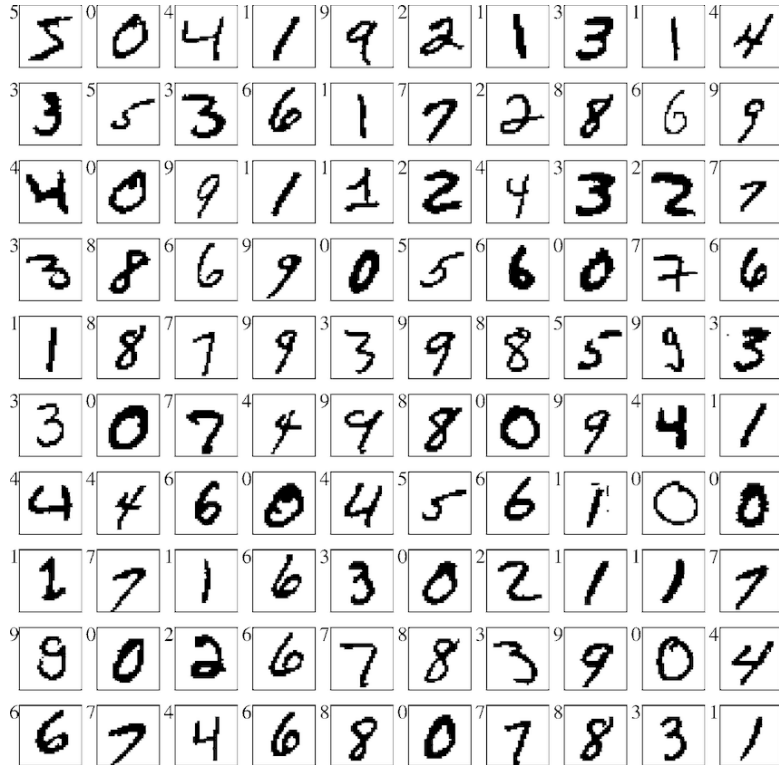


# Neural Networks: Basics

Shusen Wang

# Revisit Softmax Classifier

# Train a Softmax Classifier



## The MNIST Dataset

- $n = 60,000$  training samples  $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)$ .
- Each  $\mathbf{x}_j$  is a  $28 \times 28$  image.
- Each  $y_j$  is an integer in  $\{0, 1, 2, \dots, 9\}$ .

# Train a Softmax Classifier



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- $n = 60,000$  training samples  $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)$ .
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- Each  $y_j$  is an integer in  $\{0, 1, 2, \dots, 9\}$ .

## Task: multi-class classification

- Given a  $28 \times 28$  image, predict the digit.
- Learn a function  $\mathbf{f}: \mathbb{R}^{28 \times 28} \mapsto \mathbb{R}^{10}$ .
- The  $i$ -th entry of  $\mathbf{f}(\mathbf{x})$  indicates how likely the image  $\mathbf{x}$  is the digit  $i$ .

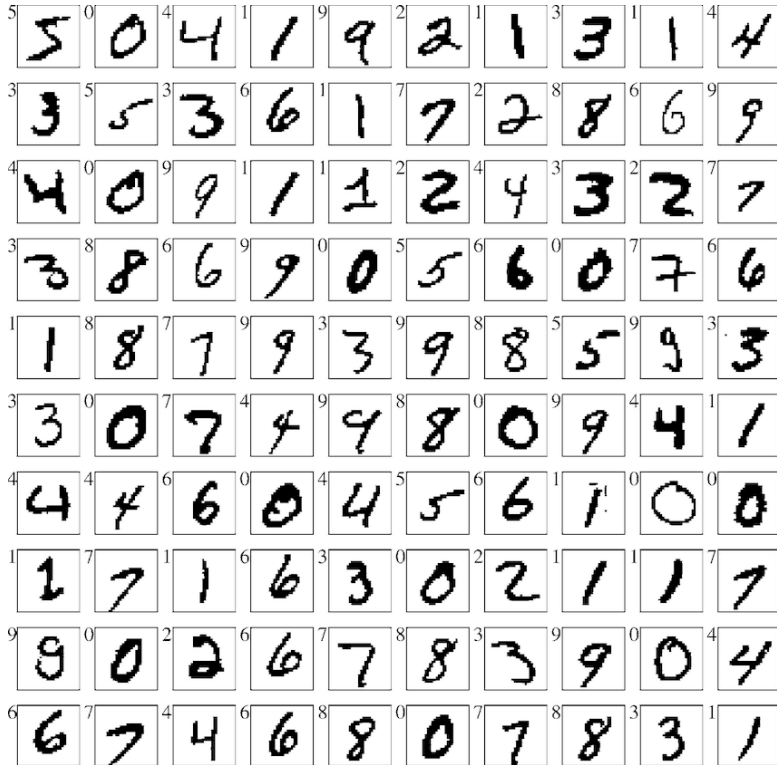
# Train a Softmax Classifier



## Linear model: softmax classifier

- Vectorize each  $28 \times 28$  image to a 784-dim vector.
- Add a feature of all ones. (So  $\mathbf{x}$  becomes 785-dim.)

# Train a Softmax Classifier



## Linear model: softmax classifier

- Vectorize each 28×28 image to a 784-dim vector.
- Add a feature of all ones. (So  $\mathbf{x}$  becomes 785-dim.)
- Let  $\mathbf{W} \in \mathbb{R}^{10 \times 785}$  contain the parameters.
- Let  $\mathbf{z} = \mathbf{W}\mathbf{x} \in \mathbb{R}^{10}$ .
- Output a 10-dim vector:

$$\mathbf{f}(\mathbf{x}) = \text{SoftMax}(\mathbf{z}).$$

# Train a Softmax Classifier



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$$\mathbf{f}(\mathbf{x}) = \text{SoftMax}(\mathbf{z}).$$

$$\text{SoftMax}(\mathbf{z}) = \frac{1}{\sum_{i=0}^9 \exp(\mathbf{z}_i)} [\exp(\mathbf{z}_0), \dots, \exp(\mathbf{z}_9)]$$

# Train a Softmax Classifier



Learn  $\mathbf{W} \in \mathbb{R}^{10 \times 785}$  from the training data

- One-hot encode of the labels
  - Originally, a label is a scalar in  $\{0, 1, 2, \dots, 9\}$ .
  - The one-hot encode  $\mathbf{y}$  is a 10-dim vector  $\{0, 1\}^{10}$ .
  - E.g., the one-hot encode of 2 is  $[0, 0, 1, 0, 0, 0, 0, 0, 0, 0]$ .



