

# Graph Neural Network – Exercise

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## Outline

**1. Objective**

**2. From MLP to GNN**

**3. Coding**

**4. Experiment on Caltech-101 and PACS Datasets**

## Outline

1. Objective

2. From MLP to GNN

3. Coding

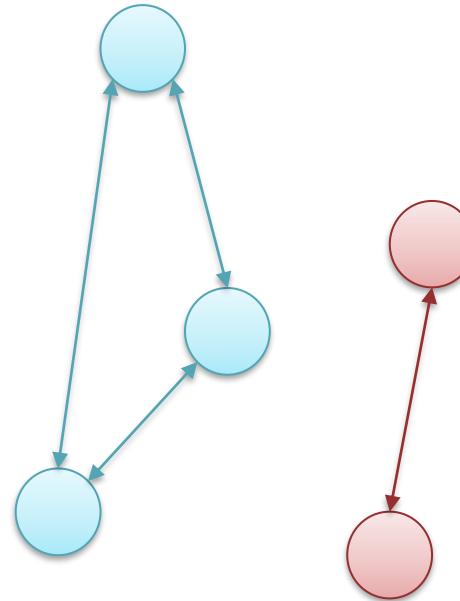
4. Experiment on Caltech-101 and PACS Datasets

# Objective

To utilize GNNs (Graph Neural Networks) for any problem, three sequential questions need to be addressed:

- What is a node?
- What is an edge?
- Can we incorporate an auxiliary loss function?

How does GNN operate?



# Objective

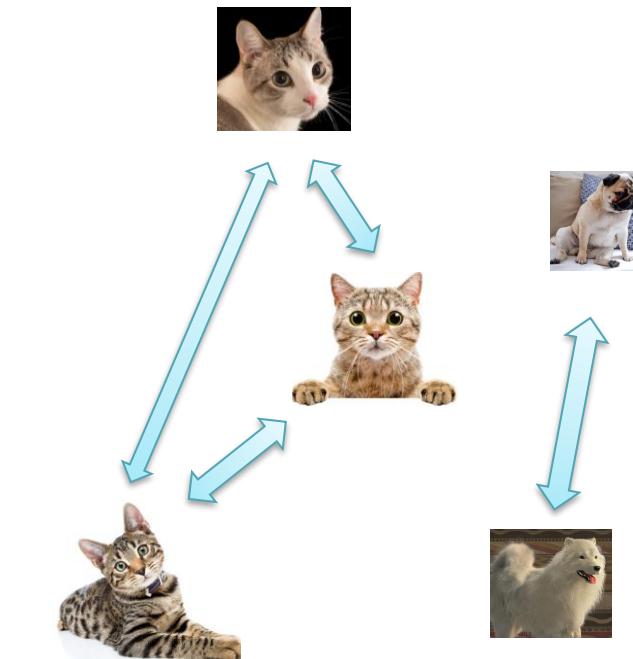
To utilize GNNs (Graph Neural Networks) for any problem, three sequential questions need to be addressed:

- What is a node?
- What is an edge?
- Can we incorporate an auxiliary loss function?

**Node:** image

**Edge:** images of the same class

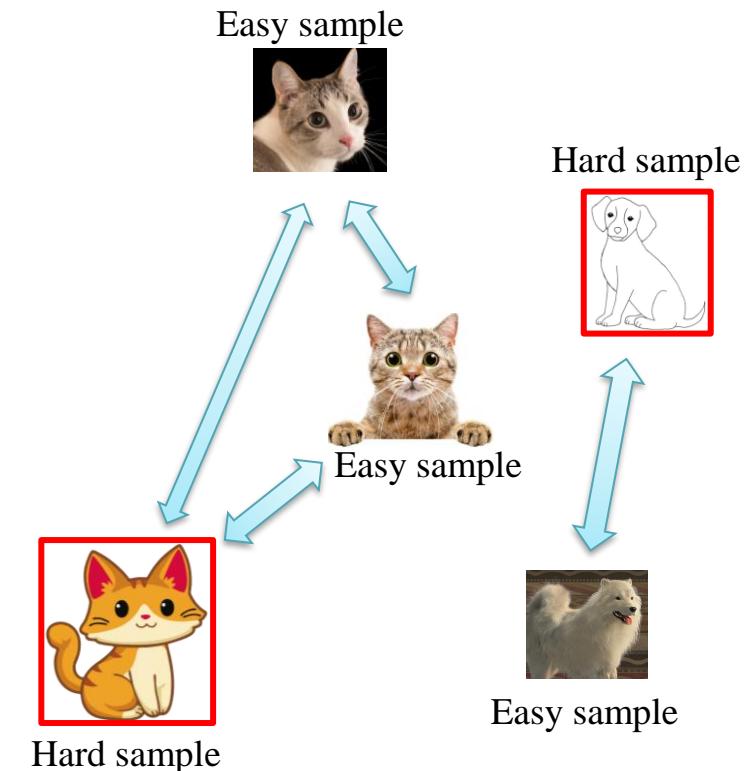
**Auxiliary loss:** yes (because it's the groundtruth)



# Objective

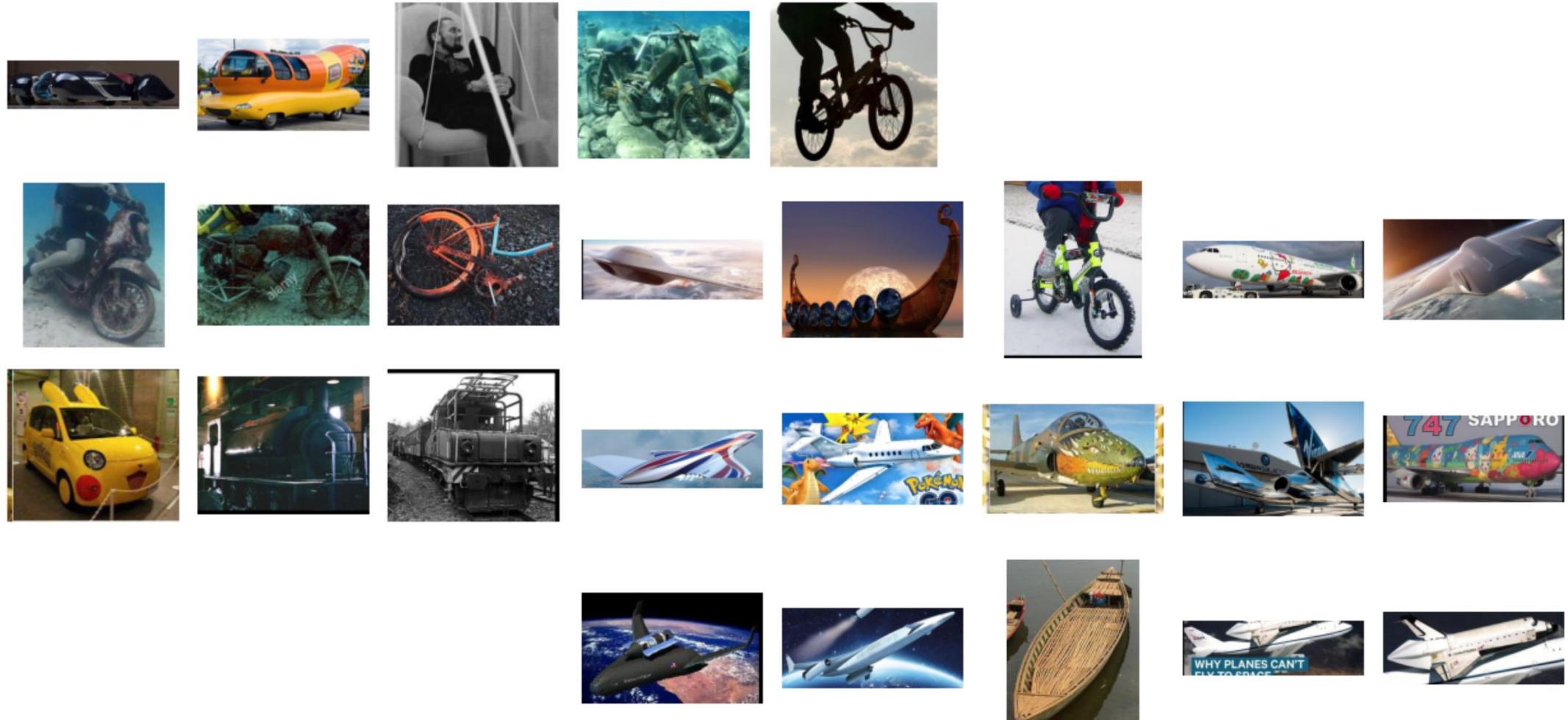
How does GNN operate?

- There are hard and easy samples for each class.
- Leverage easy samples to “provide” information for hard samples.



