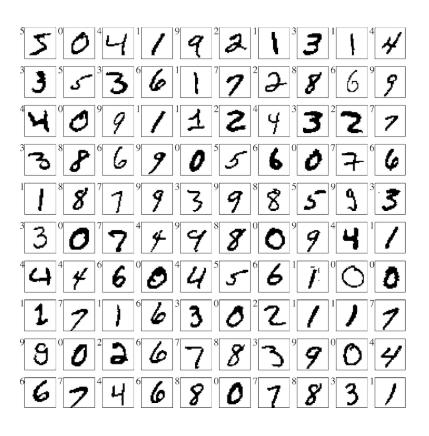
Neural Networks: Basics

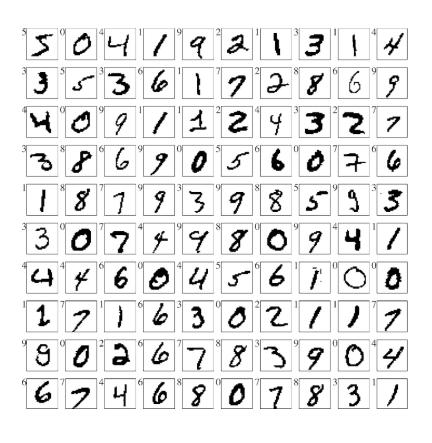
Shusen Wang

Revisit Softmax Classifier



The MNIST Dataset

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

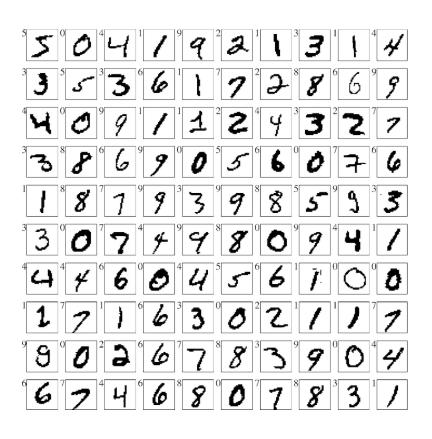


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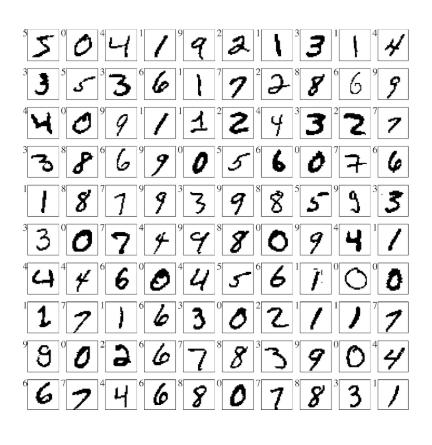
Task: multi-class classification

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



Linear model: softmax classifier

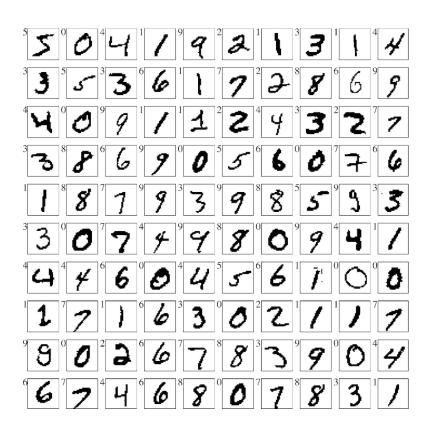
- Vectorize each 28×28 image to a 784-dim vector.
- Add a feature of all ones. (So x becomes 785-dim.)



Linear model: softmax classifier

- Vectorize each 28×28 image to a 784-dim vector.
- Add a feature of all ones. (So 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:

$$f(x) = SoftMax(z).$$

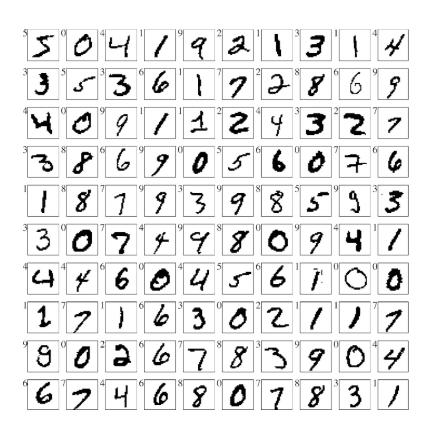


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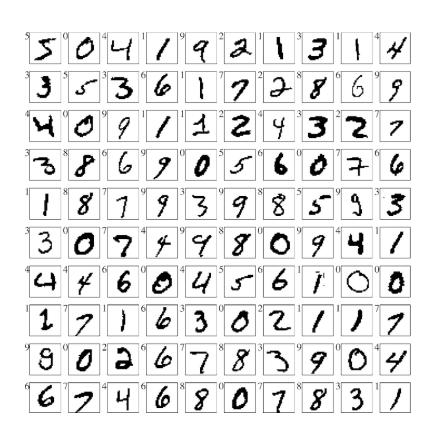
$$\mathbf{f}(\mathbf{x}) = \text{SoftMax}(\mathbf{z}).$$

$$\text{SoftMax}(\mathbf{z}) = \frac{1}{\sum_{i=0}^{9} \exp(z_i)} [\exp(z_0), \dots, \exp(z_9)]$$



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

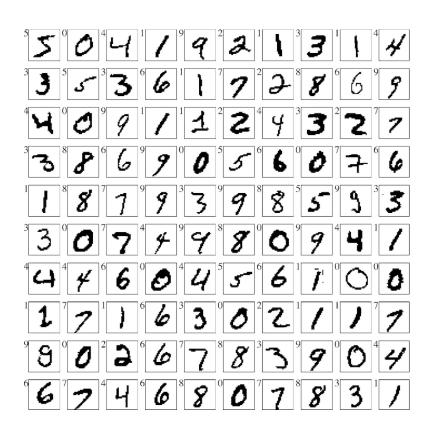
- One-hot encode of the labels
 - Originally, a label is a scalar in $\{0, 1, 2, \dots, 9\}$.
 - The one-hot encode y is a 10-dim vector $\{0,1\}^{10}$.
 - E.g., the one-hot encode of 2 is [0, 0, 1, 0, 0, 0, 0, 0, 0, 0].



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- Cross-entropy loss:

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



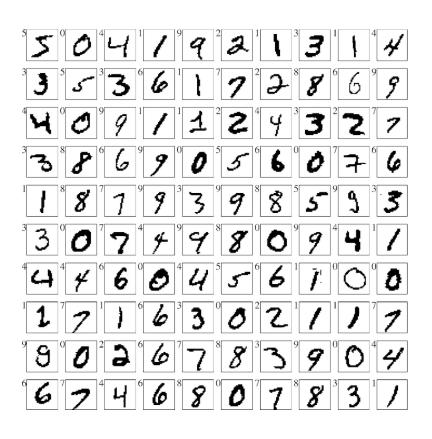
Learn $\mathbf{W} \in \mathbb{R}^{10 \times 785}$ from the training data

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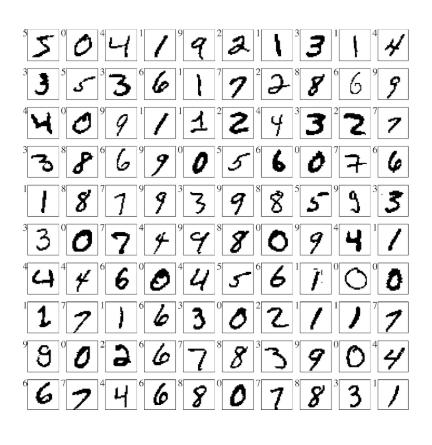
• Solve the optimization model:

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



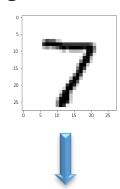
Make prediction for a test sample x'

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

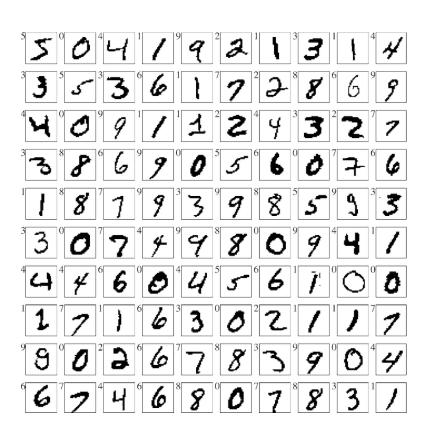


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z = [-55.7, -141.4, 18.1, 188.3, -91.3, -26.8, -183.6, 411.2, -142.1, 96.2]



Results

- The training set has 60,000 samples.
- The test set has 10,000 samples.
- The accuracy on the training set is 92.3%.
- The accuracy on the test set is 91.3%.
- Not too bad!
- The accuracy of a random guess is merely 10%.