# Train a Softmax Classifier



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- One-hot encode of the labels
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  - E.g., the one-hot encode of 2 is  $[0, 0, 1, 0, 0, 0, 0, 0, 0, 0]$ .
- Cross-entropy loss:

$$\text{CrossEntropy}(\mathbf{y}, \mathbf{f}) = -\sum_{i=0}^9 y_i \cdot \log(f_i).$$

# Train a Softmax Classifier



Learn  $\mathbf{W} \in \mathbb{R}^{10 \times 785}$  from the training data

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- Cross-entropy loss:

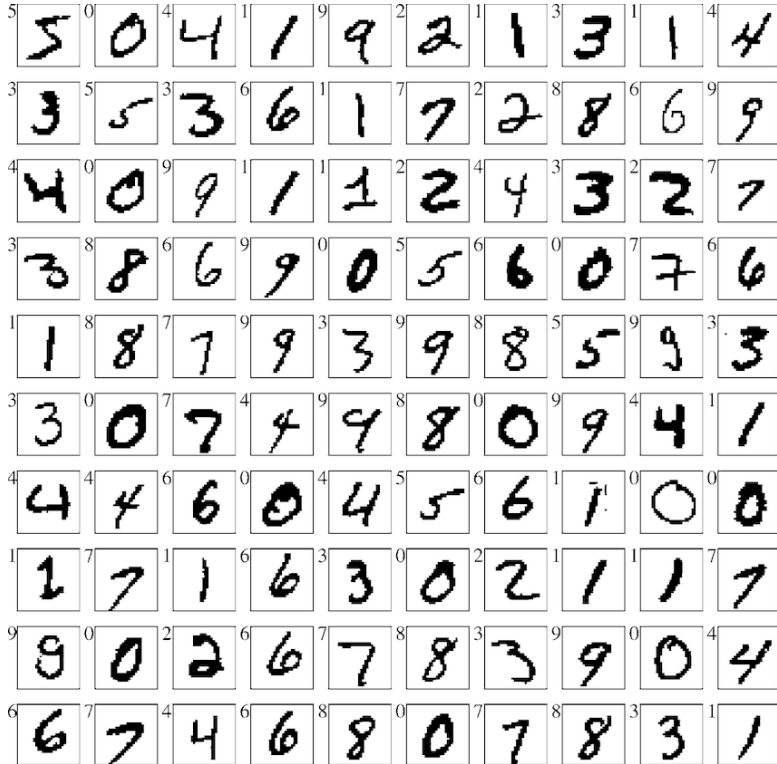
$$\text{CrossEntropy}(\mathbf{y}, \mathbf{f}) = -\sum_{i=0}^9 y_i \cdot \log(f_i).$$

- Solve the optimization model:

$$\mathbf{W}^* = \underset{\mathbf{W}}{\operatorname{argmin}} \left\{ \frac{1}{n} \sum_{j=1}^n \text{CrossEntropy}(\mathbf{y}_j, \mathbf{f}(\mathbf{x}_j)) \right\}.$$

$\mathbf{W}$  is the parameter of  $\mathbf{f}$

# Train a Softmax Classifier



## Make prediction for a test sample $\mathbf{x}'$

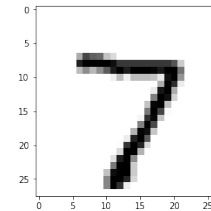
- Now we have  $\mathbf{W}^* \in \mathbb{R}^{10 \times 785}$ .
- For a test sample  $\mathbf{x}'$ , compute  $\mathbf{z} = \mathbf{W}^* \mathbf{x}' \in \mathbb{R}^{10}$ .
- Make prediction by  $\text{argmax } \mathbf{z}$ .
  - If the 7-th entry of  $\mathbf{z}$  is the largest, then the model thinks the image is digit "7".

# Train a Softmax Classifier

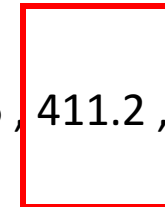


## Make prediction for a test sample $\mathbf{x}'$

- Now we have  $\mathbf{W}^* \in \mathbb{R}^{10 \times 785}$ .
- For a test sample  $\mathbf{x}'$ , compute  $\mathbf{z} = \mathbf{W}^* \mathbf{x}' \in \mathbb{R}^{10}$ .
- Make prediction by  $\text{argmax } \mathbf{z}$ .
  - If the 7-th entry of  $\mathbf{z}$  is the largest, then the model thinks the image is digit “7”.



$\mathbf{z} = [-55.7, -141.4, 18.1, 188.3, -91.3, -26.8, -183.6, 411.2, -142.1, 96.2]$



# Train a Softmax Classifier



## Results

- The training set has 60,000 samples.
- The test set has 10,000 samples.
- The accuracy on the training set is 84.64%.
- The accuracy on the test set is 83.58%.
- Not too bad!
- The accuracy of a random guess is merely 10%.

# Train a Softmax Classifier: Re-cap

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- **Input:** vector  $\mathbf{x} \in \mathbb{R}^{785}$ .
- $\mathbf{z} = \mathbf{W} \mathbf{x} \in \mathbb{R}^{10}$ .
- **Output:**  $\mathbf{f}(\mathbf{x}) = \text{SoftMax}(\mathbf{z})$ .

Trainable parameters:  $\mathbf{W} \in \mathbb{R}^{10 \times 785}$

# Train a Softmax Classifier: Re-cap

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

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- **Output:**  $\mathbf{f}(\mathbf{x}) = \text{SoftMax}(\mathbf{z})$ .

Trainable parameters:  $\mathbf{W} \in \mathbb{R}^{10 \times 785}$

Train the function by empirical risk minimization (ERM):

- **Training set:**  $(\mathbf{x}_1, \mathbf{y}_1), \dots, (\mathbf{x}_n, \mathbf{y}_n) \in \mathbb{R}^{785} \times \mathbb{R}^{10}$ .
- **Loss function:**  $\text{CrossEntropy}(\mathbf{y}, \mathbf{f}) = -\sum_{i=1}^{10} y_i \cdot \log(\mathbf{f}(\mathbf{x})_i)$ .
- **Solve ERM:** 
$$\underset{\mathbf{W}}{\operatorname{argmin}} \left\{ \frac{1}{n} \sum_{j=1}^n \text{CrossEntropy}(\mathbf{y}_j, \mathbf{f}(\mathbf{x}_j)) \right\}.$$

# Train a Softmax Classifier: Re-cap

- **How to solve**  $\underset{\mathbf{W}}{\operatorname{argmin}} \left\{ \frac{1}{n} \sum_{j=1}^n \text{CrossEntropy}(\mathbf{y}_j, \mathbf{f}(\mathbf{x}_j)) \right\} ?$
- **Stochastic gradient descent (SGD) with momentum** repeats:
  1. Randomly pick  $j$  from  $\{1, 2, \dots, n\}$ .
  2. Evaluate the gradient  $\mathbf{G}_j = \frac{\partial \text{CrossEntropy}(\mathbf{y}_j, \mathbf{f}(\mathbf{x}_j))}{\partial \mathbf{W}} \Big|_{\mathbf{W}=\mathbf{W}_{\text{old}}}$ .
  3. Update the momentum:  $\mathbf{V}_{\text{new}} = \beta \mathbf{V}_{\text{old}} + \mathbf{G}_j$ .
  4. Update  $\mathbf{W}$  by  $\mathbf{W}_{\text{new}} \leftarrow \mathbf{W}_{\text{old}} - \alpha \mathbf{V}_{\text{new}}$ .



# **Fully-Connected Neural Network (Multi-layer Perceptron)**

# Softmax Classifier

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- **Input:** vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{10}$ .
- **Output:**  $\mathbf{f}(\mathbf{x}^{(0)}) = \text{SoftMax}(\mathbf{z}^{(1)})$ .

Trainable parameter:

- $\mathbf{W}^{(0)} \in \mathbb{R}^{10 \times 785}$ .