# Objective

Examples of hard samples



## Outline

1. Objective

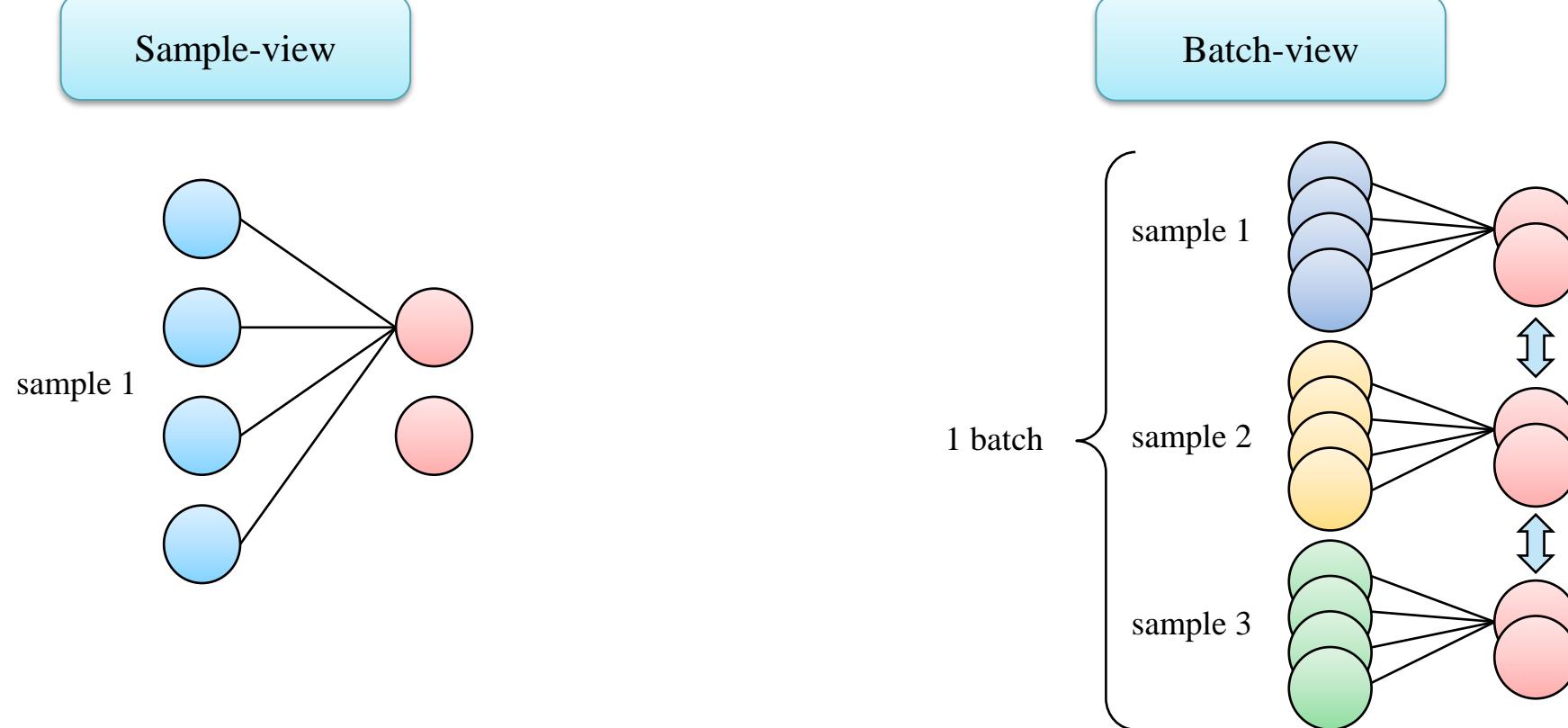
2. From MLP to GNN

3. Coding

4. Experiment on Caltech-101 and PACS Datasets

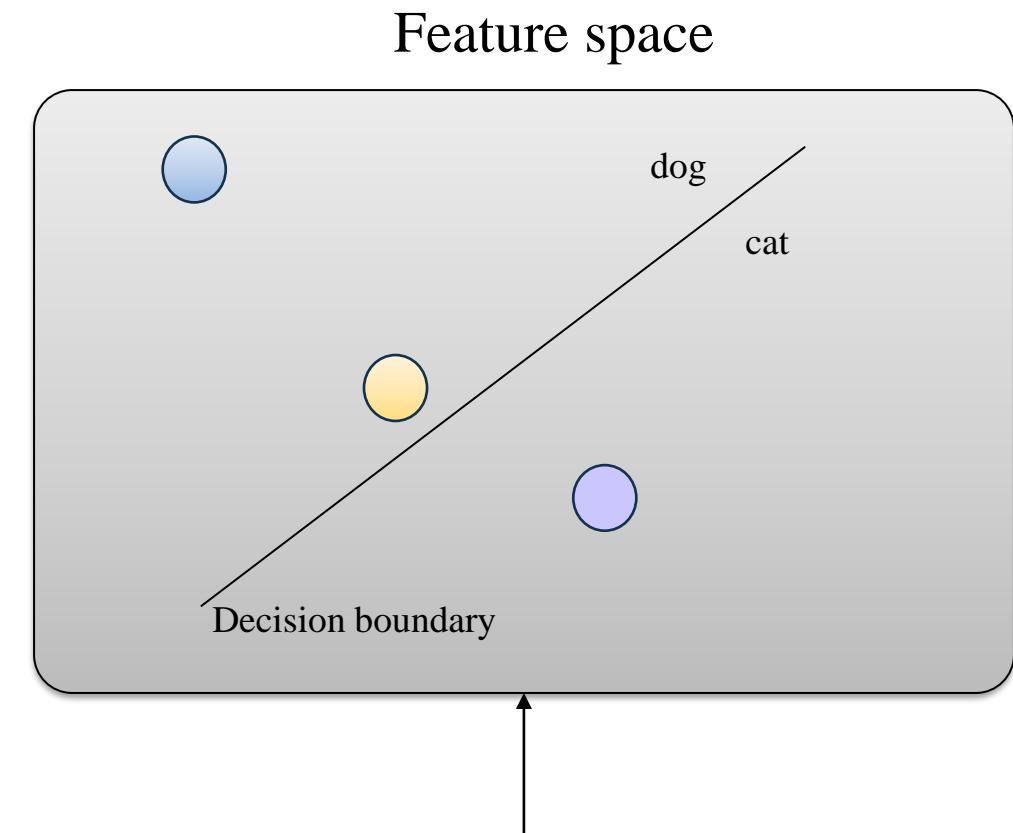
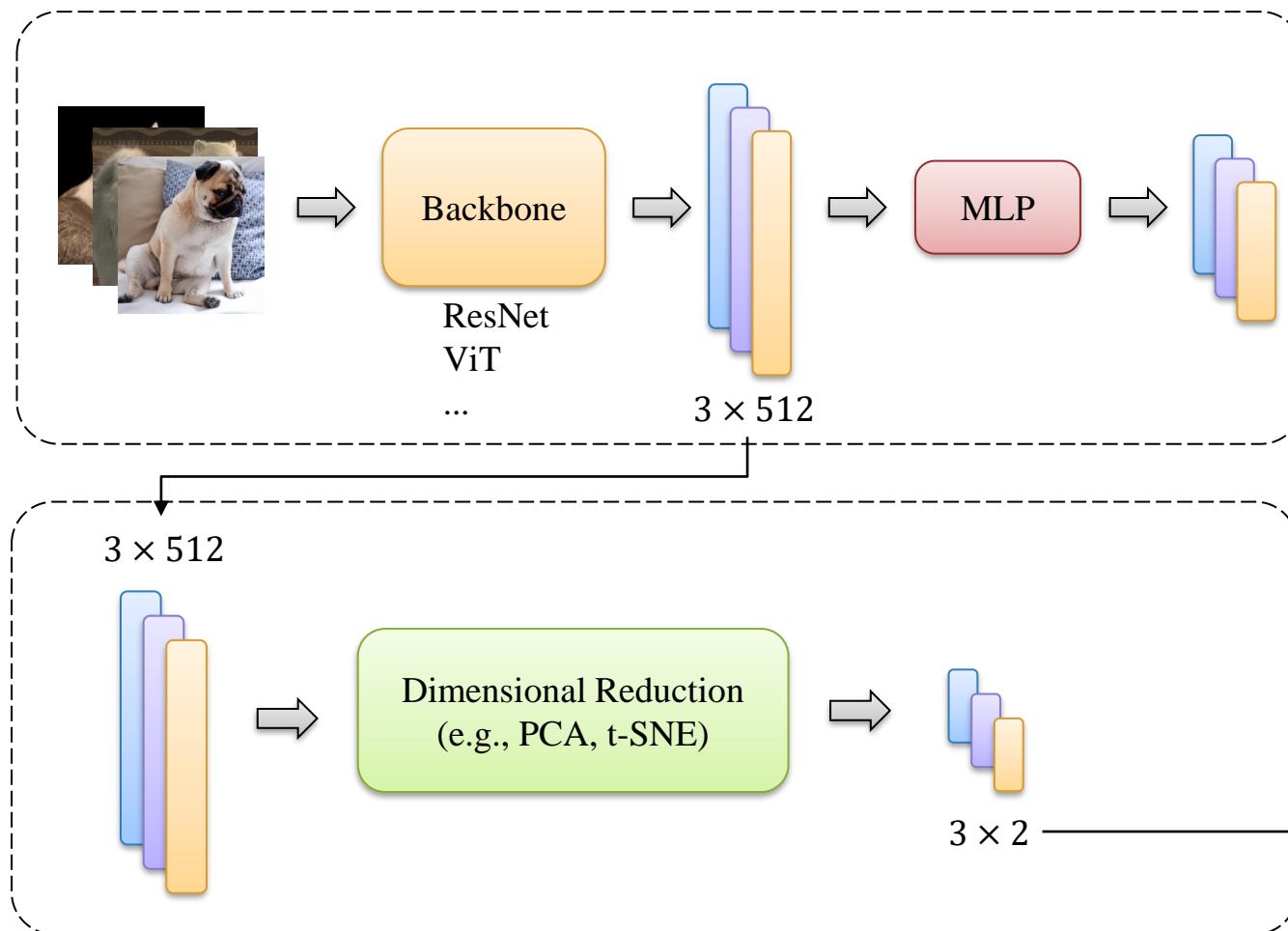
# From MLP to GNN

