

GAT

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sample_data

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mnist_train_small.csv

617.pkl

717.pkl

Digraph.gv

Digraph.gv.pdf

```

[2] def encode_onehot(labels):
    # The classes must be sorted before encoding to enable static class encoding.
    # In other words, make sure the first class always maps to index 0.
    classes = sorted(list(set(labels)))
    classes_dict = {c: np.identity(len(classes))[i, :] for i, c in enumerate(classes)}
    labels_onehot = np.array(list(map(classes_dict.get, labels)), dtype=np.int32)
    return labels_onehot

[3] def load_data(path="/content/sample_data/cora", dataset="cora"):
    """Load citation network dataset (cora only for now)"""
    print('Loading {} dataset...'.format(dataset))

    idx_features_labels = np.genfromtxt("{}_content".format(path, dataset), dtype=np.dtype(str))
    features = sp.csr_matrix(idx_features_labels[:, 1:-1], dtype=np.float32)
    labels = encode_onehot(idx_features_labels[:, -1])

    # build graph
    idx = np.array(idx_features_labels[:, 0], dtype=np.int32)
    idx_map = {j: i for i, j in enumerate(idx)}
    edges_unordered = np.genfromtxt("{}_cites".format(path, dataset), dtype=np.int32)
    edges = np.array(list(map(idx_map.get, edges_unordered.flatten())), dtype=np.int32).reshape(edges_unordered.shape)
    adj = sp.coo_matrix((np.ones(edges.shape[0]), (edges[:, 0], edges[:, 1])), shape=(labels.shape[0], labels.shape[0]), dtype=np.float32)

    # build symmetric adjacency matrix
    adj = adj + adj.T.multiply(adj.T > adj) - adj.multiply(adj.T > adj)

    features = normalize_features(features)
    adj = normalize_adj(adj + sp.eye(adj.shape[0]))

    idx_train = range(140)
    idx_val = range(200, 500)
    idx_test = range(500, 1500)

    adj = torch.FloatTensor(np.array(adj.todense()))
    features = torch.FloatTensor(np.array(features.todense()))
    labels = torch.LongTensor(np.where(labels)[1])

    idx_train = torch.LongTensor(idx_train)
    idx_val = torch.LongTensor(idx_val)
    idx_test = torch.LongTensor(idx_test)

    return adj, features, labels, idx_train, idx_val, idx_test

[4] def normalize_adj(mx):
    """Row-normalize sparse matrix"""
    rowsum = np.array(mx.sum(1))
    r_inv_sqrt = np.power(rowsum, -0.5).flatten()
    r_inv_sqrt[np.isinf(r_inv_sqrt)] = 0.
    r_mat_inv_sqrt = sp.diags(r_inv_sqrt)
    return mx.dot(r_mat_inv_sqrt).transpose().dot(r_mat_inv_sqrt)

[5] def normalize_features(mx):
    """Row-normalize sparse matrix"""
    rowsum = np.array(mx.sum(1))
    r_inv = np.power(rowsum, -1).flatten()
    r_inv[np.isinf(r_inv)] = 0.
    r_mat_inv = sp.diags(r_inv)
    mx = r_mat_inv.dot(mx)
    return mx

[6] def accuracy(output, labels):
    preds = output.max(1)[1].type_as(labels)
    correct = preds.eq(labels).double()
    correct = correct.sum()
    return correct / len(labels)

[7] import numpy as np
import torch
import torch.nn as nn
import torch.nn.functional as F

[8] class GraphAttentionLayer(nn.Module):
    """
    Simple GAT layer, similar to https://arxiv.org/abs/1710.10903
    """
    def __init__(self, in_features, out_features, dropout, alpha, concat=True):
        super(GraphAttentionLayer, self).__init__()
        self.dropout = dropout
        self.in_features = in_features
        self.out_features = out_features
        self.alpha = alpha
        self.concat = concat

        self.W = nn.Parameter(torch.empty(size=(in_features, out_features)))
        nn.init.xavier_uniform_(self.W.data, gain=1.414)
        self.a = nn.Parameter(torch.empty(size=(2*out_features, 1)))
        nn.init.xavier_uniform_(self.a.data, gain=1.414)

        self.leakyrelu = nn.LeakyReLU(self.alpha)

    def forward(self, h, adj):
        Wh = torch.mm(h, self.W) # h.shape: (N, in_features), Wh.shape: (N, out_features)
        e = self._prepare_attentional_mechanism_input(Wh)

        zero_vec = -9e15*torch.ones_like(e)
        attention = torch.where(adj > 0, e, zero_vec)
        attention = F.softmax(attention, dim=1)
        attention = F.dropout(attention, self.dropout, training=self.training)