Train a Softmax Classifier: Re-cap

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

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

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

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• Output: f(x) = SoftMax(z).

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

Train the function by empirical risk minimization (ERM):

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

Train a Softmax Classifier: Re-cap

• How to solve $\arg\min_{\mathbf{W}} \left\{ \frac{1}{n} \sum_{j=1}^{n} \operatorname{CrossEntropy} \left(\mathbf{y}_{j}, \mathbf{f}(\mathbf{x}_{j}) \right) \right\} ?$

- 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: $V_{\text{new}} = \beta V_{\text{old}} + G_{j}$.
 - 4. Update **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 $f: \mathbb{R}^{785} \mapsto \mathbb{R}^{10}$:

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

Trainable parameter:

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

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

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

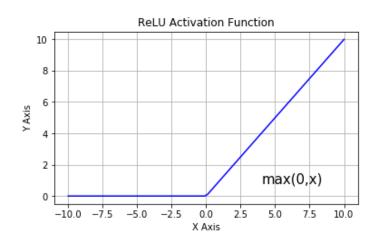
Trainable parameters:

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

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

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ReLU (activation function)



Trainable parameters:

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

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

- Input: vector $\mathbf{x}^{(0)} \in \mathbb{R}^{785}$.
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Hidden Layer 1

Trainable parameters:

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

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

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

Hidden Layer 1

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

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

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

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

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

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

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

Hidden Layer 1

Hidden Layer 2

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

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

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

Hidden Layer 1

Hidden Layer 2

Output Layer

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

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

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

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

• Output: $f(x^{(0)}) = x^{(3)}$.

Hidden Layer 1

Hidden Layer 2

Output Layer

- $W^{(0)} \in \mathbb{R}^{d_1 \times 785}$.
- $\mathbf{W}^{(1)} \in \mathbb{R}^{d_2 \times d_1}$
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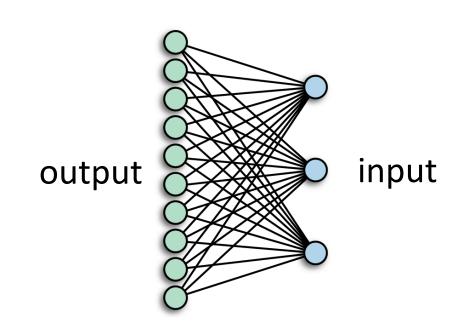
Fully-Connected Layer

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

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

"Fully-Connected" or "Dense" Layer

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



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

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

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

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

SoftMax

• Output: $f(x^{(0)}) = x^{(3)}$.

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

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SoftMax

• Output: $f(x^{(0)}) = x^{(3)}$.

 Use SoftMax because this is a multiclass classification problem.

SoftMax -

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

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

- 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 multiclass classification problem.

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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ReLU

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

- $\mathbf{z}^{(3)} = \mathbf{W}^{(2)} \mathbf{x}^{(2)} \in \mathbb{R}^{10}$.
- $\mathbf{x}^{(3)} = \operatorname{SoftMax}(\mathbf{z}^{(3)}) \in \mathbb{R}^{10}$.
- Output: $f(x^{(0)}) = x^{(3)}$.

非线性

Question: Why bothering using ReLU?

- Without the two activation functions, $z^{(3)}$ would be a linear function of $x^{(0)}$.
- 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

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

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

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

Build an optimization model:

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

E.g., the cross-entropy loss

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

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

How to solve

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

Stochastic gradient descent (SGD)

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

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

How to solve

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

Stochastic gradient descent (SGD):

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

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

- Update $W^{(0)}$: $W_{\text{new}}^{(0)} = W_{\text{old}}^{(0)} \alpha g_{j}^{(0)}$.
- Do the same for $W^{(1)}$ and $W^{(2)}$.