# From Linear Model to Neural Network

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- **Input:** vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .

Trainable parameters:

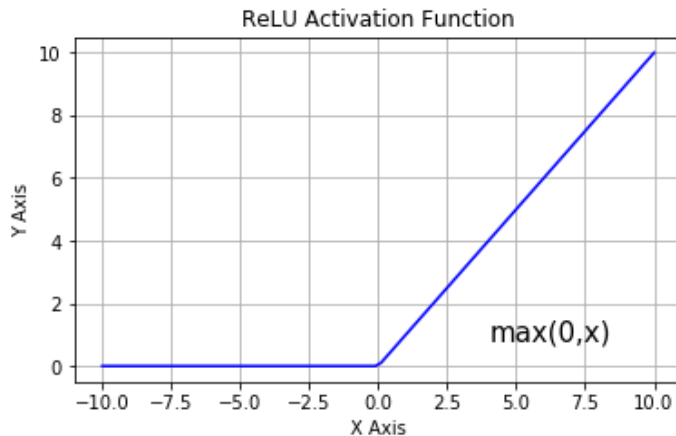
- $\mathbf{W}^{(0)} \in \mathbb{R}^{d_1 \times 785}$ ,

# From Linear Model to Neural Network

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{0, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .

ReLU (activation function)



Trainable parameters:

- $\mathbf{W}^{(0)} \in \mathbb{R}^{d_1 \times 785}$ ,

# From Linear Model to Neural Network

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- **Input:** vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .

- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .

- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .

Hidden Layer 1

Trainable parameters:

- $\mathbf{W}^{(0)} \in \mathbb{R}^{d_1 \times 785}$ ,

# From Linear Model to Neural Network

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- **Input:** vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .

- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .

- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .

Hidden Layer 1

- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .

Trainable parameters:

- $\mathbf{W}^{(0)} \in \mathbb{R}^{d_1 \times 785}$ ,
- $\mathbf{W}^{(1)} \in \mathbb{R}^{d_2 \times d_1}$ ,

It should be  $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} + \mathbf{b}^{(1)}$  in practice.  
I leave out  $\mathbf{b} \in \mathbb{R}^{d_2}$  in the slides for simplicity.

# From Linear Model to Neural Network

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- **Input:** vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .

- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
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Hidden Layer 1

- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .

Hidden Layer 2

Trainable parameters:

- $\mathbf{W}^{(0)} \in \mathbb{R}^{d_1 \times 785}$ ,
- $\mathbf{W}^{(1)} \in \mathbb{R}^{d_2 \times d_1}$ ,

# From Linear Model to Neural Network

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

• **Input:** vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .

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Hidden Layer 1

- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .

Hidden Layer 2

- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .

Output Layer

Trainable parameters:

- $\mathbf{W}^{(0)} \in \mathbb{R}^{d_1 \times 785}$ ,
- $\mathbf{W}^{(1)} \in \mathbb{R}^{d_2 \times d_1}$ ,
- $\mathbf{W}^{(2)} \in \mathbb{R}^{10 \times d_2}$ .



# From Linear Model to Neural Network

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- **Input:** vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .

- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
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- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
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Hidden Layer 2

- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .

Output Layer

- **Output:**  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

Trainable parameters:

- $\mathbf{W}^{(0)} \in \mathbb{R}^{d_1 \times 785}$ ,
- $\mathbf{W}^{(1)} \in \mathbb{R}^{d_2 \times d_1}$ ,
- $\mathbf{W}^{(2)} \in \mathbb{R}^{10 \times d_2}$ .

# Fully-Connected Layer

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .

- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .

- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .

- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .

- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .

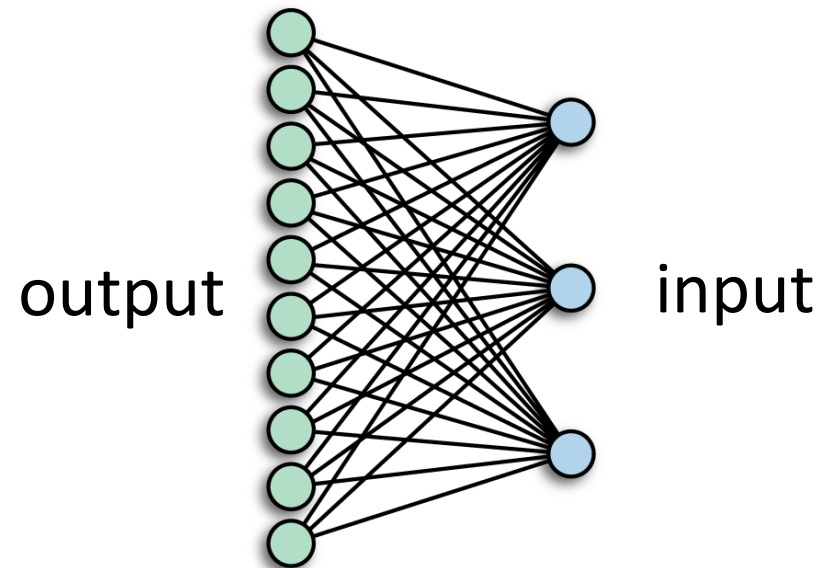
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .

- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .

- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

“Fully-Connected” or “Dense” Layer

Each entry of  $\mathbf{z}^{(1)}$  depends on (i.e., connected to) all the entries of  $\mathbf{x}^{(0)}$ .



# Activation Functions

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ . ReLU
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ . ReLU
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ . SoftMax
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

# Activation Functions

Define a function  $f: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
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- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $f(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

SoftMax

- Use **SoftMax** because this is a **multi-class classification** problem.

# Activation Functions

Define a function  $f: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .

- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .

SoftMax

- Output:  $f(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

- Use **Sigmoid or tanh function** for **binary classification problem**.

- For regression:
  - **No activation function**, if the labels are in  $\mathbb{R}$ .
  - Use **ReLU** if the labels are positive.

- Use **SoftMax** because this is a **multi-class classification problem**.

# Activation Functions

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
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- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

**Question:** Why bothering using ReLU?

- Without the two activation functions,  $\mathbf{z}^{(3)}$  would be a linear function of  $\mathbf{x}^{(0)}$ .
- A linear function can be represented by  $\mathbf{z}^{(3)} = \mathbf{W}\mathbf{x}^{(0)}$ .
- The neural network would be equally expressive as a linear model!!!

# Gradient and Backpropagation

# Train the Neural Network

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- **Input:** vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- **Output:**  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .



# Train the Neural Network

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- **Input:** vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- **Output:**  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

Build an optimization model:

$$\underset{\mathbf{W}^{(0)}, \mathbf{W}^{(1)}, \mathbf{W}^{(2)}}{\operatorname{argmin}} \left\{ \frac{1}{n} \sum_{j=1}^n \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j) \right\}$$

E.g., the cross-entropy loss

# Train the Neural Network

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- **Input:** vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- **Output:**  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to solve

$$\underset{\mathbf{W}^{(0)}, \mathbf{W}^{(1)}, \mathbf{W}^{(2)}}{\operatorname{argmin}} \left\{ \frac{1}{n} \sum_{j=1}^n \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j) \right\} ?$$

**Stochastic gradient descent (SGD)**

# Train the Neural Network

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to solve

$$\underset{\mathbf{W}^{(0)}, \mathbf{W}^{(1)}, \mathbf{W}^{(2)}}{\operatorname{argmin}} \left\{ \frac{1}{n} \sum_{j=1}^n \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j) \right\} ?$$

**Stochastic gradient descent (SGD):**

- Randomly pick  $j$  from  $\{1, 2, \dots, n\}$ .
- Compute the stochastic gradient w.r.t.  $\mathbf{W}^{(0)}$  at the current iteration  $\mathbf{W}_{\text{old}}^{(0)}$ :

$$\mathbf{g}_j^{(0)} = \left. \frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(0)}} \right|_{\mathbf{W}^{(0)} = \mathbf{W}_{\text{old}}^{(0)}}$$

- Update  $\mathbf{W}^{(0)}$ :  $\mathbf{W}_{\text{new}}^{(0)} = \mathbf{W}_{\text{old}}^{(0)} - \alpha \mathbf{g}_j^{(0)}$ .
- Do the same for  $\mathbf{W}^{(1)}$  and  $\mathbf{W}^{(2)}$ .

# Backpropagation

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to compute  $\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(k)}}$  ?

# Backpropagation

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to compute  $\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(k)}}$  ?

## Backpropagation:

- Denote  $L = \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)$ .

# Backpropagation

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
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- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- **Output:**  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to compute  $\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(k)}}$  ?

## Backpropagation:

- Denote  $L = \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)$ .
- Compute  $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .

10-dim vector

# Backpropagation

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to compute  $\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(k)}}$  ?

## Backpropagation:

- Denote  $L = \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)$ .
- Compute  $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .

$\mathbf{z}^{(3)}$  is a function of  $\mathbf{z}^{(2)}$  and  $\mathbf{W}^{(2)}$ .

Apply the chain rule.

# Backpropagation

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to compute  $\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(k)}}$  ?

## Backpropagation:

- Denote  $L = \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)$ .

- Compute  $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .

$$\frac{\partial L}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{z}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}} \quad \frac{\partial L}{\partial \mathbf{W}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{W}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}$$

$\mathbf{z}^{(3)}$  is a function of  $\mathbf{z}^{(2)}$  and  $\mathbf{W}^{(2)}$ .

Apply the chain rule.



# Backpropagation

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
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- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to compute  $\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(k)}}$  ?

## Backpropagation:

- Denote  $L = \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)$ .
- Compute  $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .
- $\frac{\partial L}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{z}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}, \quad \frac{\partial L}{\partial \mathbf{W}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{W}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .

Then free  $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$  from memory.

# Backpropagation

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to compute  $\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(k)}}$  ?

## Backpropagation:

- Denote  $L = \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)$ .
- Compute  $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .
- $\frac{\partial L}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{z}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}$ ,  $\frac{\partial L}{\partial \mathbf{W}^{(2)}}$   $= \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{W}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .

Use it to update  $\mathbf{W}^{(2)}$  (e.g., by SGD).

# Backpropagation

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
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- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to compute  $\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(k)}}$  ?

## Backpropagation:

- Denote  $L = \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)$ .
- Compute  $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .
- $\frac{\partial L}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{z}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}$ ,  $\frac{\partial L}{\partial \mathbf{W}^{(2)}}$   $= \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{W}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .

Then free  $\frac{\partial L}{\partial \mathbf{W}^{(2)}}$  from memory.

# Backpropagation

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to compute  $\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(k)}}$  ?

## Backpropagation:

- Denote  $L = \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)$ .

- Compute  $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .

$$\bullet \quad \frac{\partial L}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{z}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}, \quad \frac{\partial L}{\partial \mathbf{W}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{W}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}.$$

$$\bullet \quad \frac{\partial L}{\partial \mathbf{z}^{(1)}} = \frac{\partial \mathbf{z}^{(2)}}{\partial \mathbf{z}^{(1)}} \frac{\partial L}{\partial \mathbf{z}^{(2)}}, \quad \frac{\partial L}{\partial \mathbf{W}^{(1)}} = \frac{\partial \mathbf{z}^{(2)}}{\partial \mathbf{W}^{(1)}} \frac{\partial L}{\partial \mathbf{z}^{(2)}}.$$

Apply the chain rule again.

# Backpropagation

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
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- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to compute  $\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(k)}}$  ?

## Backpropagation:

- Denote  $L = \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)$ .
- Compute  $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .
- $\frac{\partial L}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{z}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}, \quad \frac{\partial L}{\partial \mathbf{W}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{W}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .
- $\frac{\partial L}{\partial \mathbf{z}^{(1)}} = \frac{\partial \mathbf{z}^{(2)}}{\partial \mathbf{z}^{(1)}} \frac{\partial L}{\partial \mathbf{z}^{(2)}}, \quad \frac{\partial L}{\partial \mathbf{W}^{(1)}} = \frac{\partial \mathbf{z}^{(2)}}{\partial \mathbf{W}^{(1)}} \frac{\partial L}{\partial \mathbf{z}^{(2)}}$ .

Free  $\frac{\partial L}{\partial \mathbf{z}^{(2)}}$  from memory.

# Backpropagation

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to compute  $\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(k)}}$  ?

## Backpropagation:

- Denote  $L = \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)$ .
- Compute  $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .
- $\frac{\partial L}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{z}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}, \quad \frac{\partial L}{\partial \mathbf{W}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{W}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .
- $\frac{\partial L}{\partial \mathbf{z}^{(1)}} = \frac{\partial \mathbf{z}^{(2)}}{\partial \mathbf{z}^{(1)}} \frac{\partial L}{\partial \mathbf{z}^{(2)}}, \quad \boxed{\frac{\partial L}{\partial \mathbf{W}^{(1)}}} = \frac{\partial \mathbf{z}^{(2)}}{\partial \mathbf{W}^{(1)}} \frac{\partial L}{\partial \mathbf{z}^{(2)}}$ .

Use it to update  $\mathbf{W}^{(1)}$  (e.g., by SGD).

# Backpropagation

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to compute  $\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(k)}}$  ?

## Backpropagation:

- Denote  $L = \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)$ .
- Compute  $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .
- $\frac{\partial L}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{z}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}, \quad \frac{\partial L}{\partial \mathbf{W}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{W}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .
- $\frac{\partial L}{\partial \mathbf{z}^{(1)}} = \frac{\partial \mathbf{z}^{(2)}}{\partial \mathbf{z}^{(1)}} \frac{\partial L}{\partial \mathbf{z}^{(2)}}, \quad \boxed{\frac{\partial L}{\partial \mathbf{W}^{(1)}}} = \frac{\partial \mathbf{z}^{(2)}}{\partial \mathbf{W}^{(1)}} \frac{\partial L}{\partial \mathbf{z}^{(2)}}$ .

Free  $\frac{\partial L}{\partial \mathbf{W}^{(1)}}$  from memory.

# Backpropagation

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to compute  $\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(k)}}$  ?

## Backpropagation:

- Denote  $L = \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)$ .