        h_prime = torch.matmul(attention, Wh)

        if self.concat:
            return F.leaky_relu(self.leakyrelu(h_prime), self.alpha)
        else:
            return attention, h_prime

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        return F.elu(h_prime)
    else:
        return h_prime

    def _prepare_attentional_mechanism_input(self, Wh):
        # Wh.shape (N, out_feature)
        # self.a.shape (2 * out_feature, 1)
        # Wh1&2.shape (N, 1)
        # e.shape (N, N)
        Wh1 = torch.matmul(Wh, self.a[:self.out_features, :])
        Wh2 = torch.matmul(Wh, self.a[self.out_features:, :])
        # broadcast add
        e = Wh1 + Wh2.T
        return self.leakyrelu(e)

    def __repr__(self):
        return self.__class__.__name__ + ' (' + str(self.in_features) + ' -> ' + str(self.out_features) + ')'

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[9] class SpecialSpmmFunction(torch.autograd.Function):
    """Special function for only sparse region backpropataion layer."""
    @staticmethod
    def forward(ctx, indices, values, shape, b):
        assert indices.requires_grad == False
        a = torch.sparse_coo_tensor(indices, values, shape)
        ctx.save_for_backward(a, b)
        ctx.N = shape[0]
        return torch.matmul(a, b)

    @staticmethod
    def backward(ctx, grad_output):
        a, b = ctx.saved_tensors
        grad_values = grad_b = None
        if ctx.needs_input_grad[1]:
            grad_a_dense = grad_output.matmul(b.t())
            edge_idx = a._indices()[:, 0] * ctx.N + a._indices()[:, 1]
            grad_values = grad_a_dense.view(-1)[edge_idx]
        if ctx.needs_input_grad[3]:
            grad_b = a.t().matmul(grad_output)
        return None, grad_values, None, grad_b

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[10] class SpecialSpmm(nn.Module):
    def forward(self, indices, values, shape, b):
        return SpecialSpmmFunction.apply(indices, values, shape, b)

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[11] class SpGraphAttentionLayer(nn.Module):
    """
    Sparse version GAT layer, similar to https://arxiv.org/abs/1710.10903
    """

    def __init__(self, in_features, out_features, dropout, alpha, concat=True):
        super(SpGraphAttentionLayer, self).__init__()
        self.in_features = in_features
        self.out_features = out_features
        self.alpha = alpha
        self.concat = concat

        self.W = nn.Parameter(torch.zeros(size=(in_features, out_features)))
        nn.init.xavier_normal_(self.W.data, gain=1.414)

        self.a = nn.Parameter(torch.zeros(size=(1, 2*out_features)))
        nn.init.xavier_normal_(self.a.data, gain=1.414)

        self.dropout = nn.Dropout(dropout)
        self.leakyrelu = nn.LeakyReLU(self.alpha)
        self.special_spmm = SpecialSpmm()

    def forward(self, input, adj):
        dv = 'cuda' if input.is_cuda else 'cpu'

        N = input.size()[0]
        edge = adj nonzero().t()

        h = torch.mm(input, self.W)
        # h: N x out
        assert not torch.isnan(h).any()

        # Self-attention on the nodes - Shared attention mechanism
        edge_h = torch.cat((h[edge[0], :], h[edge[1], :], ), dim=1).t()
        # edge: 2*D x E

        edge_e = torch.exp(-self.leakyrelu(self.a.mm(edge_h).squeeze()))
        assert not torch.isnan(edge_e).any()
        # edge_e: E

        e_rowsum = self.special_spmm(edge, edge_e, torch.Size([N, N]), torch.ones(size=(N,1), device=dv))
        # e_rowsum: N x 1

        edge_e = self.dropout(edge_e)
        # edge_e: E

        h_prime = self.special_spmm(edge, edge_e, torch.Size([N, N]), h)
        assert not torch.isnan(h_prime).any()
        # h_prime: N x out

        h_prime = h_prime.div(e_rowsum)
        # h_prime: N x out
        assert not torch.isnan(h_prime).any()

        if self.concat:
            # if this layer is not last layer,
            return F.elu(h_prime)
        else:
            # if this layer is last layer,
            return h_prime

    def __repr__(self):
        return self.__class__.__name__ + ' (' + str(self.in_features) + ' -> ' + str(self.out_features) + ')'

