MLG:

Machine Learning with Graphs (Strojno učenje na grafih)

Assignment:	Final Project	
Submission ti		and date: 22.03.2023

Submission Fill in and include this cover sheet with each of your assignments. It is an honor code violation to write down the wrong date and/or time. Assignments are due at 9:00am and should be submitted through Gradescope and eUcilnica. Students should check Piazza for submission details.

Late Periods Each student will have a total of two free late periods. One late period expires the morning on the day before the next class. (Assignments are usually due on Fridays, which means the first late period expires on the following Tuesday at 9:00am.) Once these late periods are exhausted, any assignments turned in late will be penalized 50% per late period. However, no assignment will be accepted more than one late period after its due date.

Honor Code We strongly encourage students to form study groups. Students may discuss and work on assignments in groups. However, each student must write down their solutions independently, i.e., each student must understand the solution well enough in order to reconstruct it by him/herself. Students should clearly mention the names of all the other students who were part of their study group. Using code or solutions obtained from the web (GitHub, Google, previous years etc.) is considered an honor code violation. We check all submissions for plagiarism. We take the honor code very seriously and expect students to do the same.

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I acknowledge and accept the Honor Code.

(Signed)___

Medium article:

https://medium.com/ @drusany.jakob/ playlist-expansionwithIn this project, we will train a GNN to perform link prediction on a heterogenous graph from the Spotify Million Playlists dataset.

Import libraries

```
!pip install torch numpy matplotlib torch_geometric torch-scatter torcheval
# https://stackoverflow.com/a/73534928
import torch
!pip install torch-sparse -f https://data.pyg.org/whl/torch-{torch.__version__}.html
import tqdm
import torch
{\tt import\ torch\_geometric}
import numpy as np
import time
import matplotlib.pyplot as plt
import torch_geometric.transforms as T
from torcheval.metrics import BinaryAccuracy
import itertools
import time
import networkx as nx
import json
import os
import networkx as nx
from tqdm import tqdm
```

Configuration

```
Dataset files
```

```
from google.colab import drive
drive.mount('/content/drive')

dataset_path = "drive/MyDrive/spotify_million_playlist_dataset/data"

Drive already mounted at /content/drive; to attempt to forcibly remount, call drive.mount("/content/drive", force_remount=True).
```

Load graph

```
def load_graph(dataset_path=dataset_path):
    """Load a nx.Graph from disk.""
   filenames = os.listdir(dataset_path)
   G = nx.DiGraph()
   for i in tqdm(range(len(filenames)), unit="files"):
       with open(os.path.join(dataset\_path, filenames[i])) as json\_file:
            playlists = json.load(json_file)["playlists"]
            for playlist in playlists:
                playlist_name = f"spotify:playlist:{playlist['pid']}"
                G.add node(
                    playlist_name,
                    node_type="playlist",
                   num_followers=playlist["num_followers"],
                   num_tracks=playlist["num_tracks"],
                   num_artists=playlist["num_artists"],
                    num_albums=playlist["num_albums"],
                    duration_ms=playlist["duration_ms"],
                   collaborative=playlist["collaborative"],
                   num_edits=playlist["num_edits"]
                for track in playlist["tracks"]:
                   G.add_node(track["track_uri"], node_type="track", duration=track["duration_ms"])
                   G.add_node(track["album_uri"], node_type="album")
                    G.add_node(track["artist_uri"], node_type="artist")
                    G.add_edge(track["track_uri"], playlist_name, edge_type="track-playlist")
                   G.add_edge(track["track_uri"], track["album_uri"], edge_type="track-album")
                    G.add_edge(track["track_uri"], track["artist_uri"], edge_type="track-artist")
    return G
def nx2hetero(G):
```

