KYOTO UNIVERSITY

Statistical Machine Learning Theory

Neural Networks

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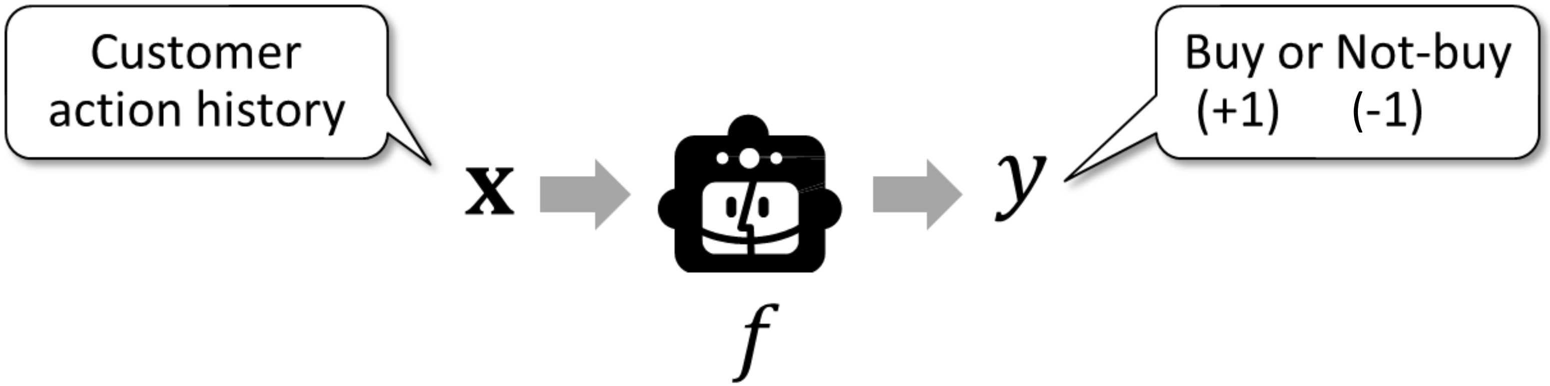
Neural networks:
Foundation of deep learning

- Linear models to non-linear models
  - “Classic” non-linear models:
    - Decision trees, kernel machines, boosting, …
- Neural networks
  - Inherently nonlinear models
  - Foundation of the successful “deep learning”
- To see what they are and how to train them, we will start from reviewing the logistic regression model

Logistic Regression

Classification problem: Supervised learning for predicting discrete variable

- Goal: Obtain a function $f: \mathcal{X} \to \mathcal{Y}$
  - $\mathcal{X} = \mathbb{R}^D$: Input domain
  - $\mathcal{Y}$: discrete output domain
    - We focus on two-class classification: $\mathcal{Y} = \{+1, -1\}$
- Training dataset: N pairs of an input and an output $\{(\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(N)}, y^{(N)})\}$

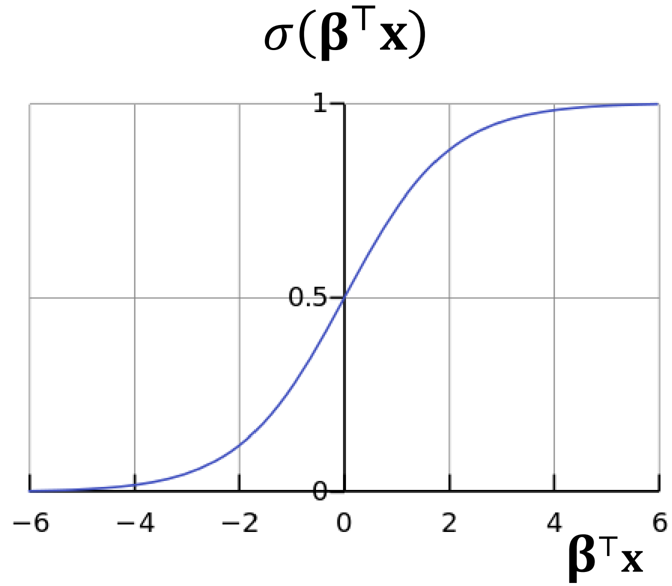


Logistic regression model: A probabilistic model for binary classification

- Logistic regression model gives the conditional probability

$$f_{\mathbf{w}}(y=+1|\mathbf{x}) = \sigma(\mathbf{w}^\top\mathbf{x}) = \frac{1}{1+\exp(-\mathbf{w}^\top\mathbf{x})}$$