```

```

[12] import torch
import torch.nn as nn
import torch.nn.functional as F

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[13] class GAT(nn.Module):
    def __init__(self, nfeat, nhid, nclass, dropout, alpha, nheads):
        """Dense version of GAT."""

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super(GAT, self).__init__()
self.dropout = dropout

self.attentions = [GraphAttentionLayer(nfeat, nhid, dropout=dropout, alpha=alpha, concat=True) for _ in range(nheads)]
for i, attention in enumerate(self.attentions):
    self.add_module('attention_{}'.format(i), attention)

self.out_att = GraphAttentionLayer(nhid * nheads, nclass, dropout=dropout, alpha=alpha, concat=False)

def forward(self, x, adj):
    x = F.dropout(x, self.dropout, training=self.training)
    x = torch.cat([att(x, adj) for att in self.attentions], dim=1)
    x = F.dropout(x, self.dropout, training=self.training)
    x = F.elu(self.out_att(x, adj))
    return F.log_softmax(x, dim=1)

```

[14] class SpGAT(nn.Module):
 def __init__(self, nfeat, nhid, nclass, dropout, alpha, nheads):
 """Sparse version of GAT."""
 super(SpGAT, self).__init__()
 self.dropout = dropout

 self.attentions = [SpGraphAttentionLayer(nfeat,
 nhid,
 dropout=dropout,
 alpha=alpha,
 concat=True) for _ in range(nheads)]
 for i, attention in enumerate(self.attentions):
 self.add_module('attention_{}'.format(i), attention)

 self.out_att = SpGraphAttentionLayer(nhid * nheads,
 nclass,
 dropout=dropout,
 alpha=alpha,
 concat=False)

 def forward(self, x, adj):
 x = F.dropout(x, self.dropout, training=self.training)
 x = torch.cat([att(x, adj) for att in self.attentions], dim=1)
 x = F.dropout(x, self.dropout, training=self.training)
 x = F.elu(self.out_att(x, adj))
 return F.log_softmax(x, dim=1)

[15] from __future__ import division
from __future__ import print_function

import os
import glob
import time
import random
import argparse
import numpy as np
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim
from torch.autograd import Variable

[16] parser = argparse.ArgumentParser()

[17] parser.add_argument('--no-cuda', action='store_true', default=False, help='Disables CUDA training.')
parser.add_argument('--fastmode', action='store_true', default=False, help='Validate during training pass.')
parser.add_argument('--sparse', action='store_true', default=False, help='GAT with sparse version or not.')
parser.add_argument('--seed', type=int, default=72, help='Random seed.')
parser.add_argument('--epochs', type=int, default=10000, help='Number of epochs to train.')
parser.add_argument('--lr', type=float, default=0.005, help='Initial learning rate.')
parser.add_argument('--weight_decay', type=float, default=5e-4, help='Weight decay (L2 loss on parameters).')
parser.add_argument('--hidden', type=int, default=8, help='Number of hidden units.')
parser.add_argument('--nb_heads', type=int, default=8, help='Number of head attentions.')
parser.add_argument('--dropout', type=float, default=0.6, help='Dropout rate (1 - keep probability.).')
parser.add_argument('--alpha', type=float, default=0.2, help='Alpha for the leaky_relu.')
parser.add_argument('--patience', type=int, default=100, help='Patience')
parser.add_argument('-f')

