



# 기계이상진단을 위한 인공지능 학습 기법

## 제 5강 분류 태스크를 이용한 이상진단 (실습)

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# 목차

- 분류 태스크를 통한 이상진단 실습
- 실습 1 : 분류기 구현 및 기법 실습
  - Framework
  - Label smoothing
  - Temperature scaling
  - t-SNE visualization
- 실습 2 : 레이블이 없는 경우의 분류기 구현
  - RotNet

# Exercise with Classification Tasks

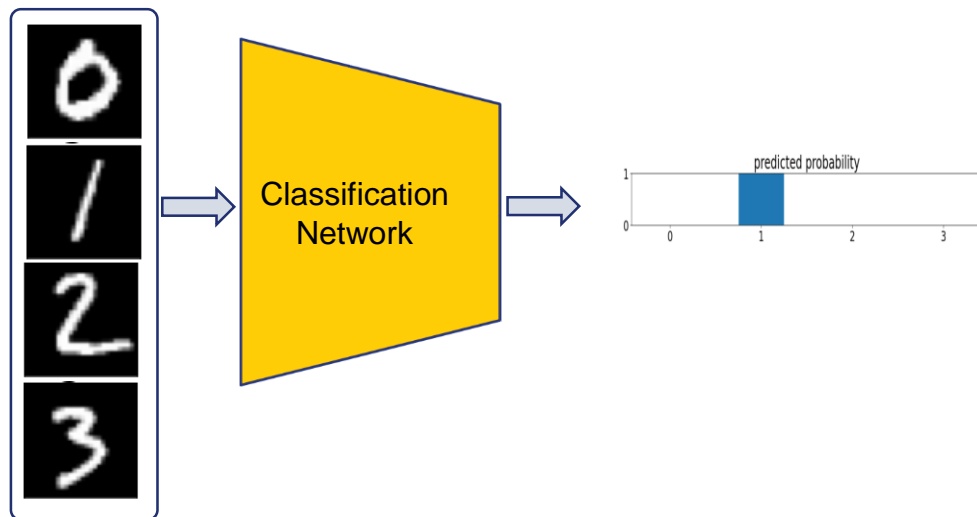
## 1. Classification of internal labels

# 실습 데이터 설명

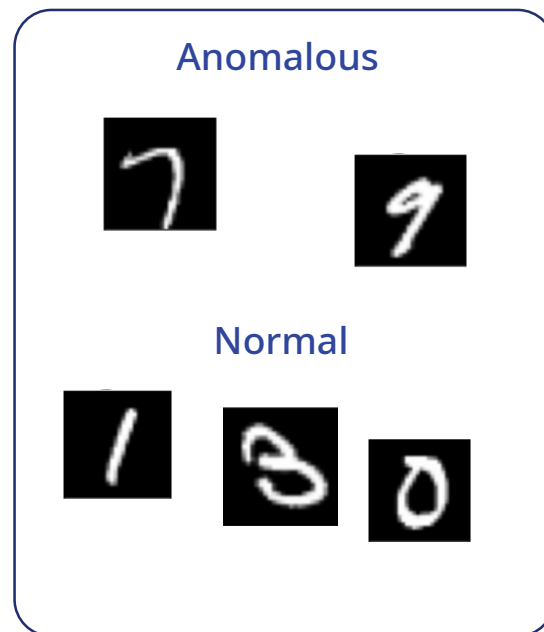
- MNIST dataset

- Normal data: 0, 1, 2, 3
- Anomalies: 7, 8, 9
- Train a CNN model to classify normal data
- Inspect the model's behavior for anomalous samples

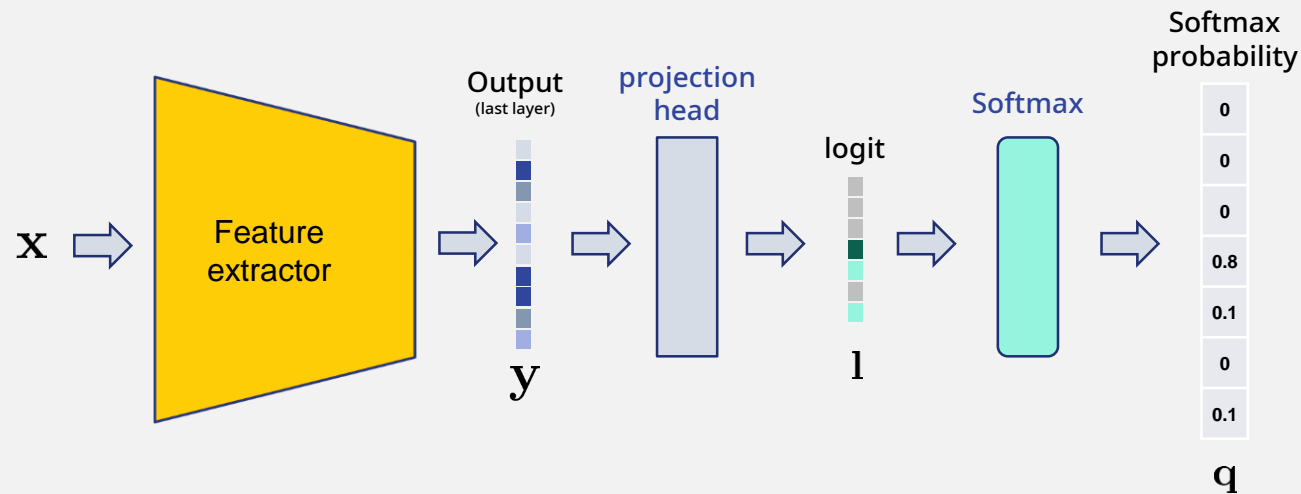
Normal dataset  
(training)



Test, Validation

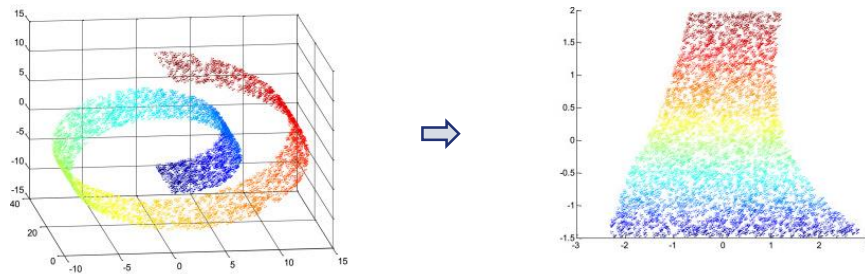


# Recap: Structure of DNN classifier



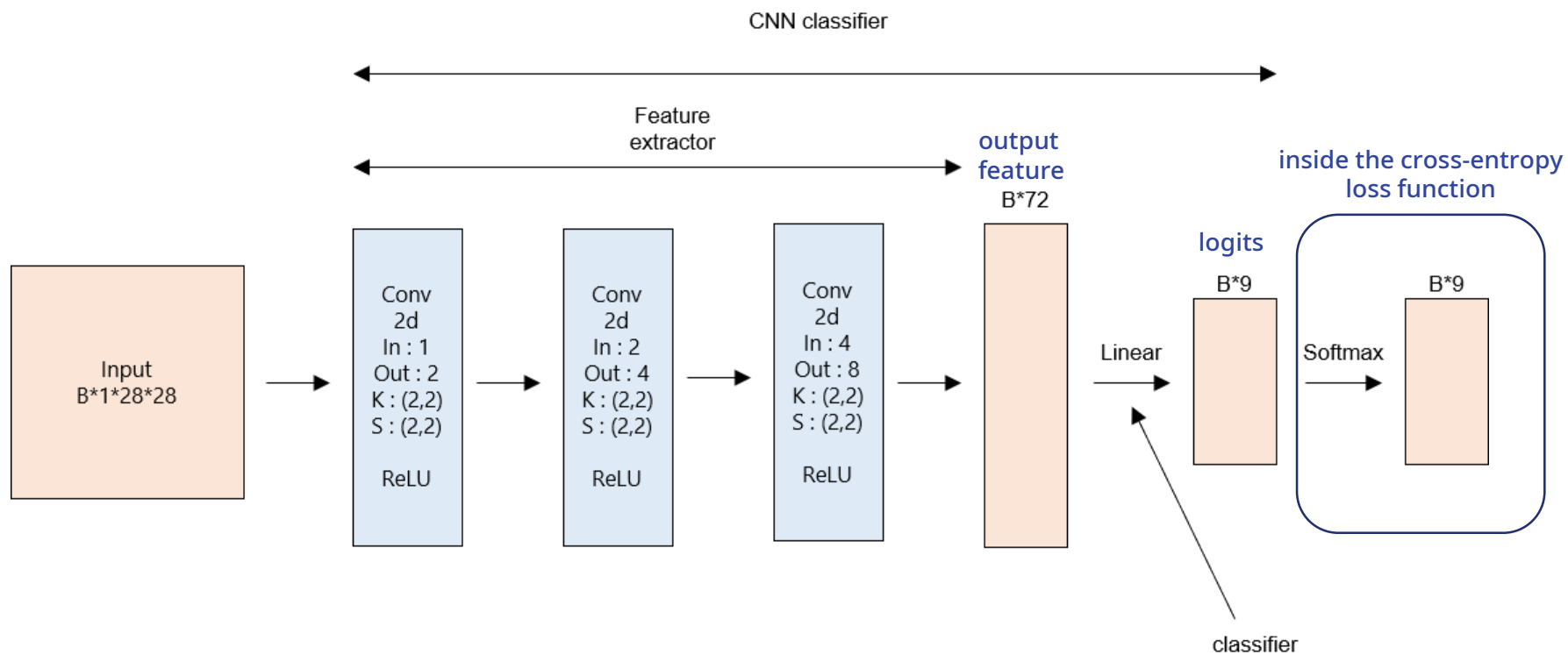
- Feature extractor

- Transform input data  $\mathbf{x}$  to feature space data  $\mathbf{y}$
- Trained to find a good mapping for classification