MLP



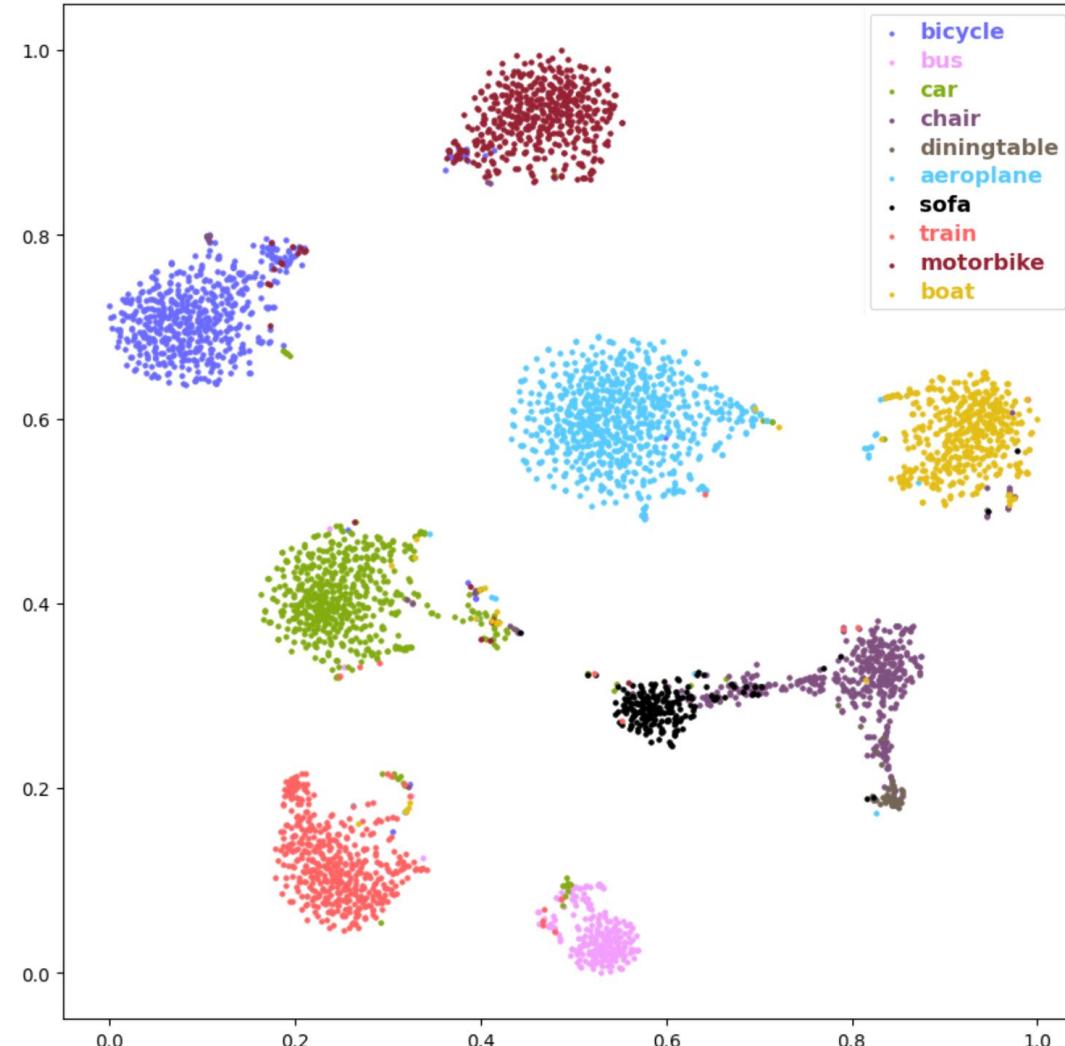
# From MLP to GNN

## Feature space



# From MLP to GNN

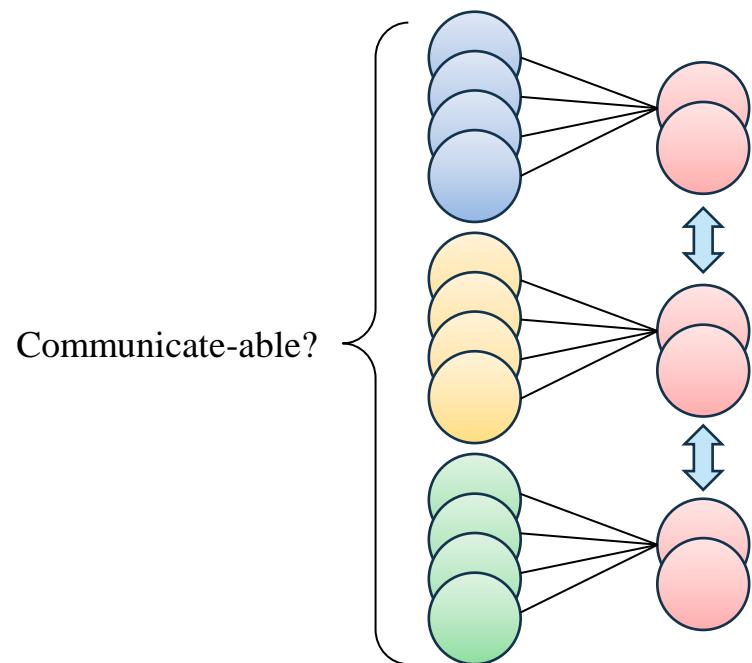
Feature space



t-SNE Visualization

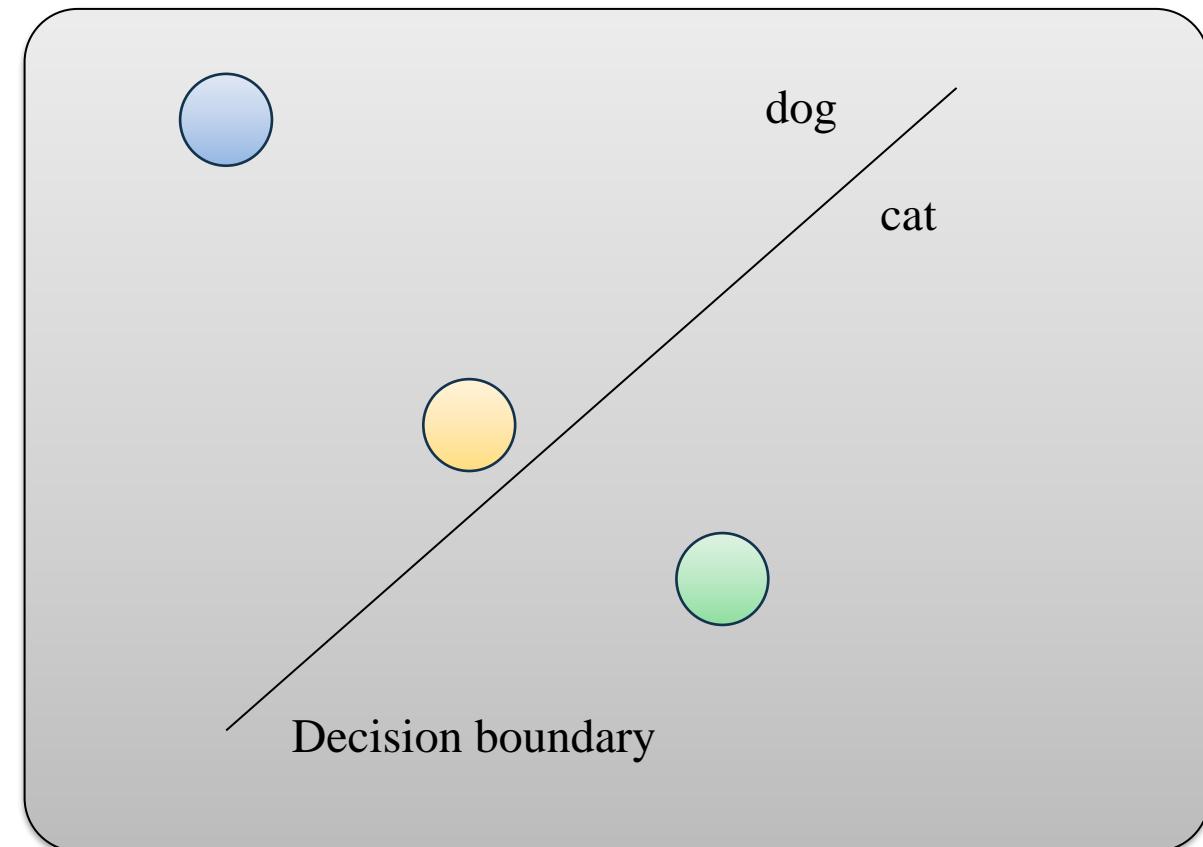
# From MLP to GNN

MLP



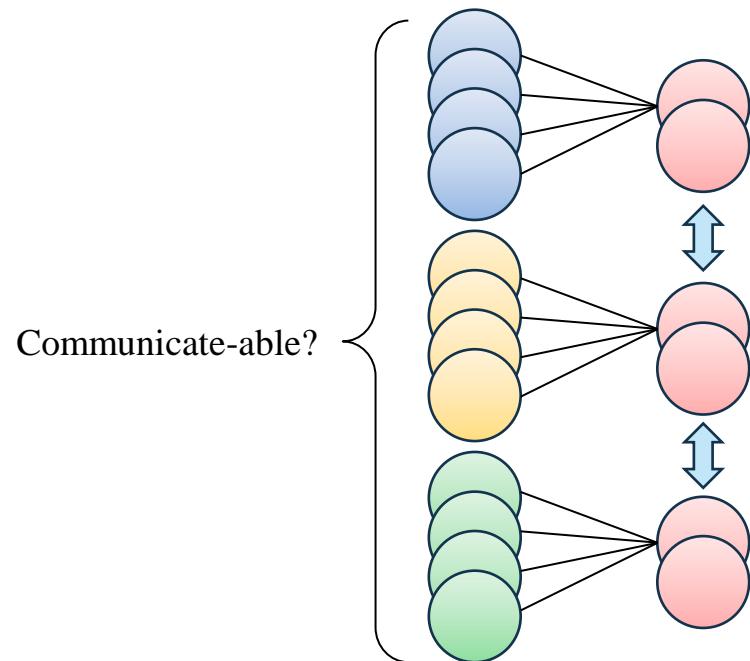
Communicate-able?