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```
"""Convert a nx.Graph into a torch_geometric.data.HeteroData object."""
ids_by_type = {
    "playlist": {},
    "track": {},
    "artist": {},
    "album": {}
}
def node_id(node_type, id):
    d = ids_by_type[node_type]
    if id not in d:
       d[id] = len(d)
    return d[id]
node_features_by_type = {
    _
"playlist": [],
    "track": [],
    "artist": [],
    "album": []
}
# comment:
# {
      "name": "musical",
#
      "collaborative": "false",
#
      "pid": 5,
      "modified_at": 1493424000,
      "num_albums": 7,
      "num_tracks": 12,
#
      "num_followers": 1,
      "num_edits": 2,
      "duration_ms": 2657366,
      "num_artists": 6,
      "tracks": [
          {
               "pos": 0,
#
               "artist_name": "Degiheugi",
               "track_uri": "spotify:track:7vqa3sDmtEaVJ2gcvxtRID",
#
               "artist_uri": "spotify:artist:3V2paBXEoZIAhfZRJmo2jL",
               "track_name": "Finalement",
               "album_uri": "spotify:album:2KrRMJ9z7Xjoz1Az406UML",
#
               "duration_ms": 166264,
#
               "album_name": "Dancing Chords and Fireflies"
          },
#
      ],
# })
for node in G.nodes(data=True):
    t = node[1]["node_type"]
    node_id(t, node[0])
    if t == "playlist":
        if node[1]["collaborative"] not in ("true", "false"):
            raise\ Value Error (f"collaborative is not a boolean: \{node[1]['collaborative']\}")
        node_features_by_type["playlist"] += [[
            node[1]["num_followers"],
            node[1]["collaborative"] == 'true',
            node[1]["num_albums"],
            node[1]["num_tracks"],
            node[1]["num_edits"],
            node[1]["duration_ms"],
            node[1]["num_artists"]
        ]]
    elif t == "track":
        distances = nx.single_source_shortest_path_length(G, node[0], cutoff=2)
        node_features_by_type["track"] += [[node[1]["duration"], len(distances)]]
    elif t == "artist":
        distances = nx.single_source_shortest_path_length(G, node[0], cutoff=2)
        node_features_by_type["artist"] += [[len(distances)]]
    elif t == "album":
        \label{eq:distances} distances = nx.single\_source\_shortest\_path\_length(G, node[0], cutoff=2)
        node_features_by_type["album"] += [[len(distances)]]
edge_index_by_type = {
    ("track", "contains", "playlist"): [],
    ("track", "includes", "album"): [], ("track", "authors", "artist"): []
existing_edges = set()
for edge in G.edges(data=True):
    track_node = edge[0]
    other node = edge[1]
    if "track" not in track_node:
        track_node, other_node = other_node, track_node
```

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```
if (track node, other node) in existing edges:
            continue
        if G[edge[0]][edge[1]]["edge_type"] == "track-playlist":
            s_id = node_id("track", track_node)
            d_id = node_id("playlist", other_node)
            edge_index_by_type[("track", "contains", "playlist")] += [(s_id, d_id)]
        elif G[edge[0]][edge[1]]["edge_type"] == "track-album":
            s_id = node_id("track", track_node)
            d_id = node_id("album", other_node)
            \verb|edge_index_by_type[("track", "includes", "album")] += [(s_id, d_id)]|
        elif G[edge[0]][edge[1]]["edge_type"] == "track-artist":
            s_id = node_id("track", track_node)
            d_id = node_id("artist", other_node)
            edge_index_by_type[("track", "authors", "artist")] += [(s_id, d_id)]
        existing_edges.add((track_node, other_node))
    # construct HeteroData
    hetero = torch_geometric.data.HeteroData()
    # add initial node features
    hetero["playlist"].x = torch.FloatTensor(node_features_by_type["playlist"]).reshape(-1,len(node_features_by_type["playlist"]]0]))
    hetero["track"].x = torch.FloatTensor(node_features_by_type["track"]).reshape(-1,len(node_features_by_type["track"][0]))
    \label{lem:hetero} hetero["artist"]. x = torch. FloatTensor(node\_features\_by\_type["artist"]). reshape(-1,len(node\_features\_by\_type["artist"]]0]))
    # add edge indices
   hetero["track", "contains", "playlist"].edge_index = torch.tensor(edge_index_by_type[("track", "contains", "playlist")]).t()
hetero["track", "includes", "album"].edge_index = torch.tensor(edge_index_by_type[("track", "includes", "album")]).t()
hetero["track", "authors", "artist"].edge_index = torch.tensor(edge_index_by_type[("track", "authors", "artist")]).t()
    # post-processing
    hetero = torch_geometric.transforms.ToUndirected()(hetero)
    hetero = torch_geometric.transforms.NormalizeFeatures()(hetero)
def ghetero2datasets(ghetero):
    """Split the dataset into train, validation and test sets."""
    transform = T.Compose([
        T.NormalizeFeatures(),
        T.RandomLinkSplit(
            num_val=0.1,
            num_test=0.1,
            disjoint_train_ratio=0.3,
            neg sampling ratio=2.0,
            {\tt add\_negative\_train\_samples=False,}
            edge_types=("track", "contains", "playlist"),
            rev_edge_types=("playlist", "rev_contains", "track"),
    1)
    return transform(ghetero) # 3-tuple: data_train, data_val, data_test
```

Preprocessing

We took a subset of our dataset by taking a subgraph of 5000 nodes.