_StorerAction(option_strings=['-f'], dest='f', nargs=None, const=None, default=None, type=None, choices=None, help=None, metavar=None)

[18] args = parser.parse_args()
args.cuda = not args.no_cuda and torch.cuda.is_available()

[19] random.seed(args.seed)
np.random.seed(args.seed)
torch.manual_seed(args.seed)
if args.cuda:
 torch.cuda.manual_seed(args.seed)

[20] adj, features, labels, idx_train, idx_val, idx_test = load_data()

Loading cora dataset...

[21] if args.sparse:
 model = SpGAT(nfeat=features.shape[1],
 nhid=args.hidden,
 nclass=int(labels.max()) + 1,
 dropout=args.dropout,
 nheads=args.nb_heads,
 alpha=args.alpha)
else:
 model = GAT(nfeat=features.shape[1],
 nhid=args.hidden,
 nclass=int(labels.max()) + 1,
 dropout=args.dropout,
 nheads=args.nb_heads,
 alpha=args.alpha)
optimizer = optim.Adam(model.parameters(),
 lr=args.lr,
 weight_decay=args.weight_decay)

[22] if args.cuda:
 model.cuda()
 features = features.cuda()
 adj = adj.cuda()
 labels = labels.cuda()

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idx_train = idx_train.cuda()
idx_val = idx_val.cuda()
idx_test = idx_test.cuda()

features, adj, labels = Variable(features), Variable(adj), Variable(labels)

[23] def train(epoch):
    t = time.time()
    model.train()
    optimizer.zero_grad()
    output = model(features, adj)
    loss_train = F.nll_loss(output[idx_train], labels[idx_train])
    acc_train = accuracy(output[idx_train], labels[idx_train])
    loss_train.backward()
    optimizer.step()

    if not args.fastmode:
        # Evaluate validation set performance separately,
        # deactivates dropout during validation run.
        model.eval()
        output = model(features, adj)

    loss_val = F.nll_loss(output[idx_val], labels[idx_val])
    acc_val = accuracy(output[idx_val], labels[idx_val])
    print('Epoch: {:.0d}'.format(epoch+1),
          'loss_train: {:.4f}'.format(loss_train.data.item()),
          'acc_train: {:.4f}'.format(acc_train.data.item()),
          'loss_val: {:.4f}'.format(loss_val.data.item()),
          'acc_val: {:.4f}'.format(acc_val.data.item()),
          'time: {:.4f}s'.format(time.time() - t))

    return loss_val.data.item()

[24] def compute_test():
    model.eval()
    output = model(features, adj)
    loss_test = F.nll_loss(output[idx_test], labels[idx_test])
    acc_test = accuracy(output[idx_test], labels[idx_test])
    print("Test set results:",
          "loss= {:.4f}".format(loss_test.data.item()),
          "accuracy= {:.4f}".format(acc_test.data.item()))

[25] # Train model
t_total = time.time()
loss_values = []
bad_counter = 0
best = args.epochs + 1
best_epoch = 0
for epoch in range(args.epochs):
    loss_values.append(train(epoch))

    torch.save(model.state_dict(), '{}.pkl'.format(epoch))
    if loss_values[-1] < best:
        best = loss_values[-1]
        best_epoch = epoch
        bad_counter = 0
    else:
        bad_counter += 1

    if bad_counter == args.patience:
        break

    files = glob.glob('*.*')
    for file in files:
        epoch_nb = int(file.split('.')[0])
        if epoch_nb < best_epoch:
            os.remove(file)

    files = glob.glob('*.pkl')
    for file in files:
        epoch_nb = int(file.split('.')[0])
        if epoch_nb > best_epoch:
            os.remove(file)