Feature space



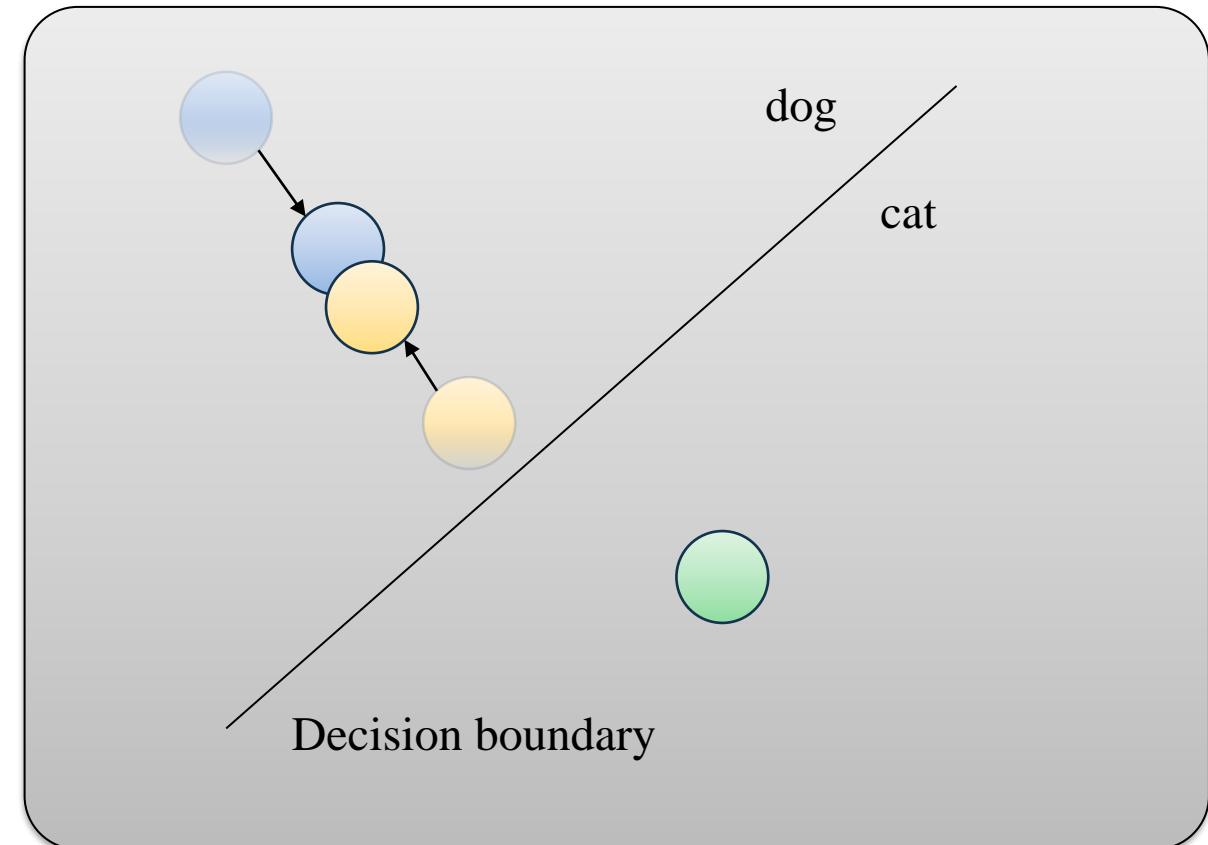
# From MLP to GNN

MLP



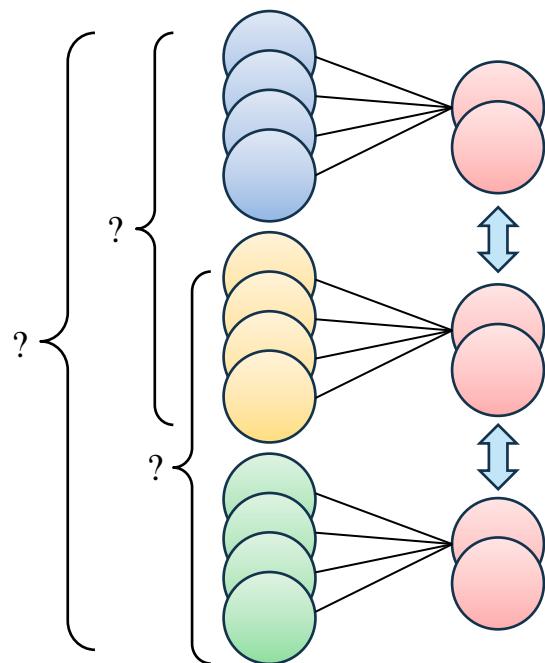
Communicate-able?

Feature space

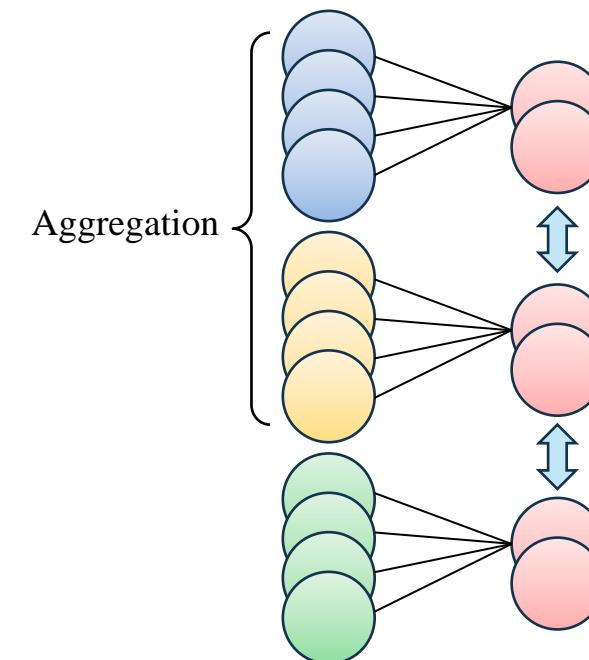


## From MLP to GNN

How to communicate?



Edge Network



Node Network

# GNN = MLP + Message Passing (MP)

GNN

$$(\text{MP}): \quad \tilde{\mathbf{h}}_u^{(l-1)} = \sum_{v \in \mathcal{N}_u \cup \{u\}} a_{u,v} \cdot \mathbf{h}_v^{(l-1)}, \quad (\text{FF}): \quad \mathbf{h}_u^{(l)} = \psi^{(l)} \left( \tilde{\mathbf{h}}_u^{(l-1)} \right) \quad (1)$$

S.t.

$\psi^{(l)}$  denotes a feature transformation mapping at the  $l$ -th layer → nn.Linear()

$a_G(u, v)$  is the affinity function

$$\mathbf{h}_u^{(0)} = \mathbf{x}_u$$

MLP

GNN models in forms of Eq. 1 degrade to an MLP with a series of FF layers after removing all the MP operations:

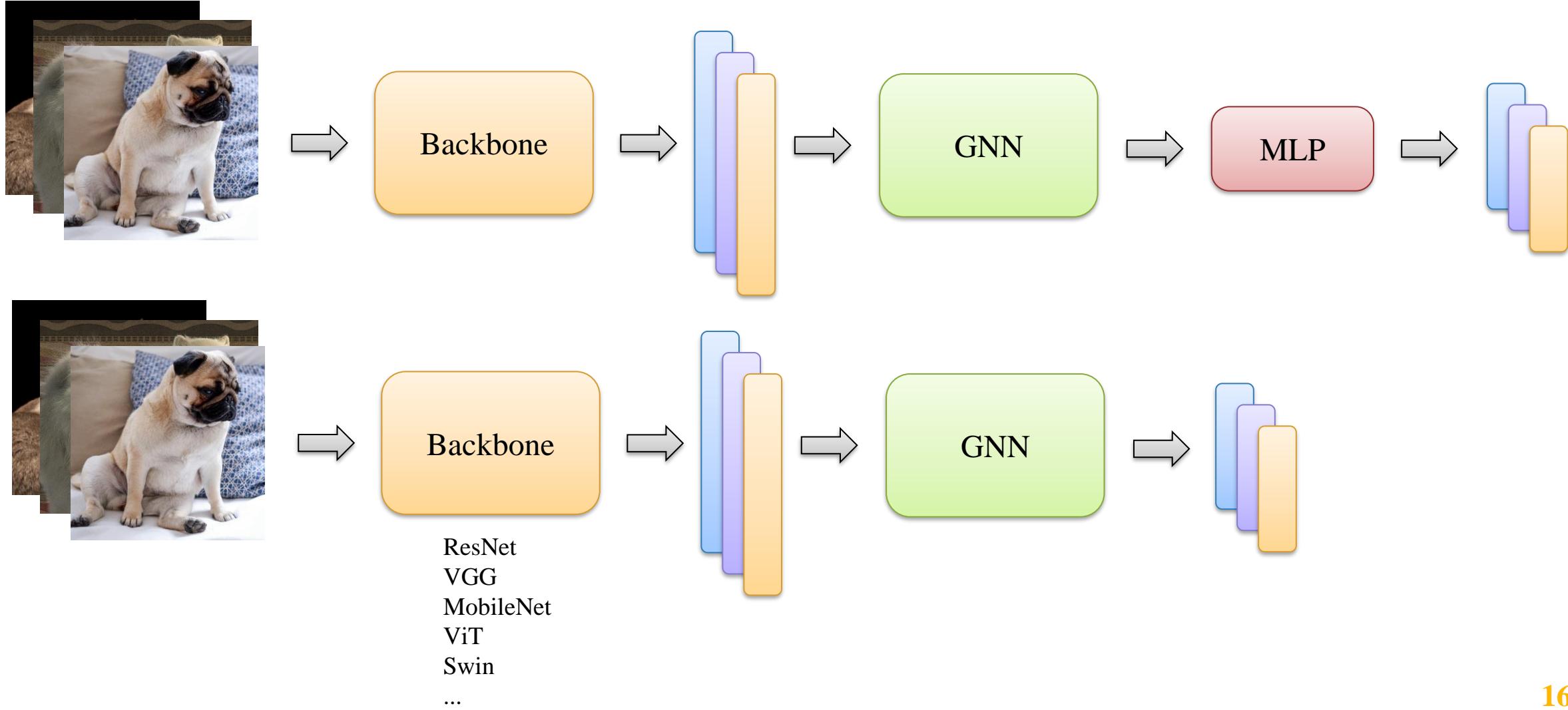
$$\hat{y}_u = \psi^{(L)}(\dots(\psi^{(1)}(\mathbf{x}_u)) = \psi(\mathbf{x}_u). \quad (2)$$

```

1 # GNN
2 fc1 = nn.Linear()
3 mp1 = MP()
4 fc2 = nn.Linear()
5 mp2 = MP()
6
7 # Forward
8 out1 = fc1(mp1(x))
9 out2 = fc2(mp2(out1))
10
11 -----
12
13 # MLP
14 fc1 = nn.Linear()
15 fc2 = nn.Linear()
16
17 # Forward
18 out1 = fc1(x)
19 out2 = fc2(out1)