Backpropagation

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

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

How to compute $\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial \mathbf{W}^{(k)}}$?

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

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

How to compute $\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial W^{(k)}}$?

Backpropagation:

• Denote $L = \text{Loss}(f(x_i), y_i)$.

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

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

How to compute $\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial W^{(k)}}$?

Backpropagation:

- Denote $L = Loss(f(x_i), y_i)$.
- Compute $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$.

10-dim vector

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

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

How to compute $\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial W^{(k)}}$?

Backpropagation:

- Denote $L = \text{Loss}(f(x_i), y_i)$.
- 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.

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

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

How to compute $\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial W^{(k)}}$?

Backpropagation:

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

•
$$\frac{\partial L}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{z}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}$$
 $\frac{\partial L}{\partial \mathbf{w}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{w}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}$

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

Apply the chain rule.

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

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

How to compute $\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial W^{(k)}}$?

Backpropagation:

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

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

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

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

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

How to compute $\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial W^{(k)}}$?

Backpropagation:

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

•
$$\frac{\partial L}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{z}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}, \qquad \frac{\partial L}{\partial \mathbf{w}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{w}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}.$$

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

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

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

How to compute $\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial W^{(k)}}$?

Backpropagation:

- Denote $L = Loss(f(x_j), y_j)$.
- Compute $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$.

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

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

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

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

How to compute $\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial \mathbf{W}^{(k)}}$?

Backpropagation:

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

•
$$\frac{\partial L}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{z}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}, \qquad \frac{\partial L}{\partial \mathbf{w}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{w}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}.$$

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

Apply the chain rule again.

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

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

How to compute $\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial W^{(k)}}$?

Backpropagation:

- Denote $L = Loss(f(x_j), y_j)$.
- Compute $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$.

•
$$\frac{\partial L}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{z}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}, \qquad \frac{\partial L}{\partial \mathbf{w}^{(2)}} = \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{w}^{(2)}} \frac{\partial L}{\partial \mathbf{z}^{(3)}}.$$

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

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

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

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

How to compute $\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial \mathbf{W}^{(k)}}$?

Backpropagation:

- Denote $L = Loss(f(x_i), y_i)$.
- Compute $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$.

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

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

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

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

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

How to compute $\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial W^{(k)}}$?

- Denote $L = Loss(f(x_i), y_i)$.
- Compute $\frac{\partial L}{\partial \mathbf{z}^{(3)}}$.

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

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

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

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

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

How to compute $\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial w^{(k)}}$?

Backpropagation:

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

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

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

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

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

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

Apply the chain rule again.

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

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

How to compute $\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial w^{(k)}}$?

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

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

•
$$\frac{\partial L}{\partial \mathbf{z}^{(1)}} = \frac{\partial \mathbf{z}^{(2)}}{\partial \mathbf{z}^{(1)}} \frac{\partial L}{\partial \mathbf{z}^{(2)}}$$
, Free $\frac{\partial L}{\partial \mathbf{z}^{(1)}}$ from memory.

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

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

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

How to compute $\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial w^{(k)}}$?

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

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

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

•
$$\left| \frac{\partial L}{\partial \mathbf{W}^{(0)}} \right| = \frac{\partial \mathbf{z}^{(1)}}{\partial \mathbf{W}^{(0)}} \frac{\partial L}{\partial \mathbf{z}^{(1)}}$$
. Use it to update $\mathbf{W}^{(0)}$.

Backpropagation: Example

反向传播 示例

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

- 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: $f(x^{(0)}) = z^{(3)}$.

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

- 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: $f(x^{(0)}) = z^{(3)}$.

Random sampling:

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

Forward pass (input → output):

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

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

- 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: $f(x^{(0)}) = z^{(3)}$.

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

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

- 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: $f(x^{(0)}) = z^{(3)}$.

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

$$\bullet \ \frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j.$$

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

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

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

$$\bullet \overline{\left|\frac{\partial L}{\partial z^{(3)}}\right|} = z^{(3)} - y_j.$$

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

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

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: $f(x^{(0)}) = z^{(3)}.$

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

$$\bullet \ \frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j.$$

•
$$\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$$

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

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: $f(x^{(0)}) = z^{(3)}$.