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```
def get_smart_playlist_subset(G, playlists_to_keep):
    keep_nodes = set()
    for node in playlists_to_keep:
       keep nodes.add(node[0])
        tracks = get_neigh_of_edge_type(G, "track-playlist", node[0])
        artists_and_albums = []
        for track in tracks:
            artists_and_albums += get_neigh_of_edge_type(G, "track-artist", track)
            artists_and_albums += get_neigh_of_edge_type(G, "track-album", track)
        keep_nodes = keep_nodes.union(set(tracks))
        keep_nodes = keep_nodes.union(set(artists_and_albums))
   return keep_nodes
def smart_split(G, splits=[100,500,1000,5000,10000]):
    ret = [None for _ in splits]
    for i in tqdm(splits):
        print(f"[{i}] started")
        start = time.time()
        playlists_to_keep = top_n_by_followers(G, i, "playlist")
        print(f"[\{i\}] \ got \ top \ n \ playlists \ in \ \{time.time() \ - \ start\} \ seconds")
        keep_nodes = get_smart_playlist_subset(G, playlists_to_keep)
        print(f"[\{i\}] \ finshed \ getting \ neighbors \ in \ \{time.time() - start\} \ seconds")
        print(f"\t(\{len(keep\_nodes)\}\ nodes\ =\ \{len(keep\_nodes)/len(G.nodes)\}\ \%\ of\ graph)")
        start = time.time()
        G_sub = nx.Graph(G.subgraph(keep_nodes))
        print(f"[{i}] finished subgraphing in {time.time() - start} seconds")
        start = time.time()
        splits[i] = G_sub
        print(f"[\{i\}] finished pickling in \{time.time() - start\} seconds")
    return ret
```

Model

```
Check if cuda is available
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
GNN embedding prediction network (three SAGEConv layers)
class GNN(torch.nn.Module):
   def __init__(self, hidden_channels):
       super(). init ()
       self. conv1 = torch\_geometric.nn. SAGEConv((-1, -1), hidden\_channels, normalize=True, dropout=True, bias=True, dropout\_prob=0.1)
       self. conv2 = torch\_geometric.nn. SAGEConv((-1, -1), hidden\_channels, normalize=True, dropout=True, bias=True, dropout\_prob=0.1)
       self.conv3 = torch_geometric.nn.SAGEConv((-1, -1), hidden_channels)
       self.reset_parameters()
   def forward(self, x, edge_index):
       x = self.conv1(x, edge_index)
       x = torch.nn.functional.leaky_relu(x, negative_slope=0.1)
       x = self.conv2(x, edge_index)
       x = torch.nn.functional.leaky_relu(x, negative_slope=0.1)
       x = self.conv3(x, edge_index)
       return x
   def reset_parameters(self):
       self.conv1.reset_parameters()
       self.conv2.reset_parameters()
       self.conv3.reset_parameters()
Link predictor (predicts using dot product)
class LinkPredictor(torch.nn.Module):
   def __init__(self):
       super().__init__()
   def forward(self, x_track, x_playlist, track_playlist_edge):
       track_embedding = x_track[track_playlist_edge[0]]
       playlist\_embedding = x\_playlist[track\_playlist\_edge[1]]
       # Apply dot-product to get a prediction per supervision edge:
       return (track_embedding * playlist_embedding).sum(dim=-1)
```

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```
Full model
```

```
class HeteroModel(torch.nn.Module):
   def __init__(self, hidden_channels, node_features, metadata):
       super().__init__()
       self.node lin = {
           k: torch.nn.Linear(v.shape[1], hidden_channels).to(device) for k, v in node_features.items()
       self.gnn = GNN(hidden_channels).to(device)
       self.gnn = torch_geometric.nn.to_hetero(self.gnn, metadata=metadata).to(device)
       self.classifier = LinkPredictor().to(device)
   def embed(self, data):
       x_dict = {
           k: self.node_lin[k](v) for k, v in data.x_dict.items()
       x_dict = self.gnn(x_dict, data.edge_index_dict)
       return x_dict
   def forward(self, data):
       x_{dict} = self.embed(data)
       pred = self.classifier(
           x_dict["track"],
           x_dict["playlist"],
           data["track", "contains", "playlist"].edge_label_index,
       return pred
   def reset_parameters(self):
       for _, v in self.node_lin.items():
           torch.nn.init.xavier_uniform_(v.weight)
       self.gnn.reset_parameters()
def dummy_generator(source):
   for e in source:
       yield e
Model train and test functions
outs = []
def test(model, data_test):
   with torch.no_grad():
       test_out = model(data_test.to(device)).to('cpu')
       truth = data_test["track", "contains", "playlist"].edge_label.to('cpu')
   test_loss = torch.nn.functional.mse_loss(
       test_out,
   metric = BinaryAccuracy()
   metric.update(test_out, truth)
   return float(test_loss), metric.compute()
def train(model, train_loader, optimizer, batch_wrapper=dummy_generator):
   model.train()
   accuracy = 0
   total_examples = total_loss = 0
    for batch in batch_wrapper(train_loader):
       optimizer.zero_grad()
       out = model(batch)
       truth = batch["track", "contains", "playlist"].edge_label
       loss = torch.nn.functional.mse_loss(
           out, truth
       loss.backward()
       optimizer.step()
       aute_gledam = out.to('cpu')
       outs.append(aute_gledam)
       metric = BinaryAccuracy()
       metric.update(aute_gledam, truth.to('cpu'))
       accuracy += metric.compute() * len(out)
```