```

# From MLP to GNN



## Outline

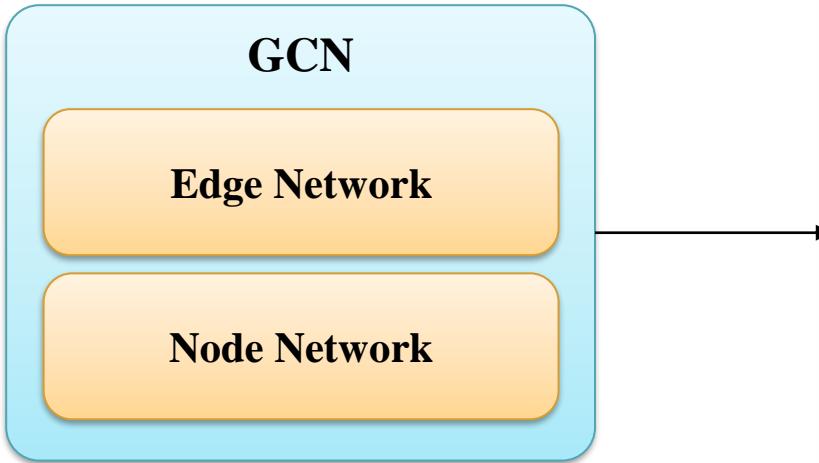
1. Objective

2. From MLP to GNN

3. Coding

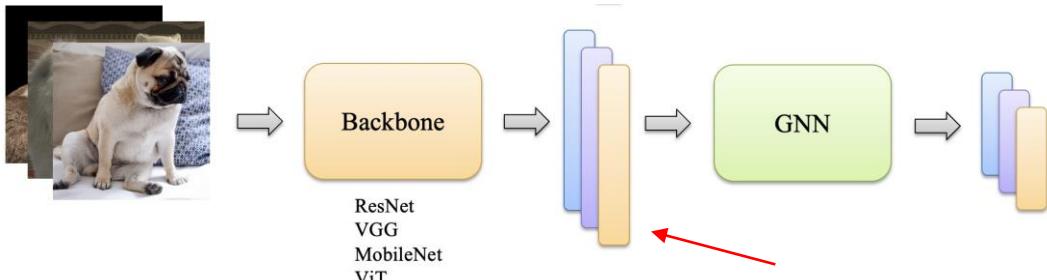
4. Experiment on Caltech-101 and PACS Datasets

# GCN



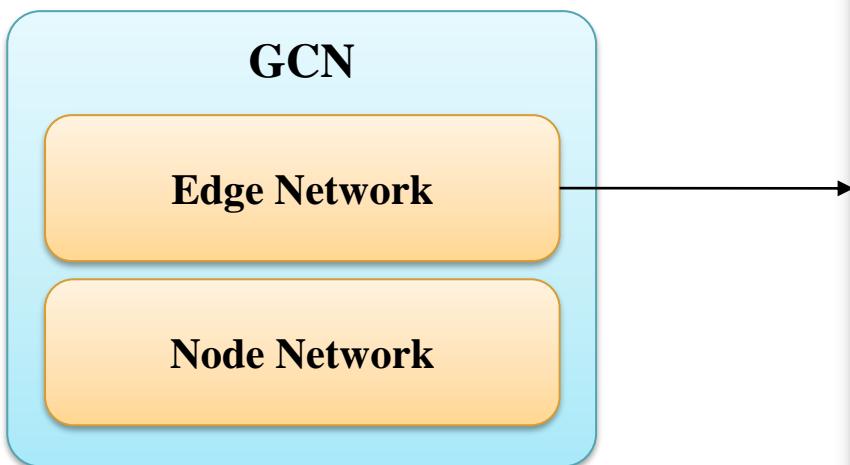
**Input** = `init_node_feat` (bs, hidden\_dim)  
**Output** = `logits_gnn` (bs, hidden\_dim)

**edge\_feat** (bs, bs): correlation matrix **after** normalizing  
**edge\_sim** (bs, bs): correlation matrix **before** normalizing (for loss function)



```
1 class GCN(nn.Module):
2     def __init__(self, in_features, edge_features, out_feature, device, ratio=(1,)):
3         super(GCN, self).__init__()
4
5         self.edge_net = EdgeNet(
6             in_features=in_features,
7             num_features=edge_features,
8             device=device,
9             ratio=ratio,
10        )
11        # set edge to node
12        self.node_net = NodeNet(
13            in_features=in_features,
14            num_features=out_feature,
15            device=device,
16            ratio=ratio,
17        )
18        # mask value for no-gradient edges
19        self.mask_val = -1
20
21    def label2edge(self, targets):
22        """convert node labels to affinity mask for backprop"""
23        num_sample = targets.size()[1]
24        label_i = targets.unsqueeze(-1).repeat(1, 1, num_sample)
25        label_j = label_i.transpose(1, 2)
26        edge = torch.eq(label_i, label_j).float()
27        target_edge_mask = (
28            torch.eq(label_i, self.mask_val) + torch.eq(label_j, self.mask_val)
29        ).type(torch.bool)
30        source_edge_mask = ~target_edge_mask
31        init_edge = edge * source_edge_mask.float()
32        return init_edge[0], source_edge_mask
33
34    def forward(self, init_node_feat):
35        # compute normalized and not normalized affinity matrix
36        edge_feat, edge_sim = self.edge_net(init_node_feat)
37        # compute node features and class logits
38        logits_gnn = self.node_net(init_node_feat, edge_feat)
39        return logits_gnn, edge_sim
```

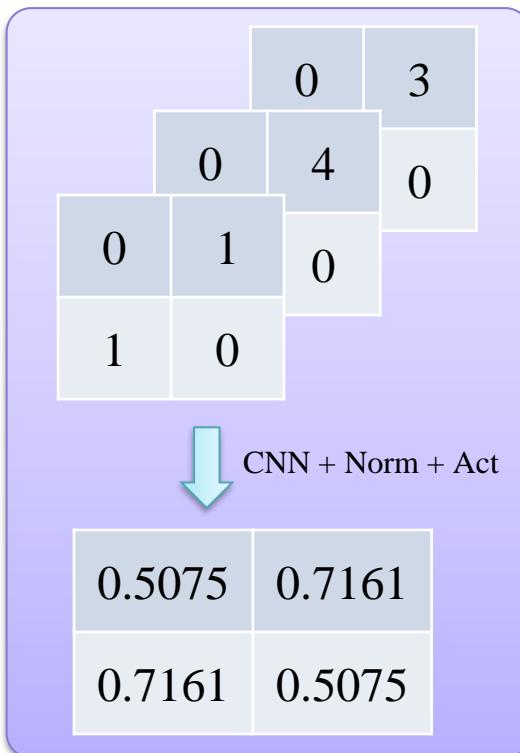
# Edge Network



```
1  class EdgeNet(nn.Module):
2      def __init__(self, in_features, num_features, device, ratio=(1,)):
3          super(EdgeNet, self).__init__()
4          num_features_list = [num_features * r for r in ratio]
5          self.device = device
6          # define layers
7          layer_list = OrderedDict()
8          for l in range(len(num_features_list)):
9              layer_list["conv{}".format(l)] = nn.Conv2d(
10                 in_channels=num_features_list[l - 1] if l > 0 else in_features,
11                 out_channels=num_features_list[l],
12                 kernel_size=1,
13                 bias=False,
14             )
15             layer_list["norm{}".format(l)] = nn.BatchNorm2d(
16                 num_features=num_features_list[l]
17             )
18             layer_list["relu{}".format(l)] = nn.LeakyReLU()
19         # add final similarity kernel
20         layer_list["conv_out"] = nn.Conv2d(
21             in_channels=num_features_list[-1], out_channels=1, kernel_size=1
22         )
23         self.sim_network = nn.Sequential(layer_list).to(device)
24
25     def forward(self, node_feat):
26         node_feat = node_feat.unsqueeze(dim=0) # (1, bs, dim)
27         num_tasks = node_feat.size(0) # 1
28         num_data = node_feat.size(1) # bs
29         x_i = node_feat.unsqueeze(2) # (1, bs, 1, dim)
30         x_j = torch.transpose(x_i, 1, 2) # (1, 1, bs, dim)
31         x_ij = torch.abs(x_i - x_j) # (1, bs, bs, dim)
32         x_ij = torch.transpose(x_ij, 1, 3) # (1, dim, bs, bs)
33         # compute similarity/dissimilarity (batch_size x feat_size x num_samples x num_samples)
34         sim_val = (
35             torch.sigmoid(self.sim_network(x_ij)).squeeze(1).squeeze(0).to(self.device)
36         ) # (bs, bs)
37         # normalize affinity matrix
38         force_edge_feat = (
39             torch.eye(num_data).unsqueeze(0).repeat(num_tasks, 1, 1).to(self.device)
40         ) # (1, bs, bs)
41         edge_feat = sim_val + force_edge_feat # (bs, bs)
42         edge_feat = edge_feat + 1e-6 # add small value to avoid nan
43         edge_feat = edge_feat / torch.sum(edge_feat, dim=1).unsqueeze(1) # normalize
44         return edge_feat, sim_val # (bs, bs), (bs, bs)
```