# 분류를 위한 신경망 모델 (initial)

- CNN 를 사용한 분류 모델



# Code outline

## 2. Hyperparameters

You can change the hyperparameter below. Parameter `ANOMALY_NUM` means which number to set as an anomaly.

```
▶ EPOCHS = 5           # Number of epochs to train
  BATCH = 32           # Minibatch size
  ORGCLASS_NUM = 10    # Num of original classes (10: 0 to 9)
  ANOMALY_NUM = [7,8,9] # (list) Digits will be used as anomalous data
  NORMAL_NUM = [0,1,2,3] # (list) Digits used as normal data

  TEMPSC = 1.0         # temperature parameter (for temperature scaling)
  LBSMOOTH = 0.0       # label smoothing parameter
```

# Code outline

- CNN model

```
▶ class ClassificationCNNModel(nn.Module):
    def __init__(self, nclass=len(NORMAL_NUM)):
        super(ClassificationCNNModel, self).__init__()
        self.feature_extractor = nn.Sequential(
            nn.Conv2d(1,2,kernel_size = (2,2), stride = (2,2)),
            nn.ReLU(),
            nn.Conv2d(2,4,kernel_size = (2,2), stride = (2,2)),
            nn.ReLU(),
            nn.Conv2d(4,8,kernel_size = (2,2), stride = (2,2)),
            nn.ReLU()
        )
        self.classifier = nn.Sequential(
            nn.Linear(72,nclass),
        )


    def forward(self, x):
        feature = self.feature_extractor(x)
        feature = feature.reshape(feature.shape[0],-1)
        out = self.classifier(feature)
        return out, feature  return the feature for feature embedding visualization (t-SNE)
```



# Code outline

- Loss function

$$l_n = - \sum_{c=1}^C w_c \log \frac{\exp(x_{n,c})}{\sum_{i=1}^C \exp(x_{n,i})} y_{n,c}$$



```
loss_fn = nn.CrossEntropyLoss(label_smoothing=LBSMOOTH) # CCE

def anomaly_score(logits): # Anomaly score = 1 - MSP
    softmaxprob = torch.softmax(logits, dim=1)
    MSP = torch.max(softmaxprob, dim=1).values # maximum softmax prob.
    return torch.tensor(1) - MSP

optimizer = torch.optim.Adam(model.parameters(), lr=1e-3) # Adam as optimizer
```

- (!) Pytorch CrossEntropyLoss includes Softmax function
- Input to the loss function is logits (not Softmax probability)
- Anomaly score = 1 – Maximum softmax probability

# Code outline (train)



```
def train(data_loader, model, loss_fn, optimizer):
    model.train()  # switch to training mode
    size = len(data_loader.dataset)
    losses = []
    for batch, dat in enumerate(data_loader):  # dat is tuple of (img, label)
        logits, _ = model(dat[0].to(device))  # logit (batch, class)

        p = F.one_hot(dat[1], ORGCLASS_NUM)[: , NORMAL_NUM]
        p = p.float().to(device)  # Generate one-hot vector from the label.
                                   # Only use normal class labels from the one-hot vector

        loss = loss_fn(logits, p)  # temperature scaling is not applied for training
        losses.append(loss.cpu().detach())

    optimizer.zero_grad()
    loss.backward()
    optimizer.step()

    if batch % 300 == 0:
        loss, current = loss.item(), batch * logits.shape[0]
        print(f"loss: {loss:>7f} [{current:>5d}/{size:>5d}]")

    return np.mean(losses)
```

# Code outline (test)

```
def test(dataloader, model, loss_fn, anomaly_score, valid_mode = True, draw_mode = False):  
    model.eval()  
    for test mode (not validation mode), return feature outputs for visualization  
  
    y_true, y_pred = [], []  
  
    normal_loss = []  
    normal_scores = []  
    anomaly_scores = []  
    outfeature = []  
    total_labels = []  
  
    with torch.no_grad(): test mode: do not update gradients  
  
        for imgs, labels in dataloader:  
  
            imgs = imgs.to(device) # upload to GPU  
            logits, features = model(imgs) # logits out (idx,class), features out (idx, num_feature )  
            logits = logits/TEMPSC # temperature scaling  
            if not valid_mode:  
                outfeature.append(features) # append features to tensor list for t-SNE plot  
                total_labels.append(labels)  
  
            score = anomaly_score(logits) # anomaly score (idx)  
            y_pred.extend(score.cpu().tolist()) # stack prediction score
```

# Code outline (test)

```
with torch.no_grad():
```

```
    for imgs, labels in dataloader:
```

```
        # We do nothing if label does not belong to NORMAL_NUM or ANOMALY_NUM
```

```
        for idata in range(logits.shape[0]):
```

```
            score_ = score[idata].item() anomaly score of each image
```

```
            if labels[idata] in NORMAL_NUM: # for normal data
```

```
                # calc CE loss for normal data
```

```
                p = F.one_hot(labels[idata], 10)[NORMAL_NUM].reshape(1, -1) make one-hot vector & reshape to 2D tensor
```

```
                logit = logits[idata, :].reshape(1, -1)
```

```
                loss = loss_fn(logit.to(device), p.float().to(device)) # Cross-Entropy loss for normal
```

```
                normal_loss.append(loss.cpu())
```

```
            # record scores
```

```
            y_true.append(0.)
```

```
            normal_scores.append(score_) append scores
```

```
        elif labels[idata] in ANOMALY_NUM: # for abnormal data
```

```
            y_true.append(1.)
```

```
            anomaly_scores.append(score_)
```

```
roc_auc = metrics.roc_auc_score(y_true, y_pred)
```

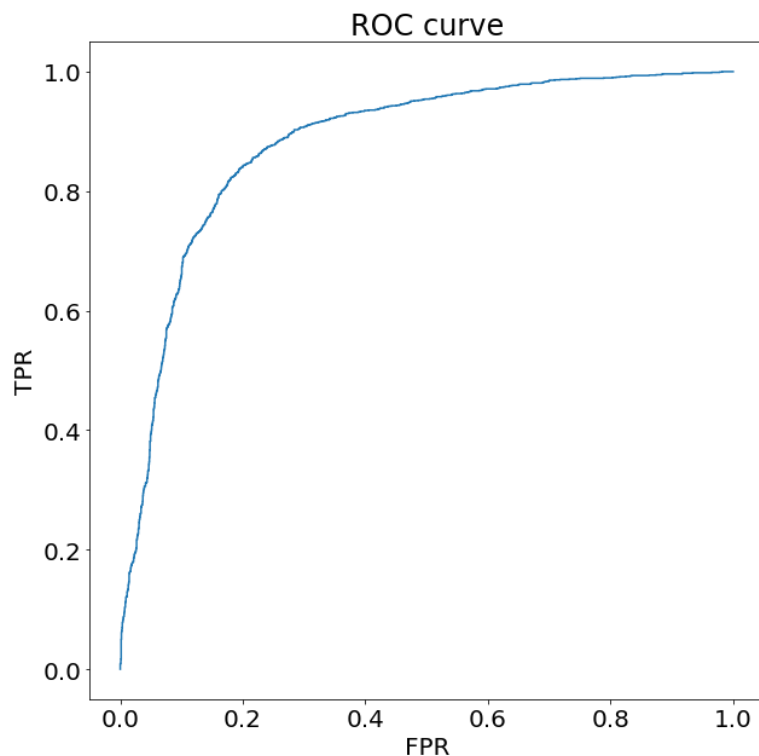
```
if not valid_mode:
```

```
    outfeature = torch.cat(outfeature, dim=0).cpu().numpy()
```

