processed_file_names(self):
16        return ['./input/yoochoose_click_binary_1M_sess.dataset']
17
18    def download(self):
19        pass
20
21    def process(self):
22        data_list = []
```

```
28     group = group.reset_index(drop=True)
29     group['sess_item_id'] = sess_item_id
30     node_features = group.loc[group.session_id==session_id,['sess_item_id','item_id']].sort_values('sess_item_
31
32     node_features = torch.LongTensor(node_features).unsqueeze(1)
33     target_nodes = group.sess_item_id.values[1:]
34     source_nodes = group.sess_item_id.values[:-1]
35
36     edge_index = torch.tensor([source_nodes, target_nodes], dtype=torch.long)
37     x = node_features
38
39     y = torch.FloatTensor([group.label.values[0]])
40
41     data = Data(x=x, edge_index=edge_index, y=y)
42     data_list.append(data)
43
44     data, slices = self.collate(data_list)
45     torch.save((data, slices), self.processed_paths[0])
46
```

split it into three sets for training, validation, and testing.

```
1  dataset = dataset.shuffle()
2  train_dataset = dataset[:800000]
3  val_dataset = dataset[800000:900000]
4  test_dataset = dataset[900000:]
5  len(train_dataset), len(val_dataset), len(test_dataset)
```

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Build a Graph Neural Network

The following custom GNN takes reference from one of the examples in PyG's official Github repository. I changed the GraphConv layer with our self-implemented SAGEConv layer illustrated above. In addition, the output layer was also modified to match with a binary classification setup.

```
1  embed_dim = 128
2  from torch_geometric.nn import TopKPooling
3  from torch_geometric.nn import global_mean_pool as gap, global_max_pool as gmp
4  import torch.nn.functional as F
5  class Net(torch.nn.Module):
6      def __init__(self):
7          super(Net, self).__init__()
8
9          self.conv1 = SAGEConv(embed_dim, 128)
10         self.pool1 = TopKPooling(128, ratio=0.8)
11         self.conv2 = SAGEConv(128, 128)
12         self.pool2 = TopKPooling(128, ratio=0.8)
13         self.conv3 = SAGEConv(128, 128)
```

```
19     self.bn1 = torch.nn.BatchNorm1d(128)
20     self.bn2 = torch.nn.BatchNorm1d(64)
21     self.act1 = torch.nn.ReLU()
22     self.act2 = torch.nn.ReLU()
23
24     def forward(self, data):
25         x, edge_index, batch = data.x, data.edge_index, data.batch
26         x = self.item_embedding(x)
27         x = x.squeeze(1)
28
29         x = F.relu(self.conv1(x, edge_index))
30
31         x, edge_index, _, batch, _ = self.pool1(x, edge_index, None, batch)
32         x1 = torch.cat([gmp(x, batch), gap(x, batch)], dim=1)
33
34         x = F.relu(self.conv2(x, edge_index))
35
36         x, edge_index, _, batch, _ = self.pool2(x, edge_index, None, batch)
37         x2 = torch.cat([gmp(x, batch), gap(x, batch)], dim=1)
38
39         x = F.relu(self.conv3(x, edge_index))
40
41         x, edge_index, _, batch, _ = self.pool3(x, edge_index, None, batch)
42         x3 = torch.cat([gmp(x, batch), gap(x, batch)], dim=1)
43
44         x = x1 + x2 + x3
45
46         x = self.lin1(x)
47         x = self.act1(x)
48         x = self.lin2(x)
49         x = self.act2(x)
50         x = F.dropout(x, p=0.5, training=self.training)
51
52         x = torch.sigmoid(self.lin3(x)).squeeze(1)
53
54         return x
```

Training our custom GNN is very easy, we simply iterate the `DataLoader` constructed from the training set and back-propagate the loss function. Here, we use Adam as the optimizer with the learning rate set to 0.005 and Binary Cross Entropy as the loss function.

```
1     def train():
2         model.train()
3
4         loss_all = 0
```

```
10     loss = criterion(output, label)
11     loss.backward()
12     loss_all += data.num_graphs * loss.item()
13     optimizer.step()
14     return loss_all / len(train_dataset)
15
16 device = torch.device('cuda')
17 model = Net().to(device)
18 optimizer = torch.optim.Adam(model.parameters(), lr=0.005)
19 crit = torch.nn.BCELoss()
20 train_loader = DataLoader(train_dataset, batch_size=batch_size)
21 for epoch in range(num_epochs):
22     train()
23
```

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validation

This label is highly unbalanced with an overwhelming amount of negative labels since most of the sessions are not followed by any buy event. In other words, a dumb model guessing all negatives would give you above 90% accuracy. Therefore, instead of accuracy, Area Under Curve (AUC) is a better metric for this task as it only cares if the positive examples are scored higher than the negative examples. We use the off-the-shelf AUC calculation function from Sklearn.

```
1 def evaluate(loader):
2     model.eval()
3
4     predictions = []
5     labels = []
6
7     with torch.no_grad():
8         for data in loader:
9
10             data = data.to(device)
11             pred = model(data).detach().cpu().numpy()
12
13             label = data.y.detach().cpu().numpy()
14             predictions.append(pred)
15             labels.append(label)
```

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Result

I trained the model for 1 epoch. and measure the training, validation, and testing AUC scores:

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

Obtain an AUC score of around 0.75 for validation and test set. The score is very likely to improve if more data is used to train the model with larger training steps.

Conclusion

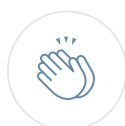
You have learned the basic usage of PyTorch Geometric, including dataset construction, custom graph layer, and training GNNs with real-world data. All the code in this post can also be found in my Github repo, where you can find another Jupyter notebook file in which I solve the second task of the RecSys Challenge 2015. I hope you have enjoyed this article. Should you have any questions or comments, please leave it below! Make sure to follow me on twitter where I share my blog post or interesting Machine Learning/ Deep Learning news! Have fun playing GNN with PyG!

Machine Learning

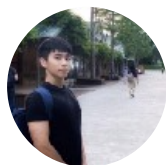
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WRITTEN BY

黃功詳 Steeve Huang

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Co-founder & CTO @ Rosetta.ai. Kaggle Competitions Master.

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