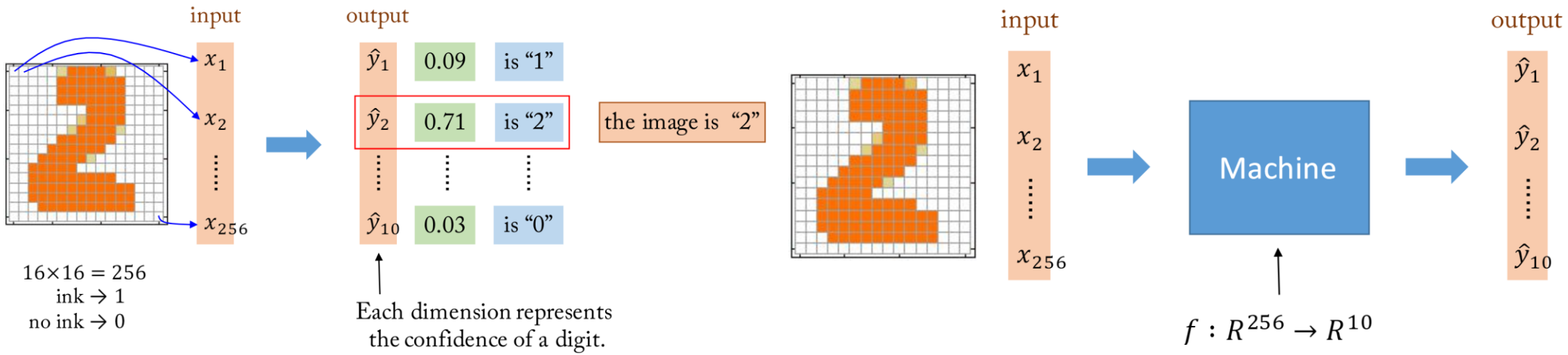
Classifying MNIST digits using MLP

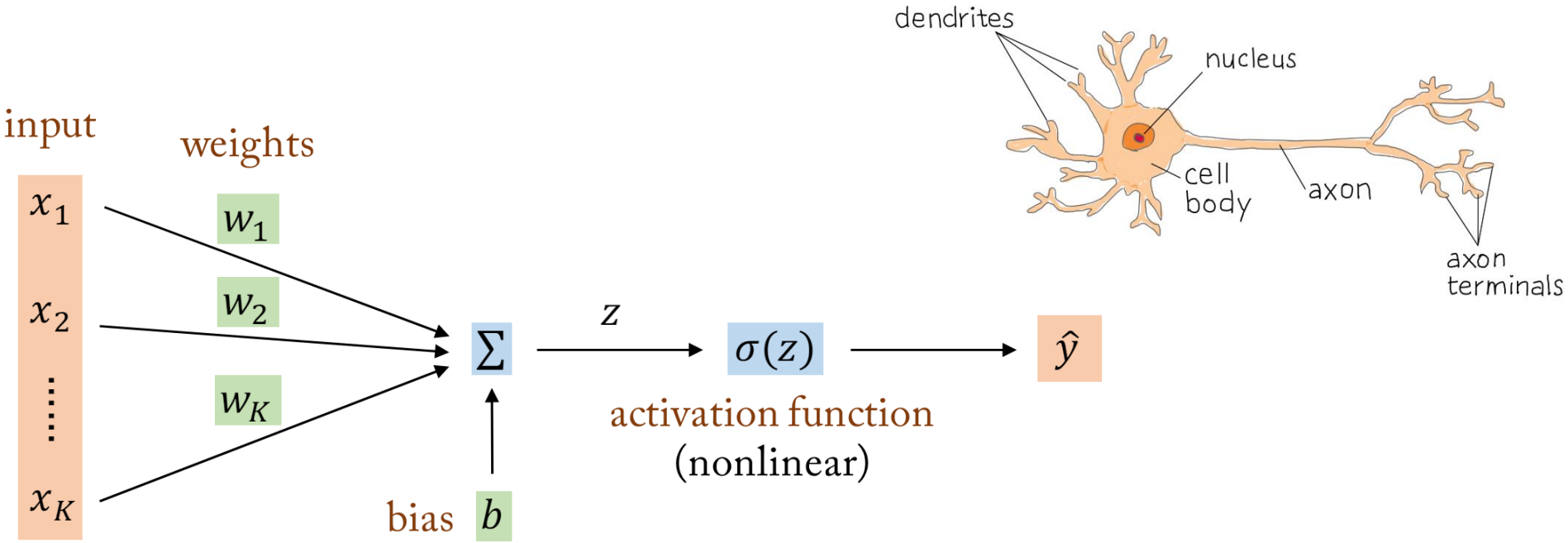
TA. Dongjae Kim

Contents

1. Deep Learning motivation



- In Traditional programming, we hand-design the function f, then compute the output $y = f(x)$.
- In Deep Learning, we collect data (x, y) and learn the function $f_\theta(x)$ that best maps $x \rightarrow y$.