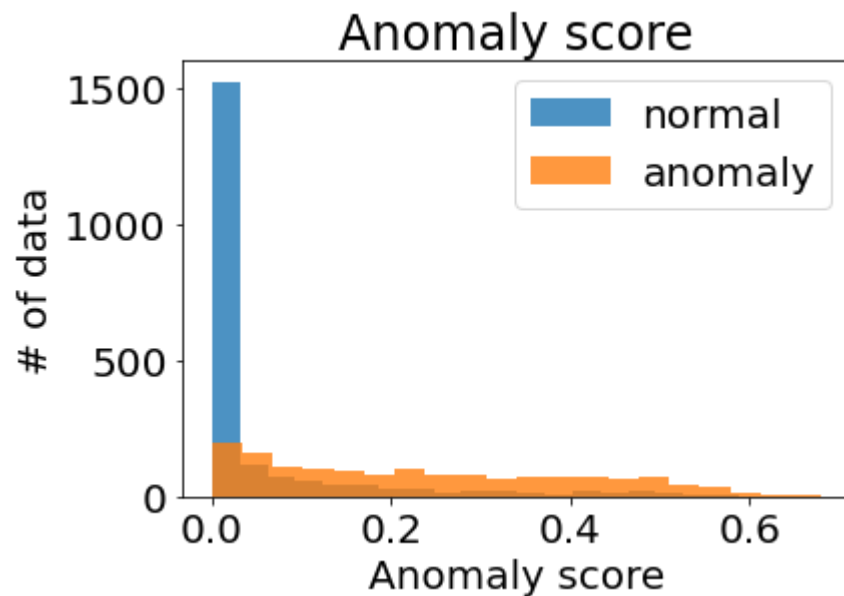
```
    total_labels = torch.cat(total_labels, dim=0).cpu().numpy()
```

# Classification result (Init)

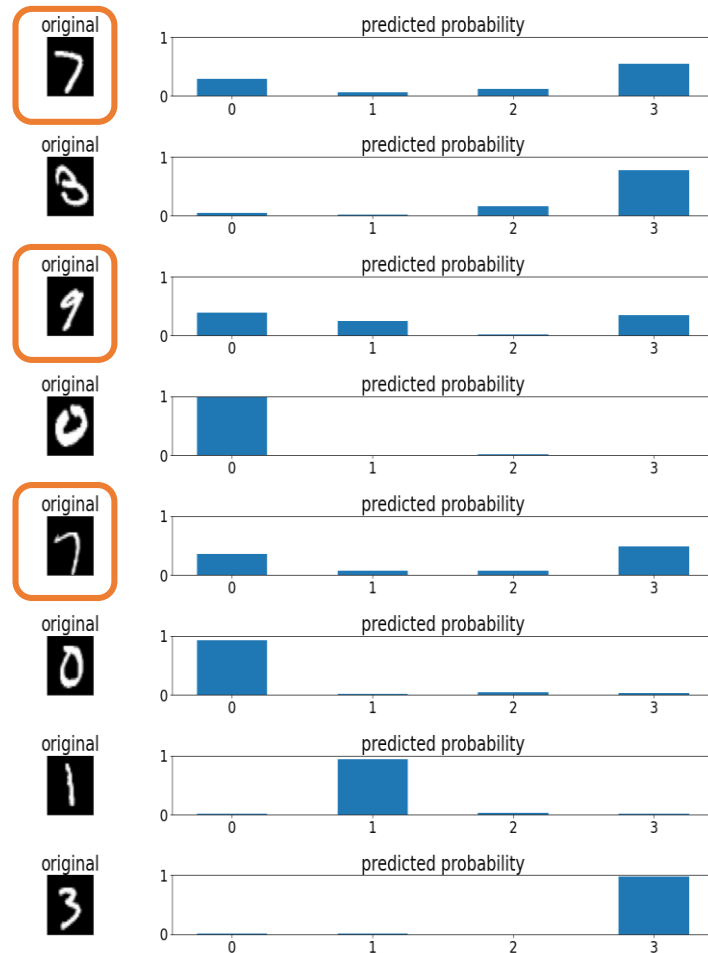
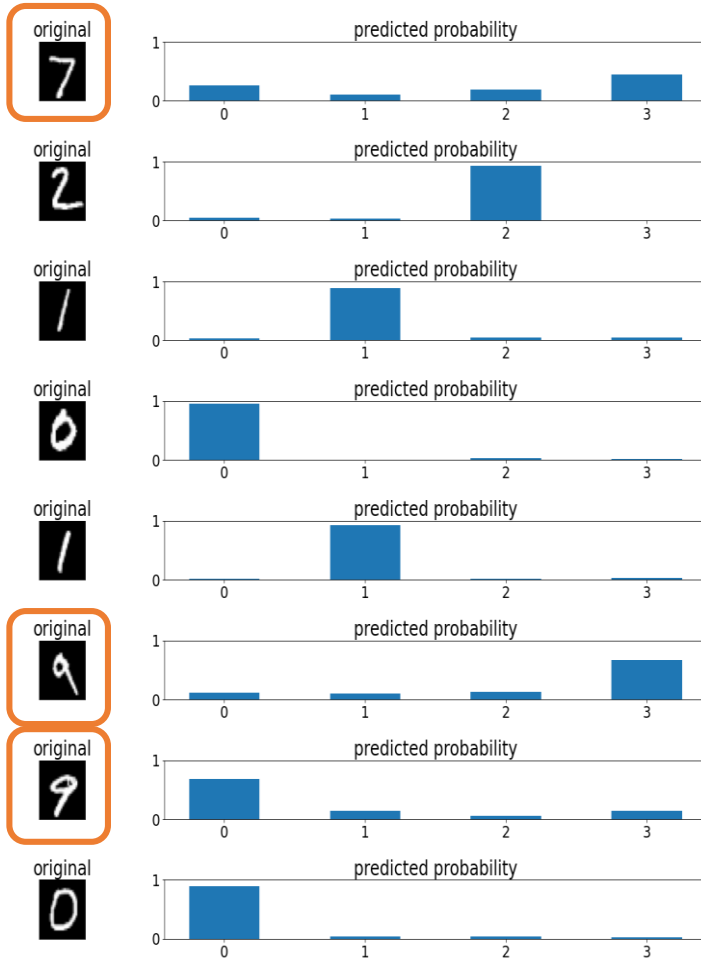
- Without label smoothing & temperature scaling