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

$$\bullet \frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j.$$

•
$$\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$$

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



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

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: $f(x^{(0)}) = z^{(3)}$.

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

$$\bullet \ \frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j.$$

$$\bullet \frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)'}} \frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$$

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

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

$$\bullet \frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j.$$

$$\bullet \frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)'}} \frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$$

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

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: $f(x^{(0)}) = z^{(3)}$.

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

$$\bullet \ \frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j.$$

•
$$\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$$
 $\frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$

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

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

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

$$\bullet \frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j.$$

•
$$\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$$
 $\frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$

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

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: $f(x^{(0)}) = z^{(3)}$.

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

$$\bullet \frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j.$$

•
$$\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)'}} \frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$$

$$\bullet \ \frac{\partial L}{\partial z^{(1)}} = \left[\frac{\partial z^{(2)}}{\partial z^{(1)}} \right] \frac{\partial L}{\partial z^{(2)}}$$

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

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: $f(x^{(0)}) = z^{(3)}$.

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

$$\bullet \frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j.$$

•
$$\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)}}$$
 $\frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$

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

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

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

$$\bullet \ \frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j.$$

•
$$\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)'}} \frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$$
.

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

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

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

- 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: $f(x^{(0)}) = z^{(3)}$.

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

$$\bullet \ \frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j.$$

•
$$\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)'}} \frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$$
.

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

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

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

$$\bullet \ \frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j.$$

•
$$\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)'}} \frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$$
.

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

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

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: $f(x^{(0)}) = z^{(3)}$.

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

$$\bullet \frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j.$$

•
$$\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)'}} \frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$$
.

•
$$\frac{\partial L}{\partial z^{(1)}} = \frac{\partial z^{(2)}}{\partial z^{(1)}} \frac{\partial L}{\partial z^{(2)'}}$$
 $\frac{\partial L}{\partial w^{(1)}} = \frac{\partial z^{(2)}}{\partial w^{(1)}} \frac{\partial L}{\partial z^{(2)}}$

•
$$\frac{\partial L}{\partial w^{(0)}} = \boxed{\frac{\partial z^{(1)}}{\partial w^{(0)}}} \frac{\partial L}{\partial z^{(1)}}$$
.

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

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

$$\bullet \frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j.$$

•
$$\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)'}} \frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$$
.

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

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

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: $f(x^{(0)}) = z^{(3)}$.

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

$$\bullet \frac{\partial L}{\partial z^{(3)}} = z^{(3)} - y_j.$$

•
$$\frac{\partial L}{\partial z^{(2)}} = \frac{\partial z^{(3)}}{\partial z^{(2)}} \frac{\partial L}{\partial z^{(3)'}} \frac{\partial L}{\partial w^{(2)}} = \frac{\partial z^{(3)}}{\partial w^{(2)}} \frac{\partial L}{\partial z^{(3)}}$$
.

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

•
$$\left| \frac{\partial L}{\partial w^{(0)}} \right| = \frac{\partial z^{(1)}}{\partial w^{(0)}} \frac{\partial L}{\partial z^{(1)}}.$$

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

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

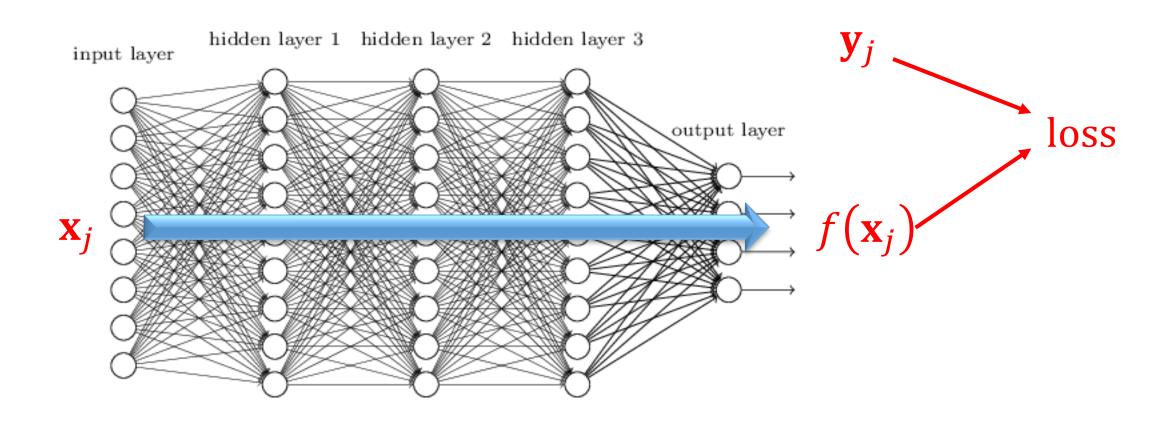
Backpropagation:

One iteration:

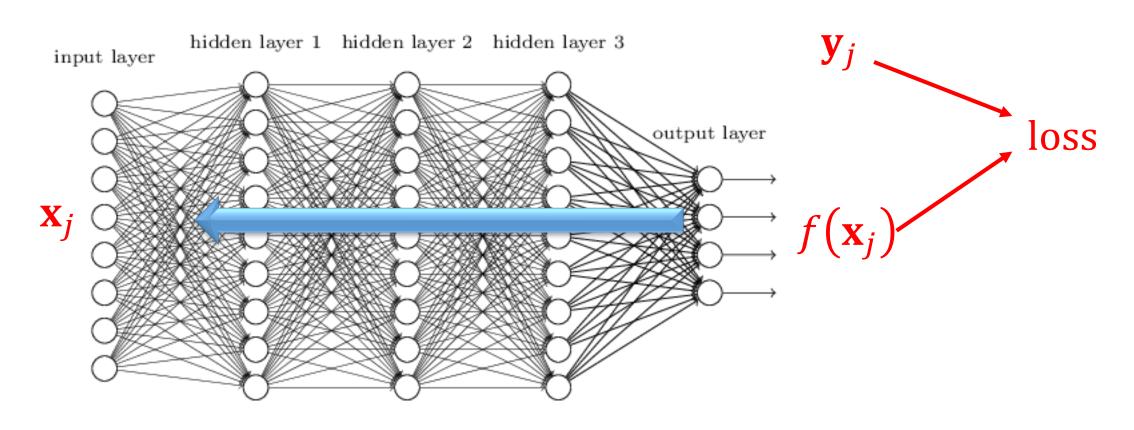
- 1. Randomly sample j from $\{1, 2, \dots, n\}$.
- 2. Forward pass: take x_j as input $(x^{(0)} = x_j)$, compute each layer $x_j = x_j = x_j$.
- 3. Backward pass:
 - i. Compute the derivatives $\frac{\partial L}{\partial z^{(3)}}$, $\frac{\partial L}{\partial w^{(2)}}$, $\frac{\partial L}{\partial z^{(2)}}$, $\frac{\partial L}{\partial w^{(1)}}$, $\frac{\partial L}{\partial z^{(1)}}$, $\frac{\partial L}{\partial w^{(0)}}$.
 - ii. Update $w^{(k)}$ using $\frac{\partial L}{\partial w^{(k)}}$.

Summary of Backpropagation

- 1. Randomly pick a sample (x_i, y_i) .
- 2. Run a forward pass (from the input $\mathbf{x}^{(0)}$ to the prediction).



- 1. Randomly pick a sample (x_i, y_i) .
- 2. Run a forward pass (from the input $\mathbf{x}^{(0)}$ to the prediction).
- 3. Run a backward pass (from the loss to $W^{(0)}$).



- 1. Randomly pick a sample (x_i, y_i) .
- 2. Run a forward pass (from the input $\mathbf{x}^{(0)}$ to the prediction).
- 3. Run a backward pass (from the loss to $W^{(0)}$).



Get the derivatives (stochastic gradients):

$$\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial W^{(2)}}, \quad \frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial W^{(1)}}, \quad \frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial W^{(0)}}.$$

- 1. Randomly pick a sample (x_i, y_i) .
- 2. Run a forward pass (from the input $\mathbf{x}^{(0)}$ to the prediction).
- 3. Run a backward pass (from the loss to $W^{(0)}$).