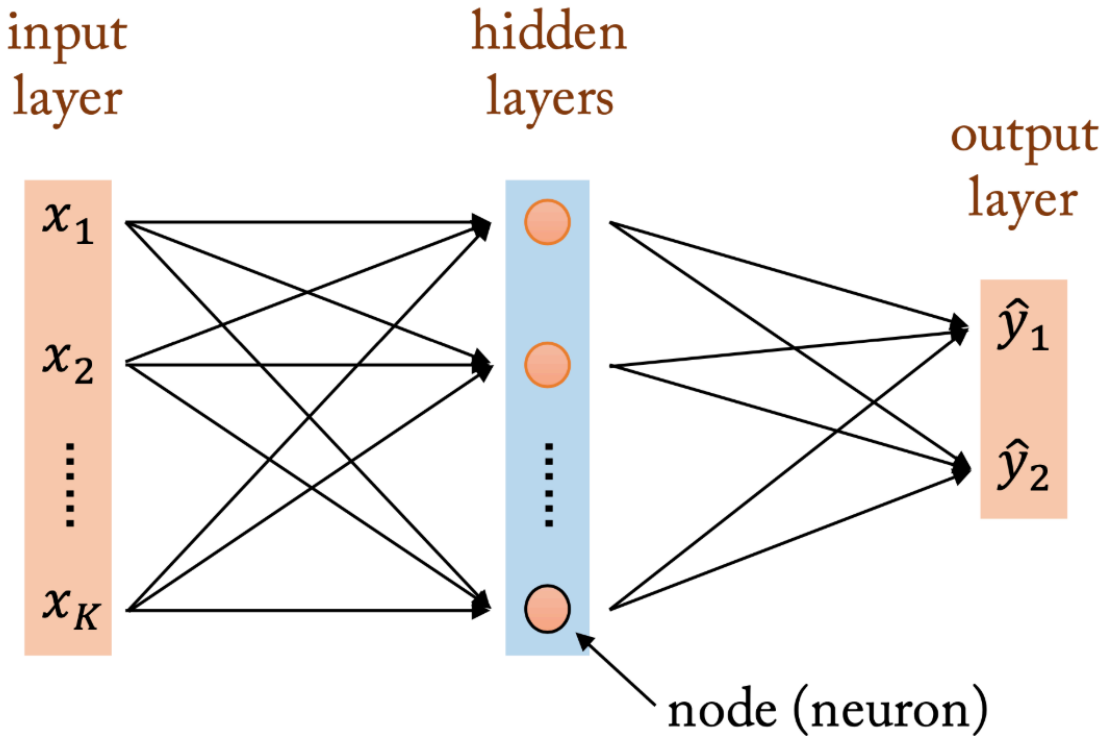


$$f : \mathbb{R}^K \rightarrow \mathbb{R}$$

$$\hat{y} = \sigma(z) = \sigma(w_1 x_1 + w_2 x_2 + \cdots + w_K x_K + b)$$

nonlinear weighted sum (linear)

3. Multilayer Perceptron (MLP)



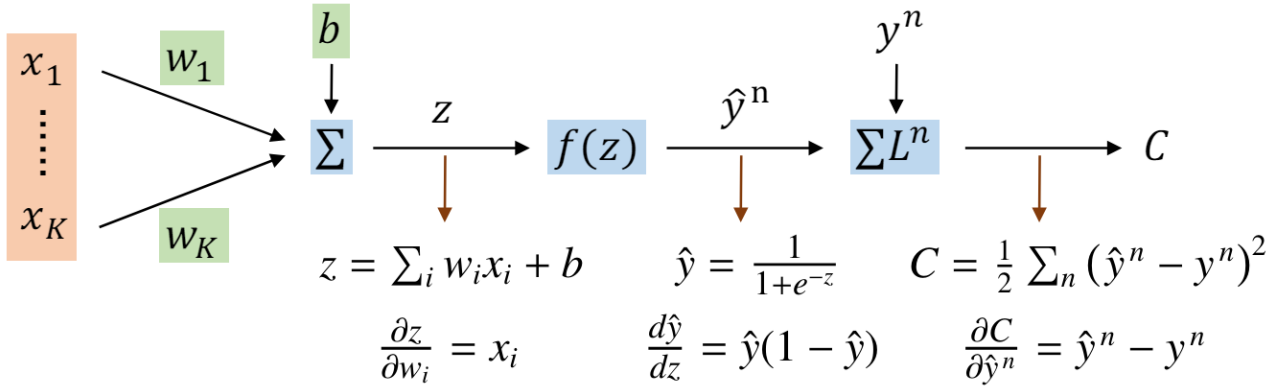
- MLP is a class of feedforward artificial neural network.
- MLP consists of an input layer, several hidden layers and an output layer.
- Except input nodes, each node is a neuron (perceptron) that uses a nonlinear activation function.