ROC-AUC: 0.868

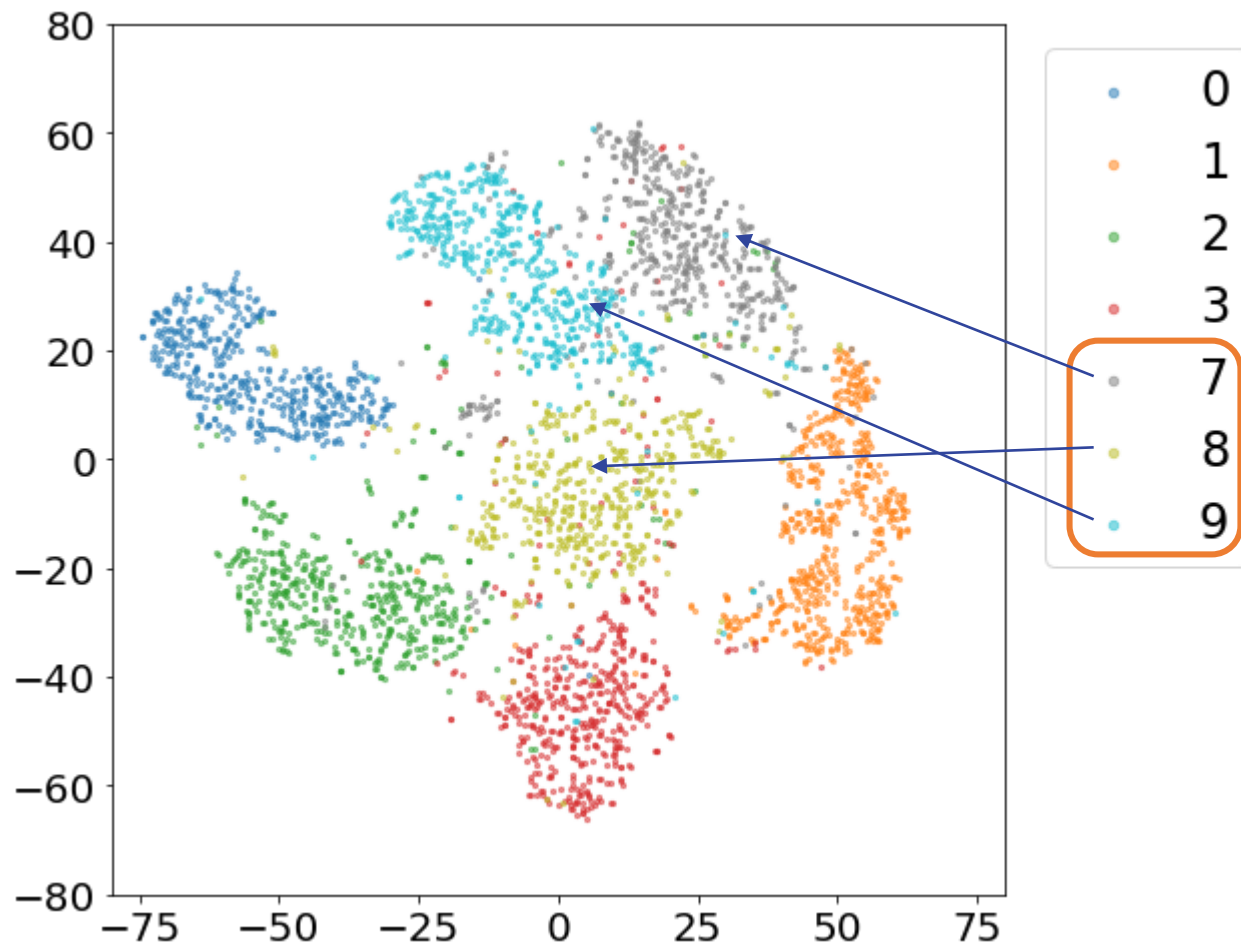


# Classification result (initial)



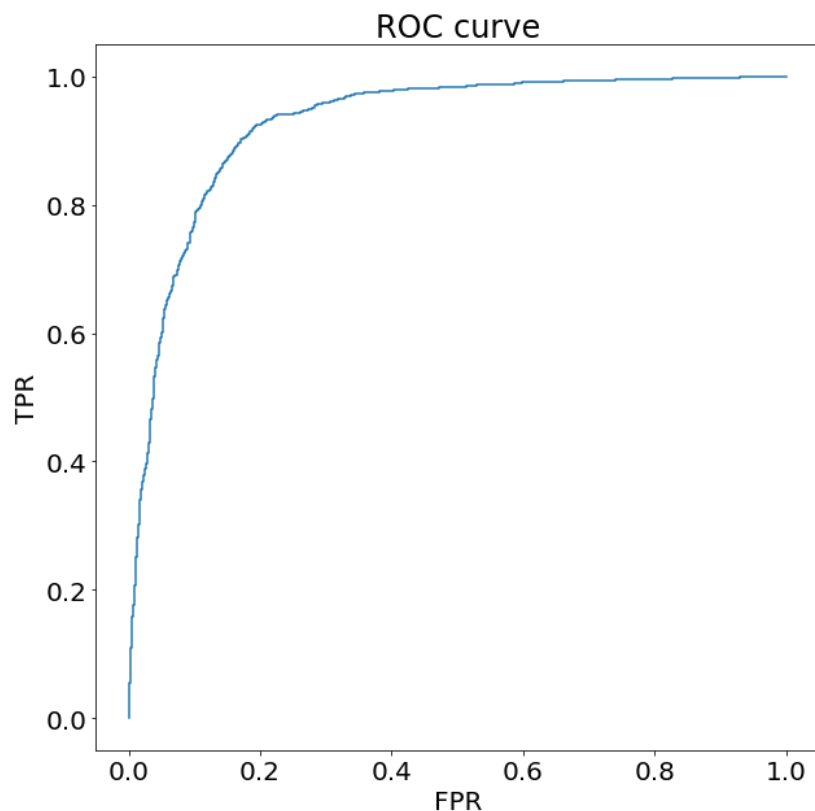
# Feature embedding visualization

- t-SNE visualization (Without label smoothing & temperature scaling)

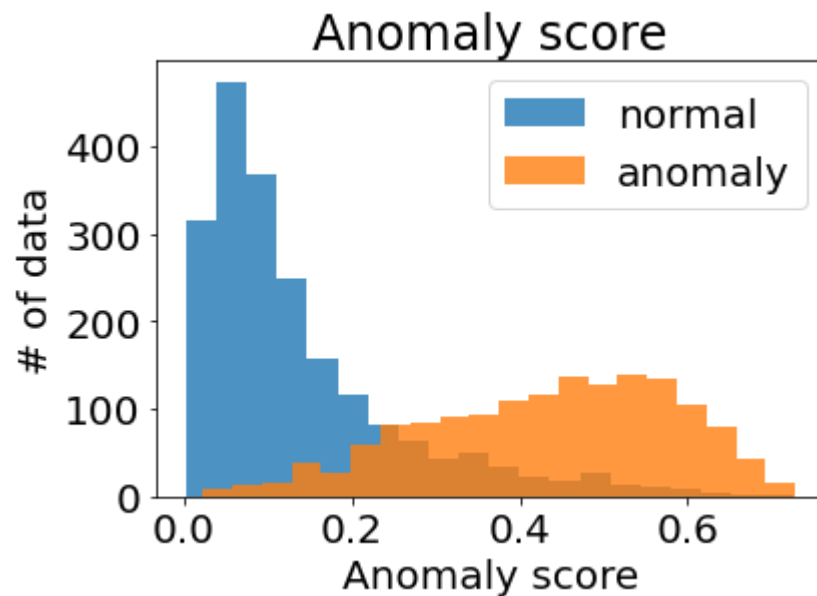


# Classification result (Label Smoothing = 0.1)

- With label smoothing (smoothing = 0.1)

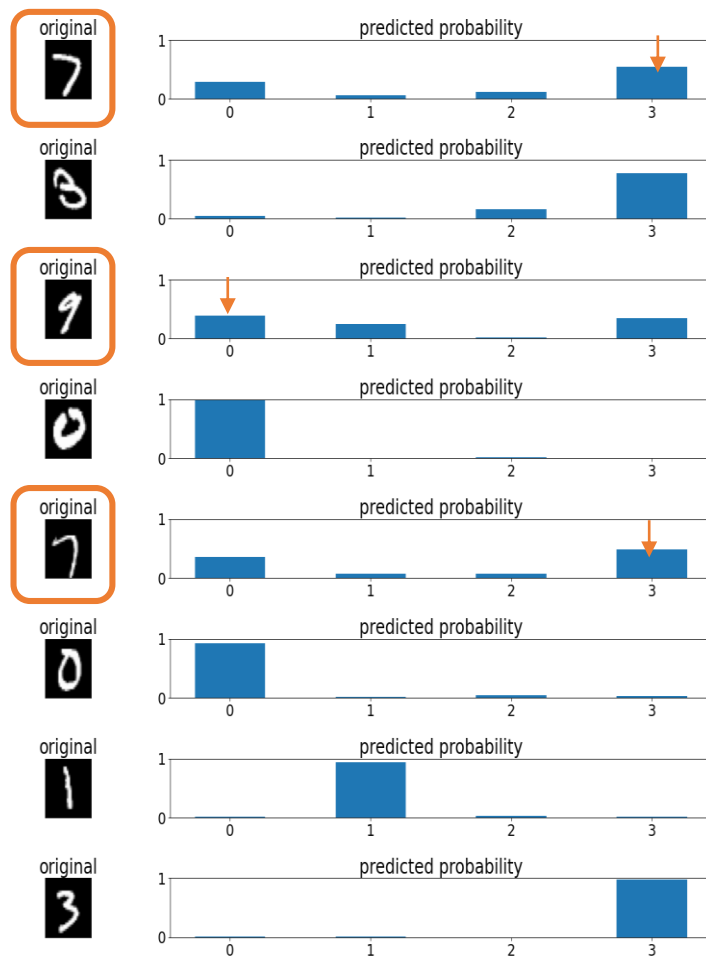
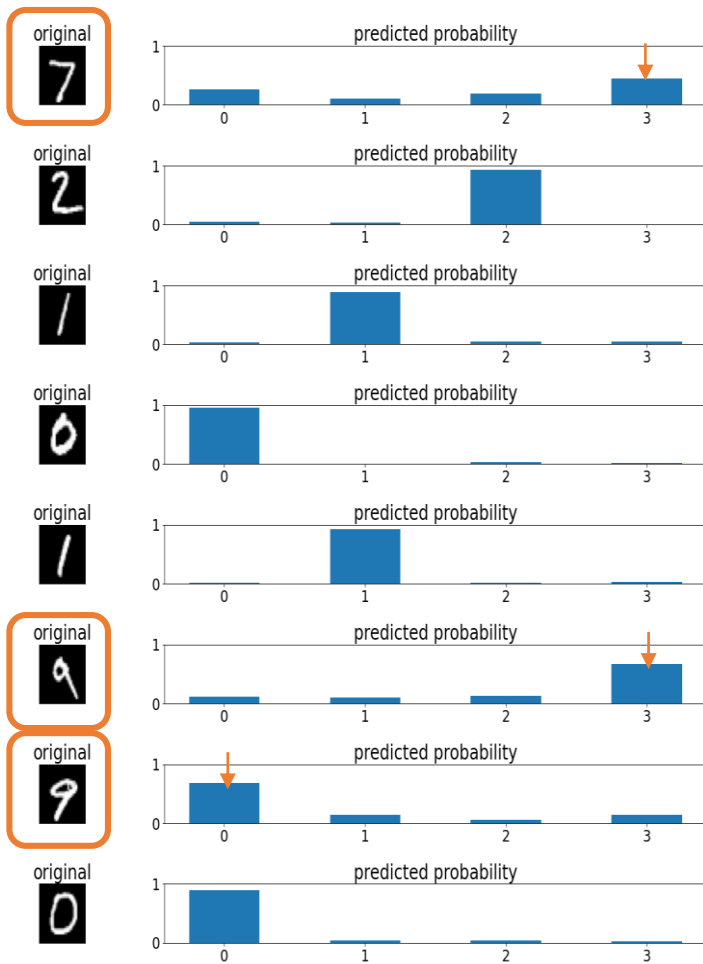