Epoch: 0661 loss_train: 0.5724 acc_train: 0.8143 loss_val: 0.6579 acc_val: 0.8100 time: 0.0737s
Epoch: 0662 loss_train: 0.5605 acc_train: 0.8357 loss_val: 0.6581 acc_val: 0.8100 time: 0.0737s
Epoch: 0663 loss_train: 0.5759 acc_train: 0.8429 loss_val: 0.6582 acc_val: 0.8100 time: 0.0737s
Epoch: 0664 loss_train: 0.6254 acc_train: 0.8214 loss_val: 0.6583 acc_val: 0.8100 time: 0.0737s
Epoch: 0665 loss_train: 0.5461 acc_train: 0.8571 loss_val: 0.6583 acc_val: 0.8100 time: 0.0738s
Epoch: 0666 loss_train: 0.5912 acc_train: 0.8357 loss_val: 0.6584 acc_val: 0.8100 time: 0.0738s
Epoch: 0667 loss_train: 0.5772 acc_train: 0.8357 loss_val: 0.6579 acc_val: 0.8100 time: 0.0738s
Epoch: 0668 loss_train: 0.5881 acc_train: 0.8143 loss_val: 0.6576 acc_val: 0.8100 time: 0.0737s
Epoch: 0669 loss_train: 0.5910 acc_train: 0.8143 loss_val: 0.6572 acc_val: 0.8100 time: 0.0736s
Epoch: 0670 loss_train: 0.5294 acc_train: 0.8571 loss_val: 0.6568 acc_val: 0.8200 time: 0.0736s
Epoch: 0671 loss_train: 0.6458 acc_train: 0.7643 loss_val: 0.6563 acc_val: 0.8200 time: 0.0737s
Epoch: 0672 loss_train: 0.5741 acc_train: 0.8571 loss_val: 0.6563 acc_val: 0.8200 time: 0.0737s
Epoch: 0673 loss_train: 0.5568 acc_train: 0.8286 loss_val: 0.6566 acc_val: 0.8200 time: 0.0737s
Epoch: 0674 loss_train: 0.6350 acc_train: 0.7929 loss_val: 0.6567 acc_val: 0.8200 time: 0.0738s
Epoch: 0675 loss_train: 0.5923 acc_train: 0.8429 loss_val: 0.6569 acc_val: 0.8233 time: 0.0738s
Epoch: 0676 loss_train: 0.5214 acc_train: 0.8500 loss_val: 0.6571 acc_val: 0.8233 time: 0.0738s
Epoch: 0677 loss_train: 0.5714 acc_train: 0.8643 loss_val: 0.6572 acc_val: 0.8233 time: 0.0737s
Epoch: 0678 loss_train: 0.6063 acc_train: 0.8000 loss_val: 0.6574 acc_val: 0.8233 time: 0.0737s
Epoch: 0679 loss_train: 0.6239 acc_train: 0.8071 loss_val: 0.6577 acc_val: 0.8267 time: 0.0737s
Epoch: 0680 loss_train: 0.5992 acc_train: 0.8500 loss_val: 0.6580 acc_val: 0.8267 time: 0.0737s
Epoch: 0681 loss_train: 0.6340 acc_train: 0.7929 loss_val: 0.6583 acc_val: 0.8267 time: 0.0737s
Epoch: 0682 loss_train: 0.5761 acc_train: 0.8500 loss_val: 0.6582 acc_val: 0.8267 time: 0.0737s
Epoch: 0683 loss_train: 0.5393 acc_train: 0.8429 loss_val: 0.6589 acc_val: 0.8300 time: 0.0738s
Epoch: 0684 loss_train: 0.6477 acc_train: 0.8286 loss_val: 0.6590 acc_val: 0.8300 time: 0.0737s
Epoch: 0685 loss_train: 0.6285 acc_train: 0.8571 loss_val: 0.6592 acc_val: 0.8267 time: 0.0737s
Epoch: 0686 loss_train: 0.6385 acc_train: 0.8429 loss_val: 0.6589 acc_val: 0.8267 time: 0.0737s
Epoch: 0687 loss_train: 0.6081 acc_train: 0.8000 loss_val: 0.6584 acc_val: 0.8300 time: 0.0737s
Epoch: 0688 loss_train: 0.6802 acc_train: 0.7857 loss_val: 0.6586 acc_val: 0.8300 time: 0.0738s
Epoch: 0689 loss_train: 0.5380 acc_train: 0.8786 loss_val: 0.6573 acc_val: 0.8300 time: 0.0737s
Epoch: 0690 loss_train: 0.5949 acc_train: 0.8214 loss_val: 0.6566 acc_val: 0.8300 time: 0.0737s
Epoch: 0691 loss_train: 0.5502 acc_train: 0.8429 loss_val: 0.6560 acc_val: 0.8300 time: 0.0738s
Epoch: 0692 loss_train: 0.6266 acc_train: 0.8214 loss_val: 0.6555 acc_val: 0.8300 time: 0.0740s
Epoch: 0693 loss_train: 0.6444 acc_train: 0.8429 loss_val: 0.6553 acc_val: 0.8300 time: 0.0737s
Epoch: 0694 loss_train: 0.4926 acc_train: 0.8571 loss_val: 0.6547 acc_val: 0.8300 time: 0.0736s
Epoch: 0695 loss_train: 0.5167 acc_train: 0.8357 loss_val: 0.6543 acc_val: 0.8267 time: 0.0736s
Epoch: 0696 loss_train: 0.6318 acc_train: 0.8357 loss_val: 0.6541 acc_val: 0.8233 time: 0.0736s
Epoch: 0697 loss_train: 0.6173 acc_train: 0.8500 loss_val: 0.6539 acc_val: 0.8200 time: 0.0738s
Epoch: 0698 loss_train: 0.7201 acc_train: 0.7571 loss_val: 0.6537 acc_val: 0.8200 time: 0.0738s
Epoch: 0699 loss_train: 0.6611 acc_train: 0.8071 loss_val: 0.6535 acc_val: 0.8200 time: 0.0738s
Epoch: 0700 loss_train: 0.6430 acc_train: 0.8143 loss_val: 0.6532 acc_val: 0.8167 time: 0.0738s
Epoch: 0701 loss_train: 0.7380 acc_train: 0.7714 loss_val: 0.6526 acc_val: 0.8167 time: 0.0737s
Epoch: 0702 loss_train: 0.6187 acc_train: 0.7929 loss_val: 0.6523 acc_val: 0.8167 time: 0.0737s
Epoch: 0703 loss_train: 0.6422 acc_train: 0.7857 loss_val: 0.6522 acc_val: 0.8167 time: 0.0737s
Epoch: 0704 loss_train: 0.5664 acc_train: 0.8286 loss_val: 0.6521 acc_val: 0.8167 time: 0.0738s
Epoch: 0705 loss_train: 0.5104 acc_train: 0.8714 loss_val: 0.6522 acc_val: 0.8167 time: 0.0736s
Epoch: 0706 loss_train: 0.5663 acc_train: 0.8571 loss_val: 0.6520 acc_val: 0.8167 time: 0.0737s