- Logistic (sigmoid) function $\sigma\colon \mathbb{R} \to (0,1)$
  - $\mathbf{w}^\top\mathbf{x}$ has the same form as linear regression and takes a real number
  - σ converts real numbers to “probabilities”



Cross entropy: Objective function to train a logistic regression model

- Cross entropy (to minimize):

For positive class data

$$
\begin{aligned}
L(\mathbf{w}) &= -\sum_{i=1}^{N} \delta\left(y^{(i)} = +1\right) \log f_{\mathbf{w}}\left(y^{(i)} = +1 \middle| \mathbf{x}^{(i)}\right) \\
&\quad -\sum_{i=1}^{N} \delta\left(y^{(i)} = -1\right) \log\left(1 - f_{\mathbf{w}}\left(y^{(i)} = +1 \middle| \mathbf{x}^{(i)}\right)\right) \\
&= \sum_{i=1}^{N} \log\left(1 + \exp\left(-y^{(i)} \mathbf{w}^{\top} \mathbf{x}^{(i)}\right)\right)
\end{aligned}
$$

For negative class data

- Cross entropy is equivalent to
  - Logistic loss: upper bound of 0-1 loss (#mistakes)
  - Negative log-likelihood (for maximum likelihood estimation)

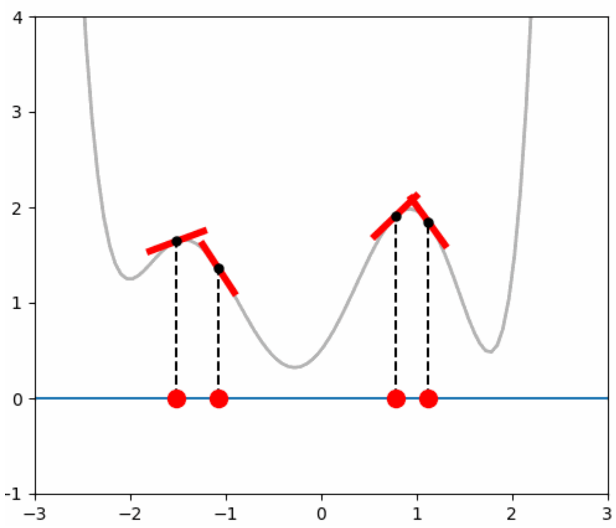
Gradient descent optimization:
A simplest parameter estimation method

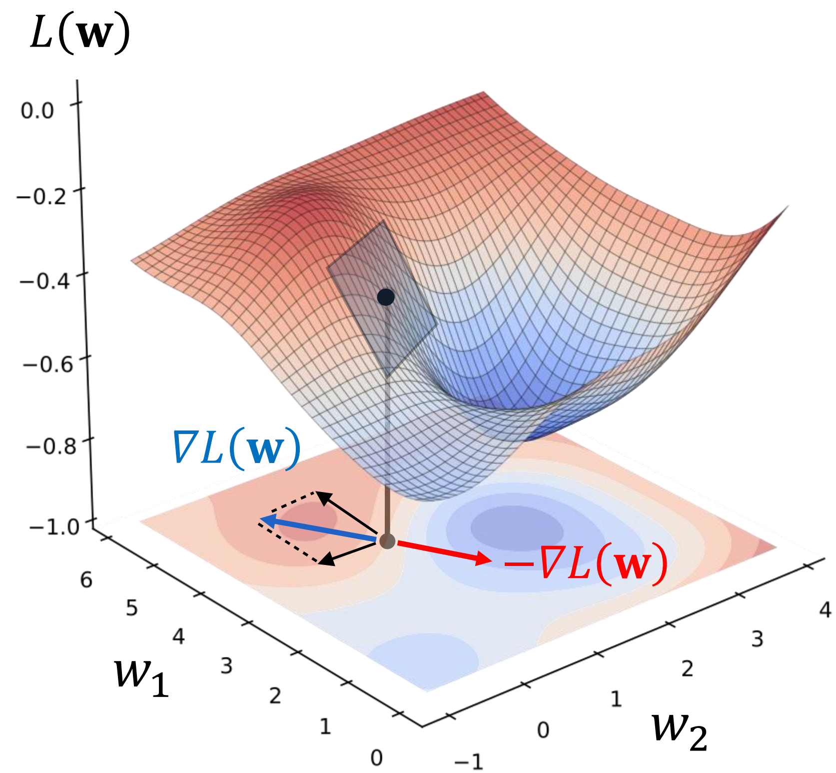
- Iteratively refine the current parameter $\mathbf{w}$ to $\mathbf{w}^{\mathrm{NEW}}$:

$$\mathbf{w}^{\mathrm{NEW}} \leftarrow \mathbf{w} - \eta \nabla L(\mathbf{w})$$

  - Gradient $\nabla L(\mathbf{w})$ is the steepest direction of the objective function $L(\mathbf{w})$
  - "learning rate" $\eta > 0$

Gradient update finds the bottoms of "valleys"





Gradient descent for logistic regression: Gradient of objective function is all you need

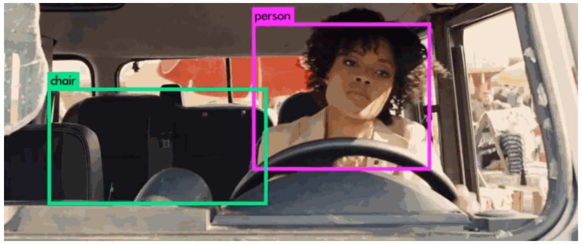
- Once we obtain the gradient, we can apply Gradient Descent
  - Objective function: $L(\mathbf{w}) = \sum_{i=1}^{n} \ln\left(1 + \exp\left(-y^{(i)} \mathbf{w}^\top \mathbf{x}^{(i)}\right)\right)$
  - Gradient of $L(\mathbf{w})$: $\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}} = \sum_{i=1}^{n} \frac{y^{(i)} \mathbf{x}^{(i)}}{1+\exp\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)}$
  - GD update: $\mathbf{w}^{\mathrm{NEW}} \leftarrow \mathbf{w} - \eta \sum_{i=1}^{n} \frac{y^{(i)} \mathbf{x}^{(i)}}{1+\exp\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)}$
- Approximation using only one data instance $\left(\mathbf{x}^{(i)}, y^{(i)}\right)$
  - Stochastic gradient descent (SGD):

$$\mathbf{w}^{\mathrm{NEW}} \leftarrow \mathbf{w} - \eta \frac{y^{(i)} \mathbf{x}^{(i)}}{1 + \exp(\mathbf{w}^\top \mathbf{x}^{(i)})}$$

Neural Networks

Success of "deep learning" :
Real world applications

Image recognition



Machine Translation

DeepL

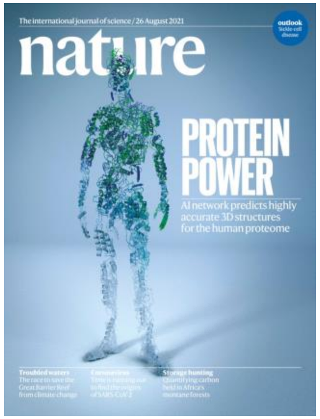
Image/movie transformation

"Deep Fake"