4. Backpropagation

- Backpropagation is the way of computing the gradient efficiently to update millions of network parameters
- Gradient Descent
  - Goal: find the optimal parameter w^*, which minimizes the total cost (MSE)

    $C = \frac{1}{2}\sum_{n=1}^{N}(\hat{y}^n - y^n)^2 \;\; where \; \hat{y}^n = f(w^T x^n + b)$
  - Backpropagation: iteratively updating the model parameters w to decrease C by using

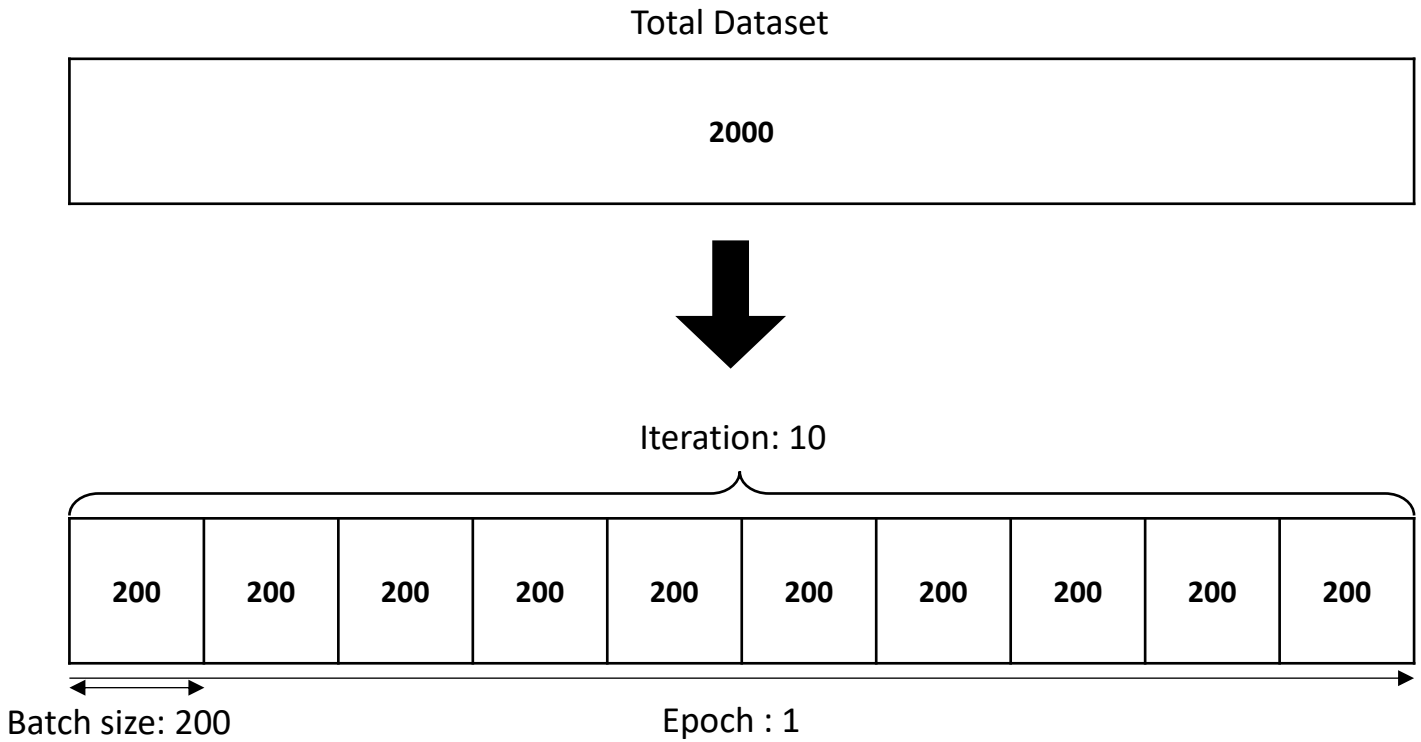
    $w_i(t+1) = w_i(t) - \eta \frac{\partial C}{\partial w_i}$



$$\frac{\partial C}{\partial w_i} = \sum_{n=1}^{N} \frac{\partial z^n}{\partial w_i}\frac{d\hat{y}^n}{dz^n}\frac{\partial C}{\partial \hat{y}^n} = \sum_{n=1}^{N} x_i^n \hat{y}^n(1-\hat{y}^n)(\hat{y}^n - y^n)$$

Chain rule

5. Batch, Minibatch, Epoch



Definitions
Batch: A subset of the training data used for one forward pass and a parameter update
Iteration: One update of the model using one batch.
Epoch: One full pass through the entire training dataset

- Batch gradient Descent: Use the entire dataset per update
- Mini-batch Gradient Descent: Use a mini-batch of dataset per update
- Stochastic Gradient Descent: Use a single data sample per update

6. After Gradient Descent Algorithm ...

모든 자료를 다 검토해서
내 위치의 산기울기를 계산해서
갈 방향을 찾겠다.

GD

스텝방향

Momentum
스텝 계산해서 움직인 후,
아까 내려 오던 관성 방향 또 가자

Nesterov Accelerated Gradient

NAG
일단 관성 방향 먼저 움직이고,
움직인 자리에 스텝을 계산하니
더 빠르더라

Nadam
Adam에 Momentum
대신 NAG를 붙이자.

SGD
전부 다봐야 한걸음은
너무 오래 걸리니까
조금만 보고 빨리 판단한다
같은 시간에 더 많이 간다

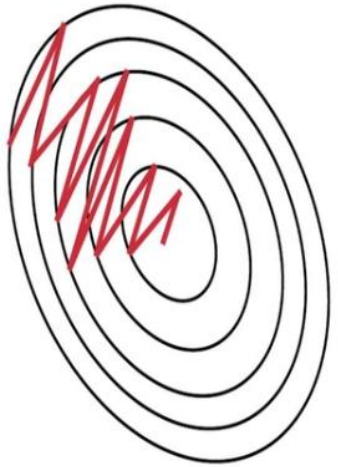
스텝사이즈

RMSProp
보폭을 줄이는 건 좋은데
이전 맥락 상황봐가며 하자.

