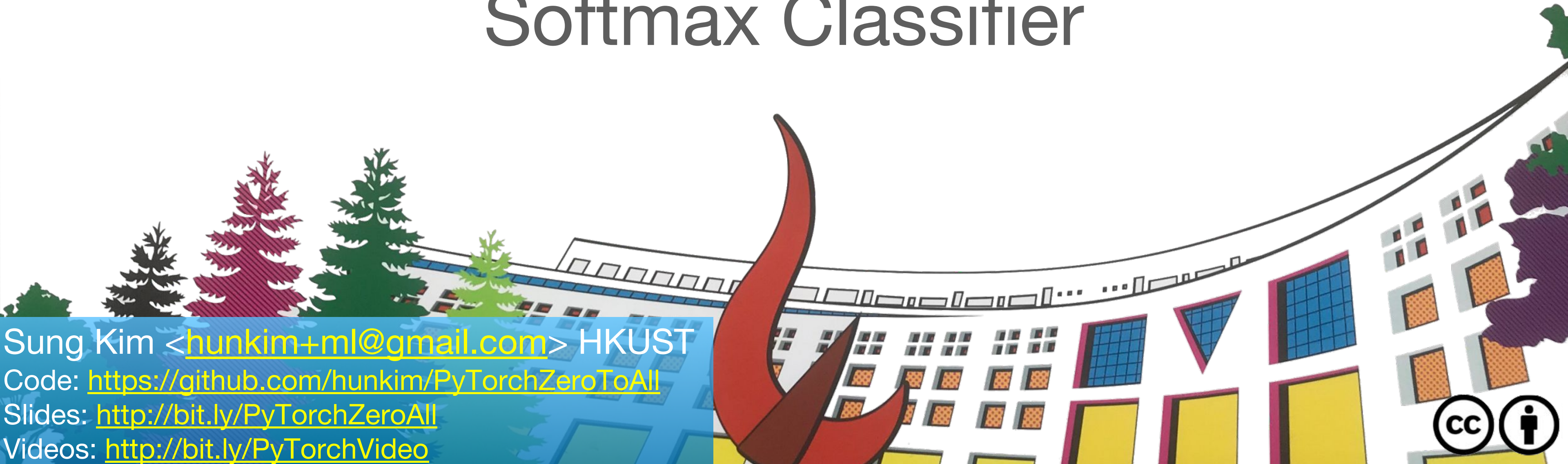
ML/DL for Everyone with PYTORCH

Lecture 9:
Softmax Classifier



Sung Kim <hunkim+ml@gmail.com> HKUST

Code: https://github.com/hunkim/PyTorchZeroToAll

Slides: http://bit.ly/PyTorchZeroAll

Videos: http://bit.ly/PyTorchVideo

Call for Comments

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Other slides: http://bit.ly/PyTorchZeroAll

Picture from http://www.tssablog.org/archives/3280

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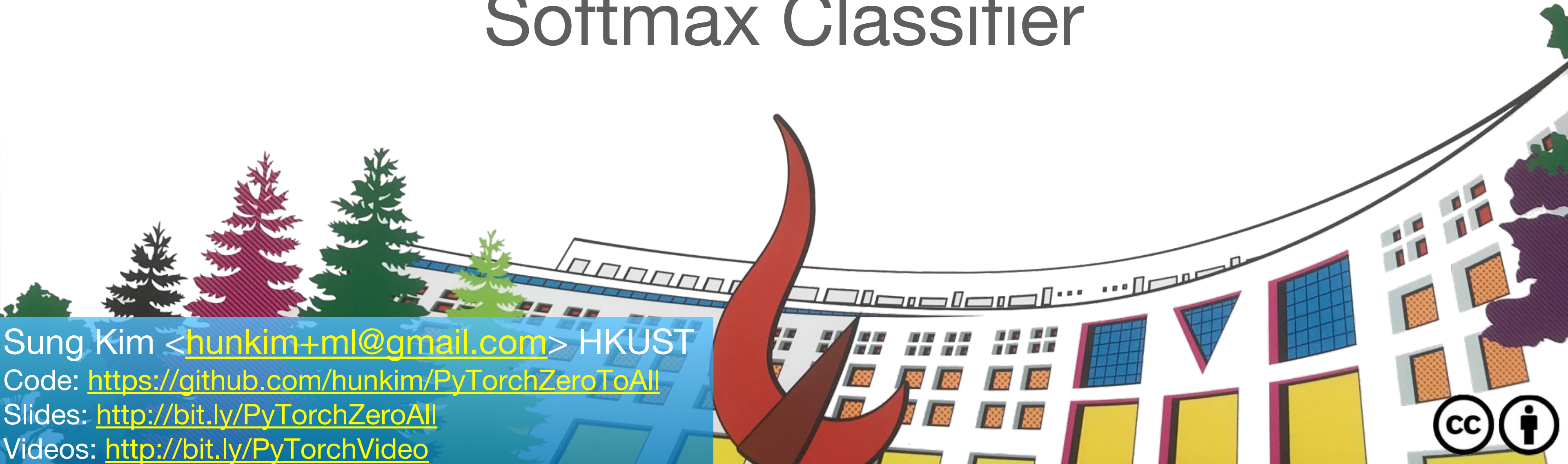
Lecture 9:
Softmax Classifier



Sung Kim <hunkim+ml@gmail.com> HKUST
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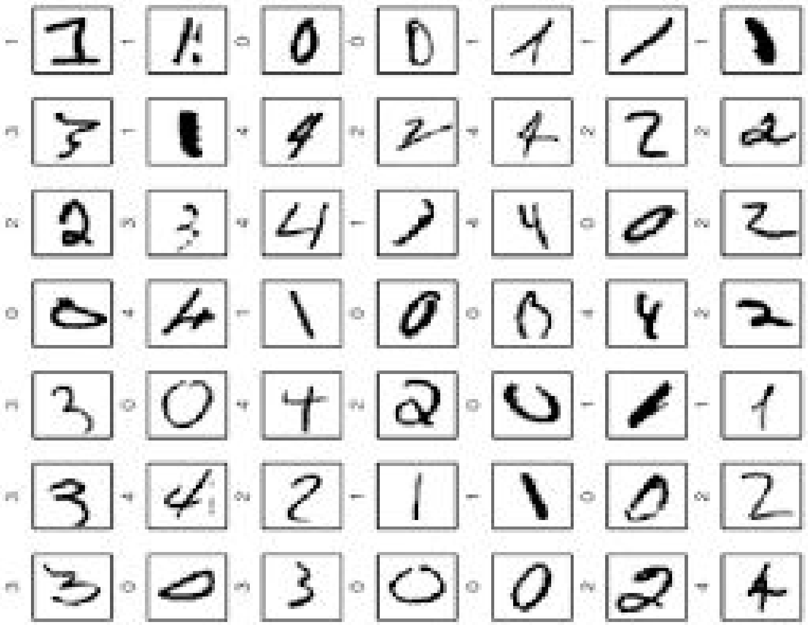
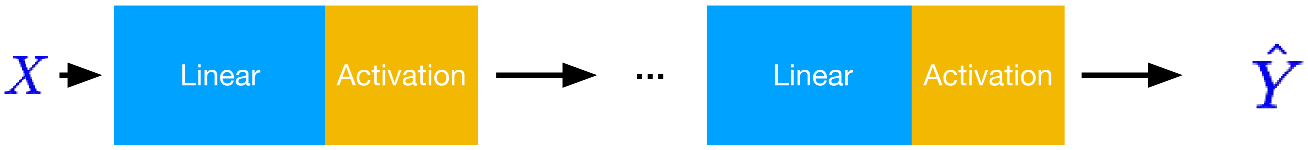
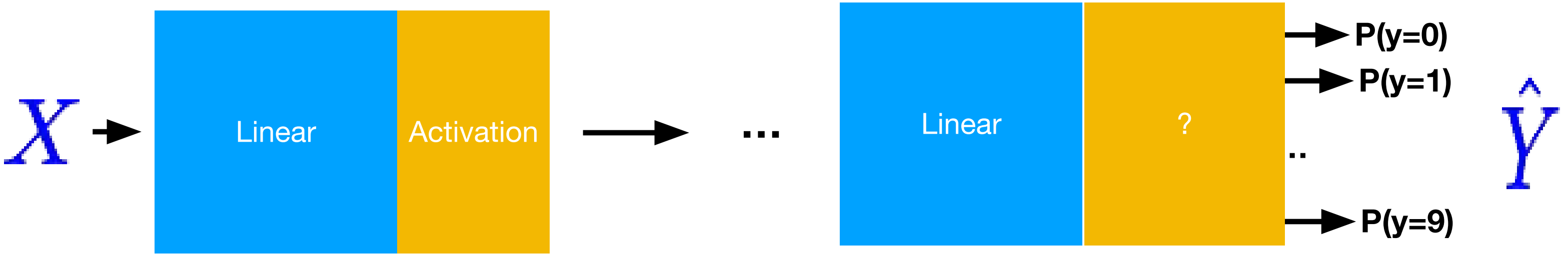
MNIST: 10 labels