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Epoch: 0700 loss_train: 0.6603 acc_train: 0.6974 loss_val: 0.6120 acc_val: 0.8107 time: 0.0737s
Epoch: 0707 loss_train: 0.6045 acc_train: 0.7929 loss_val: 0.6519 acc_val: 0.8167 time: 0.0737s
Epoch: 0708 loss_train: 0.6252 acc_train: 0.8143 loss_val: 0.6519 acc_val: 0.8167 time: 0.0737s
Epoch: 0709 loss_train: 0.5904 acc_train: 0.8143 loss_val: 0.6519 acc_val: 0.8167 time: 0.0737s
Epoch: 0710 loss_train: 0.6438 acc_train: 0.8808 loss_val: 0.6522 acc_val: 0.8133 time: 0.0737s
Epoch: 0711 loss_train: 0.5788 acc_train: 0.8429 loss_val: 0.6523 acc_val: 0.8167 time: 0.0738s
Epoch: 0712 loss_train: 0.6385 acc_train: 0.8214 loss_val: 0.6523 acc_val: 0.8167 time: 0.0738s
Epoch: 0713 loss_train: 0.6275 acc_train: 0.8214 loss_val: 0.6523 acc_val: 0.8200 time: 0.0738s
Epoch: 0714 loss_train: 0.6190 acc_train: 0.8357 loss_val: 0.6529 acc_val: 0.8200 time: 0.0736s
Epoch: 0715 loss_train: 0.5708 acc_train: 0.8429 loss_val: 0.6534 acc_val: 0.8200 time: 0.0738s
Epoch: 0716 loss_train: 0.6111 acc_train: 0.8500 loss_val: 0.6534 acc_val: 0.8200 time: 0.0740s
Epoch: 0717 loss_train: 0.5201 acc_train: 0.8500 loss_val: 0.6542 acc_val: 0.8167 time: 0.0742s
Epoch: 0718 loss_train: 0.7117 acc_train: 0.7500 loss_val: 0.6547 acc_val: 0.8167 time: 0.0738s
```