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```
total_examples += len(out)
total_loss += float(loss) * len(out)
return total_loss / total_examples, accuracy / total_examples
```

Train the model

G = load_graph()

```
ghetero = nx2hetero(G)
data_train, data_val, data_test = ghetero2datasets(ghetero)
# create training mask for playlist nodes
train_mask = torch.zeros(ghetero["playlist"].x.shape[0], dtype=torch.bool)
train\_mask[torch.randperm(train\_mask.shape[0])[:int(train\_mask.shape[0]*0.8)]] = True
ghetero["playlist"].train_mask = train_mask
ghetero["playlist"].y = torch.LongTensor([1]*ghetero["playlist"].x.shape[0]).to(device)
model = HeteroModel(64, ghetero.x_dict, ghetero.metadata()).to(device)
optimizer = torch.optim.Adam(model.parameters(), lr=0.0001, weight_decay=0.00001)
edge_label_index = data_train["track", "contains", "playlist"].edge_label_index
edge_label = data_train["track", "contains", "playlist"].edge_label
train_loader = torch_geometric.loader.LinkNeighborLoader(
    data=data_train,
    num neighbors=[-1].
    neg_sampling_ratio=0.5,
    edge_label_index=(("track", "contains", "playlist"), edge_label_index),
    edge_label=edge_label,
    batch size=20000,
    shuffle=True,
    transform=T.ToDevice(device)
epoch = 2000
render\_graph = True
losses = []
accuracies = []
test_losses = []
test_accuracies = []
epoch\_iter = tqdm(range(epoch), unit='epoch', desc='Training', bar\_format='\{desc:<5.5\}\{percentage:3.0f\}\%|\{bar:10\}\{r\_bar\}'\}|
for i in epoch_iter:
    loss, accuracy = train(model, train_loader, optimizer)
    losses.append(loss)
    accuracies.append(accuracy)
    test_loss, test_acc = test(model, data_val)
    test_losses.append(test_loss)
    test_accuracies.append(test_acc)
    epoch_iter.set_postfix_str(f"Train Loss: {loss:.4f}, Train Accuracy {accuracy:.4f}, Valid Loss {test_loss:.4f}, Valid Accuracy {test_acc:.4f}")
Render learning graph
plt.clf()
# add labels
plt.plot(np.arange(len(accuracies)), accuracies, label='Accuracy')
plt.plot(np.arange(len(losses)), losses, label='Loss')
plt.plot(np.arange(len(test_losses)), test_losses, label='Test Loss')
plt.plot(np.arange(len(test_accuracies)), test_accuracies, label='Test Accuracy')
# start plot at 0
plt.ylim(0, 1)
plt.legend()
plt.show()
```

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