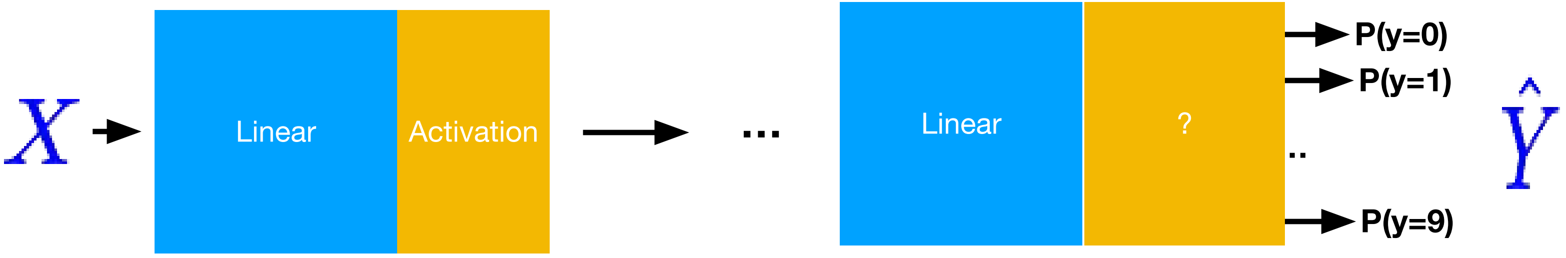
10 labels: 10 outputs



10 labels: 10 outputs

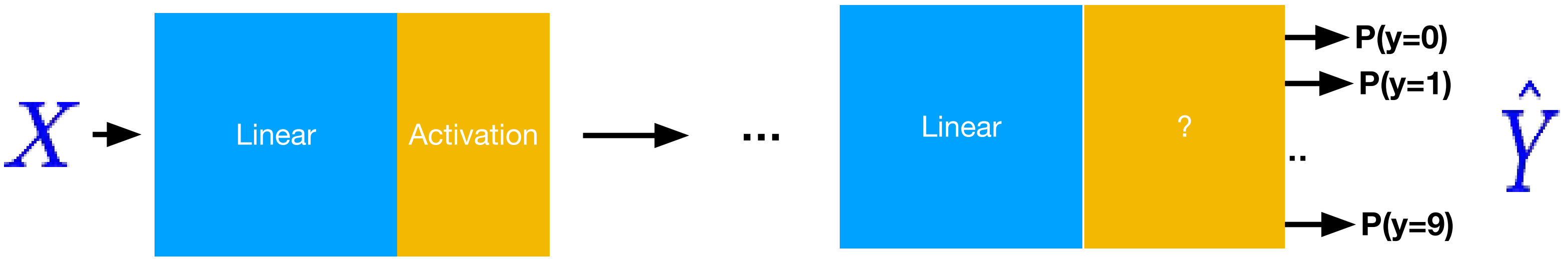


10 outputs



$$\underbrace{\begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \\ \cdots & \cdots \\ a_n & b_n \end{bmatrix}}_{x\in\mathbb{R}^{N\times 2}} \underbrace{\begin{bmatrix} w_1 \\ w_2 \end{bmatrix}}_{w\in\mathbb{R}^{2\times 1}} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \cdot\,\cdot \\ y_n \end{bmatrix}}_{y\in\mathbb{R}^{N\times 1}}$$

10 outputs

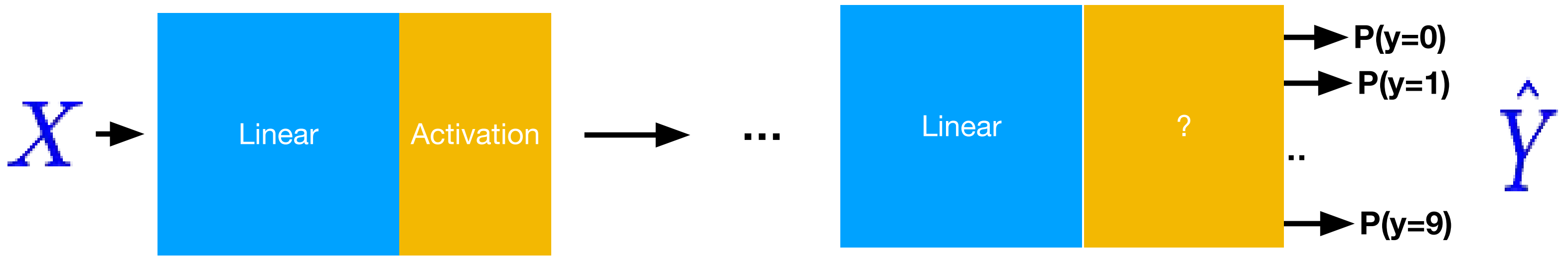


$$\underbrace{\begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \\ \cdots & \cdots \\ a_n & b_n \end{bmatrix}}_{x \in \mathbb{R}^{N\times 2}} \underbrace{\begin{bmatrix} w_1 \\ w_2 \end{bmatrix}}_{w \in \mathbb{R}^{2\times 1}} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \cdot\cdot \\ y_n \end{bmatrix}}_{y \in \mathbb{R}^{N\times 1}}$$

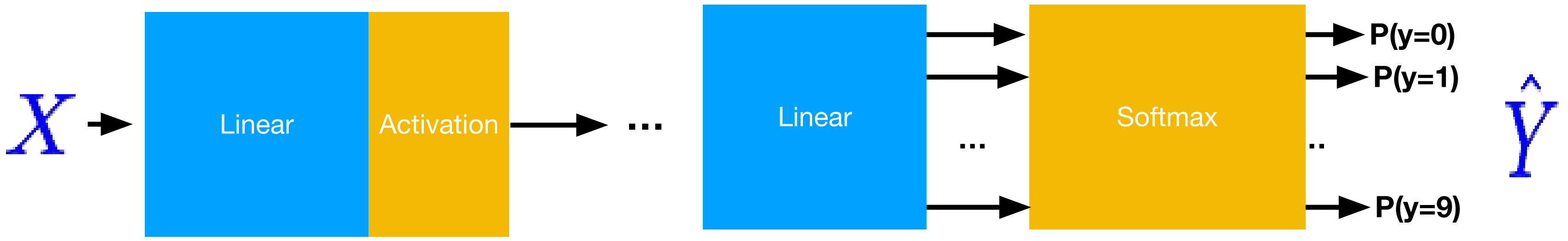
$$\underbrace{\begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \\ \cdots & \cdots \\ a_n & b_n \end{bmatrix}}_{x \in \mathbb{R}^{N\times 2}} \begin{bmatrix} \ ? \ \end{bmatrix} = y \in R^{N\times 10}$$

$$w \in \mathbb{R}^{2\times ?}$$

Probability

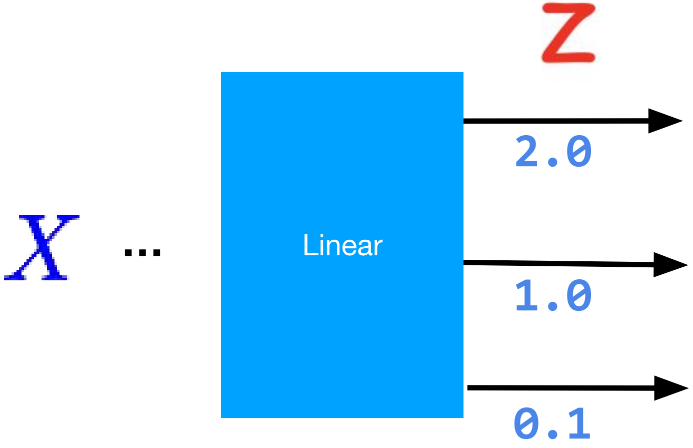


Softmax



Meet Softmax

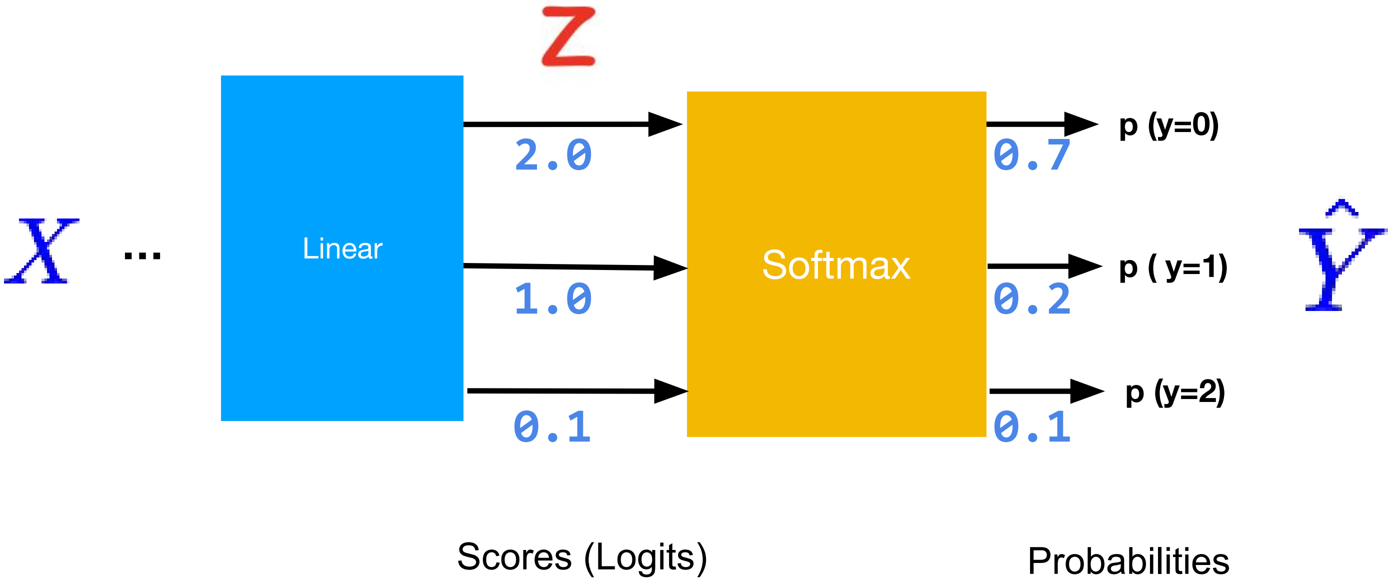
$$\sigma(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_k}} \quad \text{for } j = 1, \ldots, K.$$

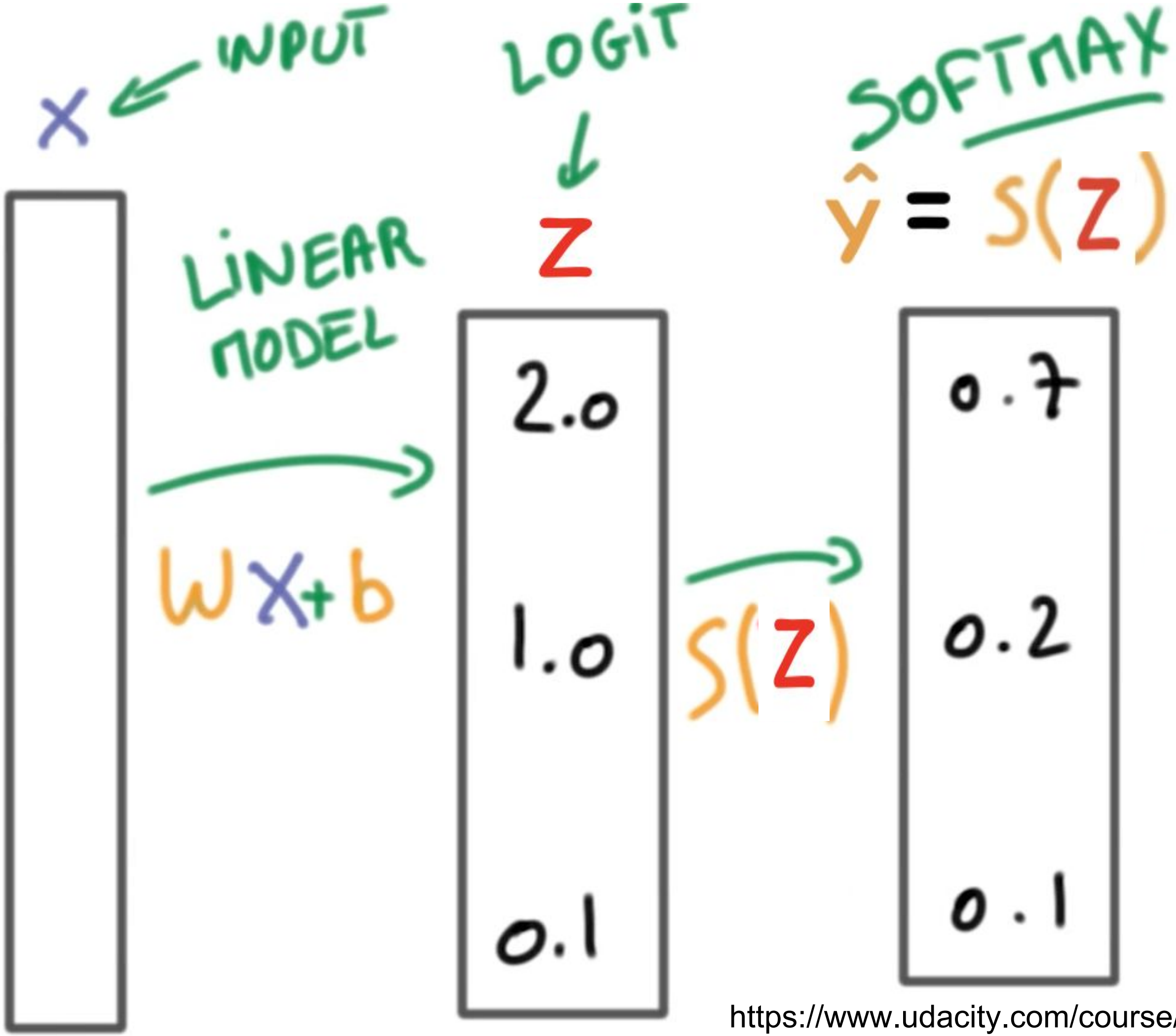


Scores (Logits)

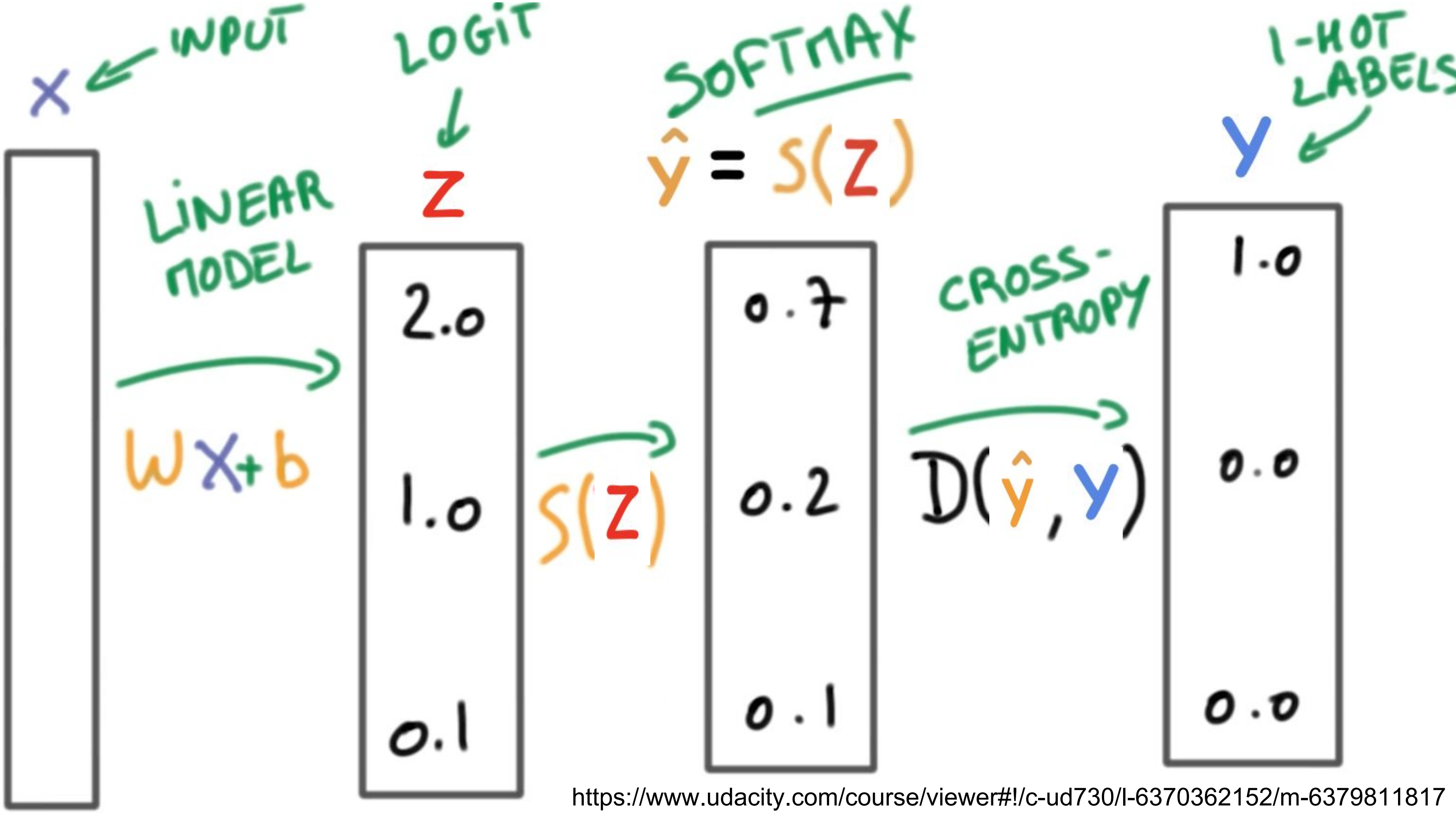
Meet Softmax

$$\sigma(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_k}} \quad \text{for } j = 1, \ldots, K.$$





https://www.udacity.com/course/viewer#!/c-ud730/l-6370362152/m-6379811817



https://www.udacity.com/course/viewer#!/c-ud730/l-6370362152/m-6379811817

Cost function: cross entropy

LOSS

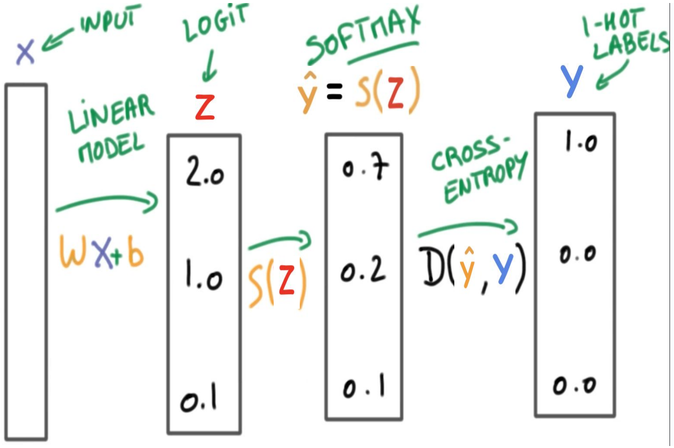
$$\mathcal{L} = \frac{1}{N}\sum_i D(\overset{\hat{y}}{S(wx_i+b)}, y_i)$$

TRAINING SET

$$D(\hat{Y}, Y) = -Y log \hat{Y}$$

https://www.udacity.com/course/viewer#!/c-ud730/l-6370362152/m-6379811817

Cost function: cross entropy

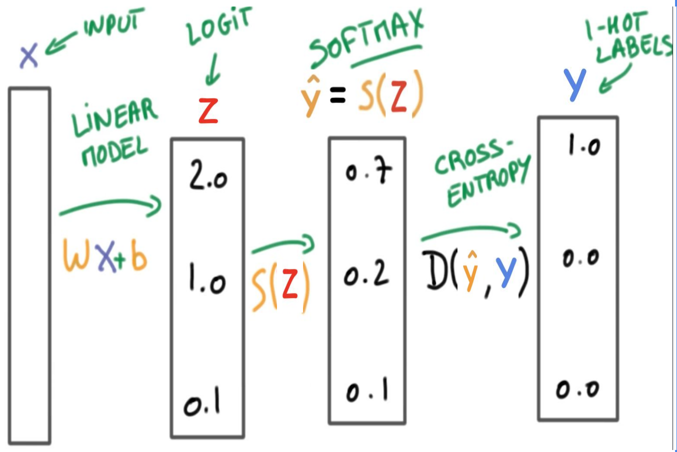


$$D(\hat{Y}, Y) = -Y log \hat{Y}$$

```python
# Cross entropy example
import numpy as np
# One hot
# 0: 1 0 0 0
# 1: 0 1 0 0
# 2: 0 0 1 0
Y = np.array([1, 0, 0])

Y_pred1 = np.array([0.7, 0.2, 0.1])
Y_pred2 = np.array([0.1, 0.3, 0.6])
print("loss1 = ", np.sum(-Y * np.log(Y_pred1)))
print("loss2 = ", np.sum(-Y * np.log(Y_pred2)))
```

https://www.udacity.com/course/viewer#!/c-ud730/l-6370362152/m-6379811817

Cross entropy in PyTorch

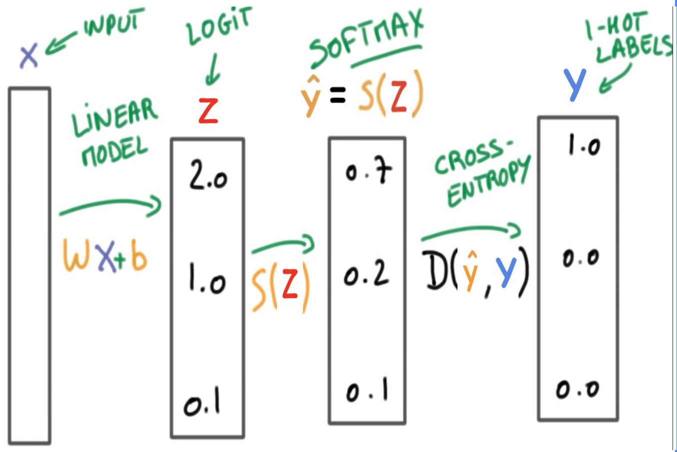


$$D(\hat{Y}, Y) = -Y log \hat{Y}$$

```
# Softmax + CrossEntropy (logSoftmax + NLLLoss)
loss = nn.CrossEntropyLoss()

# target is of size nBatch
# each element in target has to have 0 <= value < nClasses (0-2)
# Input is class, not one-hot
Y = Variable(torch.LongTensor([0]), requires_grad=False)

# input is of size nBatch x nClasses = 1 x 4
# Y_pred are logits (not softmax)
Y_pred1 = Variable(torch.Tensor([[2.0, 1.0, 0.1]]))
Y_pred2 = Variable(torch.Tensor([[0.5, 2.0, 0.3]]))

l1 = loss(Y_pred1, Y)
l2 = loss(Y_pred2, Y)

print("PyTorch Loss1 = ", l1.data,
    "\nPyTorch Loss2=", l2.data)
```

https://www.udacity.com/course/viewer#!/c-ud730/l-6370362152/m-6379811817

Cross entropy in PyTorch



$$D(\hat{Y}, Y) = -Y log \hat{Y}$$

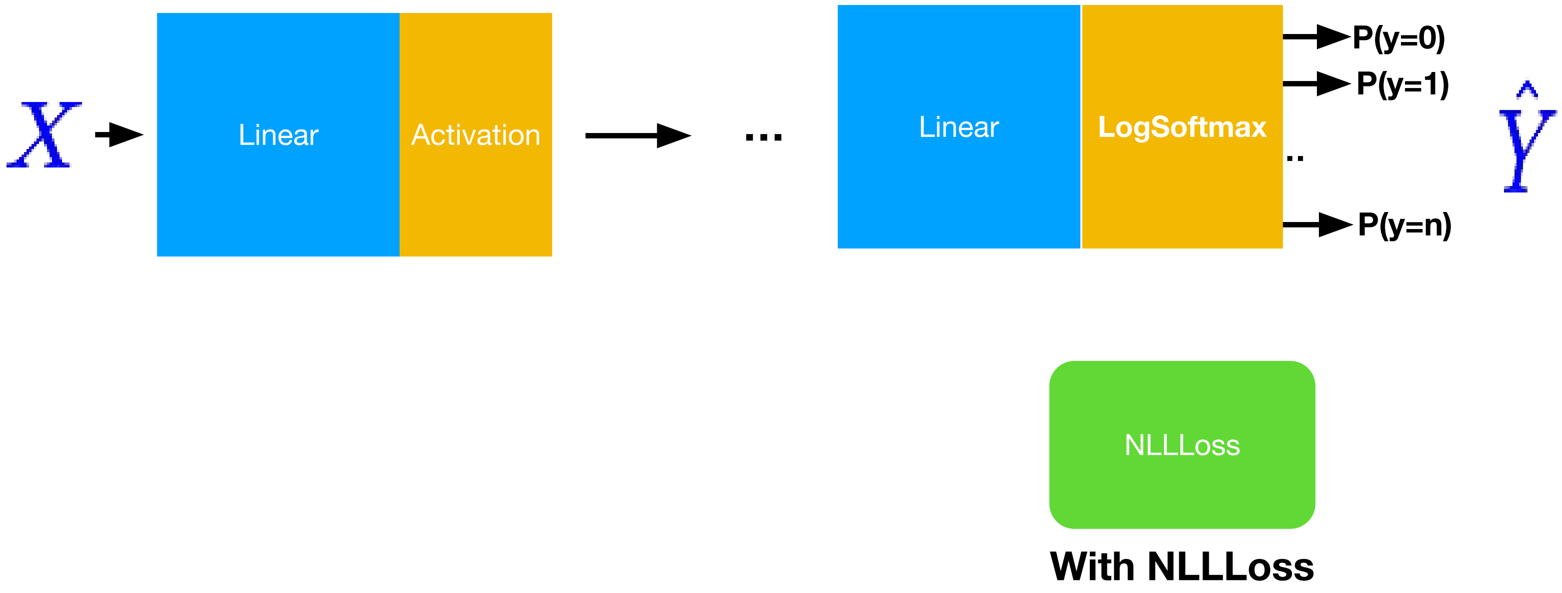
```python
# Softmax + CrossEntropy (logSoftmax + NLLLoss)
loss = nn.CrossEntropyLoss()

# target is of size nBatch
# element in target has to have 0 <= value < nClasses (0-2)
# Input is class, not one-hot
Y = Variable(torch.LongTensor([2, 0, 1]), requires_grad=False)

# input is of size nBatch x nClasses = 2 x 4
# Y_pred are logits (not softmax)
Y_pred1 = Variable(torch.Tensor([[0.1, 0.2, 0.9],
                                 [1.1, 0.1, 0.2],
                                 [0.2, 2.1, 0.1]]))


Y_pred2 = Variable(torch.Tensor([[0.8, 0.2, 0.3],
                                 [0.2, 0.3, 0.5],
                                 [0.2, 0.2, 0.5]]))

l1 = loss(Y_pred1, Y)
l2 = loss(Y_pred2, Y)

print("Batch Loss1 = ", l1.data, "\nBatch Loss2=", l2.data)
```

https://www.udacity.com/course/viewer#!/c-ud730/l-6370362152/m-6379811817

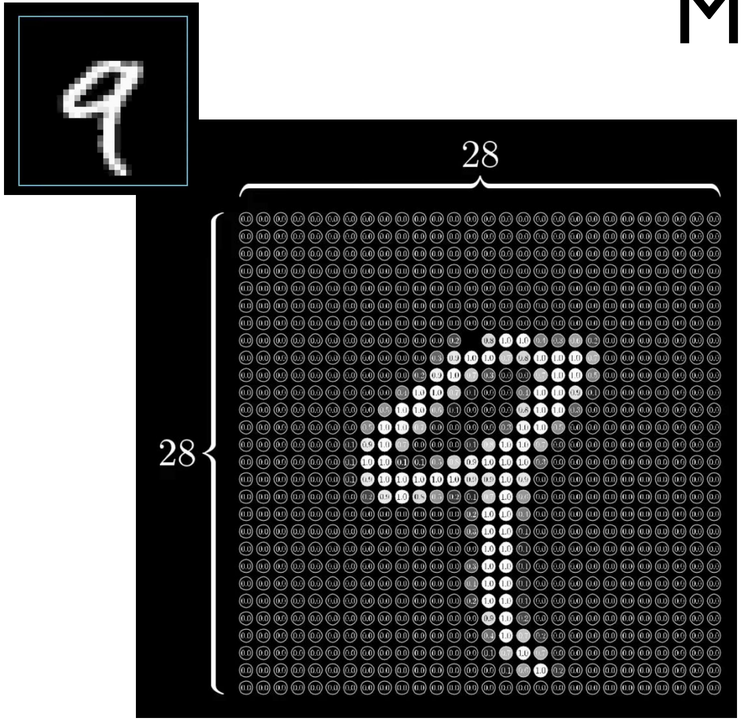
Exercise 9-1: CrossEntropyLoss VS NLLLoss

- What are the differences?
- Check out
  - http://pytorch.org/docs/master/nn.html#nllloss
  - http://pytorch.org/docs/master/nn.html#crossentropyloss
- Minimizing the Negative Log-Likelihood, in English
  http://willwolf.io/2017/05/18/minimizing_the_negative_log_likelihood_in_english/

(log)Softmax + NLLLoss



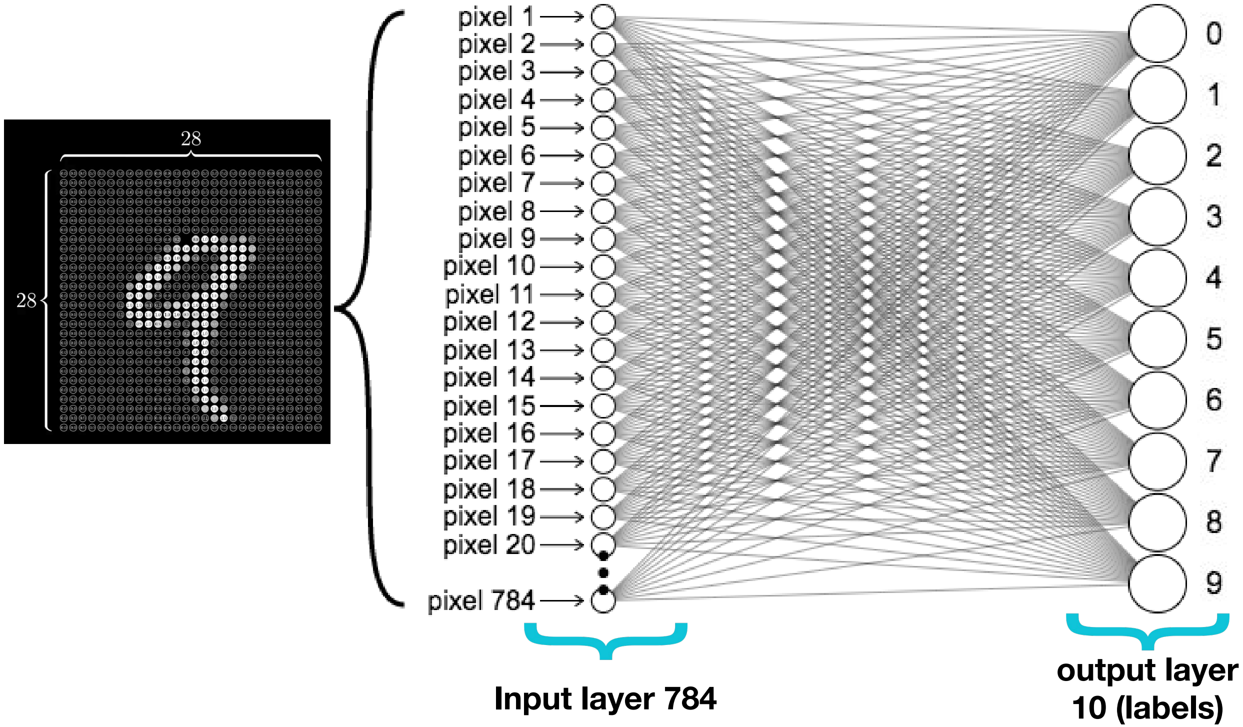
MNIST input



28x28 pixels = 784

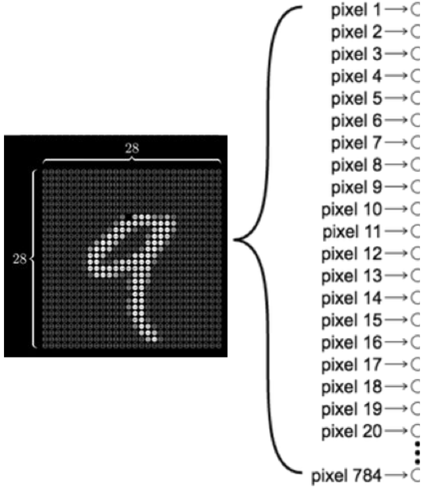
https://www.youtube.com/watch?v=aircAruvnKk&t=1s

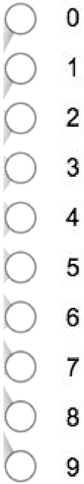
MNIST Network



https://ml4a.github.io/ml4a/looking_inside_neural_nets

MNIST Network





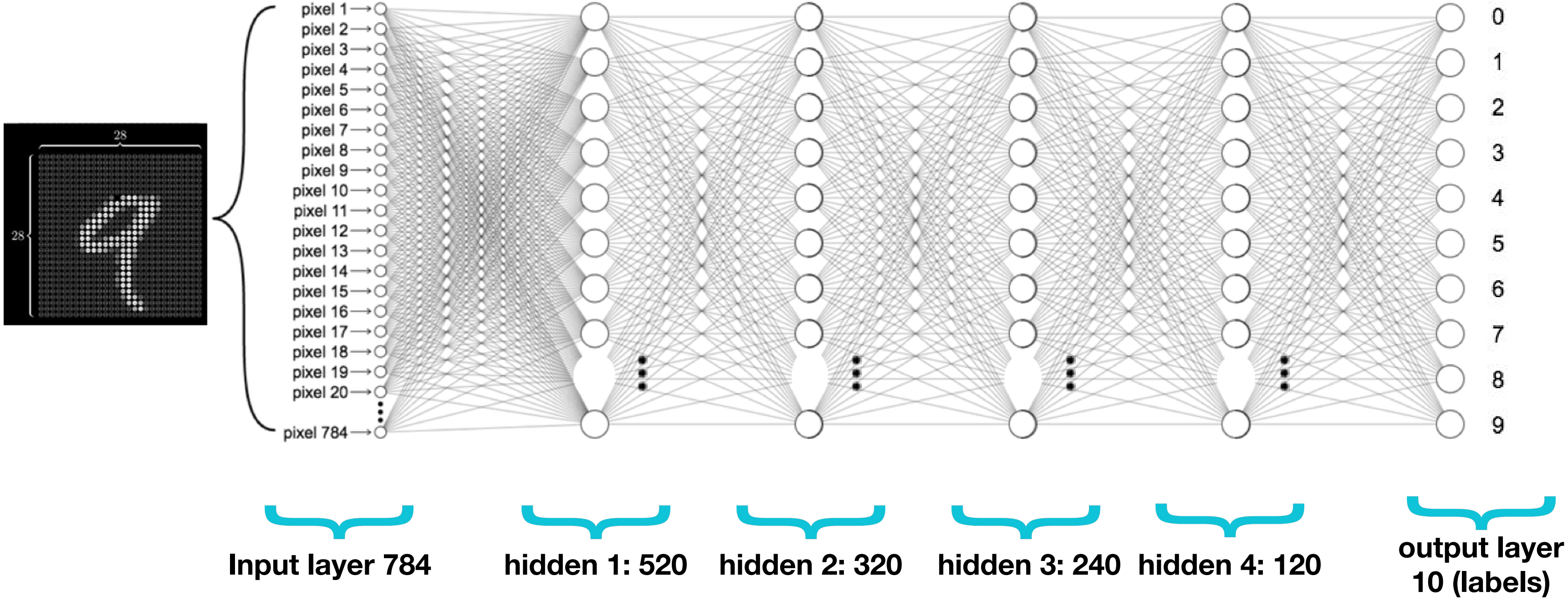
Input layer 784

Hidden layers

output layer
10 (labels)

https://ml4a.github.io/ml4a/looking_inside_neural_nets

MNIST Network



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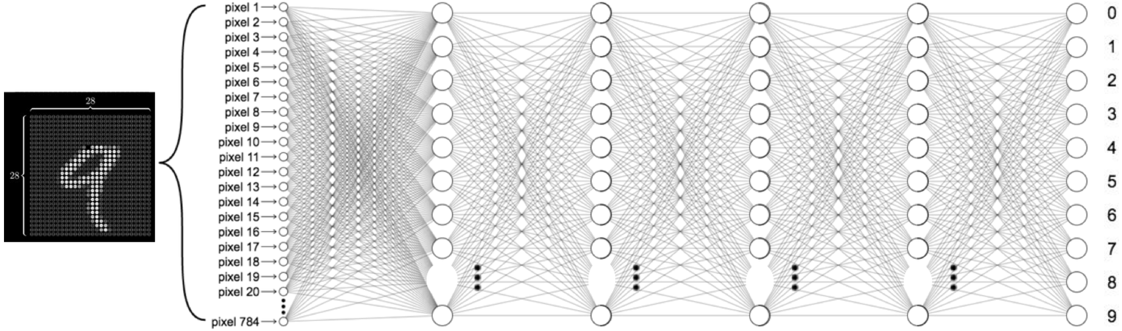
MNIST Network

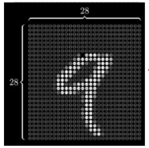


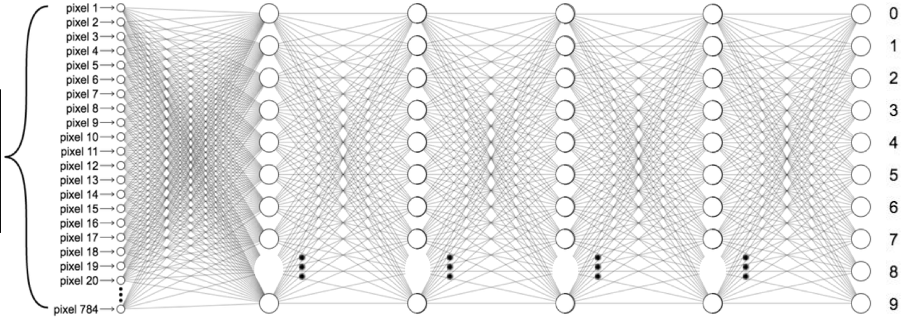

```
self.l1 = nn.Linear(784, 520)
        self.l2 = nn.Linear(520, 320)
               self.l3 = nn.Linear(320, 240)
                      self.l4 = nn.Linear(240, 120)
                             self.l5 = nn.Linear(120, 10)
```

https://ml4a.github.io/ml4a/looking_inside_neural_nets

Softmax & NLL loss

```python
class Net(nn.Module):

    def __init__(self):
        super(Net, self).__init__()
        self.l1 = nn.Linear(784, 520)
        self.l2 = nn.Linear(520, 320)
        self.l3 = nn.Linear(320, 240)
        self.l4 = nn.Linear(240, 120)
        self.l5 = nn.Linear(120, 10)

    def forward(self, x):
        # Flatten the data (n, 1, 28, 28)-> (n, 784)
        x = x.view(-1, 784)
        x = F.relu(self.l1(x))
        x = F.relu(self.l2(x))
        x = F.relu(self.l3(x))
        x = F.relu(self.l4(x))
        return self.l5(x) # No need activation
```