ROC-AUC: 0.927



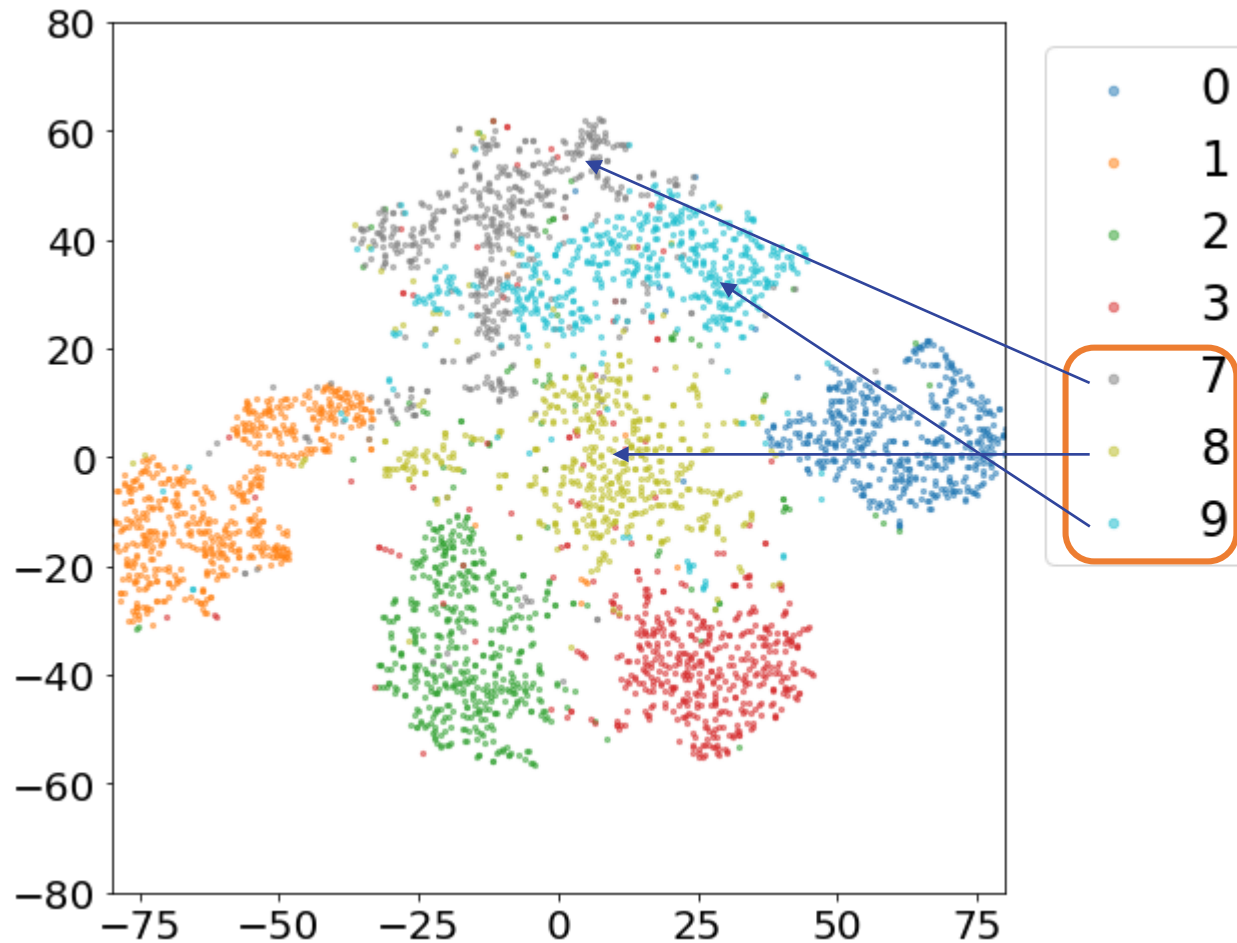


# Classification result (Label Smoothing = 0.1)



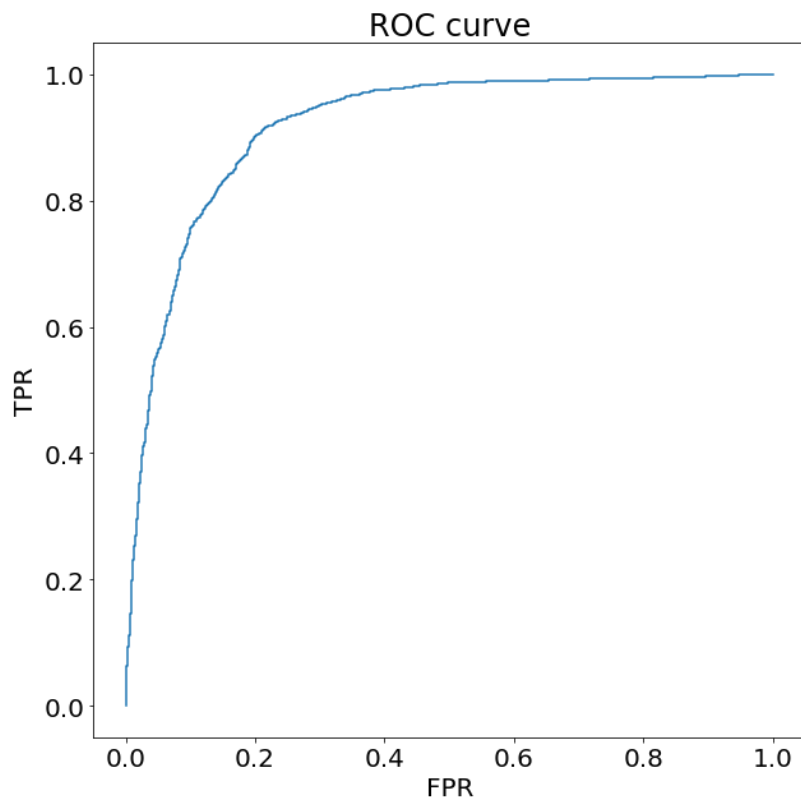
# Feature embedding visualization

- t-SNE visualization (Label Smoothing = 0.1)