- Compute  $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .

$$\frac{\partial L}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{z}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}, \quad \frac{\partial L}{\partial \mathbf{W}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{W}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}.$$

$$\frac{\partial L}{\partial \mathbf{z}^{(1)}} = \frac{\partial \mathbf{z}^{(2)}}{\partial \mathbf{z}^{(1)}} \frac{\partial L}{\partial \mathbf{z}^{(2)}}, \quad \frac{\partial L}{\partial \mathbf{W}^{(1)}} = \frac{\partial \mathbf{z}^{(2)}}{\partial \mathbf{W}^{(1)}} \frac{\partial L}{\partial \mathbf{z}^{(2)}}.$$

$$\frac{\partial L}{\partial \mathbf{W}^{(0)}} = \frac{\partial \mathbf{z}^{(1)}}{\partial \mathbf{W}^{(0)}} \frac{\partial L}{\partial \mathbf{z}^{(1)}}.$$

Apply the chain rule again.



# Backpropagation

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to compute  $\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(k)}}$  ?

## Backpropagation:

- Denote  $L = \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)$ .
- Compute  $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .
- $\frac{\partial L}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{z}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}$ ,  $\frac{\partial L}{\partial \mathbf{W}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{W}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .
- $\frac{\partial L}{\partial \mathbf{z}^{(1)}} = \frac{\partial \mathbf{z}^{(2)}}{\partial \mathbf{z}^{(1)}} \frac{\partial L}{\partial \mathbf{z}^{(2)}}$ .
- $\frac{\partial L}{\partial \mathbf{W}^{(0)}} = \frac{\partial \mathbf{z}^{(1)}}{\partial \mathbf{W}^{(0)}} \frac{\partial L}{\partial \mathbf{z}^{(1)}}$ .

Free  $\frac{\partial L}{\partial \mathbf{z}^{(1)}}$  from memory.

# Backpropagation

Define a function  $\mathbf{f}: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$ :

- Input: vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ .
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ .
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ .
- $\mathbf{x}^{(3)} = \text{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$ .
- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \mathbf{x}^{(3)}$ .

How to compute  $\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(k)}}$  ?

## Backpropagation:

- Denote  $L = \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)$ .
- Compute  $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .
- $\frac{\partial L}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{z}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}, \quad \frac{\partial L}{\partial \mathbf{W}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{W}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}$ .
- $\frac{\partial L}{\partial \mathbf{z}^{(1)}} = \frac{\partial \mathbf{z}^{(2)}}{\partial \mathbf{z}^{(1)}} \frac{\partial L}{\partial \mathbf{z}^{(2)}}, \quad \frac{\partial L}{\partial \mathbf{W}^{(1)}} = \frac{\partial \mathbf{z}^{(2)}}{\partial \mathbf{W}^{(1)}} \frac{\partial L}{\partial \mathbf{z}^{(2)}}$ .
- $\frac{\partial L}{\partial \mathbf{W}^{(0)}} = \frac{\partial \mathbf{z}^{(1)}}{\partial \mathbf{W}^{(0)}} \frac{\partial L}{\partial \mathbf{z}^{(1)}}$ . Use it to update  $\mathbf{W}^{(0)}$ .

# Backpropagation: Example

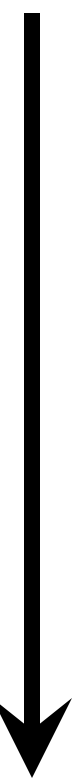
# 1D Example

**Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$**

- **Input:** scalar  $x^{(0)}$ .
- $z^{(1)} = w^{(0)} x^{(0)}$ .
- $x^{(1)} = \max\{0, z^{(1)}\}$ .
- $z^{(2)} = w^{(1)} x^{(1)}$ .
- $x^{(2)} = \max\{0, z^{(2)}\}$ .
- $z^{(3)} = w^{(2)} x^{(2)}$ .
- **Output:**  $f(x^{(0)}) = z^{(3)}$ .

# 1D Example

**Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$**

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- **Input:** scalar  $x^{(0)}$ .
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  - $x^{(2)} = \max\{0, z^{(2)}\}$ .
  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - **Output:**  $f(x^{(0)}) = z^{(3)}$ .

**Random sampling:**


- Randomly sample  $j$  from  $\{1, 2, \dots, n\}$ .

**Forward pass:**

- Take  $x_j$  as input ( $x^{(0)} = x_j$ ).
- Compute each layer  $z^{(1)}, x^{(1)}, z^{(2)}, x^{(2)}, z^{(3)}$ .

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$


- 
- **Input:** scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
  - $x^{(1)} = \max\{0, z^{(1)}\}$ .
  - $z^{(2)} = w^{(1)} x^{(1)}$ .
  - $x^{(2)} = \max\{0, z^{(2)}\}$ .
  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - **Output:**  $f(x^{(0)}) = z^{(3)}$ .

**Backpropagation:**

- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$


- 
- **Input:** scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
  - $x^{(1)} = \max\{0, z^{(1)}\}$ .
  - $z^{(2)} = w^{(1)} x^{(1)}$ .
  - $x^{(2)} = \max\{0, z^{(2)}\}$ .
  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - **Output:**  $f(x^{(0)}) = z^{(3)}$ .

**Backpropagation:**

- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2 = \frac{1}{2} (z^{(3)} - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- **Input:** scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
  - $x^{(1)} = \max\{0, z^{(1)}\}$ .
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  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - **Output:**  $f(x^{(0)}) = z^{(3)}$ .

**Backpropagation:**


- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = \boxed{z^{(3)}} - y_j$ .

The value of  $z^{(3)}$  is known  
(after the forward pass).



# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- **Input:** scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
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  - $x^{(2)} = \max\{0, z^{(2)}\}$ .
  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - **Output:**  $f(x^{(0)}) = z^{(3)}$ .

**Backpropagation:**


- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .

The value of  $z^{(3)}$  is known  
(after the forward pass).

Thus the value of  $\frac{\partial L}{\partial z^{(3)}}$  is known.

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- Input: scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
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  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - Output:  $f(x^{(0)}) = z^{(3)}$ .


**Backpropagation:**

- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .
- $\frac{\partial L}{\partial z^{(2)}} = \boxed{\frac{\partial z^{(3)}}{\partial z^{(2)}}} \frac{\partial L}{\partial z^{(3)}}$

$$\frac{\partial z^{(3)}}{\partial x^{(2)}} = w^{(2)}, \quad \frac{\partial x^{(2)}}{\partial z^{(2)}} = \begin{cases} 1, & \text{if } z^{(2)} > 0; \\ 0, & \text{else.} \end{cases}$$

# 1D Example


Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- Input: scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
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  - $z^{(2)} = w^{(1)} x^{(1)}$ .
  - $x^{(2)} = \max\{0, z^{(2)}\}$ .
  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - Output:  $f(x^{(0)}) = z^{(3)}$ .