```
[26] print("Optimization Finished!")
print("Total time elapsed: {:.4f}s".format(time.time() - t_total))

# Restore best model
print('Loading {}th epoch'.format(best_epoch))
model.load_state_dict(torch.load('{}.pkl'.format(best_epoch)))

# Testing
compute_test()
```

Optimization Finished!
Total time elapsed: 59.5648s
Loading 617th epoch
Test set results: loss= 0.6626 accuracy= 0.8410

```
[27] from graphviz import Digraph

import torch
# import models

def make_dot(var, params):
    """ Produces Graphviz representation of PyTorch autograd graph.

    Blue nodes are the Variables that require grad, orange are Tensors
    saved for backward in torch.autograd.Function

    Args:
        var: output Variable
        params: dict of (name, Variable) to add names to node that
                require grad (TODO: make optional)
    """
    param_map = {id(v): k for k, v in params.items()}
    print(param_map)

    node_attr = dict(style='filled',
                     shape='box',
                     align='left',
                     fontsize='12',
                     ranksep='0.1',
                     height='0.2')
    dot = Digraph(node_attr=node_attr, graph_attr=dict(size="12,12"))
    seen = set()

    def size_to_str(size):
        return '({},{})'.join(['%d' % v for v in size])

    def add_nodes(var):
        if var not in seen:
            if torch.is_tensor(var):
                dot.node(str(id(var)), size_to_str(var.size()), fillcolor='orange')
            elif hasattr(var, 'variable'):
                u = var.variable
                node_name = '%s\n%s' % (param_map.get(id(u)), size_to_str(u.size()))
                dot.node(str(id(var)), node_name, fillcolor='lightblue')
            else:
                dot.node(str(id(var)), str(type(var).__name__))
            seen.add(var)
        if hasattr(var, 'next_functions'):
            for u in var.next_functions:
                if u[0] is not None:
                    dot.edge(str(id(u[0])), str(id(var)))
                    add_nodes(u[0])
        if hasattr(var, 'saved_tensors'):
            for t in var.saved_tensors:
                dot.edge(str(id(t)), str(id(var)))
                add_nodes(t)
        add_nodes(var.grad_fn)
    return dot
```

```
[28] inputs = torch.randn(100, 50).cuda()
adj = torch.randn(100, 100).cuda()
model = SpGAT(50, 8, 7, 0.5, 0.01, 3)
model = model.cuda()
y = model(inputs, adj)

g = make_dot(y, model.state_dict())
g.view()
```

{140600975158944: 'attention_0.W', 140600975158624: 'attention_0.a', 140600975158784: 'attention_1.W', 140600975159024: 'attention_1.a', 140600975157424: 'attention_2.W', 'Digraph.gv.pdf'}

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