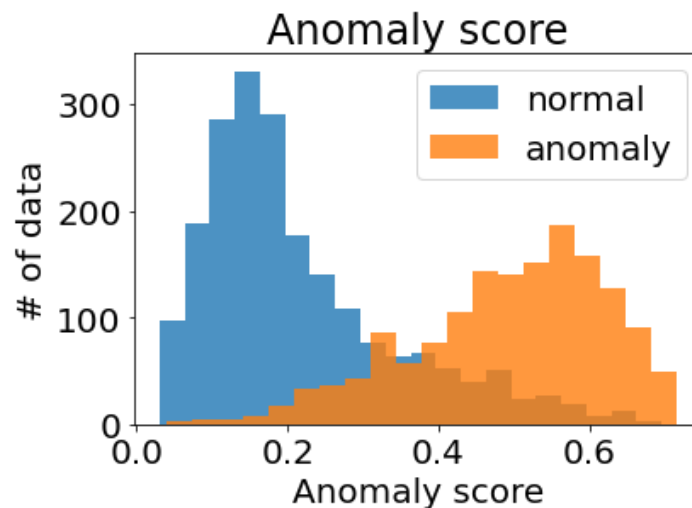


# Classification result (Label Smoothing)

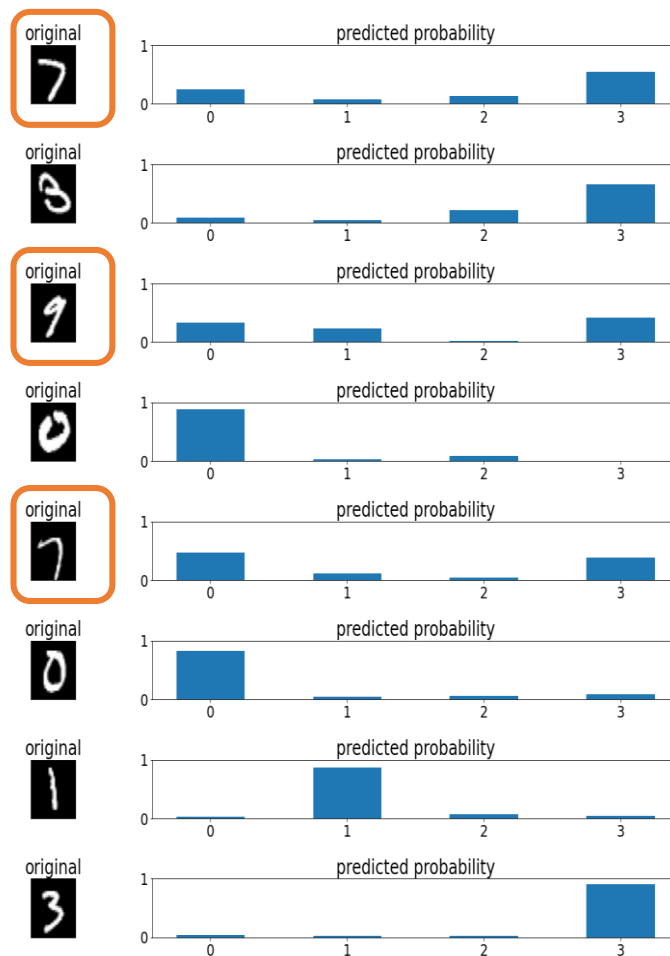
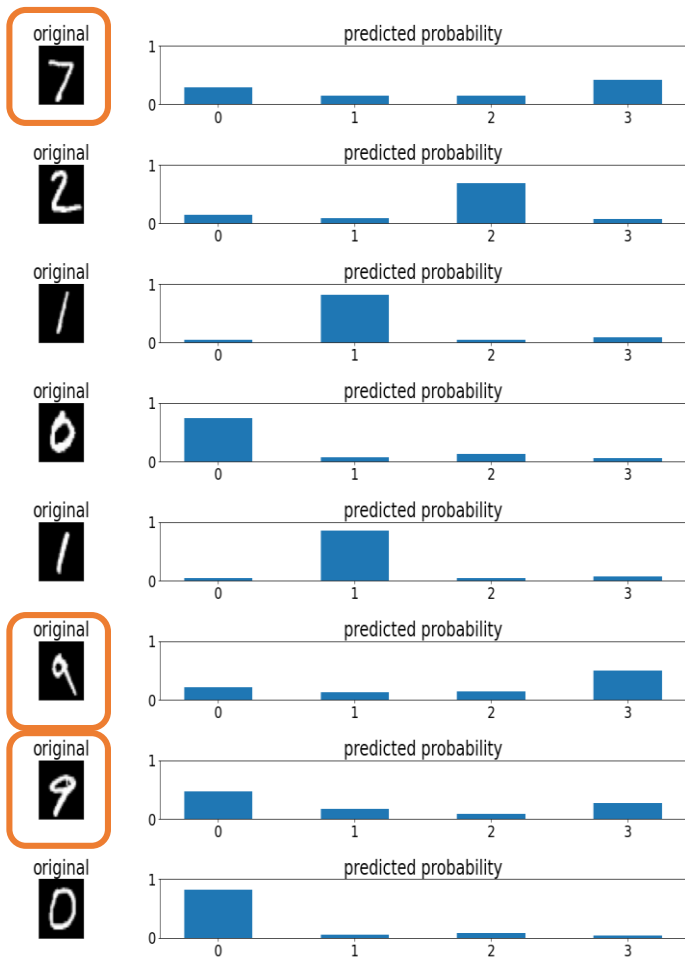
- With label smoothing (smoothing = 0.2)