**Backpropagation:**


- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .
- $\frac{\partial L}{\partial z^{(2)}} = \boxed{\frac{\partial z^{(3)}}{\partial z^{(2)}}} \frac{\partial L}{\partial z^{(3)}}$

$$\frac{\partial z^{(3)}}{\partial x^{(2)}} = w^{(2)}, \quad \frac{\partial x^{(2)}}{\partial z^{(2)}} = \begin{cases} 1, & \text{if } z^{(2)} > 0; \\ 0, & \text{else.} \end{cases}$$


$$\boxed{\frac{\partial z^{(3)}}{\partial z^{(2)}}} = \frac{\partial z^{(3)}}{\partial x^{(2)}} \frac{\partial x^{(2)}}{\partial z^{(2)}} = \begin{cases} w^{(2)}, & \text{if } z^{(2)} > 0; \\ 0, & \text{else.} \end{cases}$$

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- Input: scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
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  - $z^{(2)} = w^{(1)} x^{(1)}$ .
  - $x^{(2)} = \max\{0, z^{(2)}\}$ .
  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - Output:  $f(x^{(0)}) = z^{(3)}$ .


**Backpropagation:**

- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .
- $\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ ,  $\frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ .

$$\frac{\partial z^{(3)}}{\partial w^{(2)}} = x^{(2)}.$$

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- Input: scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
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  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - Output:  $f(x^{(0)}) = z^{(3)}$ .


**Backpropagation:**

- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .
- $\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ ,  $\frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ .

Free  $\frac{\partial L}{\partial z^{(3)}}$  from memory.

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- Input: scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
  - $x^{(1)} = \max\{0, z^{(1)}\}$ .
  - $z^{(2)} = w^{(1)} x^{(1)}$ .
  - $x^{(2)} = \max\{0, z^{(2)}\}$ .
  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - Output:  $f(x^{(0)}) = z^{(3)}$ .


Backpropagation:

- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .
- $\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ ,  $\boxed{\frac{\partial L}{\partial w^{(2)}}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ .

Update  $w^{(2)}$ :  $w^{(2)} \leftarrow w^{(2)} - \alpha \frac{\partial L}{\partial w^{(2)}}$ .

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- Input: scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
  - $x^{(1)} = \max\{0, z^{(1)}\}$ .
  - $z^{(2)} = w^{(1)} x^{(1)}$ .
  - $x^{(2)} = \max\{0, z^{(2)}\}$ .
  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - Output:  $f(x^{(0)}) = z^{(3)}$ .


**Backpropagation:**

- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .
- $\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ ,  $\frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ .

Free  $\frac{\partial z^{(3)}}{\partial w^{(2)}}$  from memory.

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- Input: scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
  - $x^{(1)} = \max\{0, z^{(1)}\}$ .
  - $z^{(2)} = w^{(1)} x^{(1)}$ .
  - $x^{(2)} = \max\{0, z^{(2)}\}$ .
  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - Output:  $f(x^{(0)}) = z^{(3)}$ .

**Backpropagation:**


- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .
- $\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ ,  $\frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ .
- $\frac{\partial L}{\partial z^{(1)}} = \frac{\partial z^{(2)}}{\partial z^{(1)}} \frac{\partial L}{\partial z^{(2)}}$

$$\frac{\partial z^{(2)}}{\partial z^{(1)}} = \frac{\partial z^{(2)}}{\partial x^{(1)}} \frac{\partial x^{(1)}}{\partial z^{(1)}} = \begin{cases} w^{(1)}, & \text{if } z^{(1)} > 0; \\ 0, & \text{else.} \end{cases}$$



# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- Input: scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
  - $x^{(1)} = \max\{0, z^{(1)}\}$ .
  - $z^{(2)} = w^{(1)} x^{(1)}$ .
  - $x^{(2)} = \max\{0, z^{(2)}\}$ .
  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - Output:  $f(x^{(0)}) = z^{(3)}$ .


**Backpropagation:**

- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .
- $\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$        $\frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ .
- $\frac{\partial L}{\partial z^{(1)}} = \frac{\partial z^{(2)}}{\partial z^{(1)}} \frac{\partial L}{\partial z^{(2)}}$        $\frac{\partial L}{\partial w^{(1)}} = \frac{\partial z^{(2)}}{\partial w^{(1)}} \frac{\partial L}{\partial z^{(2)}}$ .

$$\frac{\partial z^{(2)}}{\partial w^{(1)}} = x^{(1)}.$$

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- Input: scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
  - $x^{(1)} = \max\{0, z^{(1)}\}$ .
  - $z^{(2)} = w^{(1)} x^{(1)}$ .
  - $x^{(2)} = \max\{0, z^{(2)}\}$ .
  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - Output:  $f(x^{(0)}) = z^{(3)}$ .


**Backpropagation:**

- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .
- $\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ ,  $\frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ .
- $\frac{\partial L}{\partial z^{(1)}} = \frac{\partial z^{(2)}}{\partial z^{(1)}} \frac{\partial L}{\partial z^{(2)}}$ ,  $\frac{\partial L}{\partial w^{(1)}} = \frac{\partial z^{(2)}}{\partial w^{(1)}} \frac{\partial L}{\partial z^{(2)}}$ .

Free  $\frac{\partial L}{\partial z^{(2)}}$  from memory.

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- Input: scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
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  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - Output:  $f(x^{(0)}) = z^{(3)}$ .


Backpropagation:

- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .
- $\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ ,  $\frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ .
- $\frac{\partial L}{\partial z^{(1)}} = \frac{\partial z^{(2)}}{\partial z^{(1)}} \frac{\partial L}{\partial z^{(2)}}$ ,  $\frac{\partial L}{\partial w^{(1)}} = \frac{\partial z^{(2)}}{\partial w^{(1)}} \frac{\partial L}{\partial z^{(2)}}$ .

Update  $w^{(1)}$ :  $w^{(1)} \leftarrow w^{(1)} - \alpha \frac{\partial L}{\partial w^{(1)}}$ .

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- Input: scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
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  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - Output:  $f(x^{(0)}) = z^{(3)}$ .


Backpropagation:

- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .
- $\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ ,  $\frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ .
- $\frac{\partial L}{\partial z^{(1)}} = \frac{\partial z^{(2)}}{\partial z^{(1)}} \frac{\partial L}{\partial z^{(2)}}$ ,  $\frac{\partial L}{\partial w^{(1)}} = \frac{\partial z^{(2)}}{\partial w^{(1)}} \frac{\partial L}{\partial z^{(2)}}$ .

Free  $\frac{\partial L}{\partial w^{(1)}}$  from memory.

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- Input: scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
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  - $z^{(2)} = w^{(1)} x^{(1)}$ .
  - $x^{(2)} = \max\{0, z^{(2)}\}$ .
  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - Output:  $f(x^{(0)}) = z^{(3)}$ .


**Backpropagation:**

- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .
- $\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ ,  $\frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ .
- $\frac{\partial L}{\partial z^{(1)}} = \frac{\partial z^{(2)}}{\partial z^{(1)}} \frac{\partial L}{\partial z^{(2)}}$ ,  $\frac{\partial L}{\partial w^{(1)}} = \frac{\partial z^{(2)}}{\partial w^{(1)}} \frac{\partial L}{\partial z^{(2)}}$ .
- $\frac{\partial L}{\partial w^{(0)}} = \frac{\partial z^{(1)}}{\partial w^{(0)}} \frac{\partial L}{\partial z^{(1)}}$ .

$$\frac{\partial z^{(1)}}{\partial w^{(0)}} = x^{(0)}.$$

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- Input: scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
  - $x^{(1)} = \max\{0, z^{(1)}\}$ .
  - $z^{(2)} = w^{(1)} x^{(1)}$ .
  - $x^{(2)} = \max\{0, z^{(2)}\}$ .
  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - Output:  $f(x^{(0)}) = z^{(3)}$ .