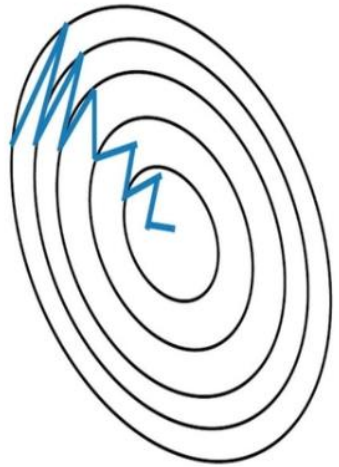
Adam
RMSProp + Momentum
방향도 스텝사이즈도 적절하게!

Adagrad
안가본곳은 성큼 빠르게 걸어 훑고
많이 가본 곳은 잘아니까
갈수록 보폭을 줄여 세밀히 탐색

AdaDelta
종종걸음 너무 작아져서
정지하는걸 막아보자.



Stochastic Gradient Descent **withhout** Momentum

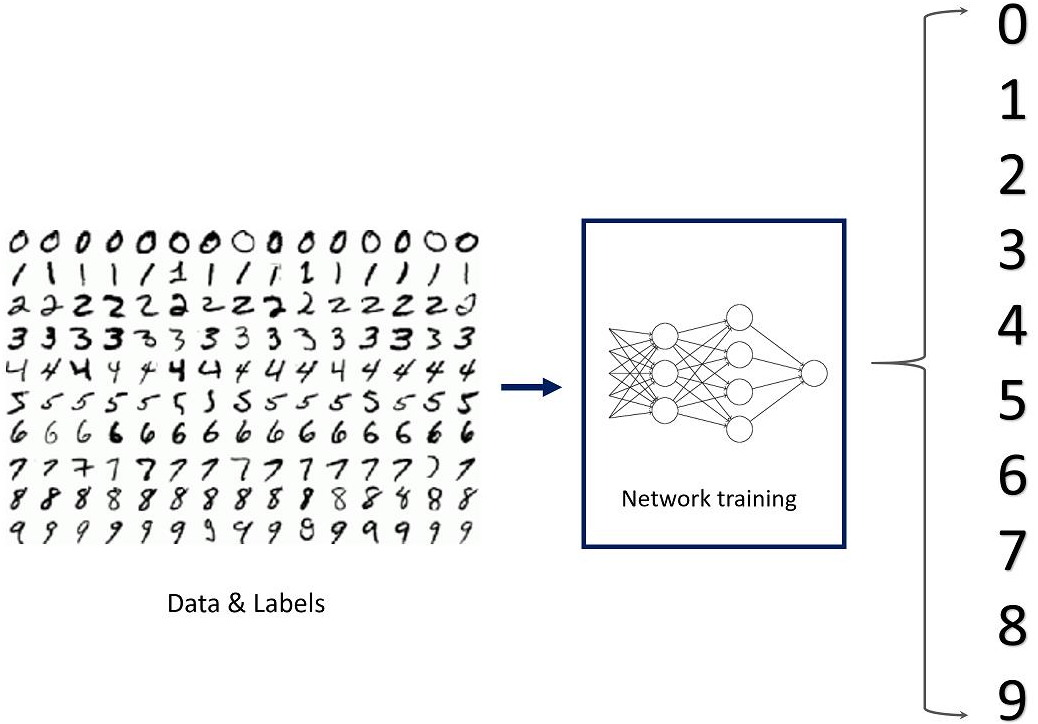


Stochastic Gradient Descent **with** Momentum

https://dev.to/nareshnishad/day-25-optimizer-algorithms-for-large-language-models-llms-1p4