Get the derivatives (stochastic gradients):

$$\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial \mathbf{W}^{(2)}}, \quad \frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial \mathbf{W}^{(1)}}, \quad \frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial \mathbf{W}^{(0)}}.$$



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

Mini-Batch

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



Get the derivatives (stochastic gradients):

$$\frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial w^{(1)}} \frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial w^{(1)}} \frac{\partial \operatorname{Loss}(f(x_j),y_j)}{\partial w^{(1)}}$$

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

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

Mini-Batch

SGD: BatchSize = 1.

Mini-Batch: BatchSize > 1.

Full Gradient: BatchSize = n.

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

需要大量的迭代来收敛

- Better than the other two, if BatchSize is properly set.
- 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 1st-order algorithms.
- Other 1st-order algorithms: SGD with momentum, AdaGrad, RMSprop...
- See the blogs:
 - http://ruder.io/optimizing-gradient-descent/
 - https://distill.pub/2017/momentum/

Summary of FC Neural Network

Network structure

Number of layers

Width of each layer

Activation functions

Network structure

Number of layers

Width of each layer

Activation functions

Example:

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

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

Network structure

Number of layers

Width of each layer

Activation functions

Example:

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

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

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

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

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

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

• Output: $f(x^{(0)}) = SoftMax(z^{(2)})$.

- 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.

Network structure

Number of layers

Width of each layer

Activation functions

Example:

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

- 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.

Network structure

Number of layers

Width of each layer

Activation functions

Example:

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

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

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

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

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

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

• Output: $f(x^{(0)}) = SoftMax(z^{(2)})$.

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

•
$$\mathbf{W}^{(1)} \in \mathbb{R}^{d_2 \times d_1}$$

•
$$\mathbf{W}^{(2)} \in \mathbb{R}^{10 \times d_2}$$

•
$$785d_1 + d_1d_2 + 10d_2$$
.

Network structure

Number of layers

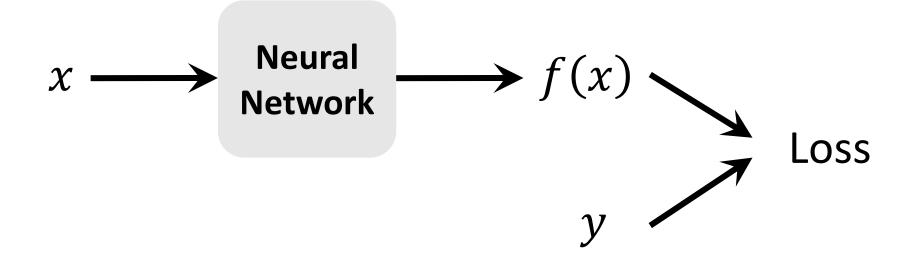
Width of each layer

Activation functions

Loss functions

Cross-entropy for classification

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



Network structure

Number of layers

Width of each layer

Activation functions

Loss functions

Cross-entropy for classification

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

Compute gradient: by a forward pass and a backward pass

Automatically performed by many deep learning systems

Batch size

Network structure

Number of layers

Width of each layer

Activation functions

Loss functions

Cross-entropy for classification

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

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 hyper-parameters)

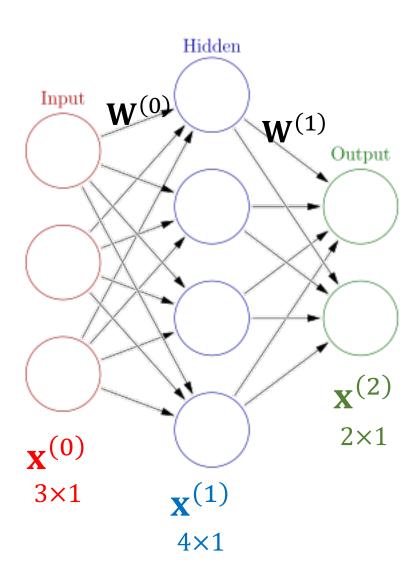
SGD

SGD with momentum

AdaGrad

RMSprop

Representing a Neural Network



- A node denotes one entry of vector x.
- A dense layer is parameterized by a matrix W.
- An edge denotes one entry of parameter matrix **W**.

Representing a Neural Network

Equivalent representation:

