STATS 507
Data Analysis in Python

Deep Learning with PyTorch

Adapted from slides by Sebastian Raschka.
Please do not distribute.

PyTorch Usage: Step 1 (Definition)

```
class MultilayerPerceptron(torch.nn.Module):

    def __init__(self, num_features, num_classes):
        super(MultilayerPerceptron, self).__init__()

        ### 1st hidden layer
        self.linear_1 = torch.nn.Linear(num_feat, num_h1)

        ### 2nd hidden layer
        self.linear_2 = torch.nn.Linear(num_h1, num_h2)

        ### Output layer
        self.linear_out = torch.nn.Linear(num_h2, num_classes)

    def forward(self, x):
        out = self.linear_1(x)
        out = F.relu(out)
        out = self.linear_2(out)
        out = F.relu(out)
        logits = self.linear_out(out)
        probas = F.log_softmax(logits, dim=1)
        return logits, probas
```

Define model parameters that will be instantiated when created an object of this class

Define how and in what order the model parameters should be used in the forward pass

PyTorch Usage: Step 2 (Creation)

```
torch.manual_seed(random_seed)
model = MultilayerPerceptron(num_features=num_features,
                             num_classes=num_classes)

model = model.to(device)

optimizer = torch.optim.SGD(model.parameters(),
                            lr=learning_rate)
```

Instantiate model
(creates the model parameters)

Optionally move model to GPU, where
device e.g. torch.device('cuda:0')

Define an optimization method

PyTorch Usage: Step 3 (Training)

Run for a specified number of epochs

Iterate over minibatches in epoch

If your model is on the GPU, data should also be on the GPU

```
for epoch in range(num_epochs):
    model.train()
    for batch_idx, (features, targets) in enumerate(train_loader):

        features = features.view(-1, 28*28).to(device)
        targets = targets.to(device)

        ### FORWARD AND BACK PROP
        logits, probas = model(features)
        cost = F.cross_entropy(probas, targets)
        optimizer.zero_grad()

        cost.backward()

        ### UPDATE MODEL PARAMETERS
        optimizer.step()

model.eval()
with torch.no_grad():
    # compute accuracy
```

PyTorch Usage: Step 3 (Training)

```
for epoch in range(num_epochs):
    model.train()
    for batch_idx, (features, targets) in enumerate(train_loader):

        features = features.view(-1, 28*28).to(device)
        targets = targets.to(device)

        ### FORWARD AND BACK PROP
        logits, probas = model(features)
        loss = F.cross_entropy(logits, targets)
        optimizer.zero_grad()

        loss.backward()

        ### UPDATE MODEL PARAMETERS
        optimizer.step()

model.eval()
with torch.no_grad():
    # compute accuracy
```

This will run the `forward()` method

Define a loss function to optimize

Set the gradient to zero
(could be non-zero from a previous forward pass)

Compute the gradients, the backward is automatically constructed by "autograd" based on the forward() method and the loss function

Use the gradients to update the weights according to the optimization method (defined on the previous slide)
E.g., for SGD, $w := w + \text{learning\_rate} \times \text{gradient}$

PyTorch Usage: Step 3 (Training)

```
for epoch in range(num_epochs):
    model.train()
    for batch_idx, (features, targets) in enumerate(train_loader):

        features = features.view(-1, 28*28).to(device)
        targets = targets.to(device)

        ### FORWARD AND BACK PROP
        logits, probas = model(features)
        loss = F.cross_entropy(logits, targets)
        optimizer.zero_grad()

        loss.backward()

        ### UPDATE MODEL PARAMETERS
        optimizer.step()

model.eval()
with torch.no_grad():
    # compute accuracy
```

For evaluation, set the model to eval mode (will be relevant later when we use DropOut or BatchNorm)

This prevents the computation graph for backpropagation from automatically being build in the background to save memory

PyTorch Usage: Step 3 (Training)

```
for epoch in range(num_epochs):
    model.train()
    for batch_idx, (features, targets) in enumerate(train_loader):

        features = features.view(-1, 28*28).to(device)
        targets = targets.to(device)

        ### FORWARD AND BACK PROP
        logits, probas = model(features)
        loss = F.cross_entropy(logits, targets)
        optimizer.zero_grad()

        loss.backward()

        ### UPDATE MODEL PARAMETERS
        optimizer.step()

model.eval()
with torch.no_grad():
    # compute accuracy
```

logits because of computational efficiency.
Basically, it internally uses a log_softmax(logits) function that is more stable than log(softmax(logits)).
More on logits coming up.

Objected-Oriented vs Functional* API

*Note that with "functional" I mean "functional programming" (one paradigm in CS)

```
import torch.nn.functional as F


class MultilayerPerceptron(torch.nn.Module):

    def __init__(self, num_features, num_classes):
        super(MultilayerPerceptron, self).__init__()

        ### 1st hidden layer
        self.linear_1 = torch.nn.Linear(num_features,
                                        num_hidden_1)

        ### 2nd hidden layer
        self.linear_2 = torch.nn.Linear(num_hidden_1,
                                        num_hidden_2)

        ### Output layer
        self.linear_out = torch.nn.Linear(num_hidden_2,
                                          num_classes)

    def forward(self, x):
        out = self.linear_1(x)
        out = F.relu(out)
        out = self.linear_2(out)
        out = F.relu(out)
        logits = self.linear_out(out)
        probas = F.log_softmax(logits, dim=1)
        return logits, probas
```

Unnecessary because these functions don't need to store a state but maybe helpful for keeping track of order of ops (when implementing "forward")

```
class MultilayerPerceptron(torch.nn.Module):

    def __init__(self, num_features, num_classes):
        super(MultilayerPerceptron, self).__init__()

        ### 1st hidden layer
        self.linear_1 = torch.nn.Linear(num_features,
                                        num_hidden_1)

        self.relu1 = torch.nn.ReLU()

        ### 2nd hidden layer
        self.linear_2 = torch.nn.Linear(num_hidden_1,
                                        num_hidden_2)

        self.relu2 = torch.nn.ReLU()

        ### Output layer
        self.linear_out = torch.nn.Linear(num_hidden_2,
                                          num_classes)

        self.softmax = torch.nn.Softmax()

    def forward(self, x):
        out = self.linear_1(x)
        out = self.relu1(out)
        out = self.linear_2(out)
        out = self.relu2(out)
        logits = self.linear_out(out)
        probas = self.softmax(logits, dim=1)
        return logits, probas
```

Objected-Oriented vs Functional API

Using "Sequential"

```
import torch.nn.functional as F


class MultilayerPerceptron(torch.nn.Module):

    def __init__(self, num_features, num_classes):
        super(MultilayerPerceptron, self).__init__()

        ### 1st hidden layer
        self.linear_1 = torch.nn.Linear(num_features,
                                        num_hidden_1)

        ### 2nd hidden layer
        self.linear_2 = torch.nn.Linear(num_hidden_1,
                                        num_hidden_2)

        ### Output layer
        self.linear_out = torch.nn.Linear(num_hidden_2,
                                          num_classes)

    def forward(self, x):
        out = self.linear_1(x)
        out = F.relu(out)
        out = self.linear_2(out)
        out = F.relu(out)
        logits = self.linear_out(out)
        probas = F.log_softmax(logits, dim=1)
        return logits, probas
```

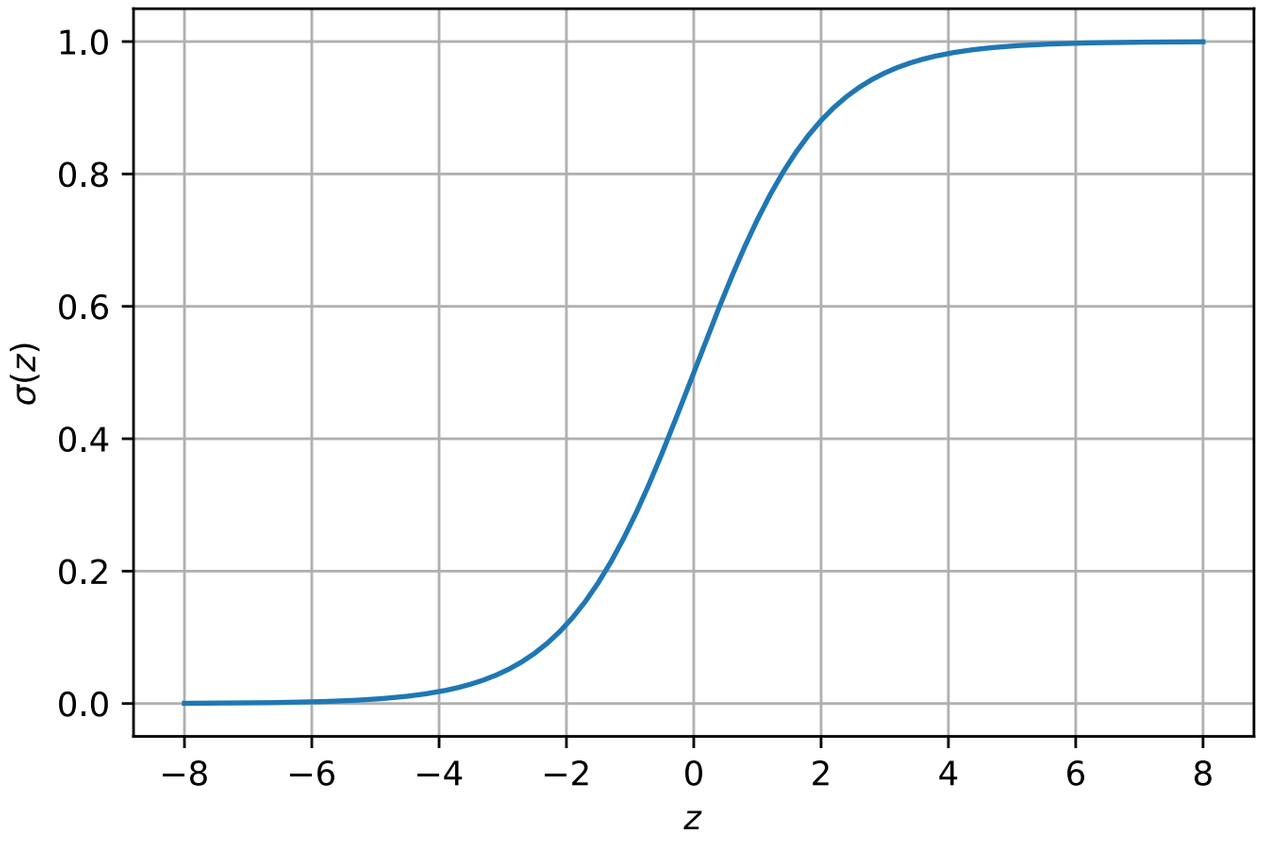
```
class MultilayerPerceptron(torch.nn.Module):

    def __init__(self, num_features, num_classes):
        super(MultilayerPerceptron, self).__init__()

        self.my_network = torch.nn.Sequential(
            torch.nn.Linear(num_features, num_hidden_1),
            torch.nn.ReLU(),
            torch.nn.Linear(num_hidden_1, num_hidden_2),
            torch.nn.ReLU(),
            torch.nn.Linear(num_hidden_2, num_classes)
        )

    def forward(self, x):
        logits = self.my_network(x)
        probas = F.softmax(logits, dim=1)
        return logits, probas
```

Much more compact and clear, but "forward" may be harder to debug if there are errors (we cannot simply add breakpoints or insert "print" statements

Logistic Regression for Binary Classification

Logistic Sigmoid Function

$$\sigma(z) = \frac{e^z}{1 + e^z} = \frac{1}{1 + e^{-z}}$$



Logistic Regression

$$P(y|\mathbf{x}) = \begin{cases} \sigma(\mathbf{w}^\top \mathbf{x}) & \text{if } y = 1 \\ 1\text{-}\sigma(\mathbf{w}^\top \mathbf{x}) & \text{if } y = 0 \end{cases}$$

want $\quad P(y = 0|\mathbf{x}) \approx 1 \quad \text{if } y = 0$

$$P(y = 1|\mathbf{x}) \approx 1 \quad \text{if } y = 1$$

Logistic Regression

rewritten more compactly

$$P(y|\mathbf{x}) = a^y(1-a)^{(1-y)}$$

where $a = \sigma(z)$

Logistic Regression

And for multiple training examples (iid), we want to maximize:

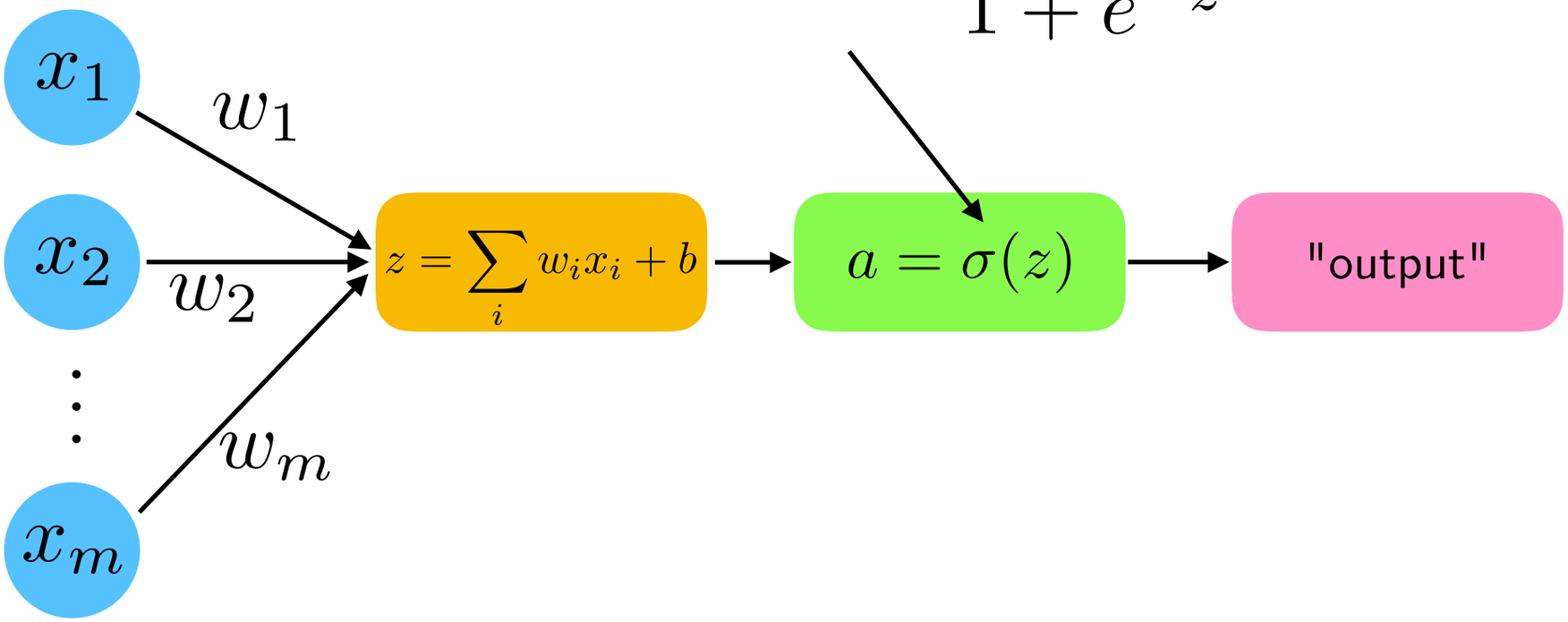
$$P\left(y^{[i]},...,y^{[n]}|\mathbf{x}^{[1]},...,\mathbf{x}^{[n]}\right) = \prod_{i=1}^{n} P\left(y^{[i]}|\mathbf{x}^{[i]}\right)$$

You may remember this as *Maximum Likelihood Estimation* from your other stats classes.

Logistic Regression Neuron

For binary classes $y \in \{0, 1\}$

"logistic sigmoid" $\sigma(z) = \dfrac{1}{1 + e^{-z}}$



Likelihood "Loss"

$$
\begin{aligned}
L(\mathbf{w}) &= P(\mathbf{y} \mid \mathbf{x}; \mathbf{w}) \\
&= \prod_{i=1}^{n} P\big(y^{(i)} \mid x^{(i)}; \mathbf{w}\big) \\
&= \prod_{i=1}^{n} \Big(\sigma\big(z^{(i)}\big)\Big)^{y^{(i)}} \Big(1 - \sigma\big(z^{(i)}\big)\Big)^{1-y^{(i)}}
\end{aligned}
$$

Log-Likelihood "Loss"

$$
\begin{aligned}
L(\mathbf{w}) &= P(\mathbf{y} \mid \mathbf{x}; \mathbf{w}) \\
&= \prod_{i=1}^{n} P\big(y^{(i)} \mid x^{(i)}; \mathbf{w}\big) \\
&= \prod_{i=1}^{n} \Big(\sigma\big(z^{(i)}\big)\Big)^{y^{(i)}} \Big(1 - \sigma\big(z^{(i)}\big)\Big)^{1-y^{(i)}}
\end{aligned}
$$

In practice, it is easier to maximize the (natural) log of this equation, which is called the log-likelihood function:

$$
\begin{aligned}
l(\mathbf{w}) &= \log L(\mathbf{w}) \\
&= \sum_{i=1}^{n} \Big[y^{(i)} \log\big(\sigma\big(z^{(i)}\big)\big) + \big(1 - y^{(i)}\big) \log\big(1 - \sigma\big(z^{(i)}\big)\big)\Big]
\end{aligned}
$$

Negative Log-Likelihood Loss

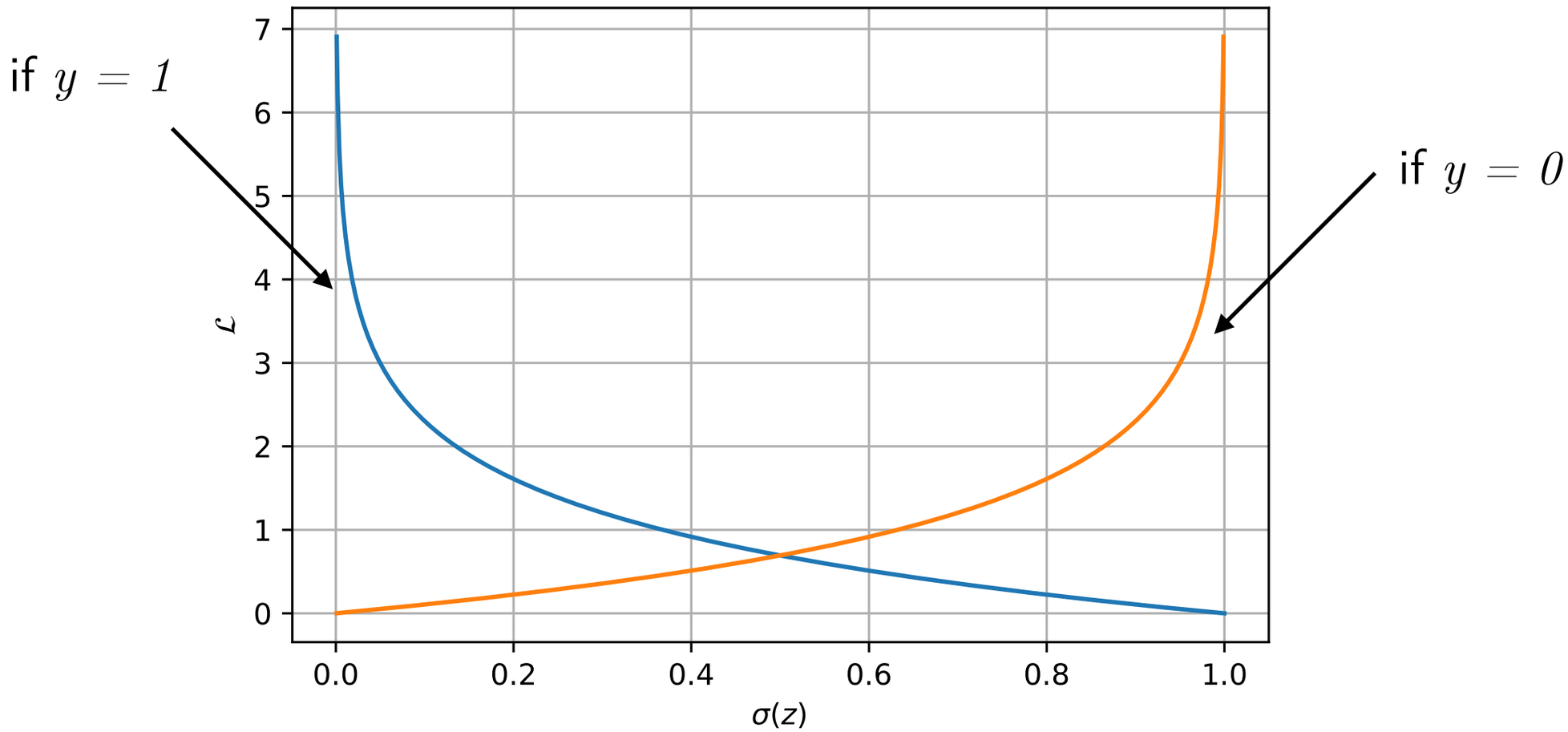
In practice, it is even more convenient to minimize negative log-likelihood instead of maximizing log-likelihood:

$$\mathcal{L}(\mathbf{w}) = -l(\mathbf{w})$$

$$= -\sum_{i=1}^{n} \left[y^{(i)} \log \left(\sigma\left(z^{(i)}\right) \right) + \left(1 - y^{(i)}\right) \log \left(1 - \sigma\left(z^{(i)}\right)\right) \right]$$

(in code, we also usually add a $1/n$ scaling factor for further convenience, where n is the number of training examples or number of examples in a minibatch)

Loss for a Single Training Example



$$\mathcal{L}(\mathbf{w}) = -y^{(i)} \log\left(\sigma\left(z^{(i)}\right)\right) + \left(1 - y^{(i)}\right) \log\left(1 - \sigma\left(z^{(i)}\right)\right)$$

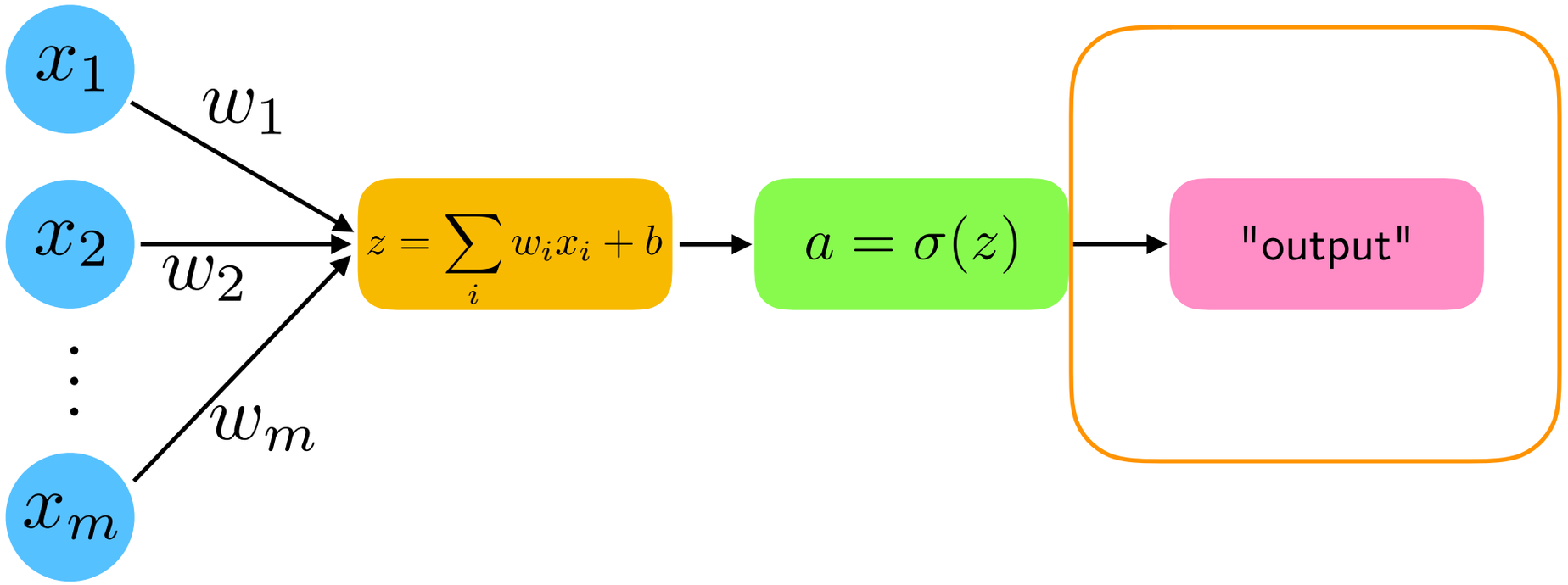
Logistic Regression Loss

- So, "doing logistic regression" is similar to what we have done before
- Previously we minimized the MSE loss:

$$\text{MSE} = \frac{1}{n}\sum_i (a^{[i]} - y^{[i]})^2$$

- However, the difference is that in Logistic Regression, we maximize the likelihood
  - Maximizing likelihood is the same as maximizing the log-likelihood, but the latter is numerically more stable
  - Maximizing the log-likelihood is the same as minimizing the negative log-likelihood, which is convenient, so we don't have to change our code and can still use gradient descent (instead of gradient ascent)

Class Label Predictions with Logistic Regression



In logistic regression, we can use

$$\hat{y} := \begin{cases} 1 & \text{if } \sigma(z) > 0.5 \\ 0 & \text{otherwise} \end{cases}$$

which is the same as

$$\hat{y} := \begin{cases} 1 & \text{if } z > 0.0 \\ 0 & \text{otherwise} \end{cases}$$

- We can think of this part as a "separate" part that converts the neural network values into a class label, for example; e.g., via a threshold function

- Predicted class labels are not used during training

Logistic Regression for Multi-class Classification:

Multinomial Logistic Regression/ Softmax Regression

MNIST - 60k Handwritten Digits

http://yann.lecun.com/exdb/mnist/

Balanced dataset:

- 10 classes (digits 0-9)
- 10k digits per class

Image dimensions: 28x28x1

In NCHW, an image batch of 128 examples would be a tensor with dimensions (128, 1, 28, 28)

- Training set images: train-images-idx3-ubyte.gz (9.9 MB, 47 MB unzipped, and 60,000 examples)
- Training set labels: train-labels-idx1-ubyte.gz (29 KB, 60 KB unzipped, and 60,000 labels)
- Test set images: t10k-images-idx3-ubyte.gz (1.6 MB, 7.8 MB, unzipped and 10,000 examples)
- Test set labels: t10k-labels-idx1-ubyte.gz (5 KB, 10 KB unzipped, and 10,000 labels)

MNIST - 60k Handwritten Digits

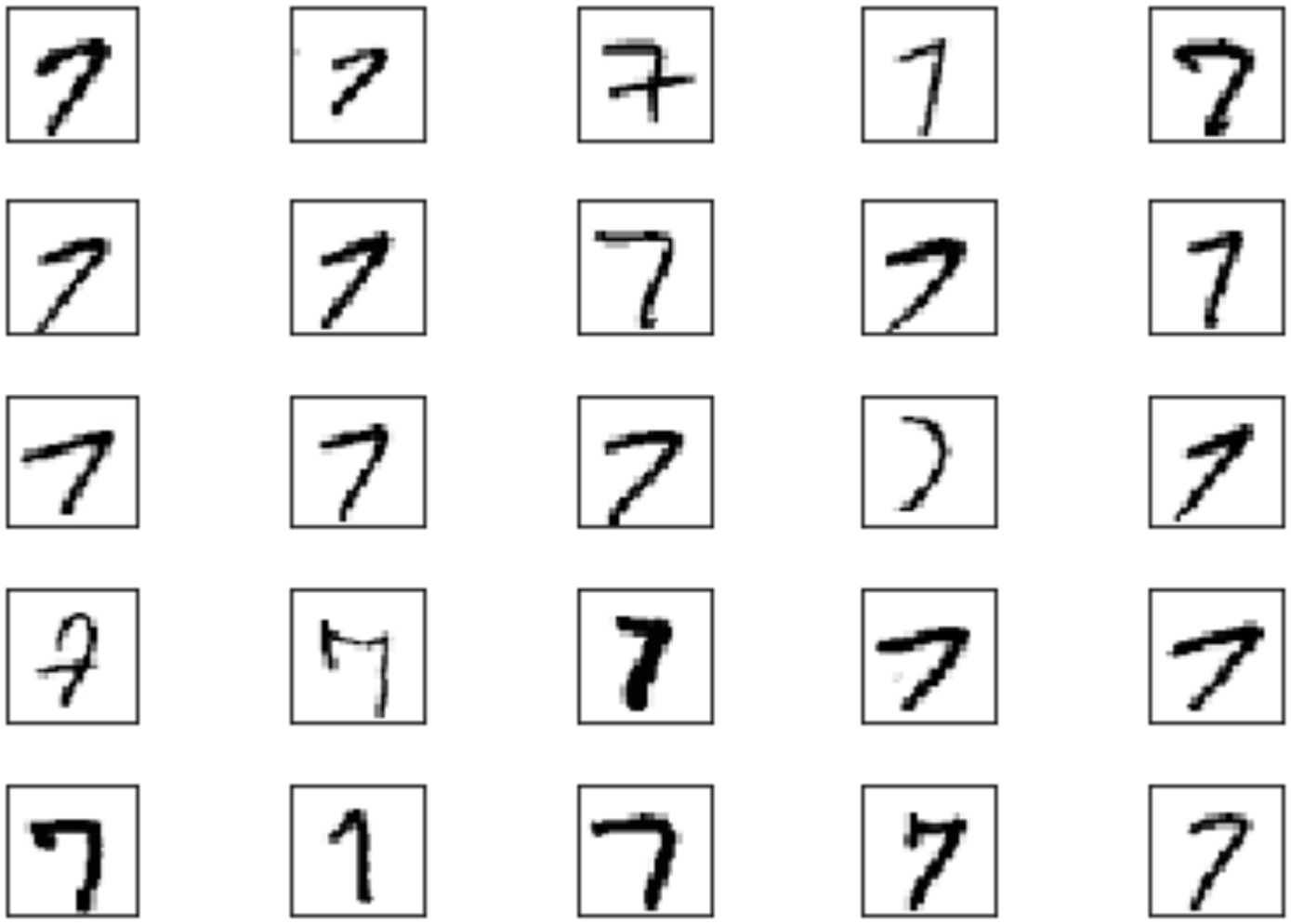


Illustration of different "7"s

Data Representation (unstructured data; images)

Softmax regression: "traditional method"


```
[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
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0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.20392157, 0.2627451, 0.2627451, 0.31764707, 0.99607843, 0.99607843, 0.99607843
, 0.99607843, 1.0, 0.99607843, 0.99607843, 0.99607843, 0.30980393, 0.14509805, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0
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9215686, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.7764706, 0.15294118, 0.0, 0.0, 0
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, 0.023529412, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
0.0, 0.0, 0.0, 0.6627451, 0.99215686, 0.99215686, 0.99215686, 0.03137255, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0
.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.49803922, 0.5529412, 0.84705883, 0.99215686, 0.99
215686, 0.59607846, 0.015686275, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.
0, 0.0, 0.06666667, 0.07450981, 0.5411765, 0.972549, 0.99215686, 0.99215686, 0.99215686, 0.627451, 0.05490196, 0.0,
0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.1882353, 0.33333334, 0.33333334, 0.33333334
, 0.8980392, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.92941177, 0.3647059, 0.0, 0.0, 0.0, 0.0,
0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.18039216, 0.8156863, 0.99215686, 0.99215686, 0.99215686, 0
.99215686, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.91764706, 0.32941177, 0.0, 0.0, 0.0, 0.0,
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.99215686, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.59607846, 0.03529412, 0.0, 0.0
, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.34901962, 0.61960787, 0.61960787, 0.61960787,
0.61960787, 0.61960787, 0.61960787, 0.9529412, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.54901963, 0.011764
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215686, 0.96862745, 0.45882353, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0
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, 0.99215686, 0.24705882, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.5372549, 0.984313
7, 0.98039216, 0.9607843, 0.9647059, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.9490196, 0.43921
57, 0.03137255, 0.003921569, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.5529412, 0.992
15686, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.7921569, 0.50980395, 0.41960785, 0
.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.14117648, 0.30980393, 0.99215
686, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.32941177, 0.14901961, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0
, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0
, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0
, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0
, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0]
```
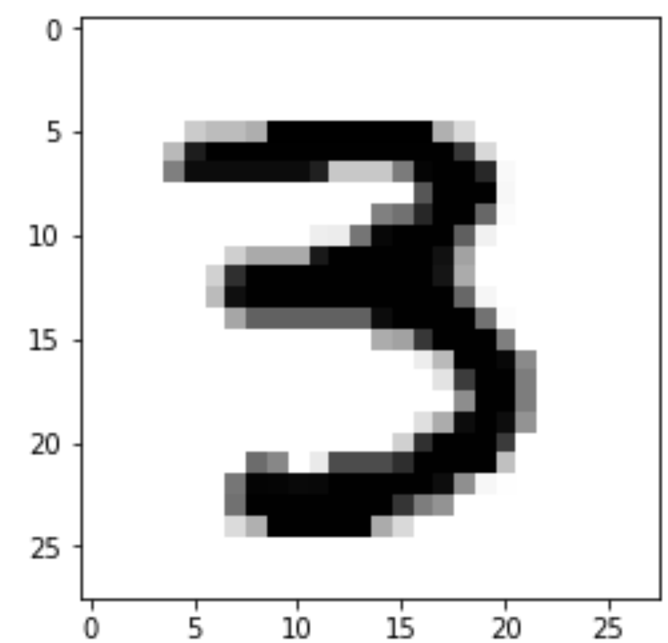
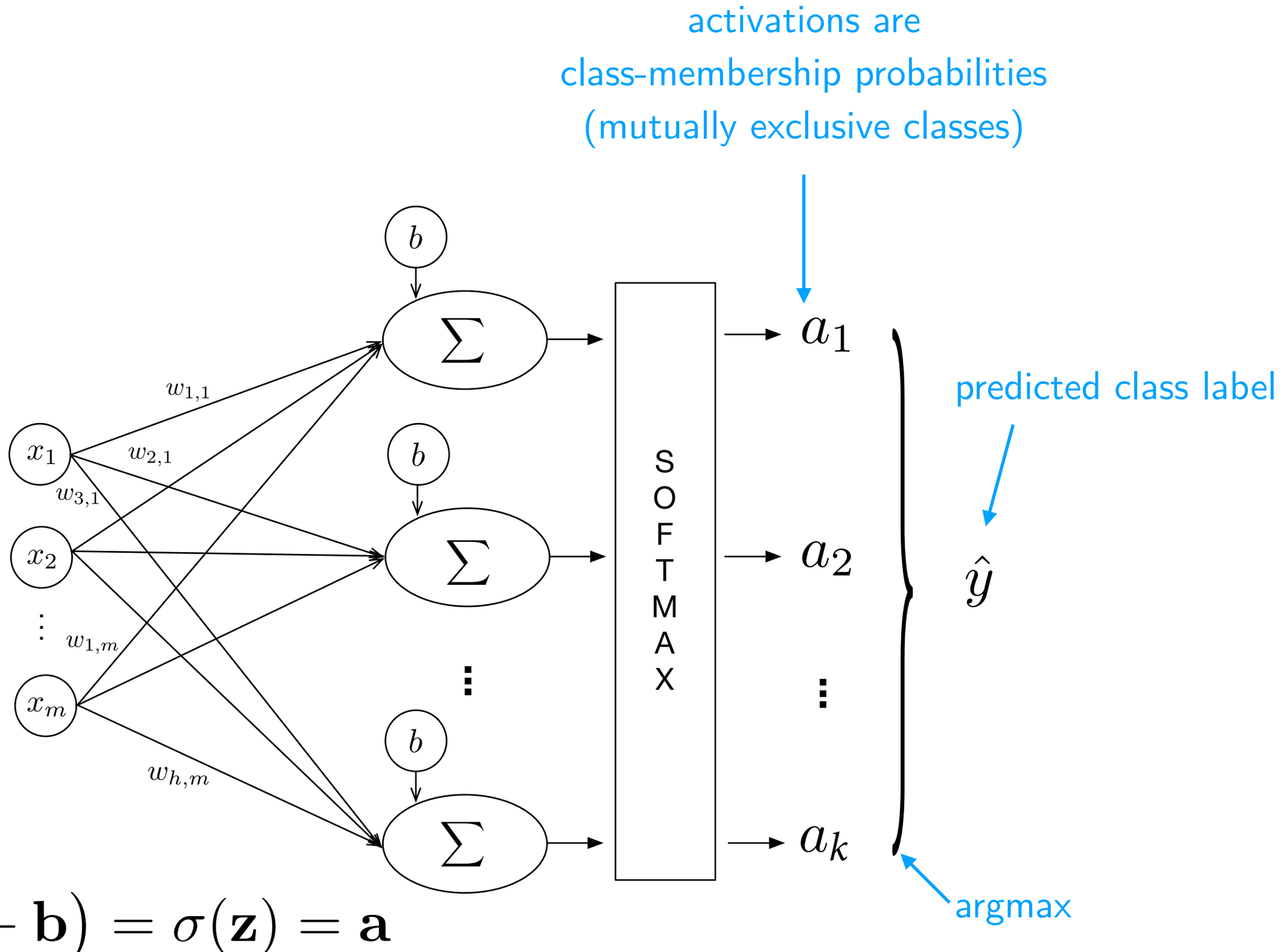


Represent digit as a long vector of pixels



Note that I normalized pixels by factor 1/255 here

Multinomial Logistic Regression / Softmax Regression



$$\sigma\big(\mathbf{W}\mathbf{x} + \mathbf{b}\big) = \sigma(\mathbf{z}) = \mathbf{a}$$

Softmax Activation

$$\sigma(\vec{z})_i = \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}$$

σ = softmax

$\vec{z}$ = input vector

e^{z_i} = standard exponential function for input vector

K = number of classes in the multi-class classifier

source: Google search sidebar

(Basically, softmax is just an exponential function that normalizes the outputs so that they sum up to 1)

Onehot Encoding

class labels
0
1
3
2

class_0	class_1	class_2	class_3
1	0	0	0
0	1	0	0
0	0	0	1
0	0	1	0

Loss Function

$$\mathcal{L} = \sum_{i=1}^{n} \sum_{j=1}^{k} -y_j^{[i]} \log\left(a_j^{[i]}\right)$$

(Multi-category) Cross Entropy for k different class labels

This assumes one-hot encoded labels!

Loss Function

$$\mathcal{L}_{\text{binary}} = -\sum_{i=1}^{n} \left(y^{[i]} \log(a^{[i]}) + (1 - y^{[i]}) \log(1 - a^{[i]}) \right)$$

This assumes one-hot encoded labels!

$$\mathcal{L}_{\text{multiclass}} = \sum_{i=1}^{n} \sum_{j=1}^{k} -y_j^{[i]} \log \left(a_j^{[i]} \right)$$

(Multi-category) Cross Entropy for k different class labels

Cross Entropy Loss Function Example

$$\mathbf{Y}_{\text{onehot}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{A}_{\text{softmax outputs}} = \begin{bmatrix} 0.3792 & 0.3104 & 0.3104 \\ 0.3072 & 0.4147 & 0.2780 \\ 0.4263 & 0.2248 & 0.3490 \\ 0.2668 & 0.2978 & 0.4354 \end{bmatrix}$$

(4 training examples, 3 classes)

Cross Entropy Loss Function Example

1 training example

$$\mathbf{Y}_{\text{onehot}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{A}_{\text{softmax outputs}} = \begin{bmatrix} 0.3792 & 0.3104 & 0.3104 \\ 0.3072 & 0.4147 & 0.2780 \\ 0.4263 & 0.2248 & 0.3490 \\ 0.2668 & 0.2978 & 0.4354 \end{bmatrix}$$

(4 training examples, 3 classes)

$$\mathcal{L}_{\text{multiclass}} = \sum_{i=1}^{n} \sum_{j=1}^{k} -y_j^{[i]} \log\left(a_j^{[i]}\right)$$

$$\begin{aligned} \mathcal{L}^{[1]} &= [(-1) \cdot \log(0.3792)] \\ &\quad + [(-0) \cdot \log(0.3104)] \\ &\quad + [(-0) \cdot \log(0.3104)] \\ &= 0.969692... \end{aligned}$$

Cross Entropy Loss Function Example

$$\mathbf{Y}_{\text{onehot}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{A}_{\text{softmax outputs}} = \begin{bmatrix} 0.3792 & 0.3104 & 0.3104 \\ 0.3072 & 0.4147 & 0.2780 \\ 0.4263 & 0.2248 & 0.3490 \\ 0.2668 & 0.2978 & 0.4354 \end{bmatrix}$$

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$$\begin{aligned} \mathcal{L}^{[2]} &= [(-0) \cdot \log(0.3072)] \\ &\quad + [(-1) \cdot \log(0.4147)] \\ &\quad + [(-0) \cdot \log(0.2780)] \\ &= 0.880200... \end{aligned}$$

$$\begin{aligned} \mathcal{L}^{[3]} &= [(-0) \cdot \log(0.4263)] \\ &\quad + [(-0) \cdot \log(0.2248)] \\ &\quad + [(-1) \cdot \log(0.3490)] \\ &= 1.05268... \end{aligned}$$

$$\begin{aligned} \mathcal{L}^{[4]} &= [(-0) \cdot \log(0.2668)] \\ &\quad + [(-0) \cdot \log(0.2978)] \\ &\quad + [(-1) \cdot \log(0.4354)] \\ &= 0.831490... \end{aligned}$$

Cross Entropy Loss Function Example

$$\mathbf{Y}_{\text{onehot}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{A}_{\text{softmax outputs}} = \begin{bmatrix} 0.3792 & 0.3104 & 0.3104 \\ 0.3072 & 0.4147 & 0.2780 \\ 0.4263 & 0.2248 & 0.3490 \\ 0.2668 & 0.2978 & 0.4354 \end{bmatrix}$$

$$\begin{aligned} \mathcal{L}^{[1]} &= [(-1) \cdot \log(0.3792)] \\ &\quad + [(-0) \cdot \log(0.3104)] \\ &\quad + [(-0) \cdot \log(0.3104)] \\ &= 0.969692... \end{aligned}$$

$$\begin{aligned} \mathcal{L}^{[2]} &= [(-0) \cdot \log(0.3072)] \\ &\quad + [(-1) \cdot \log(0.4147)] \\ &\quad + [(-0) \cdot \log(0.2780)] \\ &= 0.880200... \end{aligned}$$

$$\begin{aligned} \mathcal{L}^{[3]} &= [(-0) \cdot \log(0.4263)] \\ &\quad + [(-0) \cdot \log(0.2248)] \\ &\quad + [(-1) \cdot \log(0.3490)] \\ &= 1.05268... \end{aligned}$$

$$\begin{aligned} \mathcal{L}^{[4]} &= [(-0) \cdot \log(0.2668)] \\ &\quad + [(-0) \cdot \log(0.2978)] \\ &\quad + [(-1) \cdot \log(0.4354)] \\ &= 0.831490... \end{aligned}$$

$$\mathcal{L}_{\text{multiclass}} = \sum_{i=1}^{n} \sum_{j=1}^{k} -y_j^{[i]} \log\left(a_j^{[i]}\right)$$

$$\approx 0.9335$$

Intermission

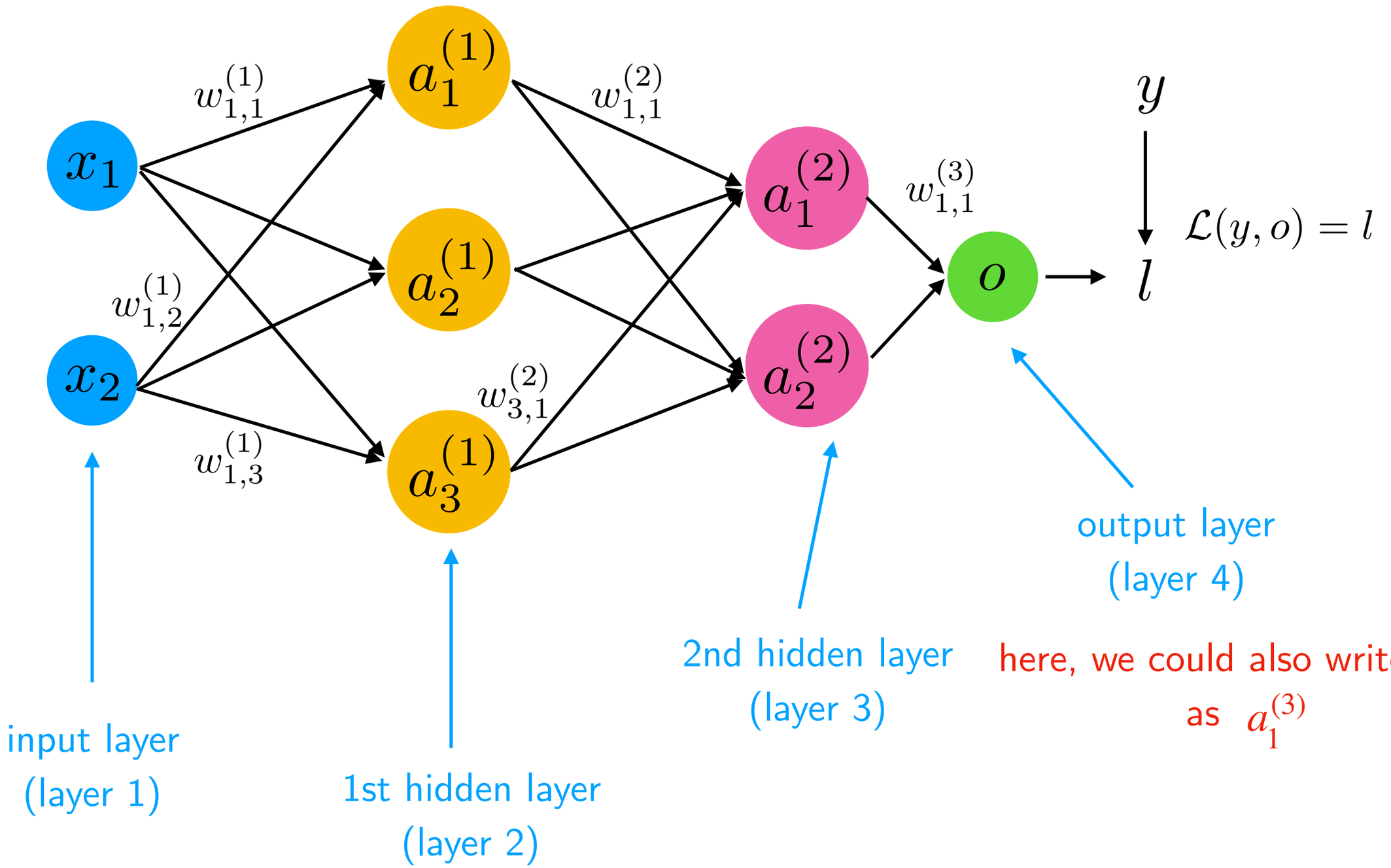
Next, multilayer perceptrons / deep learning

Multilayer Perceptrons

Graph with Fully-Connected Layers

= Multilayer Perceptron

Nothing new, really



input layer
(layer 1)

1st hidden layer
(layer 2)

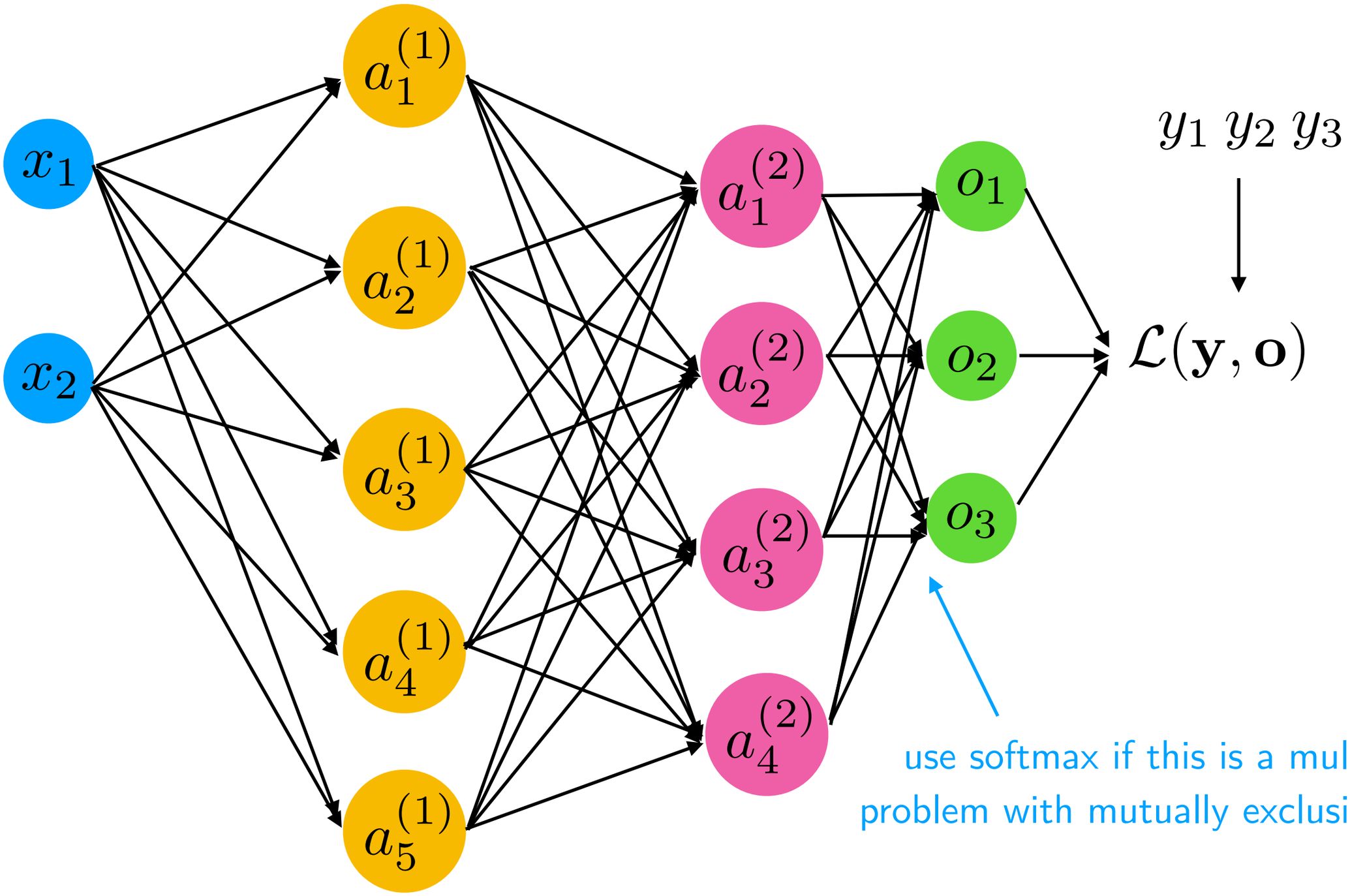
2nd hidden layer
(layer 3)

output layer
(layer 4)

here, we could also write o
as $a_1^{(3)}$

Graph with Fully-Connected Layers

= Multilayer Perceptron

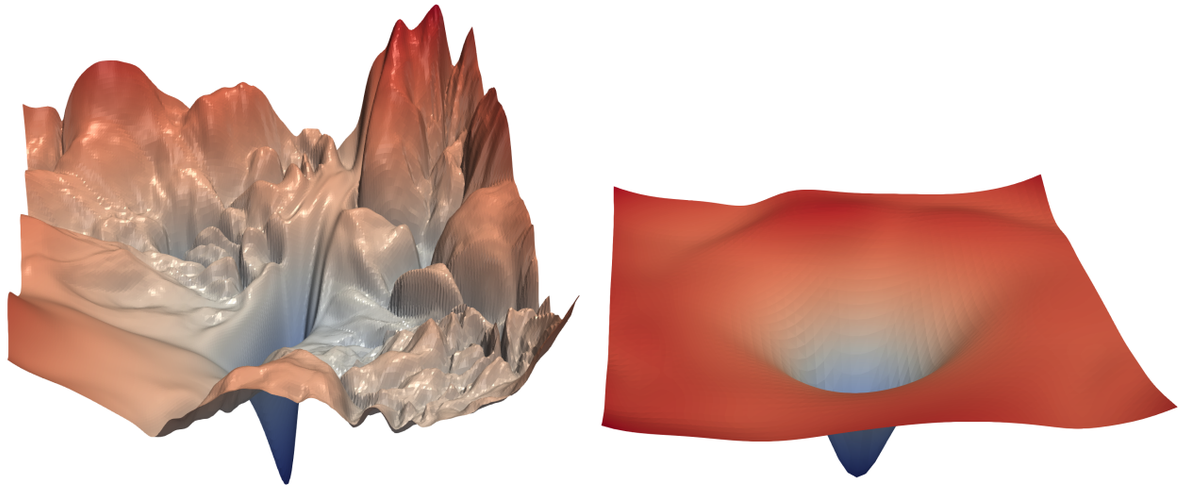


Note That the Loss is Not Convex Anymore

- Linear regression, Logistic Regression, and Softmax Regression had convex loss functions with respect to the weights

- This is not the case anymore; in practice, we usually end up at different local minima if we repeat the training (e.g., by changing the random seed for weight initialization or shuffling the dataset while leaving all setting the same)

- In practice though, we WANT to explore different starting weights, however, because some lead to better solutions than others



(a) without skip connections (b) with skip connections

Figure 1: The loss surfaces of ResNet-56 with/without skip connections. The proposed filter normalization scheme is used to enable comparisons of sharpness/flatness between the two figures.