Input layer 784

hidden 1: 520

hidden 2: 320

hidden 3: 240

hidden 3: 120

output layer 10 (labels)

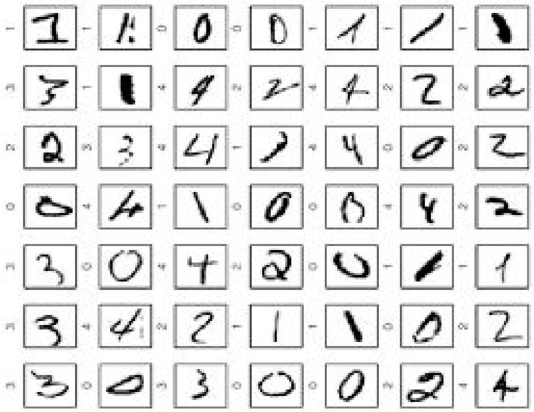
Softmax & NLL loss

```python
class Net(nn.Module):

    def __init__(self):
        super(Net, self).__init__()
        self.l1 = nn.Linear(784, 520)
        self.l2 = nn.Linear(520, 320)
        self.l3 = nn.Linear(320, 240)
        self.l4 = nn.Linear(240, 120)
        self.l5 = nn.Linear(120, 10)

    def forward(self, x):
        # Flatten the data (n, 1, 28, 28)-> (n, 784)
        x = x.view(-1, 784)
        x = F.relu(self.l1(x))
        x = F.relu(self.l2(x))
        x = F.relu(self.l3(x))
        x = F.relu(self.l4(x))
        return self.l5(x) # No need activation
```

```python
criterion = nn.CrossEntropyLoss()
…
for batch_idx, (data, target) in enumerate(train_loader):
    data, target = Variable(data), Variable(target)
    optimizer.zero_grad()
    output = model(data)
    loss = criterion(output, target)
    loss.backward()
    optimizer.step()
```

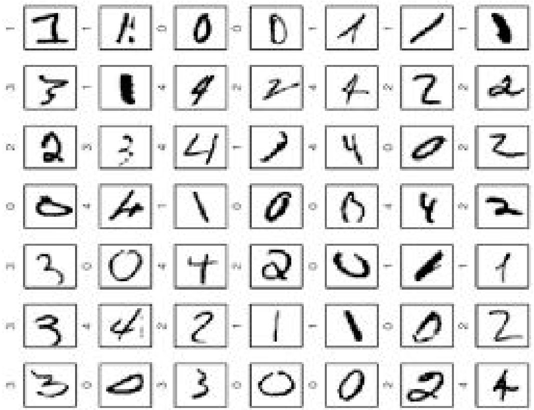
MNIST Softmax

```python
# Training settings
batch_size = 64
train_loader = torch.utils.data.DataLoader(
    datasets.MNIST('../data', train=True, download=True, transform=transforms.Compose([
        transforms.ToTensor(), transforms.Normalize((0.1307,), (0.3081,))])),
    batch_size=batch_size, shuffle=True)
test_loader = torch.utils.data.DataLoader(
    datasets.MNIST('../data', train=False, transform=transforms.Compose([
        transforms.ToTensor(),transforms.Normalize((0.1307,), (0.3081,))])),
    batch_size=batch_size, shuffle=True)

class Net(nn.Module):
   def __init__(self):
        super(Net, self).__init__()
        self.l1 = nn.Linear(784, 520)
        self.l2 = nn.Linear(520, 320)
        self.l3 = nn.Linear(320, 240)
        self.l4 = nn.Linear(240, 120)
        self.l5 = nn.Linear(120, 10)

    def forward(self, x):
        x = x.view(-1, 784)  # Flatten the data (n, 1, 28, 28)-> (n, 784)
        x = F.relu(self.l1(x))
        x = F.relu(self.l2(x))
        x = F.relu(self.l3(x))
        x = F.relu(self.l4(x))
        return self.l5(x)

model = Net()

criterion = nn.CrossEntropyLoss()
optimizer = optim.SGD(model.parameters(), lr=0.01, momentum=0.5)

def train(epoch):
    model.train()
    for batch_idx, (data, target) in enumerate(train_loader):
        data, target = Variable(data), Variable(target)
        optimizer.zero_grad()
        output = model(data)
        loss = criterion(output, target)
        loss.backward()
        optimizer.step()
        if batch_idx % 10 == 0:
            print('Train Epoch: {} [{}/{} ({:.0f}%)]\tLoss: {:.6f}'.format(
                epoch, batch_idx * len(data), len(train_loader.dataset),
                100. * batch_idx / len(train_loader), loss.data[0]))
```



```python
# Training settings
batch_size = 64
train_loader = torch.utils.data.DataLoader(
    datasets.MNIST('../data', train=True, download=True, transform=transforms.Compose([
        transforms.ToTensor(), transforms.Normalize((0.1307,), (0.3081,))])),
    batch_size=batch_size, shuffle=True)
test_loader = torch.utils.data.DataLoader(
    datasets.MNIST('../data', train=False, transform=transforms.Compose([
        transforms.ToTensor(),transforms.Normalize((0.1307,), (0.3081,))])),
    batch_size=batch_size, shuffle=True)

class Net(nn.Module):
   def __init__(self):
        super(Net, self).__init__()
        self.l1 = nn.Linear(784, 520)
        self.l2 = nn.Linear(520, 320)
        self.l3 = nn.Linear(320, 240)
        self.l4 = nn.Linear(240, 120)
        self.l5 = nn.Linear(120, 10)

    def forward(self, x):
        x = x.view(-1, 784)  # Flatten the data (n, 1, 28, 28)-> (n, 784)
        x = F.relu(self.l1(x))
        x = F.relu(self.l2(x))
        x = F.relu(self.l3(x))
        x = F.relu(self.l4(x))
        return self.l5(x)

model = Net()

criterion = nn.CrossEntropyLoss()
optimizer = optim.SGD(model.parameters(), lr=0.01, momentum=0.5)

def train(epoch):
    model.train()
    for batch_idx, (data, target) in enumerate(train_loader):
        data, target = Variable(data), Variable(target)
        optimizer.zero_grad()
        output = model(data)
        loss = criterion(output, target)
        loss.backward()
        optimizer.step()
        if batch_idx % 10 == 0:
            print('Train Epoch: {} [{}/{} ({:.0f}%)]\tLoss: {:.6f}'.format(
                epoch, batch_idx * len(data), len(train_loader.dataset),
                100. * batch_idx / len(train_loader), loss.data[0]))
```