**Backpropagation:**

- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .
- $\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ ,  $\frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ .
- $\frac{\partial L}{\partial z^{(1)}} = \frac{\partial z^{(2)}}{\partial z^{(1)}} \frac{\partial L}{\partial z^{(2)}}$ ,  $\frac{\partial L}{\partial w^{(1)}} = \frac{\partial z^{(2)}}{\partial w^{(1)}} \frac{\partial L}{\partial z^{(2)}}$ .
- $\frac{\partial L}{\partial w^{(0)}} = \frac{\partial z^{(1)}}{\partial w^{(0)}} \frac{\partial L}{\partial z^{(1)}}$ .

Free  $\frac{\partial L}{\partial z^{(1)}}$  from memory.

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

- 
- Input: scalar  $x^{(0)}$ .
  - $z^{(1)} = w^{(0)} x^{(0)}$ .
  - $x^{(1)} = \max\{0, z^{(1)}\}$ .
  - $z^{(2)} = w^{(1)} x^{(1)}$ .
  - $x^{(2)} = \max\{0, z^{(2)}\}$ .
  - $z^{(3)} = w^{(2)} x^{(2)}$ .
  - Output:  $f(x^{(0)}) = z^{(3)}$ .

**Backpropagation:**

- Loss:  $L = \frac{1}{2} (f(x_j) - y_j)^2$ .
- $\frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j$ .
- $\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ ,  $\frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$ .
- $\frac{\partial L}{\partial z^{(1)}} = \frac{\partial z^{(2)}}{\partial z^{(1)}} \frac{\partial L}{\partial z^{(2)}}$ ,  $\frac{\partial L}{\partial w^{(1)}} = \frac{\partial z^{(2)}}{\partial w^{(1)}} \frac{\partial L}{\partial z^{(2)}}$ .
- $\frac{\partial L}{\partial w^{(0)}} = \frac{\partial z^{(1)}}{\partial w^{(0)}} \frac{\partial L}{\partial z^{(1)}}$ .

Update  $w^{(0)}$ :  $w^{(0)} \leftarrow w^{(0)} - \alpha \frac{\partial L}{\partial w^{(0)}}$ .

# 1D Example

Define a function  $f: \mathbb{R} \mapsto \mathbb{R}$

Backpropagation:

## One iteration:

1. Randomly sample  $j$  from  $\{1, 2, \dots, n\}$ .

2. **Forward pass:** take  $x_j$  as input ( $x^{(0)} = x_j$ ), compute each layer  $z^{(1)}, x^{(1)}, z^{(2)}, x^{(2)}, z^{(3)}$ .

3. **Backward pass:**

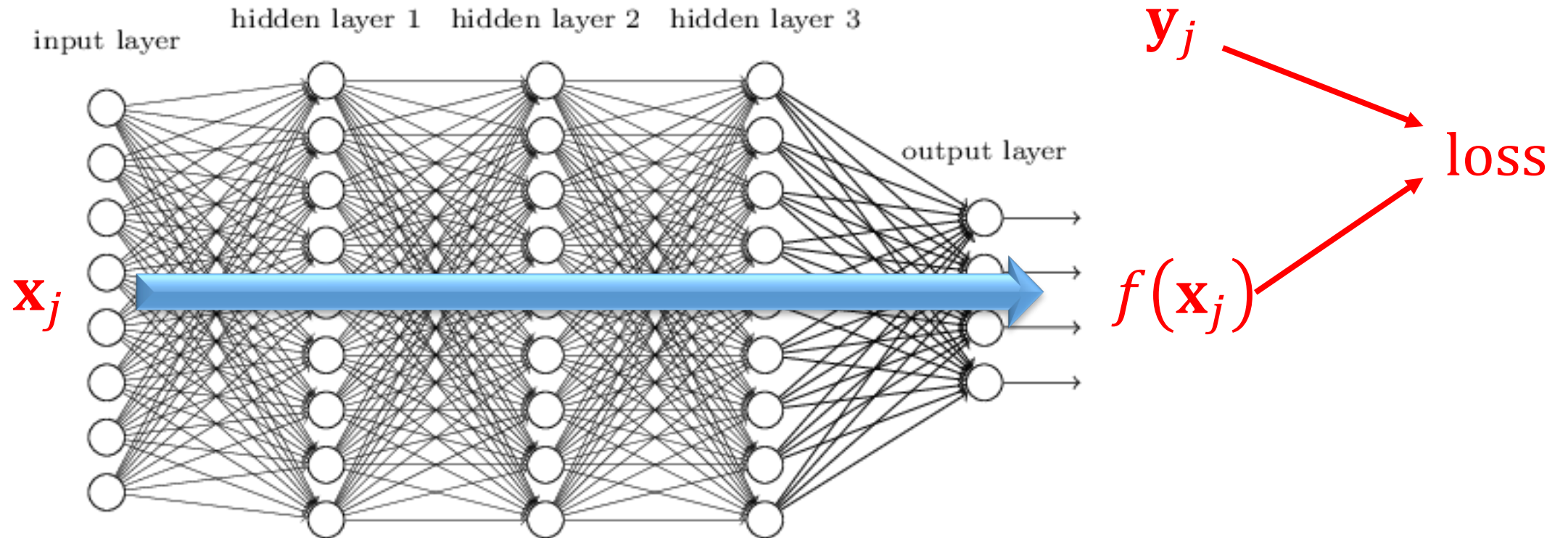
- Compute the derivatives  $\frac{\partial L}{\partial z^{(3)}}, \frac{\partial L}{\partial w^{(2)}}, \frac{\partial L}{\partial z^{(2)}}, \frac{\partial L}{\partial w^{(1)}}, \frac{\partial L}{\partial z^{(1)}}, \frac{\partial L}{\partial w^{(0)}}$ .
- Update  $w^{(k)}$  using  $\frac{\partial L}{\partial w^{(k)}}$ .