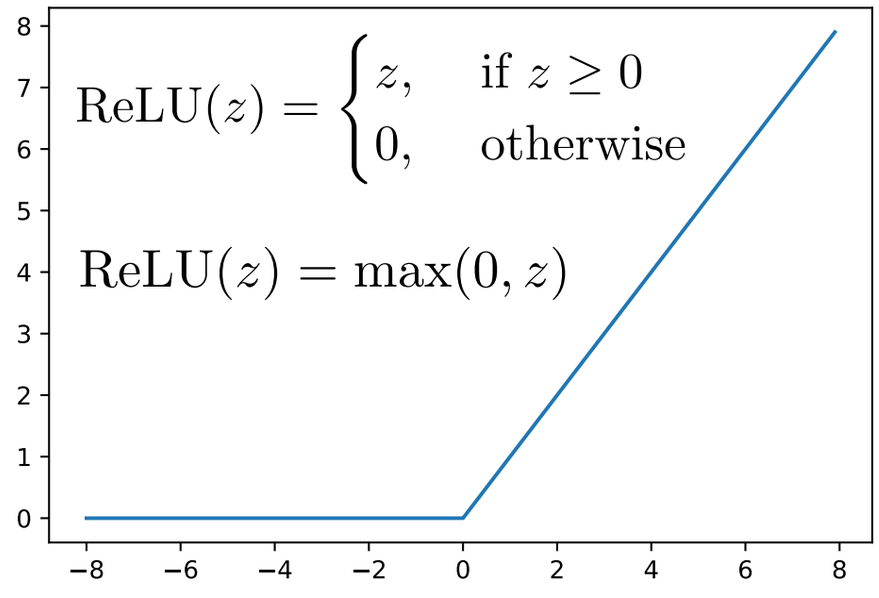
32nd Conference on Neural Information Processing Systems (NIPS 2018), Montréal, Canada.

Image Source: Li, H., Xu, Z., Taylor, G., Studer, C. and Goldstein, T., 2018. Visualizing the loss landscape of neural nets. In *Advances in Neural Information Processing Systems* (pp. 6391-6401).

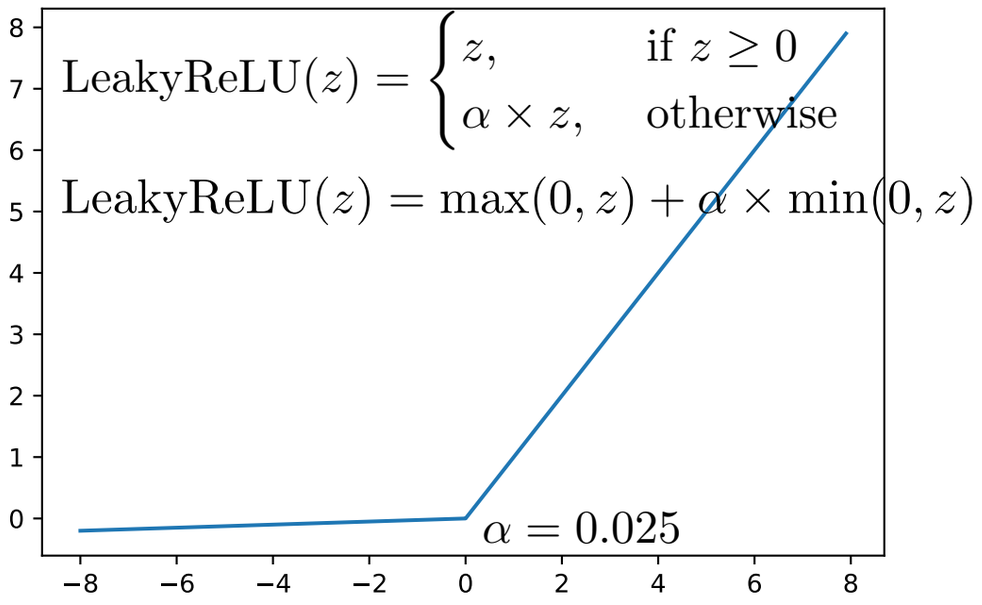
Activation Functions / Nonlinearities

A Selection of Common Activation Functions

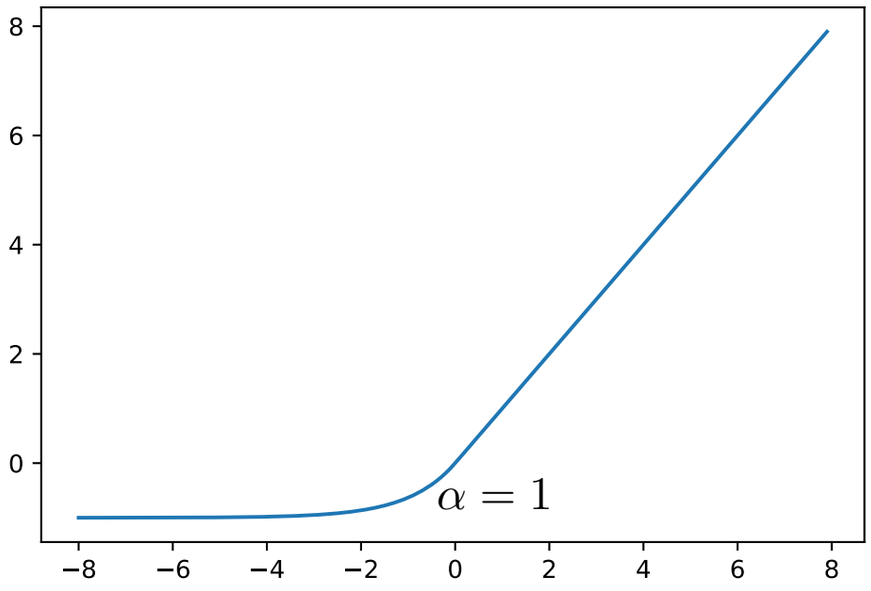
ReLU (Rectified Linear Unit)



Leaky ReLU



ELU (Exponential Linear Unit)



$$\mathrm{ELU}(z) = \max(0, z) + \min(0, \alpha \times (\exp(z) - 1))$$

Wide vs Deep Architectures (Breadth vs Depth)

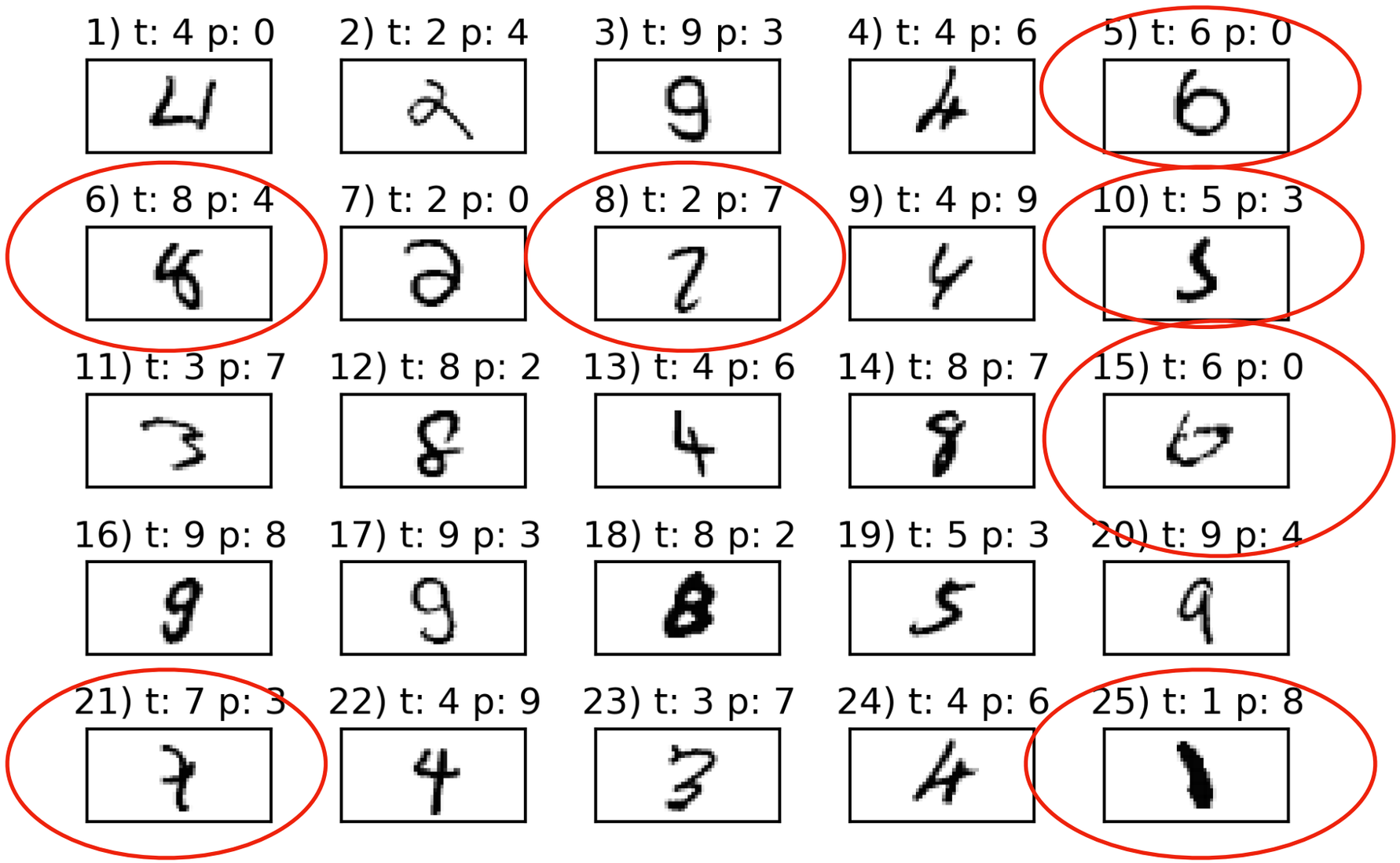
MLP's with one wide hidden layer are universal function approximators [1-3]. So why do we want to use deeper architectures?

[1] Balázs Csanád Csáji (2001) Approximation with Artificial Neural Networks; Faculty of Sciences; Eötvös Loránd University, Hungary
[2] Cybenko, G. (1989) "Approximations by superpositions of sigmoidal functions", Mathematics of Control, Signals, and Systems, 2(4), 303–314. doi:10.1007/BF02551274
[3] Hornik, K., Stinchcombe, M., & White, H. (1989). Multilayer feedforward networks are universal approximators. Neural networks, *2*(5), 359-366.

Wide vs Deep Architectures (Breadth vs Depth)

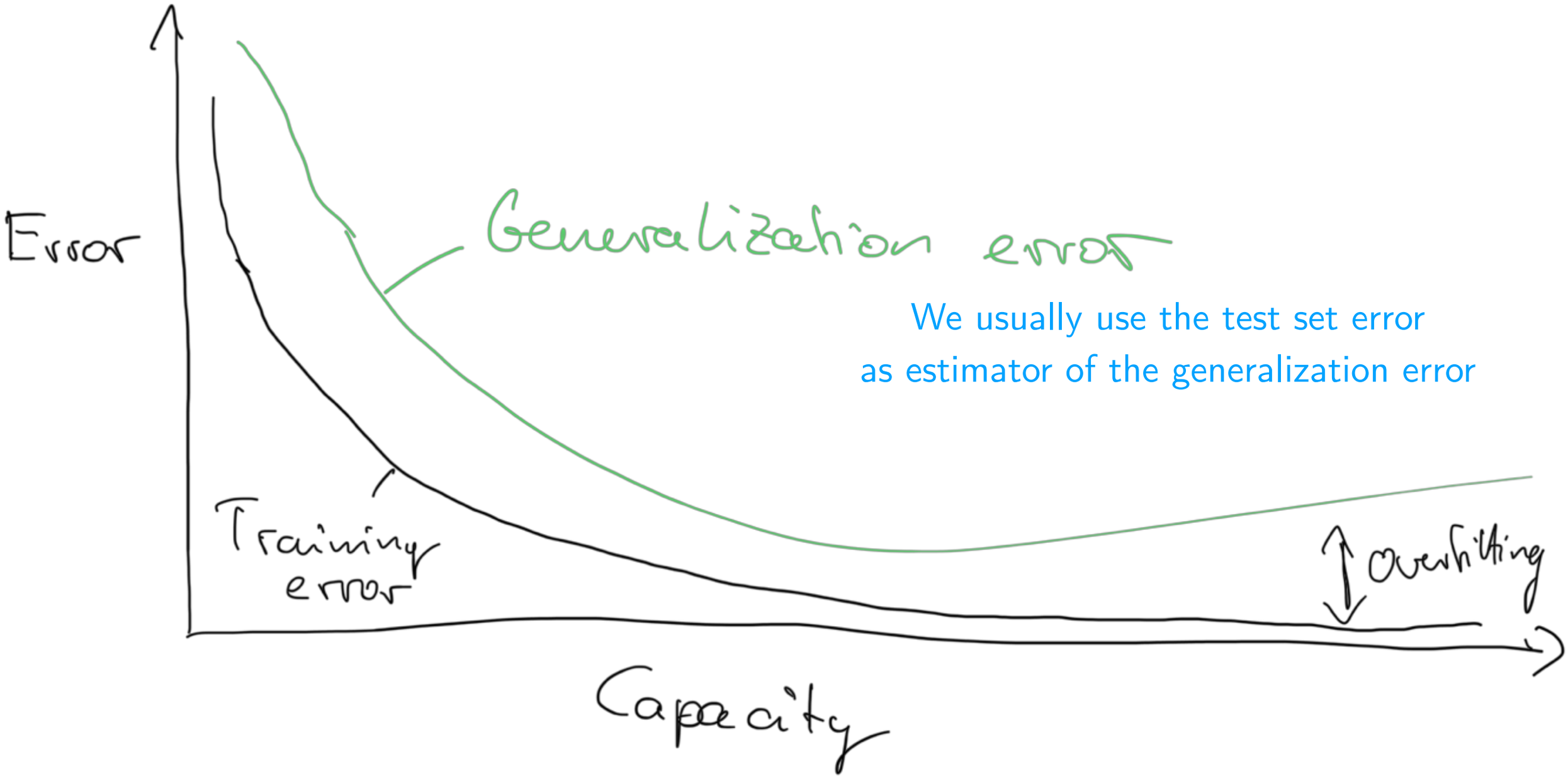
- Can achieve the same expressiveness with more layers but fewer parameters (combinatorics); fewer parameters => less overfitting
- Also, having more layers provides some form of regularization: later layers are constrained on the behavior of earlier layers
- However, more layers => vanishing/exploding gradients
- Later: different layers for different levels of feature abstraction (DL is really more about feature learning than just stacking multiple layers)

Recommended Practice: Looking at Some Failure Cases



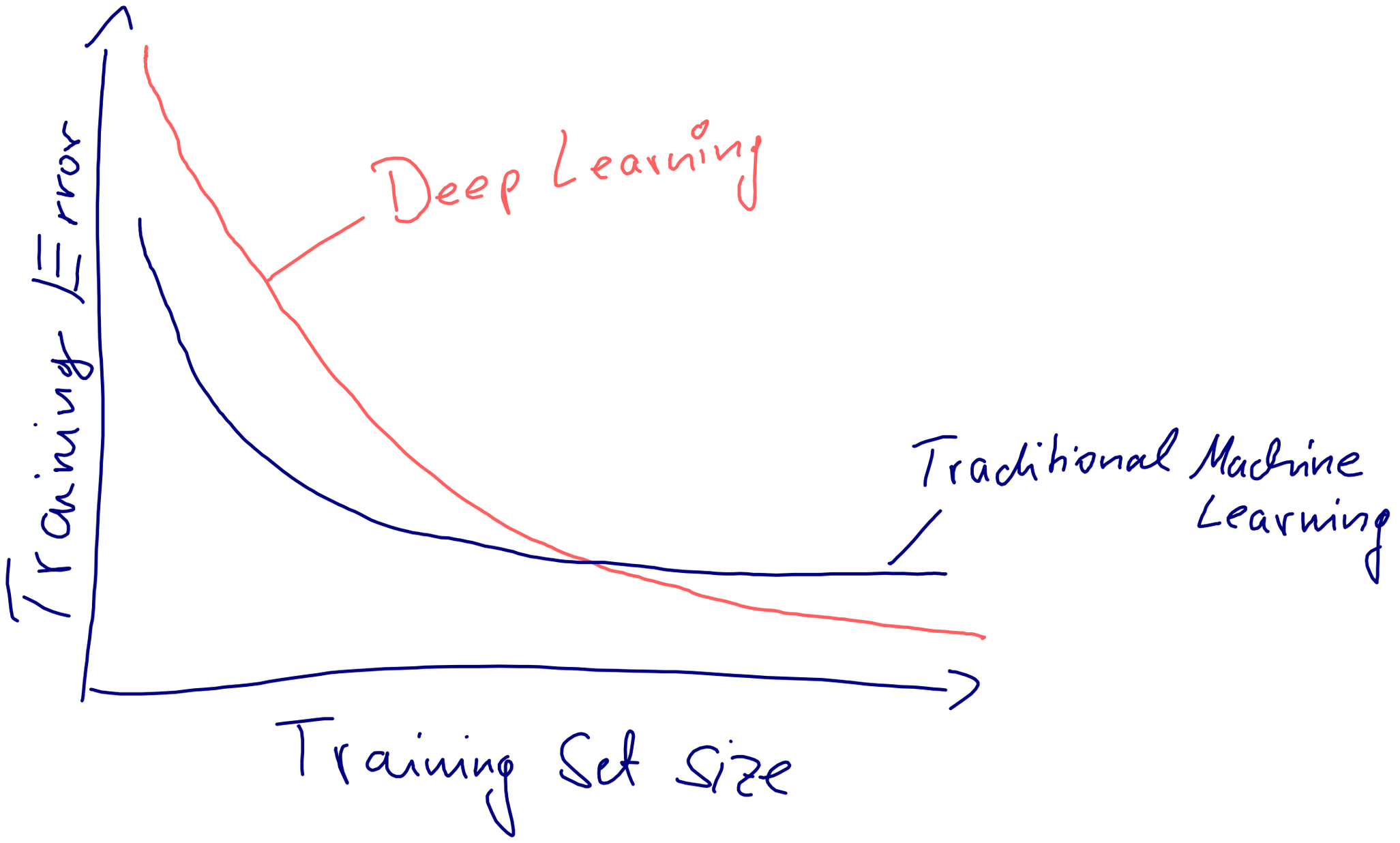
Failure cases of a ~93% accuracy (not very good, but beside the point)
2-layer (1-hidden layer) MLP on MNIST
(where *t=target* class and *p=predicted class*)

Overfitting and Underfitting



We usually use the test set error
as estimator of the generalization error

Deep Learning Works Best with Large Datasets



Parameters vs Hyperparameters

Parameters

- weights (weight parameters)
- biases (bias units)

Hyperparameters

- minibatch size
- data normalization schemes
- number of epochs
- number of hidden layers
- number of hidden units
- learning rates
- (random seed, why?)
- loss function
- various weights (weighting terms)
- activation function types
- regularization schemes (more later)
- weight initialization schemes (more later)
- optimization algorithm type (more later)
- ...

Selecting good hyperparameters requires some trial-and-error.
Hyperparameter tuning can be automated.

Regularization

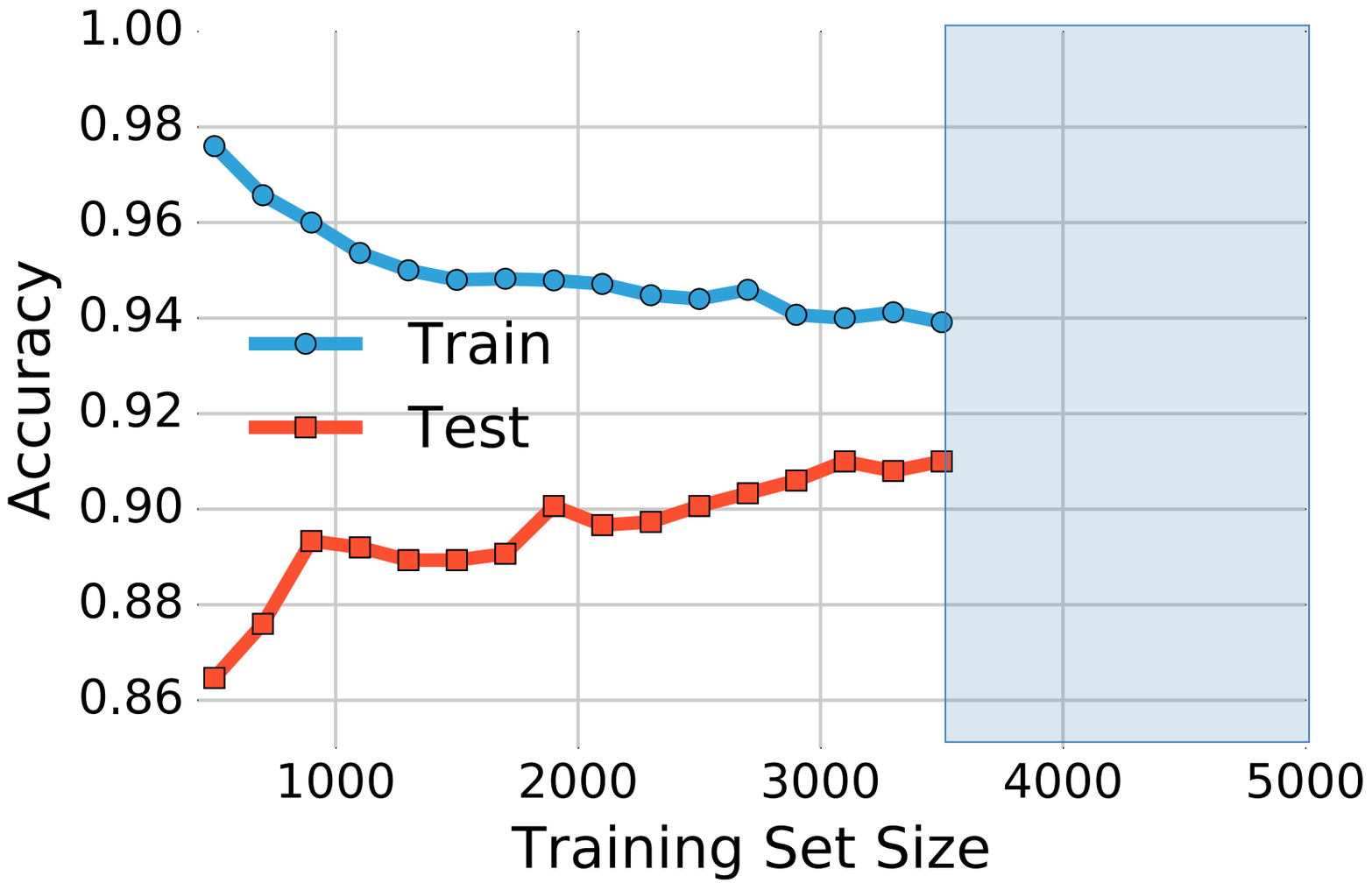
Overview: Regularization / Regularizing Effects

- Early stopping
- L_1/L_2 regularization (norm penalties)
- Dropout

Goal: reduce overfitting

usually achieved by reducing model capacity and/or reduction of the variance of the predictions

Best Way to Reduce Overfitting is Collecting More Data



Softmax on MNIST subset (kept test set size constant)

Best Way to Reduce Overfitting is Collecting More Data

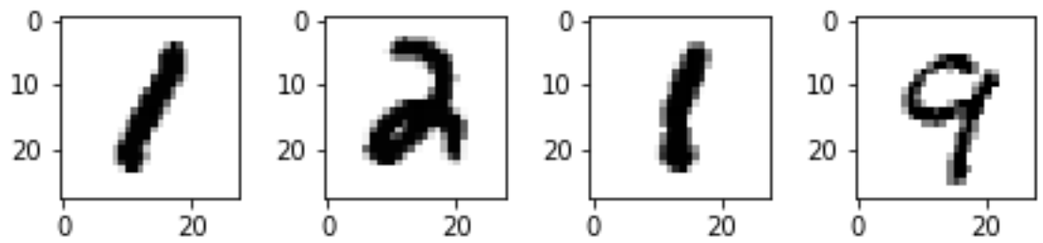
- Collecting more data is always helpful
- If not possible, data augmentation can be helpful (e.g., for images: random rotation, crop, translation ...)
- Additionally, reducing the capacity (e.g., regularization) helps