# Edge Network

	[1 2 3]	[2 6 6]
[1 2 3]	[0 0 0]	[1 4 3]
[2 6 6]	[1 4 3]	[0 0 0]



```

1  class EdgeNet(nn.Module):
2      def __init__(self, in_features, num_features, device, ratio=(1,)):
3          super(EdgeNet, self).__init__()
4          num_features_list = [num_features * r for r in ratio]
5          self.device = device
6          # define layers
7          layer_list = OrderedDict()
8          for l in range(len(num_features_list)):
9              layer_list["conv{}".format(l)] = nn.Conv2d(
10                 in_channels=num_features_list[l - 1] if l > 0 else in_features,
11                 out_channels=num_features_list[l],
12                 kernel_size=1,
13                 bias=False,
14             )
15             layer_list["norm{}".format(l)] = nn.BatchNorm2d(
16                 num_features=num_features_list[l]
17             )
18             layer_list["relu{}".format(l)] = nn.LeakyReLU()
19         # add final similarity kernel
20         layer_list["conv_out"] = nn.Conv2d(
21             in_channels=num_features_list[-1], out_channels=1, kernel_size=1
22         )
23         self.sim_network = nn.Sequential(layer_list).to(device)
24
25     def forward(self, node_feat):
26         node_feat = node_feat.unsqueeze(dim=0) # (1, bs, dim)
27         num_tasks = node_feat.size(0) # 1
28         num_data = node_feat.size(1) # bs
29         x_i = node_feat.unsqueeze(2) # (1, bs, 1, dim)
30         x_j = torch.transpose(x_i, 1, 2) # (1, 1, bs, dim)
31         x_ij = torch.abs(x_i - x_j) # (1, bs, bs, dim)
32         x_ij = torch.transpose(x_ij, 1, 3) # (1, dim, bs, bs)
33         # compute similarity/dissimilarity (batch_size x feat_size x num_samples x num_samples)
34         sim_val = (
35             torch.sigmoid(self.sim_network(x_ij)).squeeze(1).squeeze(0).to(self.device)
36         ) # (bs, bs)
37         # normalize affinity matrix
38         force_edge_feat = (
39             torch.eye(num_data).unsqueeze(0).repeat(num_tasks, 1, 1).to(self.device)
40         ) # (1, bs, bs)
41         edge_feat = sim_val + force_edge_feat # (bs, bs)
42         edge_feat = edge_feat + 1e-6 # add small value to avoid nan
43         edge_feat = edge_feat / torch.sum(edge_feat, dim=1).unsqueeze(1) # normalize
44         return edge_feat, sim_val # (bs, bs), (bs, bs)

```

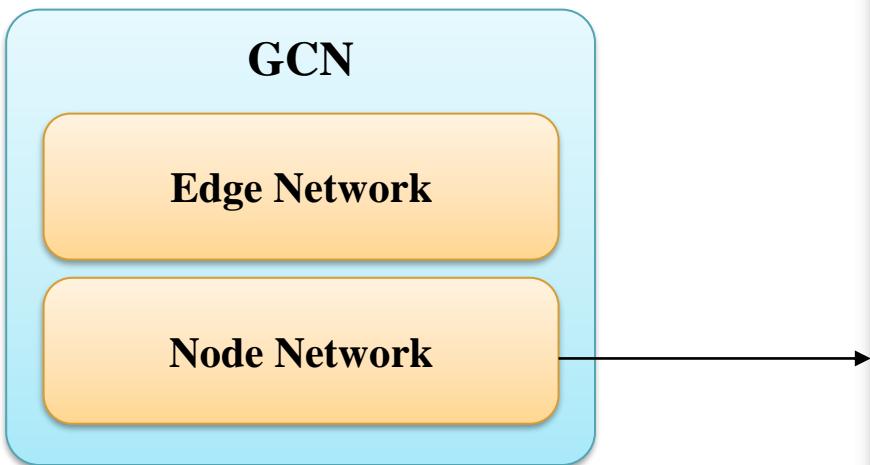
# Edge Network

1.5075	0.7161
0.7161	1.5075
0.8487	0.1513
0.1513	0.8487

Self-loop

```
1 class EdgeNet(nn.Module):
2     def __init__(self, in_features, num_features, device, ratio=(1,)):
3         super(EdgeNet, self).__init__()
4         num_features_list = [num_features * r for r in ratio]
5         self.device = device
6         # define layers
7         layer_list = OrderedDict()
8         for l in range(len(num_features_list)):
9             layer_list["conv{}".format(l)] = nn.Conv2d(
10                 in_channels=num_features_list[l - 1] if l > 0 else in_features,
11                 out_channels=num_features_list[l],
12                 kernel_size=1,
13                 bias=False,
14             )
15             layer_list["norm{}".format(l)] = nn.BatchNorm2d(
16                 num_features=num_features_list[l]
17             )
18             layer_list["relu{}".format(l)] = nn.LeakyReLU()
19         # add final similarity kernel
20         layer_list["conv_out"] = nn.Conv2d(
21             in_channels=num_features_list[-1], out_channels=1, kernel_size=1
22         )
23         self.sim_network = nn.Sequential(layer_list).to(device)
24
25     def forward(self, node_feat):
26         node_feat = node_feat.unsqueeze(dim=0) # (1, bs, dim)
27         num_tasks = node_feat.size(0) # 1
28         num_data = node_feat.size(1) # bs
29         x_i = node_feat.unsqueeze(2) # (1, bs, 1, dim)
30         x_j = torch.transpose(x_i, 1, 2) # (1, 1, bs, dim)
31         x_ij = torch.abs(x_i - x_j) # (1, bs, bs, dim)
32         x_ij = torch.transpose(x_ij, 1, 3) # (1, dim, bs, bs)
33         # compute similarity/dissimilarity (batch_size x feat_size x num_samples x num_samples)
34         sim_val = (
35             torch.sigmoid(self.sim_network(x_ij)).squeeze(1).squeeze(0).to(self.device)
36         ) # (bs, bs)
37         # normalize affinity matrix
38         force_edge_feat = (
39             torch.eye(num_data).unsqueeze(0).repeat(num_tasks, 1, 1).to(self.device)
40         ) # (1, bs, bs)
41         edge_feat = sim_val + force_edge_feat # (bs, bs)
42         edge_feat = edge_feat + 1e-6 # add small value to avoid nan
43         edge_feat = edge_feat / torch.sum(edge_feat, dim=1).unsqueeze(1) # normalize
44         return edge_feat, sim_val # (bs, bs), (bs, bs)
```

# Node Network



```
1  class NodeNet(nn.Module):
2      def __init__(self, in_features, num_features, device, ratio=(1,)):
3          super(NodeNet, self).__init__()
4          num_features_list = [num_features * r for r in ratio]
5          self.device = device
6          # define layers
7          layer_list = OrderedDict()
8          for l in range(len(num_features_list)):
9              layer_list["conv{}".format(l)] = nn.Conv2d(
10                 in_channels=num_features_list[l - 1] if l > 0 else in_features * 2,
11                 out_channels=num_features_list[l],
12                 kernel_size=1,
13                 bias=False,
14             )
15             layer_list["norm{}".format(l)] = nn.BatchNorm2d(
16                 num_features=num_features_list[l]
17             )
18             if l < (len(num_features_list) - 1):
19                 layer_list["relu{}".format(l)] = nn.LeakyReLU()
20         self.network = nn.Sequential(layer_list).to(device)
21
22     def forward(self, node_feat, edge_feat):
23         """node_feat: (bs, dim), edge_feat: (bs, bs)"""
24         node_feat = node_feat.unsqueeze(dim=0) # (1, bs, dim)
25         num_tasks = node_feat.size(0) # 1
26         num_data = node_feat.size(1) # bs
27         # get eye matrix (batch_size x node_size x node_size) only use inter dist.
28         diag_mask = 1.0 - torch.eye(num_data).unsqueeze(0).repeat(num_tasks, 1, 1).to(
29             self.device
30         ) # (1, bs, bs)
31         # set diagonal as zero and normalize
32         edge_feat = F.normalize(edge_feat * diag_mask, p=1, dim=-1) # (bs, bs)
33         # compute attention and aggregate
34         aggr_feat = torch.bmm(edge_feat.squeeze(1), node_feat) # (bs, dim)
35         node_feat = torch.cat([node_feat, aggr_feat], -1).transpose(
36             1, 2
37         ) # (1, 2*dim, bs)
38         # non-linear transform
39         node_feat = self.network(node_feat.unsqueeze(-1)).transpose(
40             1, 2
41         ) # (1, bs, dim)
42         node_feat = node_feat.squeeze(-1).squeeze(0) # (bs, dim)
43         return node_feat
```