ROC-AUC: 0.918

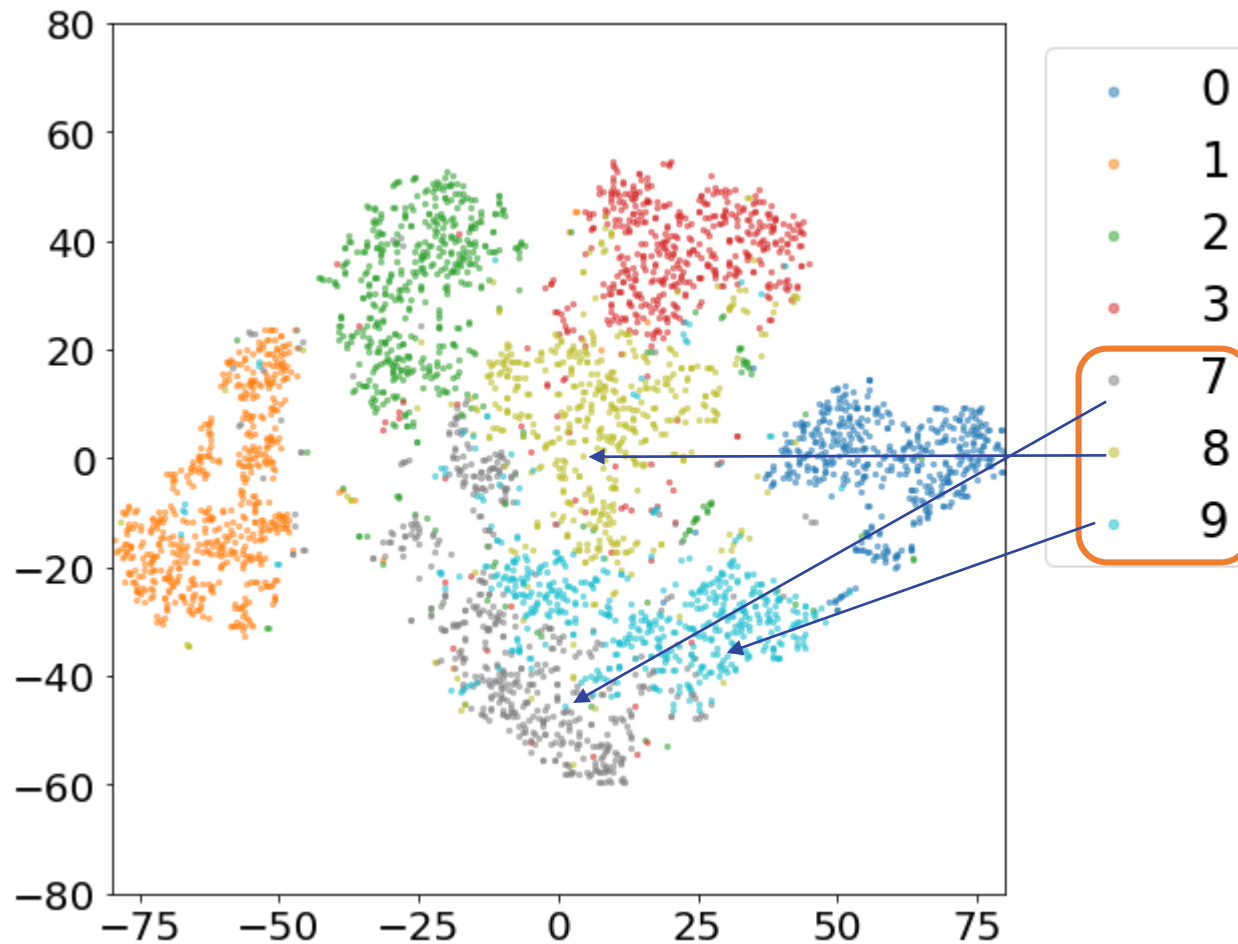


# Classification result (Label smoothing = 0.2)



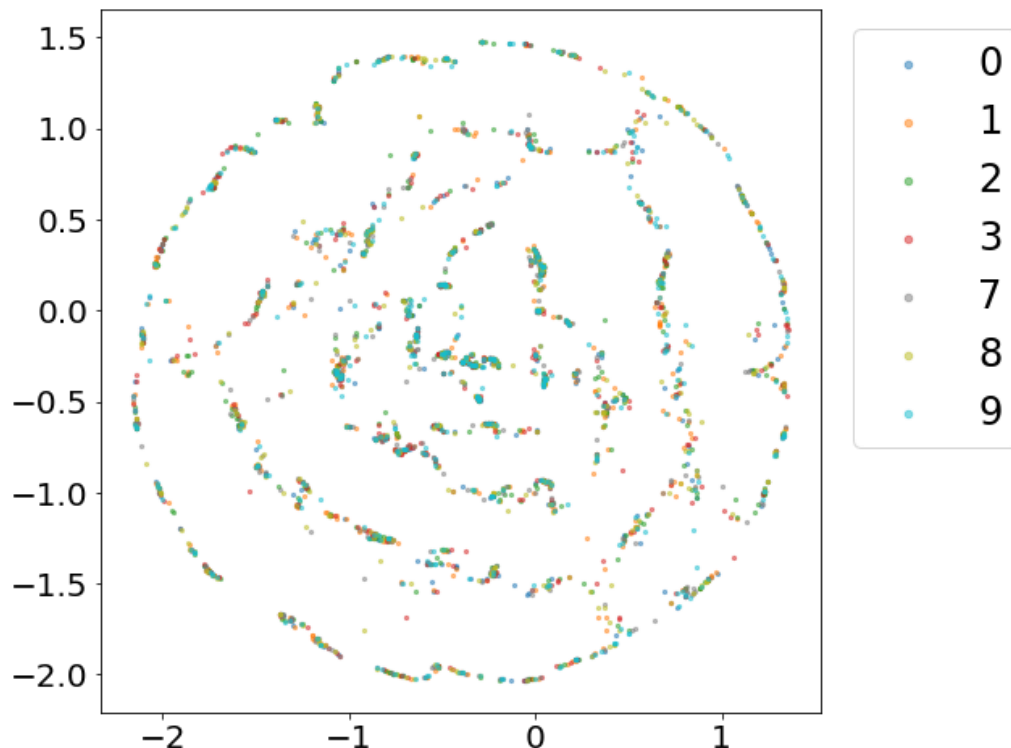
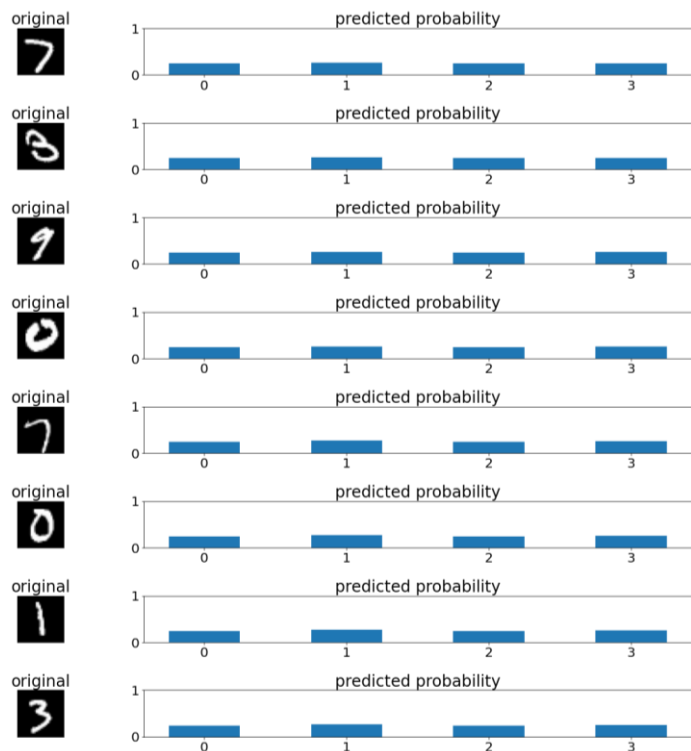
# Feature embedding visualization

- t-SNE visualization



# Excessive label smoothing

- Label Smoothing = 0.3

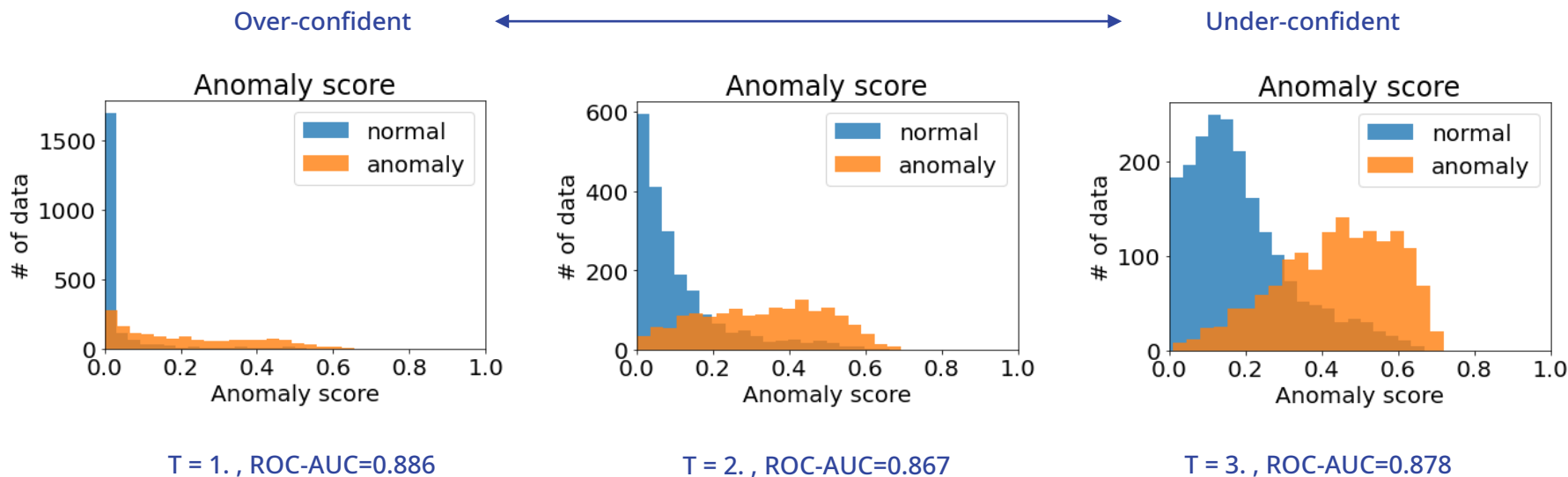


# Temperature Scaling

Calibration of trained model

# Effect of temperature scaling

- Histograms for different temperatures



```
TEMPSC = 3.0    # temperature parameter (for temperature scaling)
LBSMOOTH = 0.1  # label smoothing parameter
```



# Label smoothing vs. Temp. scaling

- Label smoothing

- Change the **target probability**
- Trained models are different

- Effect

- Prevent an over-confident **model**
- Enlarge inter-class feature distances
- Optimal parameter: by repeating training

- Temperature scaling

- Scale the **logit**
- Does not change the model & training
- Calibration of the trained model

- Effect

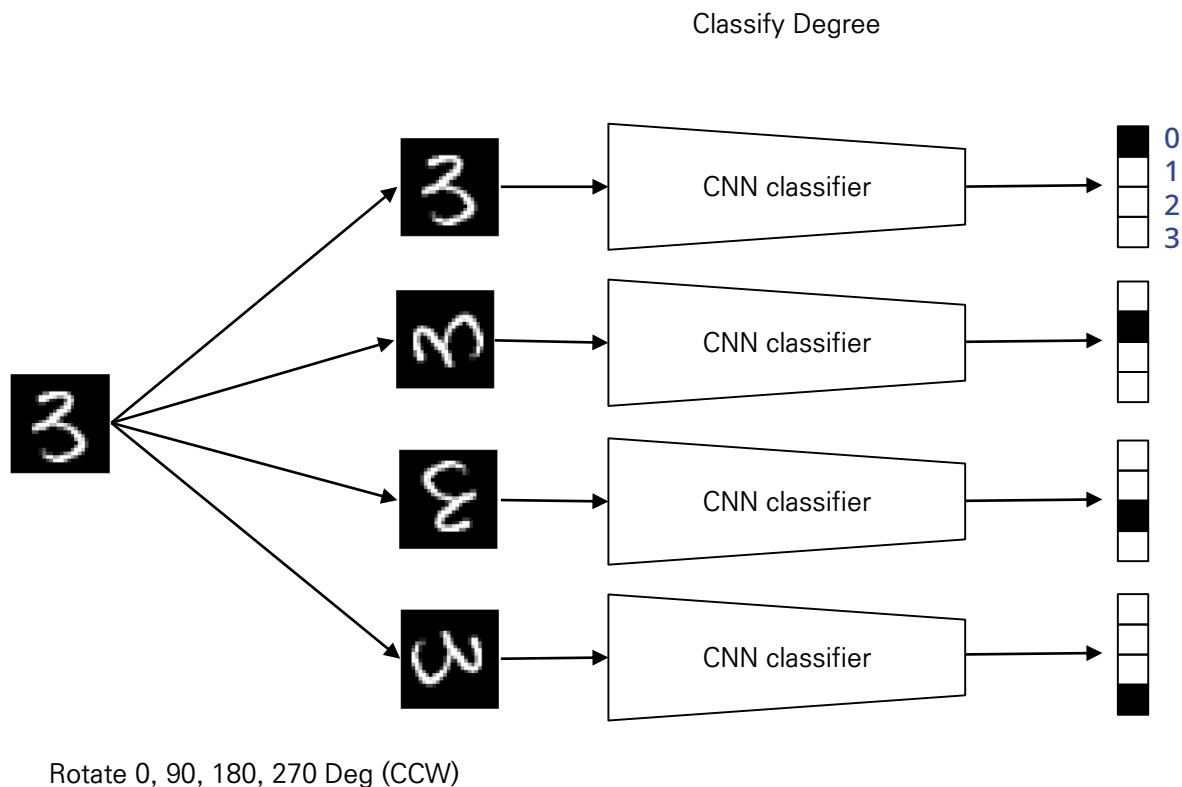
- Prevent an over-confident **scoring**
- Features do not change
- Optimal parameter can be found by tuning with a validation dataset