Data Augmentation in PyTorch via TorchVision

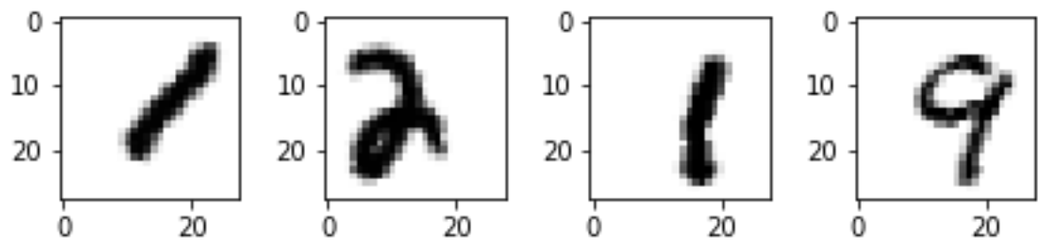
```
training_transforms = torchvision.transforms.Compose([
    #torchvision.transforms.RandomRotation(degrees=20),
    #torchvision.transforms.Resize(size=(34, 34)),
    #torchvision.transforms.RandomCrop(size=(28, 28)),
    torchvision.transforms.RandomAffine(degrees=(-20, 20), translate=(0.15, 0.15),
                                        resample=PIL.Image.BILINEAR),
    torchvision.transforms.ToTensor(),
    torchvision.transforms.Normalize(mean=(0.5, 0.5, 0.5), std=(0.5, 0.5, 0.5)),
    # normalize does (x_i - mean) / std
    # if images are [0, 1], they will be [-1, 1] afterwards
])

test_transforms = torchvision.transforms.Compose([
    torchvision.transforms.ToTensor(),
    torchvision.transforms.Normalize(mean=(0.5, 0.5, 0.5), std=(0.5, 0.5, 0.5)),
])

# for more see
# https://pytorch.org/docs/stable/torchvision/transforms.html

train_dataset = datasets.MNIST(root='data',
                               train=True,
                               transform=training_transforms,
                               download=True)

test_dataset = datasets.MNIST(root='data',
                              train=False,
                              transform=test_transforms)
```

Data Augmentation in PyTorch via TorchVision

Original

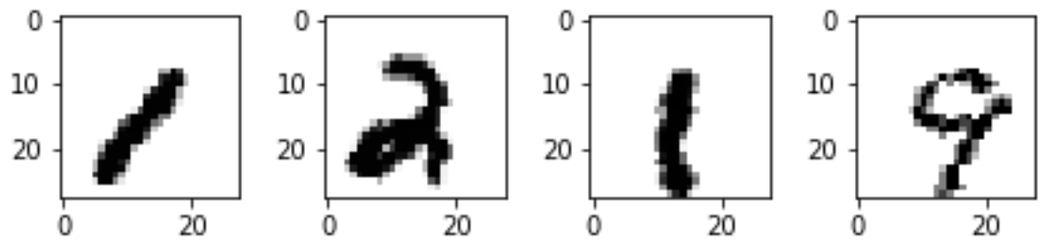


Augmented



note that it is random

Augmented w/o



`resample=PIL.Image.BILINEAR`

note that it is random

Now: Other Ways for Dealing with Overfitting if Collecting More Data is not Feasible

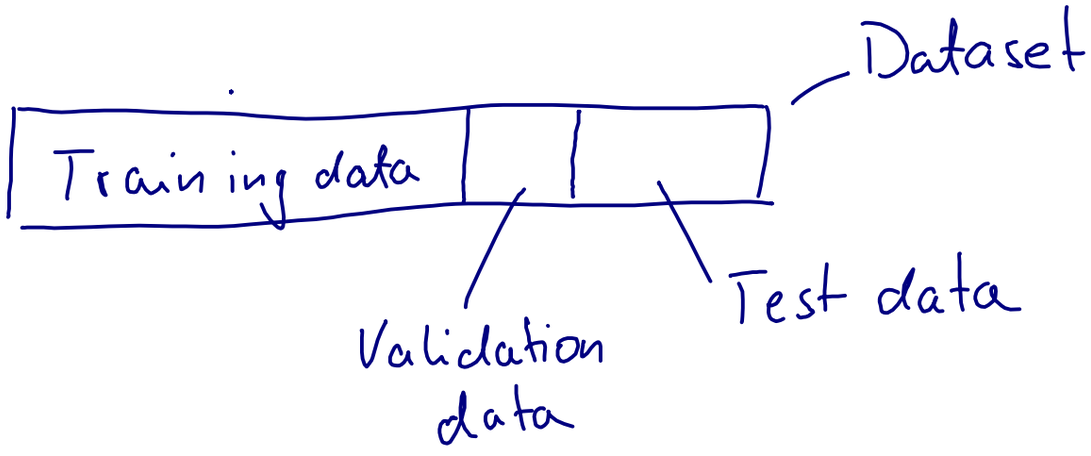
=> Reducing Network's Capacity by Other Means

- smaller architecture: fewer hidden layers & units, dropout, (dead ReLUs, L1 norm penalty)
- smaller weights: Early stopping, norm penalties
- adding noise: Dropout

Early Stopping

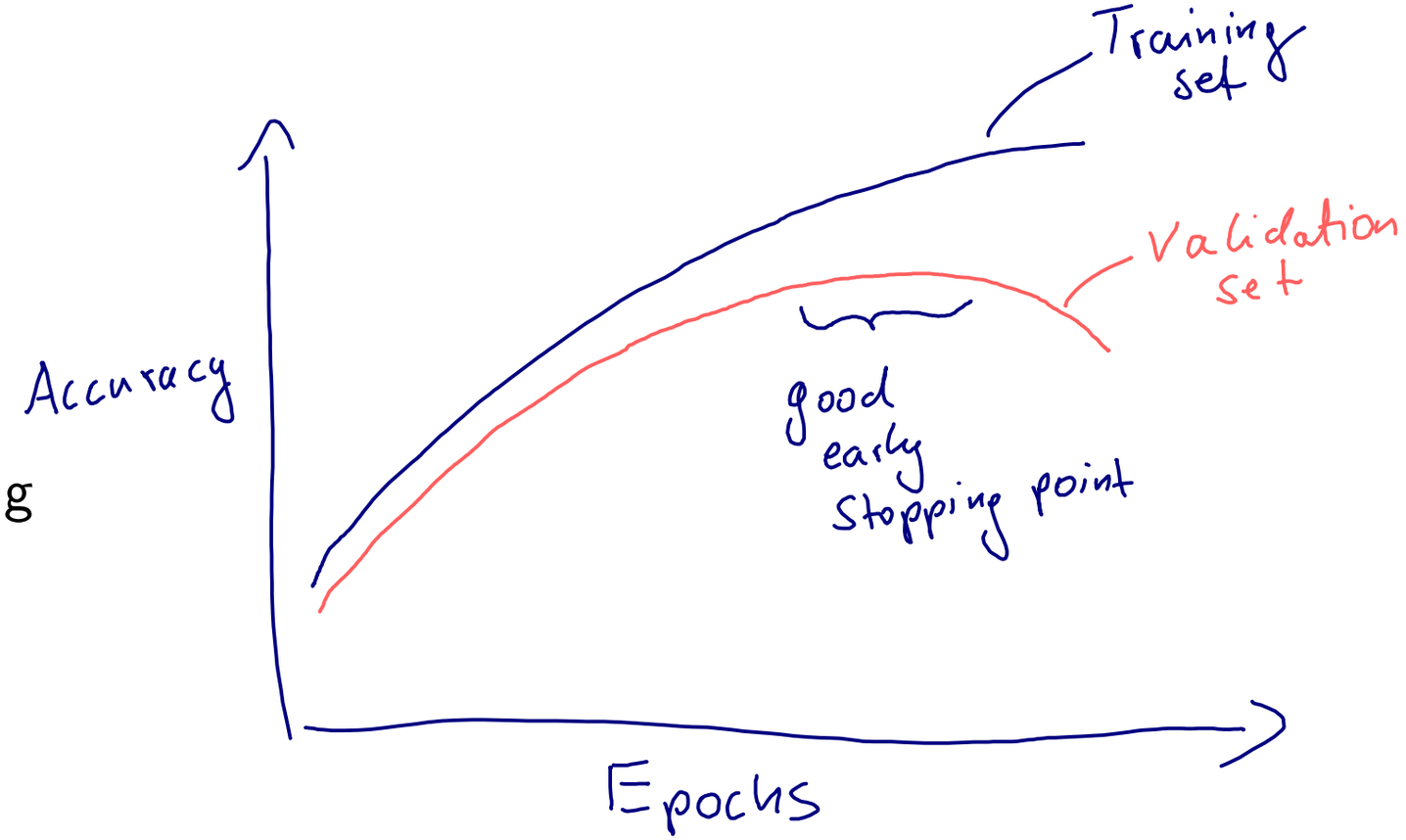
Step 1: Split your dataset into 3 parts (always recommended)

- use test set only once at the end (for unbiased estimate of generalization performance)
- use validation accuracy for tuning (always recommended)



Step 2: Early stopping (not very common anymore)

- reduce overfitting by observing the training/validation accuracy gap during training and then stop at the "right" point



L_2 Regularization

As you already know it from various statistics classes:

- L_2-regularization => Ridge regression (Thikonov regularization)

Basically, a "weight shrinkage" or a "penalty against complexity"

L_2 Regularization

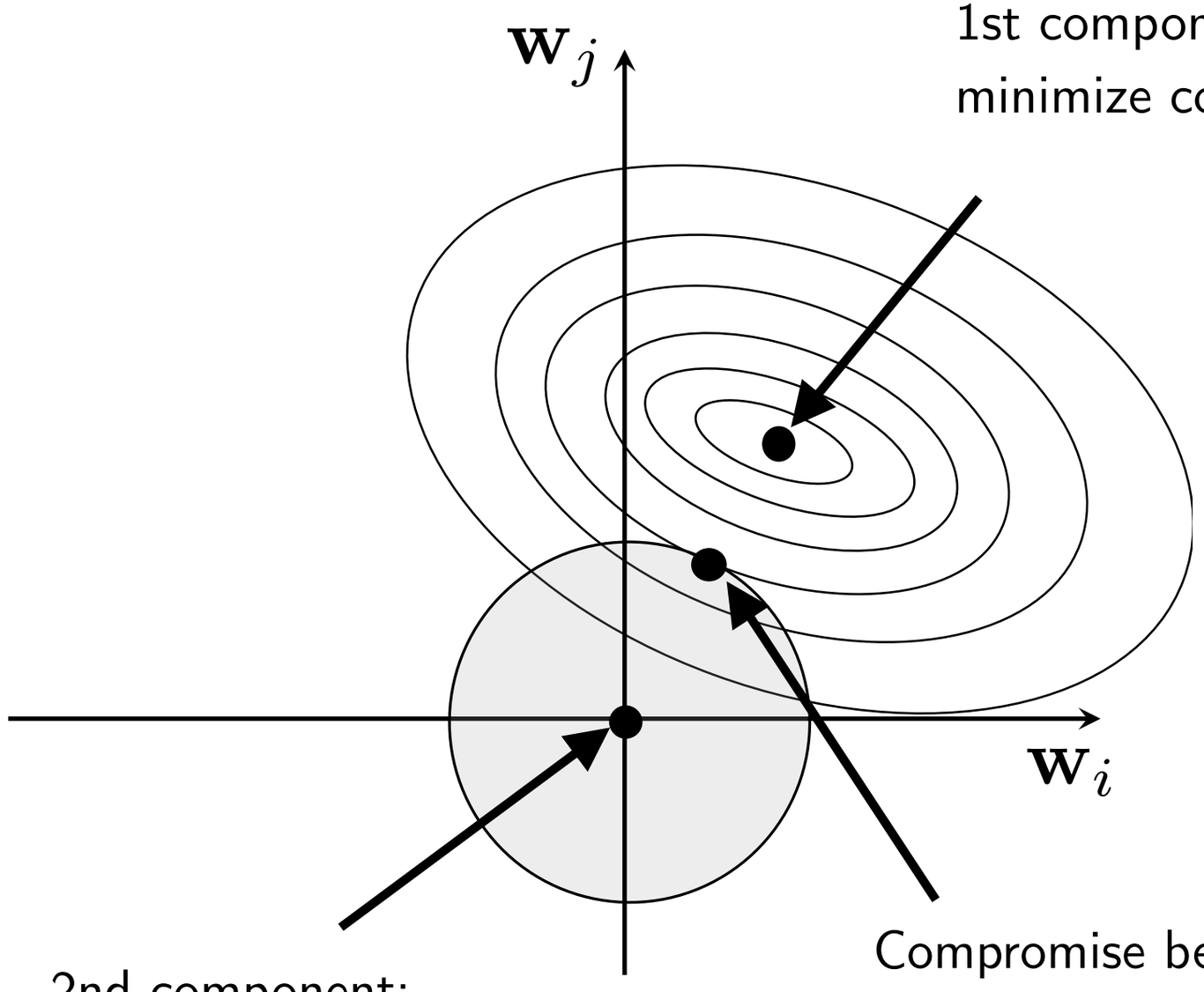
$$\text{Cost}_{\mathbf{w},\mathbf{b}} = \frac{1}{n}\sum_{i=1}^{n}\mathcal{L}(y^{[i]}, \hat{y}^{[i]})$$

$$\text{L2-Regularized-Cost}_{\mathbf{w},\mathbf{b}} = \frac{1}{n}\sum_{i=1}^{n}\mathcal{L}(y^{[i]}, \hat{y}^{[i]}) + \frac{\lambda}{n}\sum_{j} w_j^2$$

where: $\sum_{j} w_j^2 = ||\mathbf{w}||_2^2$

and λ is a hyperparameter

Geometric Interpretation of L_2 Regularization



1st component:
minimize cost function

2nd component:
minimize penalty term

Compromise between penalty
and cost

L_2 Regularization for Neural Nets

$$\text{L2-Regularized-Cost}_{\mathbf{w},\mathbf{b}} = \frac{1}{n}\sum_{i=1}^{n}\mathcal{L}(y^{[i]}, \hat{y}^{[i]}) + \frac{\lambda}{n}\sum_{l=1}^{L}||\mathbf{w}^{(l)}||_F^2$$

sum over layers

where $||\mathbf{w}^{(l)}||_F^2$ is the Frobenius norm (squared):

$$||\mathbf{w}^{(l)}||_F^2 = \sum_i \sum_j (w_{i,j}^{(l)})^2$$

L_2 Regularization for Logistic Regression in PyTorch

Manually:

```
optimizer = torch.optim.SGD(model.parameters(), lr=0.1)

for epoch in range(num_epochs):

    #### Compute outputs ####
    out = model(X_train_tensor)

    #### Compute gradients ####
    ##########################################################
    ## Apply L2 regularization (weight decay)
    cost = F.binary_cross_entropy(out, y_train_tensor, reduction='sum')
    cost = cost + 0.5 * LAMBDA * torch.mm(model.linear.weight,
                                          model.linear.weight.t())

    # note that PyTorch also regularizes the bias, hence, if we want
    # to reproduce the behavior of SGD's "weight_decay" param, we have to add
    # the bias term as well:
    cost = cost + 0.5 * LAMBDA * model.linear.bias**2
    #----------------------------------------------------------

    optimizer.zero_grad()
    cost.backward()
```