# Add GCN into Existing Code

```
1 from torchvision.models import mobilenet_v3_small
2
3 class Model(nn.Module):
4     def __init__(self, num_classes=2):
5         super(Model, self).__init__()
6         self.backbone = mobilenet_v3_small(pretrained=True)
7         self.backbone.classifier = nn.Sequential()
8
9         self.head = nn.Linear(576, num_classes)
10
11    def forward(self, x):
12        x = self.backbone(x)
13        x = self.head(x)
14        return x
```



```
1 from torchvision.models import mobilenet_v3_small
2
3 class Model(nn.Module):
4     def __init__(self, num_classes=7):
5         super(Model, self).__init__()
6         self.backbone = mobilenet_v3_small(pretrained=True)
7         self.backbone.classifier = nn.Sequential()
8
9         self.gcn = GCN(
10             in_features=576,
11             edge_features=576,
12             out_feature=num_classes,
13             device="cuda",
14             ratio=(1,),
15         )
16
17     def forward(self, x):
18        x = self.backbone(x)
19        x, edge_sim = self.gcn(x)
20        return x, edge_sim
```

# Add GCN into Existing Code

```
1 criterion = nn.CrossEntropyLoss()
2
3 for i, (inputs, labels) in enumerate(trainloader):
4     # Move inputs and labels to the device
5     inputs, labels = inputs.to(device), labels.to(device)
6
7     # Zero the parameter gradients
8     optimizer.zero_grad()
9
10    # Forward pass
11    outputs = model(inputs)
12
13    # loss
14    loss = criterion(outputs, labels)
15
16    # Backward pass and optimization
17    loss.backward()
18    optimizer.step()
```



```
1 criterion = nn.CrossEntropyLoss()
2 criterion_edge = nn.BCELoss()
3
4 for i, (inputs, labels) in enumerate(trainloader):
5     # Move inputs and labels to the device
6     inputs, labels = inputs.to(device), labels.to(device)
7
8     # Zero the parameter gradients
9     optimizer.zero_grad()
10
11    # Forward pass
12    outputs, edge_sim = model(inputs)
13
14    ##### Cls loss
15    loss_cls = criterion(outputs, labels)
16
17    ##### Edge loss
18    edge_gt, edge_mask = model.gcn.label2edge(labels.unsqueeze(dim=0))
19    loss_edge = criterion_edge(
20        edge_sim.masked_select(edge_mask), edge_gt.masked_select(edge_mask)
21    )
22
23    ##### Total loss
24    loss = 0.3 * loss_cls + loss_edge
25
26    # Backward pass and optimization
27    loss.backward()
28    optimizer.step()
```

# Create Label for Edge Network

```
1 criterion = nn.CrossEntropyLoss()
2 criterion_edge = nn.BCELoss()
3
4 for i, (inputs, labels) in enumerate(trainloader):
5     # Move inputs and labels to the device
6     inputs, labels = inputs.to(device), labels.to(device)
7
8     # Zero the parameter gradients
9     optimizer.zero_grad()
10
11    # Forward pass
12    outputs, edge_sim = model(inputs)
13
14    ##### Cls loss
15    loss_cls = criterion(outputs, labels)
16
17    ##### Edge loss
18    edge_gt, edge_mask = model.gcn.label2edge(labels.unsqueeze(dim=0))
19    loss_edge = criterion_edge(
20        edge_sim.masked_select(edge_mask), edge_gt.masked_select(edge_mask)
21    )
22
23    ##### Total loss
24    loss = 0.3 * loss_cls + loss_edge
25
26    # Backward pass and optimization
27    loss.backward()
28    optimizer.step()
```



The diagram illustrates the creation of edge labels from class labels. It shows a row of labels [1, 5, 3, 1] above a 4x4 matrix labeled "edge\_gt". The matrix contains binary values: the first row has 1s at indices 0, 2, and 3; the second row has 1s at indices 1 and 3; the third row has 1s at indices 2 and 3; and the fourth row has 1s at indices 0 and 3.

labels	1	5	3	1
edge_gt	1	0	0	1
	0	1	0	0
	0	0	1	0
	1	0	0	1

**QUIZ!**

**TIME**

## Quiz

1. Đâu là lưu ý khi áp dụng GNN vào các bài toán bắt kì?

- A. Label là gì?
- B. Độ lớn dataset
- C. Độ phức tạp của model
- D. Edge là gì?

2. Đâu là lưu ý khi áp dụng GNN vào các bài toán bắt kì?

- A. Label là gì?
- B. Node là gì?
- C. Số lượng param
- D. Loss là gì?

3. Đâu là lưu ý khi áp dụng GNN vào các bài toán bắt kì?

- A. Có cần hàm loss phụ trợ hay không?
- B. Model có tính toán song song hay không?
- C. Loss là gì?
- D. Loại hàm loss của model hiện tại.

4. Sau khi chắc chắn GNN có thể sử dụng, điều gì ta cần cân nhắc tiếp theo là phù hợp nhất?

- A. Không cần gì
- B. Độ lớn của model sau khi thêm GNN
- C. Hiểu rõ cách GNN tổng hợp thông tin
- D. Tốc độ của model sau khi thêm GNN

5. Nếu input của GNN có shape [batch\_size, dim\_1] và output có shape [batch\_size, dim\_2] thì nhận định nào sau đây là **SAI**:

- A. dim\_2 có thể bằng dim\_1 \* 2
- B. dim\_2 có thể bằng số lượng class
- C. dim\_1 và dim\_2 không bắt buộc bằng nhau
- D. dim\_1 và dim\_2 phải bằng nhau

## Outline

1. Objective

2. From MLP to GNN

3. Coding

4. Experiment on Caltech-101 and PACS Datasets

# The Caltech-101 Dataset

**Caltech-101** consists of pictures of objects belonging to 101 classes.

Each image is labeled with a single object.

Each class contains roughly 40 to 800 images, totaling around 9k images.

Images are of variable sizes, with typical edge lengths of 200-300 pixels.



# The Caltech101 Dataset

```
1 batch_size = 256
2 train_transform = transforms.Compose(
3     [
4         transforms.Resize((224, 224)),
5         transforms.Grayscale(num_output_channels=3),
6         transforms.ToTensor(),
7         transforms.Normalize([0.4914, 0.4822, 0.4465],
8                             [0.2470, 0.2435, 0.2616]),
9     ]
10 )
11
12 dataset = Caltech101(root=".data", download=True,
13                      transform=train_transform)
14
15 # # split dataset
16 n_train = int(len(dataset) * 0.8)
17 n_val = len(dataset) - n_train
18
19 train_dataset, val_dataset = random_split(dataset, [n_train, n_val])
20
21 trainloader = DataLoader(train_dataset,
22                         batch_size=batch_size,
23                         shuffle=True)
24 testloader = DataLoader(val_dataset,
25                         batch_size=batch_size,
26                         shuffle=False)
```

	Best Val Acc
MLP	86.75
GNN	91.76 ( $\uparrow$ 5.01)

# The PACS Dataset

**PACS** is an image dataset for domain generalization.

It consists of four domains, namely

- Photo (1,670 images),
- Art Painting (2,048 images),
- Cartoon (2,344 images) and
- Sketch (3,929 images).

Each domain contains seven categories.

art paint



cartoon



sketch



photo



CSDN @白马金霸侠少年

## MLP vs. GNN

Use 1 domain for training

```
1 # Clone github repository with data
2 if not os.path.isdir("./Homework3-PACS"):
3     !git clone https://github.com/MachineLearning2020/Homework3-PACS
4
5
6 transf = transforms.Compose(
7     [
8         transforms.CenterCrop(224),
9         transforms.ToTensor(),
10        transforms.Normalize([0.485, 0.456, 0.406],
11                            [0.229, 0.224, 0.225]),
12    ]
13 )
14
15 # Define datasets root
16 DIR_PHOTO = "Homework3-PACS/PACS/photo"
17 DIR_ART = "Homework3-PACS/PACS/art_painting"
18 DIR_CARTOON = "Homework3-PACS/PACS/cartoon"
19 DIR_SKETCH = "Homework3-PACS/PACS/sketch"
20
21 # Prepare Pytorch train/test Datasets
22 photo_dataset = ImageFolder(DIR_PHOTO, transform=transf)
23 art_dataset = ImageFolder(DIR_ART, transform=transf)
24 cartoon_dataset = ImageFolder(DIR_CARTOON, transform=transf)
25 sketch_dataset = ImageFolder(DIR_SKETCH, transform=transf)
```

photo2art

```
1 # Split dataset into train and test
2 train_size = int(0.8 * len(photo_dataset))
3 test_size = len(photo_dataset) - train_size
4
5 train_dataset, test_dataset = torch.utils.data.random_split(
6     photo_dataset, [train_size, test_size]
7 )
8
9 # Concatenate all datasets
10 test_datasets = torch.utils.data.ConcatDataset([test_dataset, art_dataset])
11
12 # Create Dataloaders
13 trainloader = DataLoader(
14     train_dataset, batch_size=128, shuffle=True, num_workers=4, drop_last=True
15 )
16 testloader = DataLoader(
17     test_datasets, batch_size=128, shuffle=False, num_workers=4
18 )
```