MLP with MNIST

1. MNIST

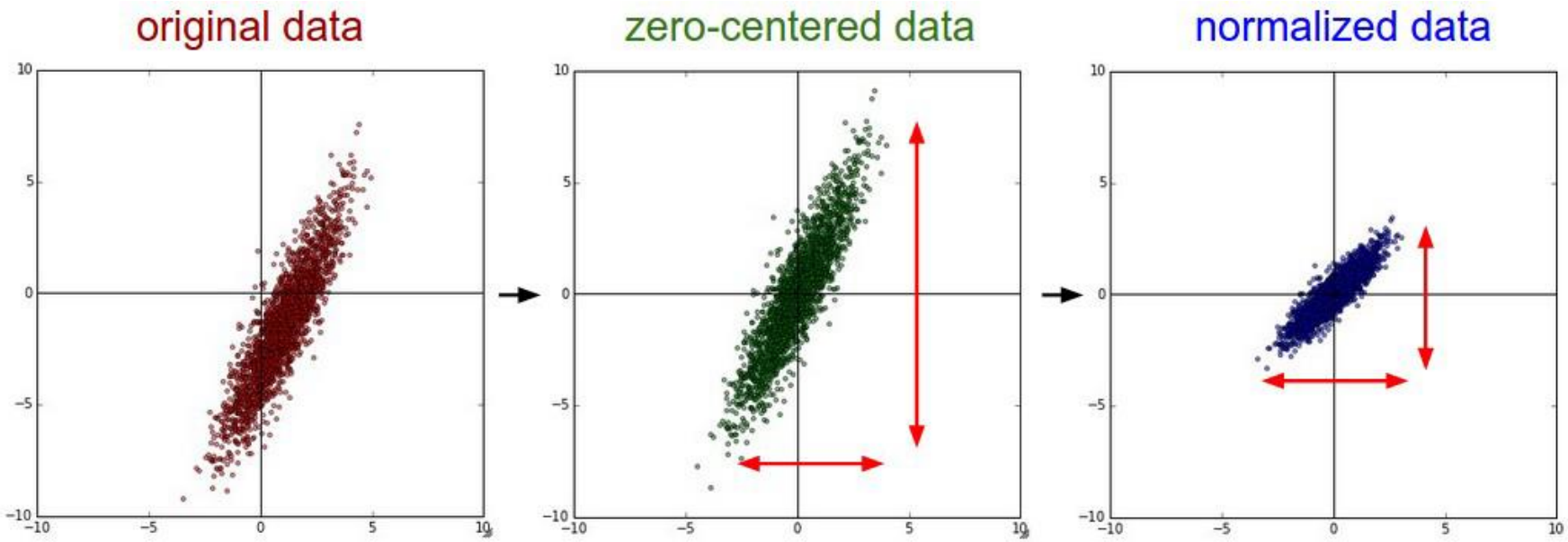


- Modified National Institute of Standards and Technology database
  - 60,000 images for the training and 10,000 images for the test.
  - Size : 28x28 pixels
  - Only 1 channel (Gray scale)

2. Preparing Data

1. Load
    - Use easy loading function in torchvision library
    - Need to create custom loading function when trying to load your own dataset.
2. Normalize
    - Standardize features by removing the mean and scaling to unit variance
    - Divide by the maximum value
3. Convert to one-hot encoding/vector
    - Need when training a neural network which classifies given data

3. Normalize

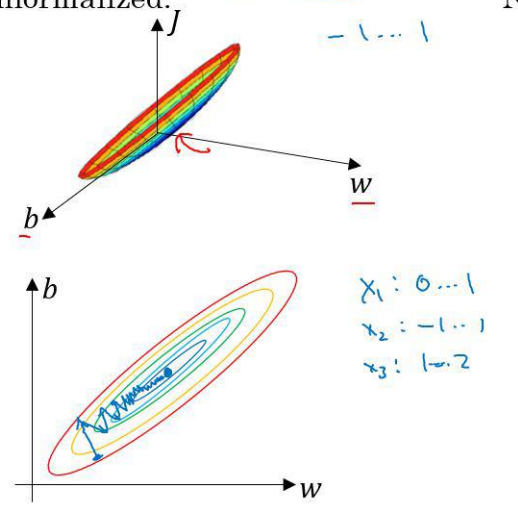


- Common data preprocessing pipeline.
  - Left: Original toy, 2-dimensional input data.
  - Middle: The data is zero-centered by subtracting the mean in each dimension. The data cloud is now centered around the origin.
  - Right: Each dimension is additionally **scaled by its standard deviation**.
- The red lines indicate the extent of the data - they are of unequal length in the middle, but of equal length on the right.

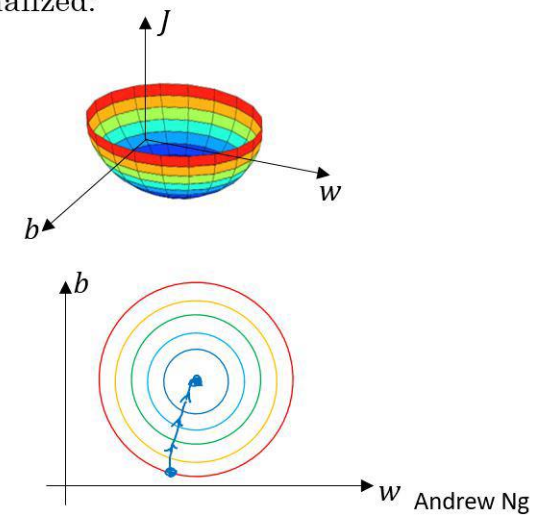
Why normalize inputs?

$$J(w,b) = \frac{1}{m}\sum_{i=1}^{m} \mathcal{L}\left(\hat{y}^{(i)}, y^{(i)}\right)$$

Unnormalized:



Normalized:

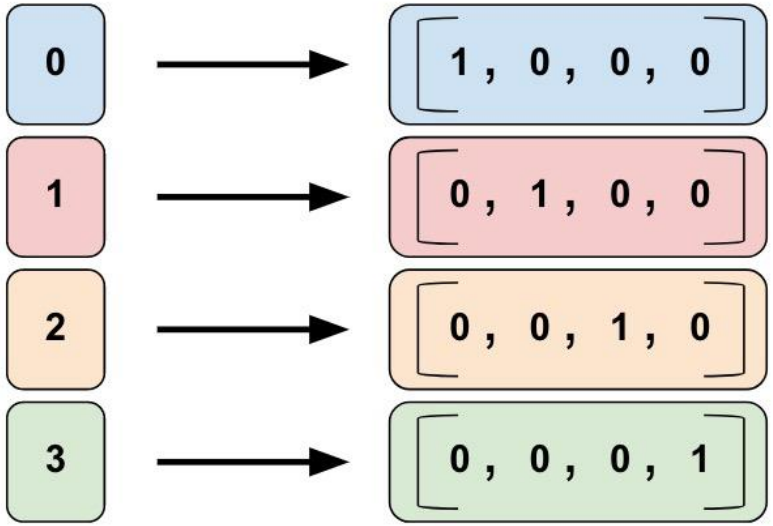


Andrew Ng

$$\nabla J(w) = \left[\frac{\partial J}{\partial w_1}, \frac{\partial J}{\partial w_2}\right]$$

```
transform = transforms.Compose([
    transforms.ToTensor(),
    transforms.Normalize((0.5,), (0.5,))
])
```

4. Convert to one-hot encoding/vector



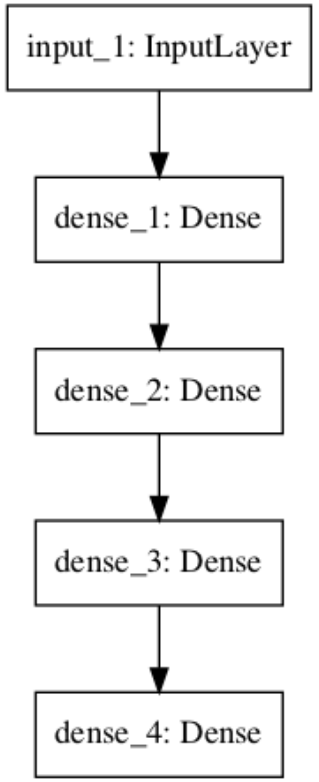

```python
class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.fc1 = nn.Linear(784, 512) # (input vector, output)
        self.fc2 = nn.Linear(512, 512)
        self.fc3 = nn.Linear(512, num_classes)
        self.dropout = nn.Dropout(0.2)

    def forward(self, x):
        x = x.view(-1, 784) # (batch size, 28, 28) -> (batch size, 784)
        x = torch.relu(self.fc1(x))
        x = self.dropout(x)
        x = torch.relu(self.fc2(x))
        x = self.dropout(x)
        x = self.fc3(x)
        return torch.log_softmax(x, dim=1)
```

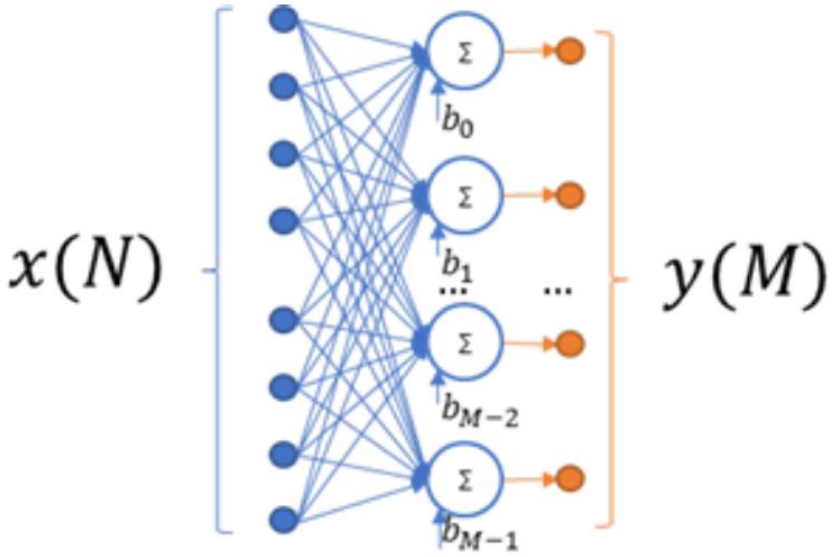
5. Creating a model

- Define custom PyTorch class (torch)
  - Easy way of creating a network.
  - Convenient, but hard to use when creating complex networks.
- Dense Layer
  - Fully connected layer.
  - Consists of weights and biases
- Activation Functions
  - Defines the output of the node
  - ReLU, tanh, sigmoid
- Dropout Layer
  - Prevents overfitting
  - Randomly removes the connections between weights
- Softmax
  - Converts the scores to the probabilities
  - Usually locates at the end of the network

```python
class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.fc1 = nn.Linear(784, 512)
        self.fc2 = nn.Linear(512, 512)
        self.fc3 = nn.Linear(512, num_classes)
        self.dropout = nn.Dropout(0.2)

    def forward(self, x):
        x = x.view(-1, 784)
        x = torch.relu(self.fc1(x))
        x = self.dropout(x)
        x = torch.relu(self.fc2(x))
        x = self.dropout(x)
        x = self.fc3(x)
        return torch.log_softmax(x, dim=1)

model = Net()
```