(Note that I am using 0.5 here because PyTorch does it; Could be considered "convenient " as the exponent "2" cancels in the derivative. This implementation exactly matches the one on the next slide)

L_2 Regularization for Logistic Regression in PyTorch

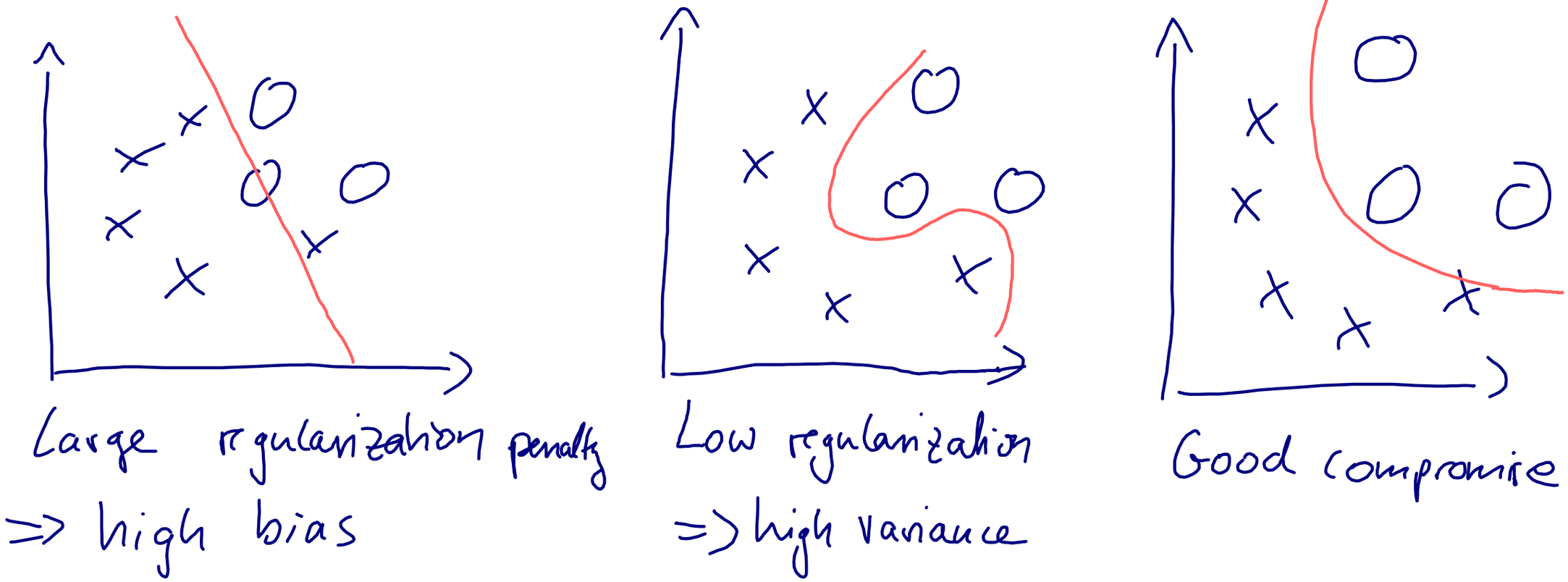
Automatically:

```
##########################################################
## Apply L2 regularization
optimizer = torch.optim.SGD(model.parameters(),
                            lr=0.1,
                            weight_decay=LAMBDA)
#----------------------------------------------------------
```

```
for epoch in range(num_epochs):

    #### Compute outputs ####
    out = model(X_train_tensor)

    #### Compute gradients ####
    cost = F.binary_cross_entropy(out, y_train_tensor, reduction='sum')
    optimizer.zero_grad()
    cost.backward()
```

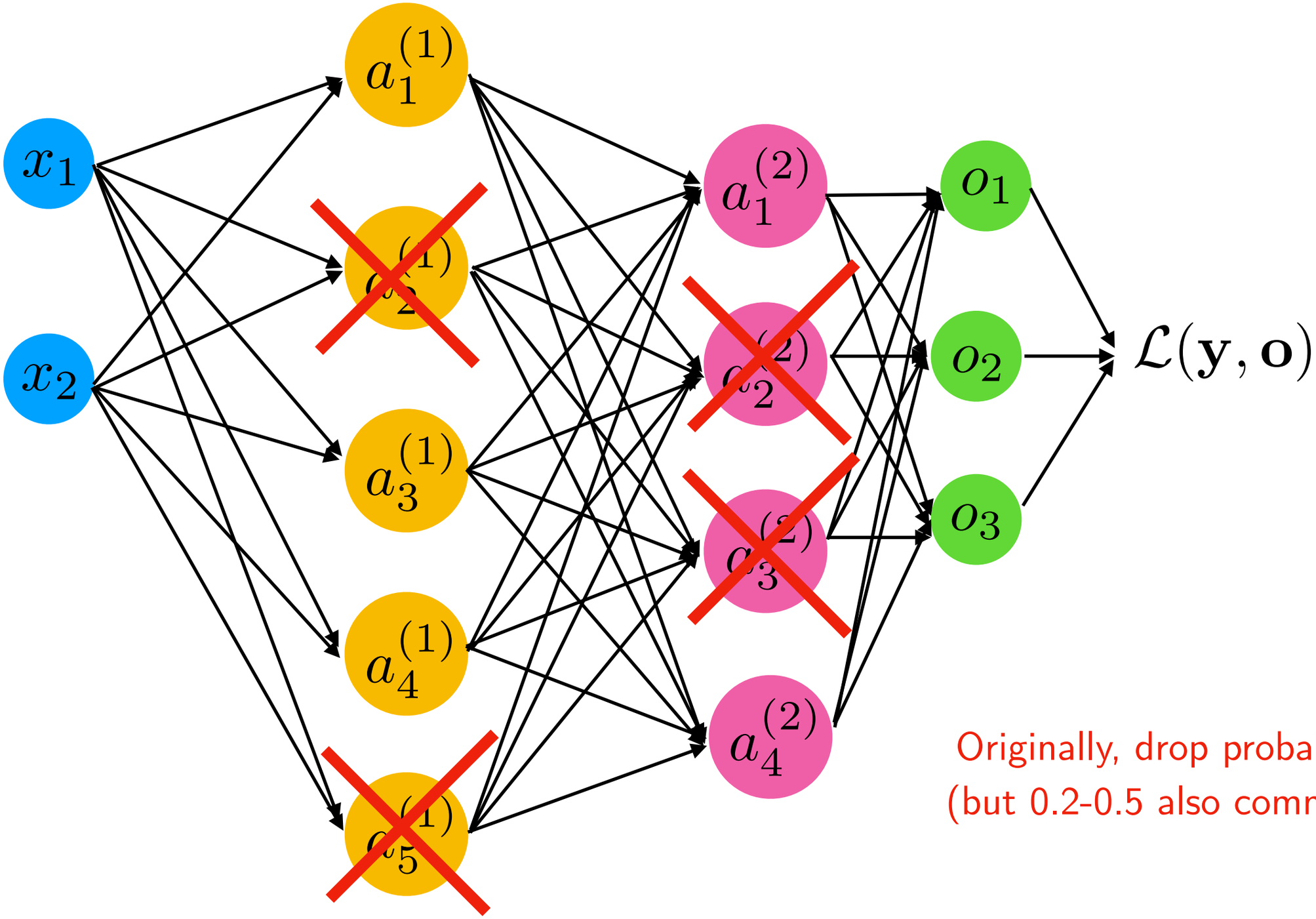
Effect of Norm Penalties on the Decision Boundary

Assume a nonlinear model



Dropout

Dropout in a Nutshell: Dropping Nodes



Originally, drop probability 0.5
(but 0.2-0.5 also common now)

Dropout in a Nutshell: Dropping Nodes

How do we drop the nodes practically/efficiently?

<u>Bernoulli Sampling (during training):</u>

- p := drop probability
- $\mathbf{v}$:= random sample from uniform distribution in range [0, 1]
- $\forall i \in \mathbf{v} : v_i := 0 \text{ if } v_i < p \text{ else } v_i$
- $\mathbf{a} := \mathbf{a} \odot \mathbf{v}$

Then, after training to make predictions (DL jargon: "inference")

$\mathbf{a} := \mathbf{a} \odot (1 - p)$

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$\mathbf{a} := \mathbf{a} \odot (1 - p)$ Q for you: Why is this required?

Why does Dropout work well?

- Network will learn not to rely on particular connections too heavily
- Thus, will consider more connections (because it cannot rely on individual ones)
- The weight values will be more spread-out (may lead to smaller weights like with L2 norm)
- Side note: You can certainly use different dropout probabilities in different layers (assigning them proportional to the number of units in a layer is not a bad idea, for example)

Dropout in PyTorch

Here, is is very important that you use `model.train()` and `model.eval()`!

```
for epoch in range(NUM_EPOCHS):
    model.train()
    for batch_idx, (features, targets) in enumerate(train_loader):

        features = features.view(-1, 28*28).to(DEVICE)

        ### FORWARD AND BACK PROP
        logits, probas = model(features)

        cost = F.cross_entropy(logits, targets)
        optimizer.zero_grad()

        cost.backward()
        minibatch_cost.append(cost)
        ### UPDATE MODEL PARAMETERS
        optimizer.step()

    model.eval()
    with torch.no_grad():
        cost = compute_loss(model, train_loader)
        epoch_cost.append(cost)
        print('Epoch: %03d/%03d Train Cost: %.4f' % (
                epoch+1, NUM_EPOCHS, cost))
        print('Time elapsed: %.2f min' % ((time.time() - start_time)/60))
```

Dropout in PyTorch ([more] Object-Oriented API)

```
class MultilayerPerceptron(torch.nn.Module):

    def __init__(self, num_features, num_classes, drop_proba,
                 num_hidden_1, num_hidden_2):
        super(MultilayerPerceptron, self).__init__()

        self.my_network = torch.nn.Sequential(
            torch.nn.Linear(num_features, num_hidden_1),
            torch.nn.ReLU(),
            torch.nn.Dropout(drop_proba),
            torch.nn.Linear(num_hidden_1, num_hidden_2),
            torch.nn.ReLU(),
            torch.nn.Dropout(drop_proba),
            torch.nn.Linear(num_hidden_2, num_classes)
        )

    def forward(self, x):
        logits = self.my_network(x)
        probas = F.softmax(logits, dim=1)
        return logits, probas
```

Dropout in PyTorch (Functional API)

```
class MultilayerPerceptron(torch.nn.Module):

    def __init__(self, num_features, num_classes, drop_proba,
                 num_hidden_1, num_hidden_2):
        super(MultilayerPerceptron, self).__init__()

        self.drop_proba = drop_proba
        self.linear_1 = torch.nn.Linear(num_features,
                                        num_hidden_1)

        self.linear_2 = torch.nn.Linear(num_hidden_1,
                                        num_hidden_2)

        self.linear_out = torch.nn.Linear(num_hidden_2,
                                          num_classes)

    def forward(self, x):
        out = self.linear_1(x)
        out = F.relu(out)
        out = F.dropout(out, p=self.drop_proba, training=self.training)
        out = self.linear_2(out)
        out = F.relu(out)
        out = F.dropout(out, p=self.drop_proba, training=self.training)
        logits = self.linear_out(out)
        probas = F.log_softmax(logits, dim=1)
        return logits, probas
```

Dropout: Practical Tips

- Don't use Dropout if your model does not overfit
- However, in that case above, it is then recommended to increase the capacity to make it overfit, and then use dropout to be able to use a larger capacity model (but make it not overfit)