# RotNet

Classifying Rotations of Images

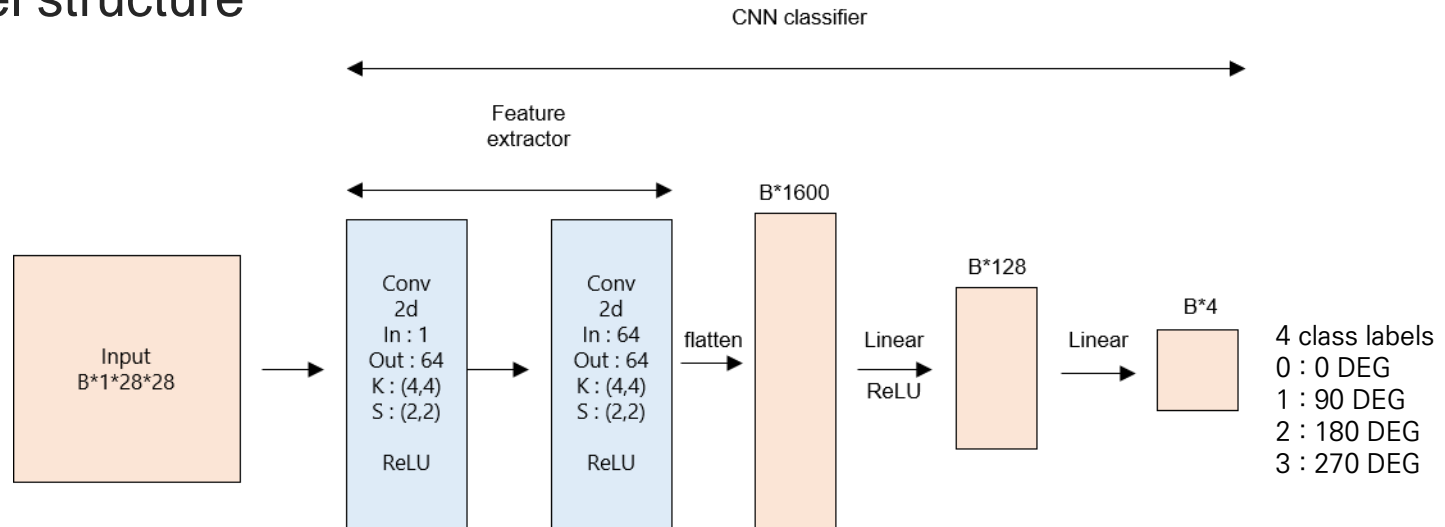
# RotNet

- Does not require internal labels
  - Apply rotation transform to each image
  - Model is forced to predict rotation angles (labels)



# RotNet Structure

- Model structure



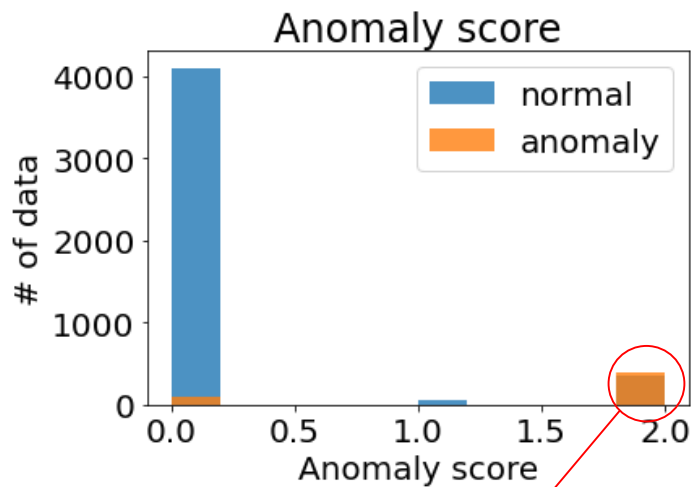
- Loss function & Anomaly score

- Loss function : Cross Entropy
- Anomaly score :
  - <ex> : pred : 0 , true : 1  $\rightarrow$  Anomaly score : 1
  - <ex> : pred : 0 , true : 3  $\rightarrow$  Anomaly score : 1 (Think that degree circulates [0,360).)

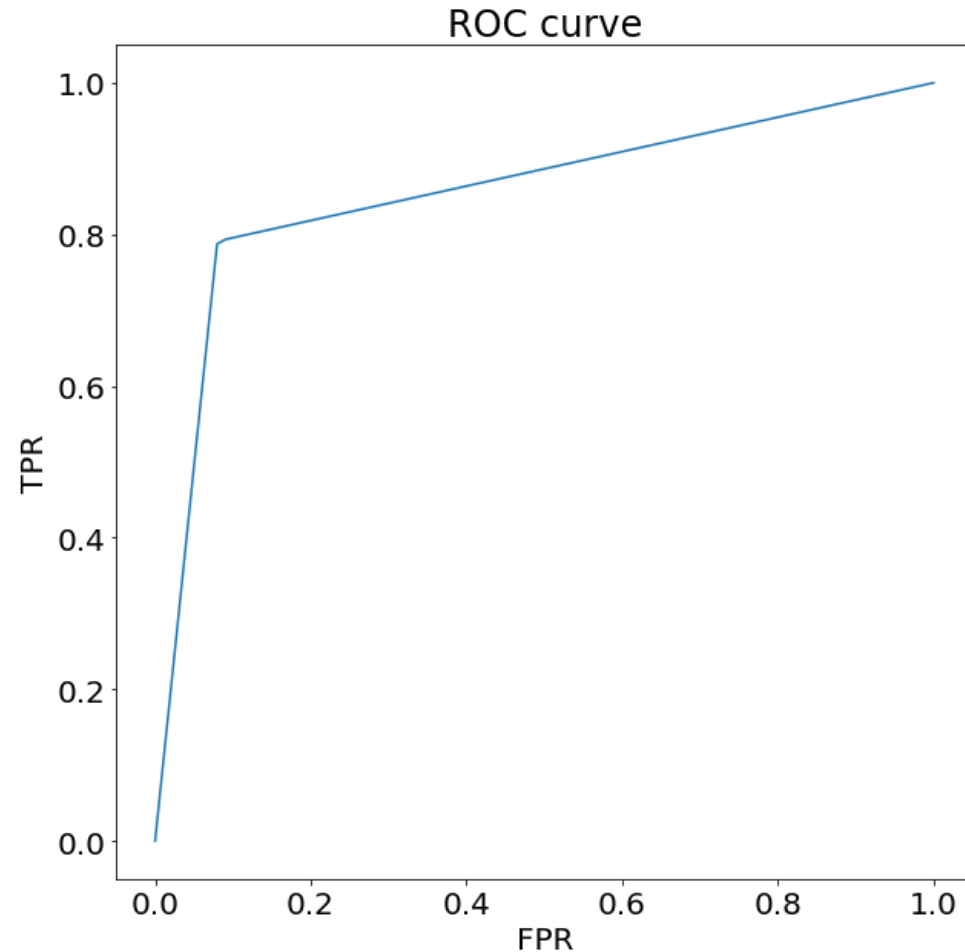
$$\min(|pred - true|, 4 - |pred - true|)$$

# Anomaly Detection using Self-supervised learning

- Rotnet



Why this happen?



ROC AUC = 0.856

# Anomaly Detection using Self-supervised learning

Blue for predicted class label and orange for true class label