6. Dense Layer






```python
class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.fc1 = nn.Linear(784, 512)
        self.fc2 = nn.Linear(512, 512)
        self.fc3 = nn.Linear(512, num_classes)
        self.dropout = nn.Dropout(0.2)

    def forward(self, x):
        x = x.view(-1, 784)
        x = torch.relu(self.fc1(x))
        x = self.dropout(x)
        x = torch.relu(self.fc2(x))
        x = self.dropout(x)
        x = self.fc3(x)
        return torch.log_softmax(x, dim=1)

model = Net()
```

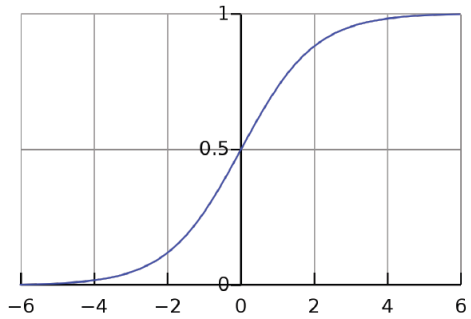
$$y_i = x_j W_{i,j} + b_i$$

Where:

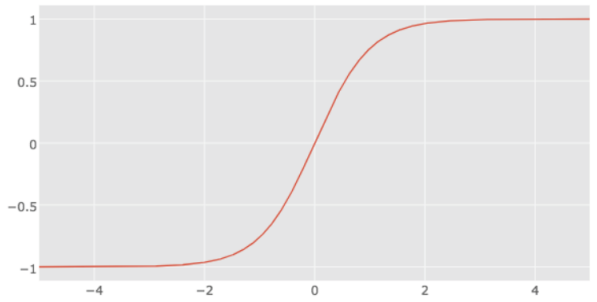
- x_j - j_{th} value in input tensor.
- y_i - i_{th} value in output tensor.
- W_{ij} - weight of j_{th} input element for i_{th} neuron.
- b_j - bias for i_{th} neuron.

7. Activation Functions

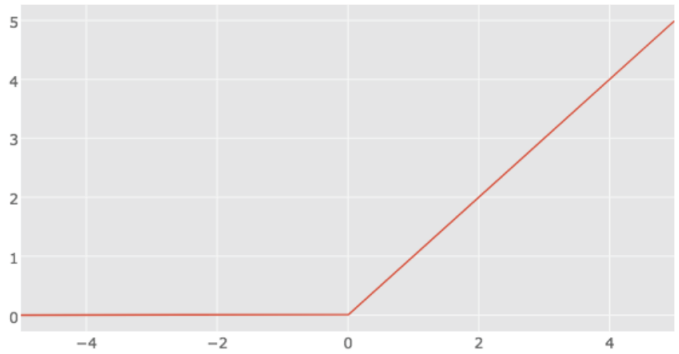
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$
$$\sigma'(x) = \sigma(x)\big(1 - \sigma(x)\big)$$