	Best Val Acc
MLP	54.58
GNN	66.46 (↑ 11.8)

## MLP vs. GNN

photo2art

Best Val Acc	
MLP	54.58
GNN	66.46 ( $\uparrow$ 11.8)

photo2sketch

Best Val Acc	
MLP	22.12
GNN	29.35 ( $\uparrow$ 7.23)

photo\_cartoon2art

Best Val Acc	
MLP	70.15
GNN	85.62 ( $\uparrow$ 15.47)

photo2all

Best Val Acc	
MLP	26.6
GNN	31.44 ( $\uparrow$ 4.48)

# MLP vs. GNN

Use all domains for training and testing

```
1 # Clone github repository with data
2 if not os.path.isdir("./Homework3-PACS"):
3     !git clone https://github.com/MachineLearning2020/Homework3-PACS
4
5
6 transf = transforms.Compose(
7     [
8         transforms.CenterCrop(224),
9         transforms.ToTensor(),
10        transforms.Normalize([0.485, 0.456, 0.406],
11                            [0.229, 0.224, 0.225]),
12    ]
13 )
14
15 # Define datasets root
16 DIR_PHOTO = "Homework3-PACS/PACS/photo"
17 DIR_ART = "Homework3-PACS/PACS/art_painting"
18 DIR_CARTOON = "Homework3-PACS/PACS/cartoon"
19 DIR_SKETCH = "Homework3-PACS/PACS/sketch"
20
21 # Prepare Pytorch train/test Datasets
22 photo_dataset = ImageFolder(DIR_PHOTO, transform=transf)
23 art_dataset = ImageFolder(DIR_ART, transform=transf)
24 cartoon_dataset = ImageFolder(DIR_CARTOON, transform=transf)
25 sketch_dataset = ImageFolder(DIR_SKETCH, transform=transf)
```

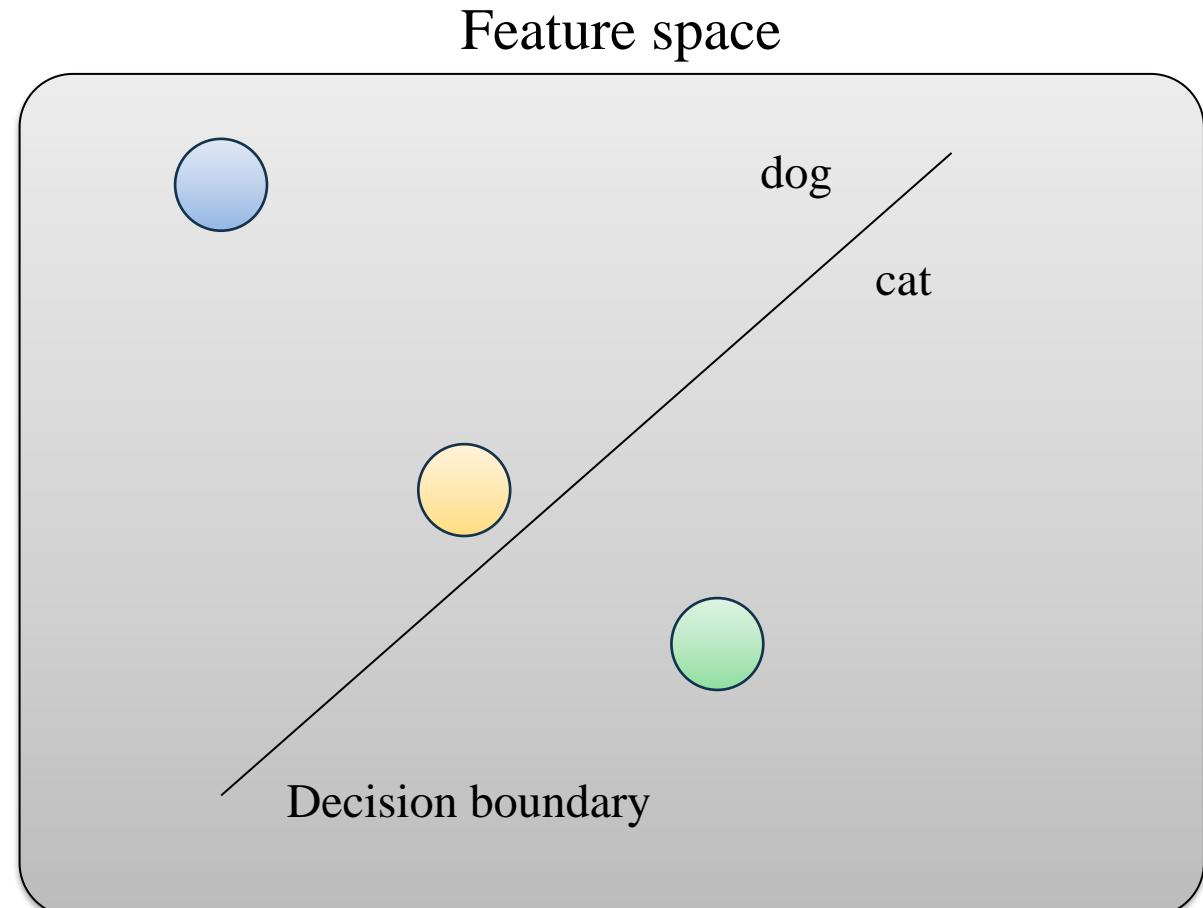
all2all

```
1 # concat all datasets
2 full_dataset = torch.utils.data.ConcatDataset([photo_dataset,
3
4
5
6
7 # Split dataset into train and test
8 train_size = int(0.8 * len(full_dataset))
9 test_size = len(full_dataset) - train_size
10
11 train_dataset, test_dataset = random_split(full_dataset, [train_size, test_size])
12
13 # Create DataLoaders
14 trainloader = DataLoader(
15     train_dataset, batch_size=128, shuffle=True, num_workers=4, drop_last=True
16 )
17 testloader = DataLoader(
18     test_datasets, batch_size=128, shuffle=False, num_workers=4
19 )
```

	Best Val Acc
MLP	90.40
GNN	91.35 ( $\uparrow$ 0.95)

# Limitations

- Require clean data
- Require batch size  $> 1$
- Slower training and inference  
(computational expensive)



# Summary

To utilize GNNs (Graph Neural Networks) for any problem, three sequential questions need to be addressed:

- What is a node?
- What is an edge?
- Can we incorporate an auxiliary loss function?

How does GNN operate?

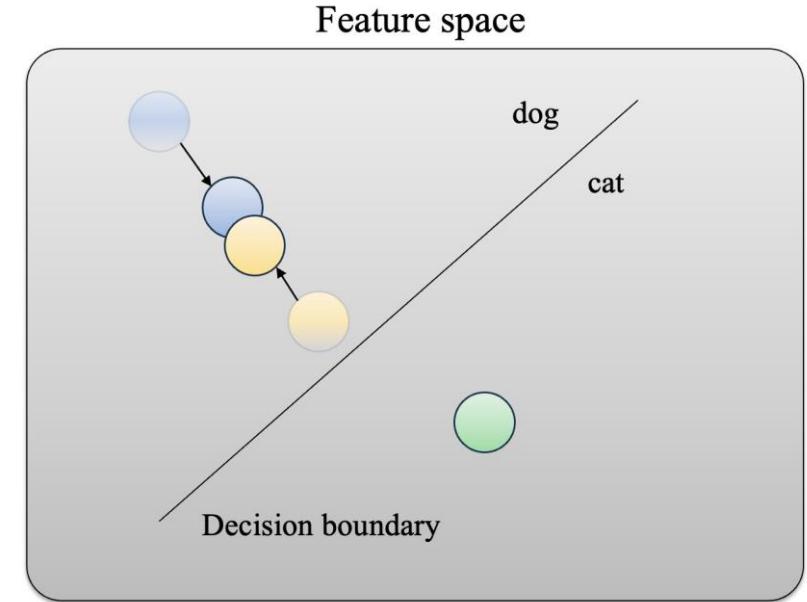
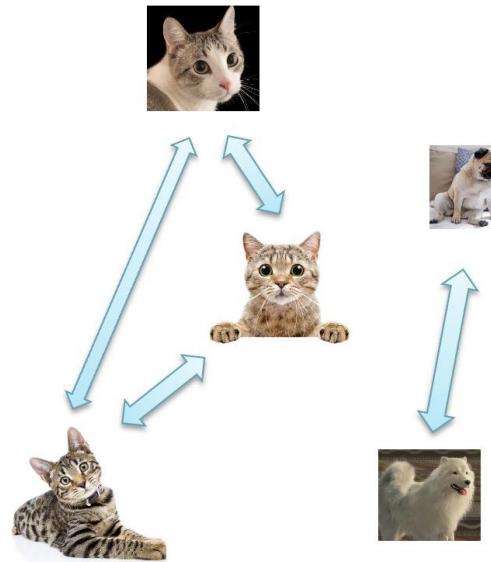


photo2art	
	Best Val Acc
MLP	54.58
GNN	66.46 ( $\uparrow$ 11.8)

photo2sketch	
	Best Val Acc
MLP	22.12
GNN	29.35 ( $\uparrow$ 7.23)

all2all	
	Best Val Acc
MLP	90.40
GNN	91.35 ( $\uparrow$ 0.95)

photo_cartoon2art	
	Best Val Acc
MLP	70.15
GNN	85.62 ( $\uparrow$ 15.47)

photo2all	
	Best Val Acc
MLP	26.6
GNN	31.44 ( $\uparrow$ 4.48)

Caltech101	
	Best Val Acc
MLP	86.75
GNN	91.76 ( $\uparrow$ 5.01)

# Thanks!

## Any questions?