Accuracy?




```
train_loader = torch.utils.data.DataLoader(
    datasets.MNIST('../data', train=True, download=True, transform=transforms.Compose([
        transforms.ToTensor(),
        transforms.Normalize((0.1307,), (0.3081,))
    ])),
    batch_size=batch_size, shuffle=True)
test_loader = torch.utils.data.DataLoader(
    datasets.MNIST('../data', train=False, transform=transforms.Compose([
        transforms.ToTensor(),
        transforms.Normalize((0.1307,), (0.3081,))
    ])),
    batch_size=batch_size, shuffle=True)
```

```
def train(epoch):
    ...
```

```
def test():
    model.eval()
    test_loss = 0
    correct = 0
    for data, target in test_loader:
        data, target = Variable(data, volatile=True), Variable(target)
        output = model(data)
        # sum up batch loss
        test_loss += criterion(output, target, size_average=False).data[0]
        # get the index of the max log-probability
        pred = torch.max(output.data, 1)[1]
        correct += pred.eq(target.data.view_as(pred)).cpu().sum()

    test_loss /= len(test_loader.dataset)
    print('\nTest set: Average loss: {:.4f}, Accuracy: {}/{} ({:.0f}%)\n'.format(
        test_loss, correct, len(test_loader.dataset),
        100. * correct / len(test_loader.dataset)))
```


```
train_loader = torch.utils.data.DataLoader(
    datasets.MNIST('../data', train=True, download=True, transform=transforms.Compose([
        transforms.ToTensor(),
        transforms.Normalize((0.1307,), (0.3081,))
    ])),
    batch_size=batch_size, shuffle=True)
test_loader = torch.utils.data.DataLoader(
    datasets.MNIST('../data', train=False, transform=transforms.Compose([
        transforms.ToTensor(),
        transforms.Normalize((0.1307,), (0.3081,))
    ])),
    batch_size=batch_size, shuffle=True)
```

```
def train(epoch):
    ...
```

```
def test():
    model.eval()
    test_loss = 0
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        output = model(data)
        # sum up batch loss
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        # get the index of the max log-probability
        pred = torch.max(output.data, 1)[1]
        correct += pred.eq(target.data.view_as(pred)).cpu().sum()

    test_loss /= len(test_loader.dataset)
    print('\nTest set: Average loss: {:.4f}, Accuracy: {}/{} ({:.0f}%)\n'.format(
        test_loss, correct, len(test_loader.dataset),
        100. * correct / len(test_loader.dataset)))
```

```
Y_pred_scores = Variable(
 torch.Tensor([[0.3, 0.2, 0.9, 0.1]]))

# torch.max returns both the max values and indices
Y_pred_val, Y_pred_idx =
             torch.max(Y_pred_scores.data,1)

Y_pred_idx = torch.max(Y_pred_scores.data,1)[1]
```

```python
def train(epoch):
    model.train()
    for batch_idx, (data, target) in enumerate(train_loader):
        data, target = Variable(data), Variable(target)
        optimizer.zero_grad()
        output = model(data)
        loss = criterion(output, target)
        loss.backward()
        optimizer.step()
        if batch_idx % 10 == 0:
            print('Train Epoch: {} [{}/{} ({:.0f}%)]\tLoss: {:.6f}'.format(
                epoch, batch_idx * len(data), len(train_loader.dataset),
                100. * batch_idx / len(train_loader), loss.data[0]))


def test():
    model.eval()
    test_loss = 0
    correct = 0
    for data, target in test_loader:
        data, target = Variable(data, volatile=True), Variable(target)
        output = model(data)
        # sum up batch loss
        test_loss += criterion(output, target, size_average=False).data[0]
        # get the index of the max log-probability
        pred = output.data.max(1, keepdim=True)[1]
        correct += pred.eq(target.data.view_as(pred)).cpu().sum()

    test_loss /= len(test_loader.dataset)
    print('\nTest set: Average loss: {:.4f}, Accuracy: {}/{} ({:.0f}%)\n’.
        format(test_loss, correct, len(test_loader.dataset),
        100. * correct / len(test_loader.dataset)))

for epoch in range(1, 10):
    train(epoch)
    test()
```

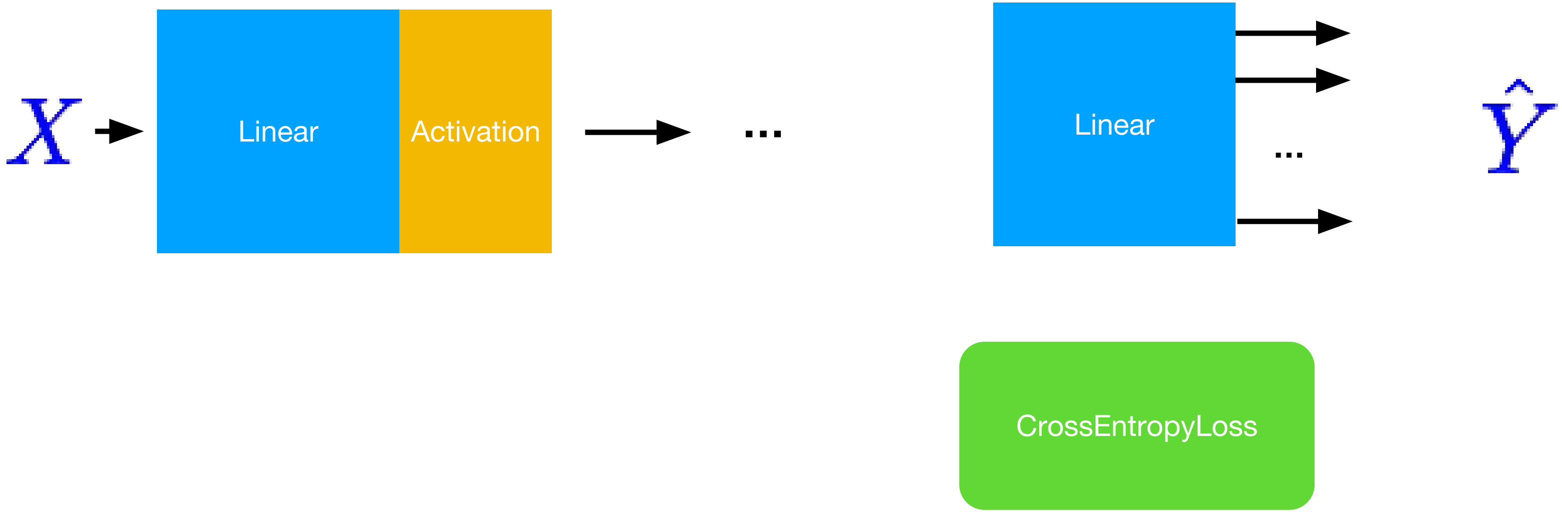
Accuracy?

```
Train Epoch: 1 [0/60000 (0%)]       Loss: 2.313209
Train Epoch: 1 [640/60000 (1%)]     Loss: 2.303560
Train Epoch: 1 [1280/60000 (2%)]    Loss: 2.296464
Train Epoch: 1 [1920/60000 (3%)]    Loss: 2.297758
Train Epoch: 1 [2560/60000 (4%)]    Loss: 2.308579
Train Epoch: 1 [3200/60000 (5%)]    Loss: 2.300100
Train Epoch: 1 [3840/60000 (6%)]    Loss: 2.300800
Train Epoch: 1 [4480/60000 (7%)]    Loss: 2.301295
Train Epoch: 1 [5120/60000 (9%)]    Loss: 2.295039
...
Train Epoch: 9 [51200/60000 (85%)]     Loss: 0.069267
Train Epoch: 9 [51840/60000 (86%)]     Loss: 0.044378
Train Epoch: 9 [52480/60000 (87%)]     Loss: 0.163481
Train Epoch: 9 [53120/60000 (88%)]     Loss: 0.243676
Train Epoch: 9 [53760/60000 (90%)]     Loss: 0.045024
Train Epoch: 9 [54400/60000 (91%)]     Loss: 0.064958
Train Epoch: 9 [55040/60000 (92%)]     Loss: 0.071447
Train Epoch: 9 [55680/60000 (93%)]     Loss: 0.043712
Train Epoch: 9 [56320/60000 (94%)]     Loss: 0.099484
Train Epoch: 9 [56960/60000 (95%)]     Loss: 0.159727
Train Epoch: 9 [57600/60000 (96%)]     Loss: 0.109291
Train Epoch: 9 [58240/60000 (97%)]     Loss: 0.116370
Train Epoch: 9 [58880/60000 (98%)]     Loss: 0.127303
Train Epoch: 9 [59520/60000 (99%)]     Loss: 0.030254

Test set: Average loss: -12.1596, Accuracy: 9697/10000 (97%)
```

Multiple label prediction?

Just use CrossEntropyLoss!



With CrossEntropyLoss

Exercise 9-2

- Build a classifier for Otto Group Product
  - https://www.kaggle.com/c/otto-group-product-classification-challenge/data
  - Use train.csv.zip (1.59 MB)
- Use DataLoader

WHAT NEXT

Lecture 10: CNN