Sigmoid



Tanh

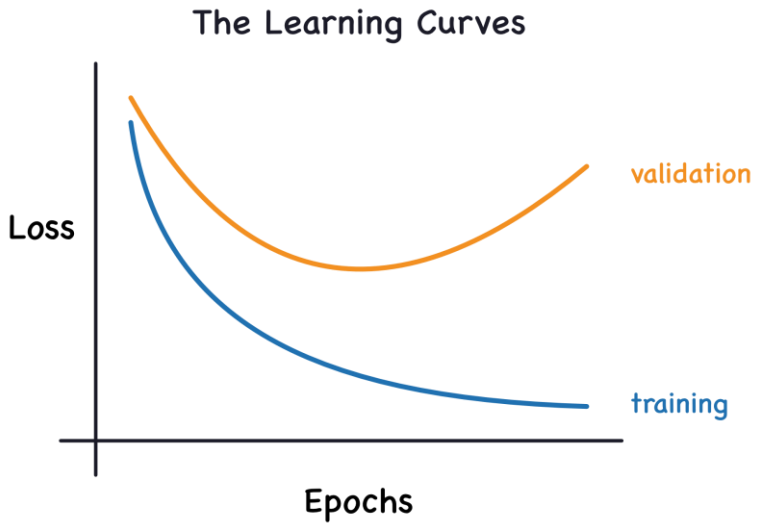


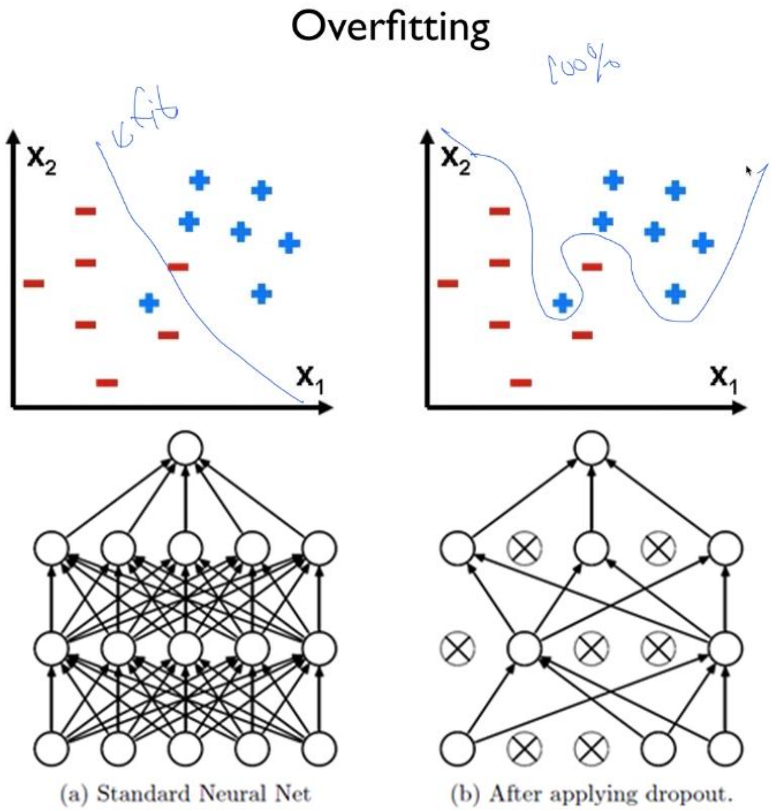
ReLU (Rectified Linear Unit)

```python
class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.fc1 = nn.Linear(784, 512)
        self.fc2 = nn.Linear(512, 512)
        self.fc3 = nn.Linear(512, num_classes)
        self.dropout = nn.Dropout(0.2)

    def forward(self, x):
        x = x.view(-1, 784)
        x = torch.relu(self.fc1(x))
        x = self.dropout(x)
        x = torch.relu(self.fc2(x))
        x = self.dropout(x)
        x = self.fc3(x)
        return torch.log_softmax(x, dim=1)

model = Net()
```

- Defines the output strength of the signal to the following layer
- Select proper and better activation functions by trial and errors

8. Dropout Layer

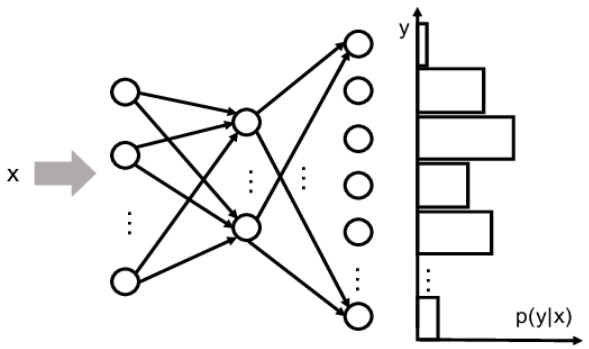





```python
class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.fc1 = nn.Linear(784, 512)
        self.fc2 = nn.Linear(512, 512)
        self.fc3 = nn.Linear(512, num_classes)
        self.dropout = nn.Dropout(0.2)

    def forward(self, x):
        x = x.view(-1, 784)
        x = torch.relu(self.fc1(x))
        x = self.dropout(x)
        x = torch.relu(self.fc2(x))
        x = self.dropout(x)
        x = self.fc3(x)
        return torch.log_softmax(x, dim=1)

model = Net()
```

- Prevents overfitting when the network has many hidden layers
- Skips / removes the connections between weights

9. Softmax



$$P(y=j \mid \theta^{(i)}) = \frac{e^{\theta^{(i)}}}{\sum_{j=0}^{k} e^{\theta_k^{(i)}}}$$

Softmax function

where $\theta = w_0x_0 + w_1x_1 + \ldots + w_kx_k = \sum_{i=0}^{k} w_ix_i = w^Tx$

```python
class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.fc1 = nn.Linear(784, 512)
        self.fc2 = nn.Linear(512, 512)
        self.fc3 = nn.Linear(512, num_classes)
        self.dropout = nn.Dropout(0.2)

    def forward(self, x):
        x = x.view(-1, 784)
        x = torch.relu(self.fc1(x))
        x = self.dropout(x)
        x = torch.relu(self.fc2(x))
        x = self.dropout(x)
        x = self.fc3(x)
        return torch.log_softmax(x, dim=1)

model = Net()
```

- Softmax layer is used as the output layer
- Converts the scores to the probabilities
- We select the index of the largest probability as a classification result

```
criterion = nn.CrossEntropyLoss()
optimizer = optim.RMSprop(model.parameters())

for epoch in range(epochs):
    for i, (images, labels) in enumerate(train_loader):
        outputs = model(images) # images.shape == [128, 1, 28, 28]
        loss = criterion(outputs, labels)

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

        if (i+1) % 100 == 0:
            print(f'Epoch [{epoch+1}/{epochs}], Step [{i+1}/{len(train_loader)}], Loss: {loss.item():.4f}')
```

Choose an appropriate loss function for current task (loss function ex: MSE, …)

Sets the optimizer (ex: GD, …)

Clears the gradients of all optimized parameters

Computes the gradient of the loss with respect to the model parameters

Updates the model parameters based on the computed gradients

11. Test a network

```
model.eval()
with torch.no_grad():
    correct = 0
    total = 0
    # To store a few test images for visualization
    examples = []
    num_examples = 16

    for images, labels in test_loader:
        outputs = model(images)
        _, predicted = torch.max(outputs.data, 1)
        total += labels.size(0)
        correct += (predicted == labels).sum().item()
```

Question