# **Summary of Backpropagation**

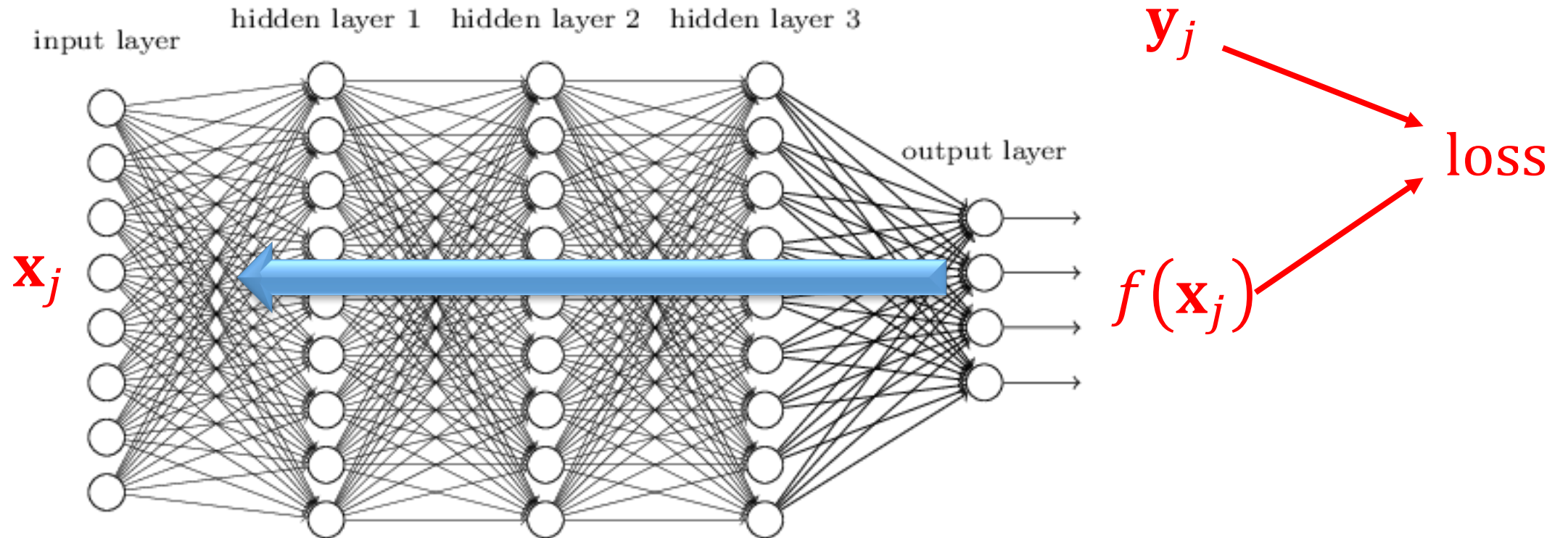
# Backpropagation: Take-Home Message

1. Randomly pick a sample  $(\mathbf{x}_j, \mathbf{y}_j)$ .
2. Run a forward pass (from the input  $\mathbf{x}^{(0)}$  to the loss function).



# Backpropagation: Take-Home Message

1. Randomly pick a sample  $(\mathbf{x}_j, \mathbf{y}_j)$ .
2. Run a forward pass (from the input  $\mathbf{x}^{(0)}$  to the loss function).
3. Run a backward pass (from the **loss** to  $\mathbf{W}^{(0)}$ ).



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Get the derivatives (stochastic gradients):

$$\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(2)}}, \quad \frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(1)}}, \quad \frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(0)}}.$$

# Backpropagation: Take-Home Message

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Update  $\mathbf{W}^{(0)}, \mathbf{W}^{(1)}, \mathbf{W}^{(2)}$  using the derivatives.

# Mini-Batch

1. Randomly pick a sample  ~~$(\mathbf{x}_j, \mathbf{y}_j)$~~ . Several random samples.
2. Run a forward pass (from the input  $\mathbf{x}^{(0)}$  to the loss function).
3. Run a backward pass (from the loss to  $\mathbf{W}^{(0)}$ ).



Get the derivatives (stochastic gradients):

$$\frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(2)}}, \quad \frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(1)}}, \quad \frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(0)}}.$$

$$\frac{1}{|\mathcal{J}|} \sum_{j \in \mathcal{J}} \frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(2)}}, \quad \frac{1}{|\mathcal{J}|} \sum_{j \in \mathcal{J}} \frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(1)}}, \quad \frac{1}{|\mathcal{J}|} \sum_{j \in \mathcal{J}} \frac{\partial \text{Loss}(\mathbf{f}(\mathbf{x}_j), \mathbf{y}_j)}{\partial \mathbf{W}^{(0)}}.$$

Mini-batch should always be used! Set  $|\mathcal{J}|$  to 16, 32, 64, ...

# Mini-Batch

**SGD:**  $\text{BatchSize} = 1$ .

- Per-iteration cost is low.
- Lots of iterations to converge.

**Mini-Batch:**  $\text{BatchSize} > 1$ .

- Better than the other two, if  $\text{BatchSize}$  is properly set.

**Full Gradient:**  $\text{BatchSize} = n$ .

- Per-iteration cost is  $n$  times higher than SGD.
- Convex problem: less number of iterations.
- Neural network: it doesn't work!

# First-Order Optimization

- First-order optimization: update the parameters using gradient.
- Gradient descent algorithm (including SGD, mini-batch SGD, and full gradient descent, conjugate gradient) are typical 1<sup>st</sup>-order algorithms.
- Other 1<sup>st</sup>-order algorithms: SGD with momentum, AdaGrad, RMSprop...
- See the blogs:
  - <http://runder.io/optimizing-gradient-descent/>
  - <https://distill.pub/2017/momentum/>



# Summary of FC Neural Network

# Build a Fully-Connected Neural Network

- Network structure

Number of layers

Width of each layer

Activation functions

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## Example:

- **Input:** vector  $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$ . **Input layer**
- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ . **Hidden Layer 1**
- $\mathbf{x}^{(1)} = \max\{\mathbf{0}, \mathbf{z}^{(1)}\} \in \mathbb{R}^{d_1}$ .
- $\mathbf{z}^{(2)} = \mathbf{W}^{(1)} \mathbf{x}^{(1)} \in \mathbb{R}^{d_2}$ . **Hidden Layer 2**
- $\mathbf{x}^{(2)} = \max\{\mathbf{0}, \mathbf{z}^{(2)}\} \in \mathbb{R}^{d_2}$ .
- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$ . **Output layer**
- **Output:**  $\mathbf{f}(\mathbf{x}^{(0)}) = \text{SoftMax}(\mathbf{z}^{(2)})$ .

- Three layers (2 hidden and 1 output).
  - Input layer doesn't count (no parameter).

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  - Layer 1:  $d_1$ ,
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- $\mathbf{z}^{(1)} = \mathbf{W}^{(0)} \mathbf{x}^{(0)} \in \mathbb{R}^{d_1}$ .
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- Three layers (2 hidden and 1 output).
  - Input layer doesn't count (no parameter).
- Width of each layer:
  - Layer 1:  $d_1$ ,
  - Layer 2:  $d_2$ ,
  - Output layer: 10.
- Activation functions:
  - Layer 1: ReLU,
  - Layer 2: ReLU,
  - Output layer: Softmax.

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## Example:

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- Output:  $\mathbf{f}(\mathbf{x}^{(0)}) = \text{SoftMax}(\mathbf{z}^{(2)})$ .

- Trainable parameters:
  - $\mathbf{W}^{(0)} \in \mathbb{R}^{d_1 \times 785}$ ,
  - $\mathbf{W}^{(1)} \in \mathbb{R}^{d_2 \times d_1}$ ,
  - $\mathbf{W}^{(2)} \in \mathbb{R}^{10 \times d_2}$ .
- Number of parameters:
  - $785d_1 + d_1d_2 + 10d_2$ .

# Build a Fully-Connected Neural Network

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- Loss functions

Cross-entropy for multi-class classification

Sigmoid/tanh for binary classification

L1 or squared L2 for regression (the labels are continuous)

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- Compute gradient: by a forward pass and a backward pass

Automatically performed by many deep learning systems

Batch size



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- Compute gradient: by a forward pass and a backward pass

Automatically performed by many deep learning systems

Batch size

- Choose an optimization algorithm (and tune its parameters)

SGD

SGD with momentum

AdaGrad

RMSprop