AlphaGo

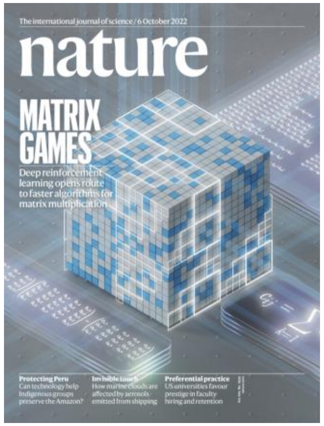
AlphaGo

AlphaFold2



AlphaFold

AlphaTensor



AlphaTensor

OpenAI ChatGPT

Midjourney

OpenAI DALL·E 3

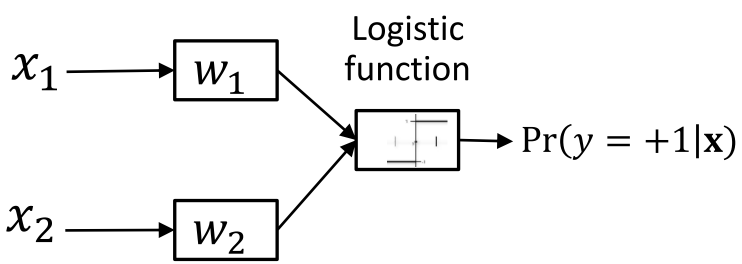
Stable Diffusion

"Generative" AI

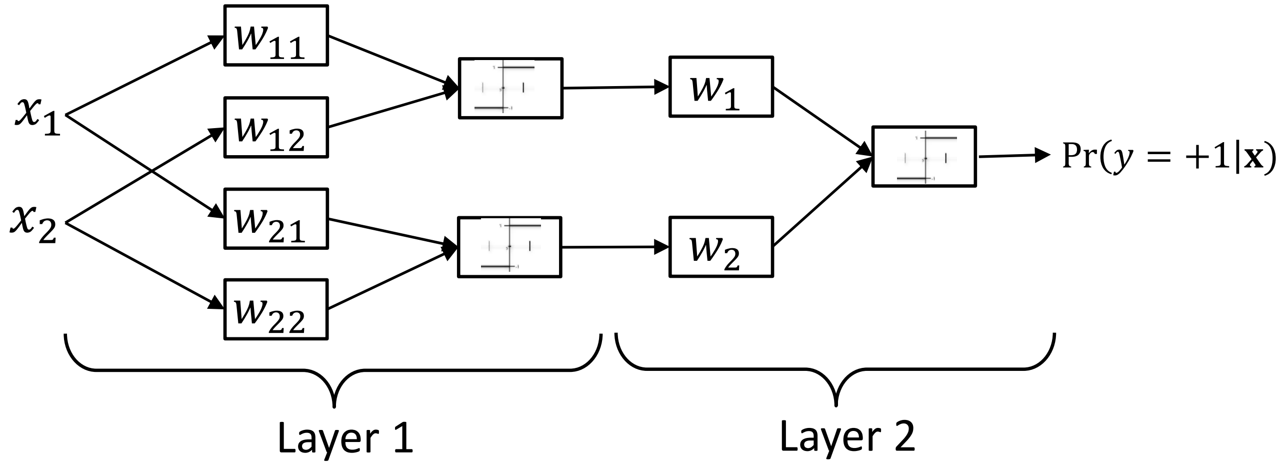
Neural networks: Multi-layered logistic regression models

- (Very roughly speaking,) a neural network is multi-layered logistic regression models
  - Outputs of some logistic regression models are inputs to other logistic regression models
- The form of final output is still $\Pr(y = +1|\mathbf{x})$

Logistic regression



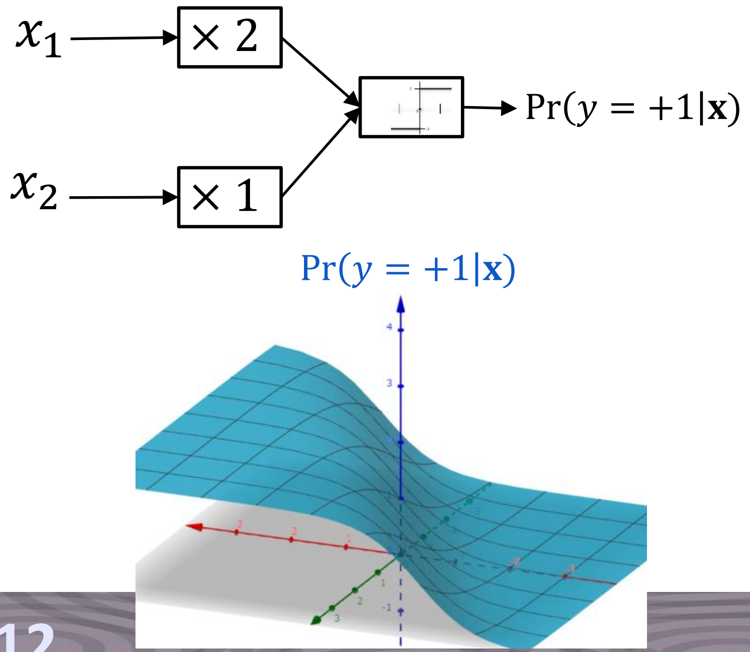
Neural network (2 layers)



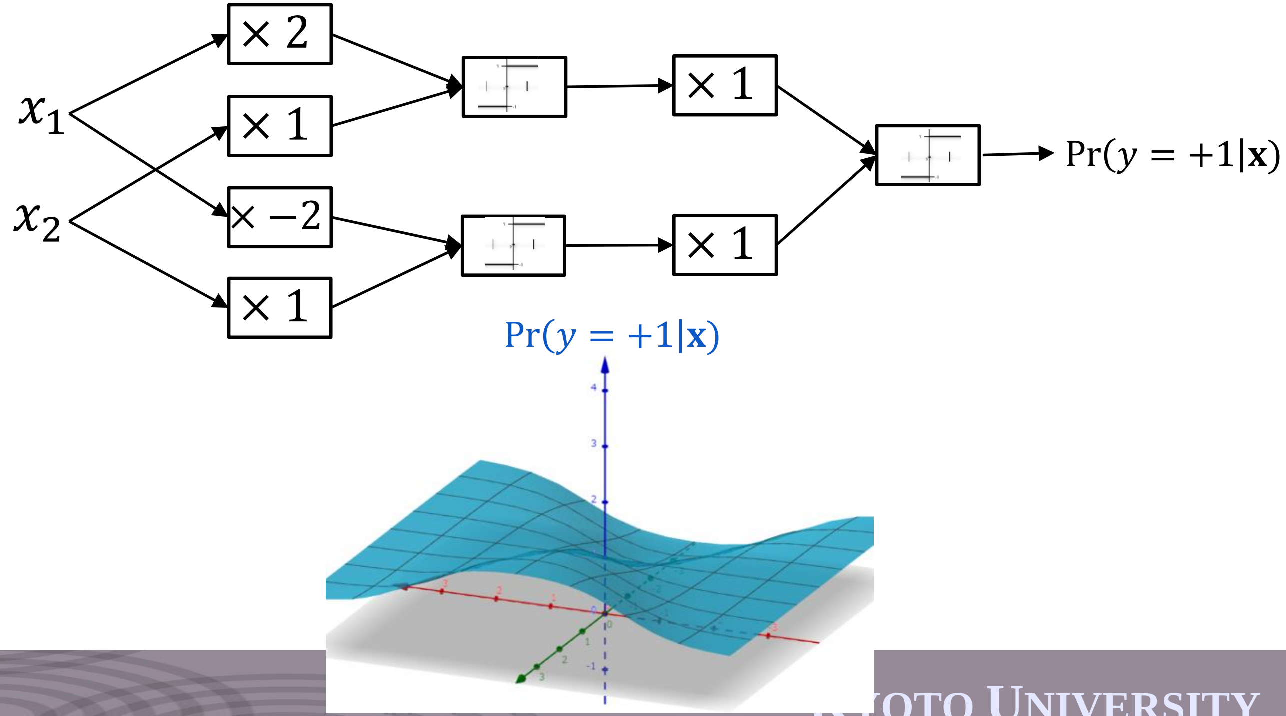
Why do we need to stack layers?
Nonlinear classification

- (1-layer) logistic regression only allow linear classification (AND/OR)
- Gains *non-linear* expressive power by stacking two layers (XOR)
- Universal approximation theorem: neural network can represent arbitrary functions by introducing many intermediate units

Logistic regression



Neural network (2 layers)

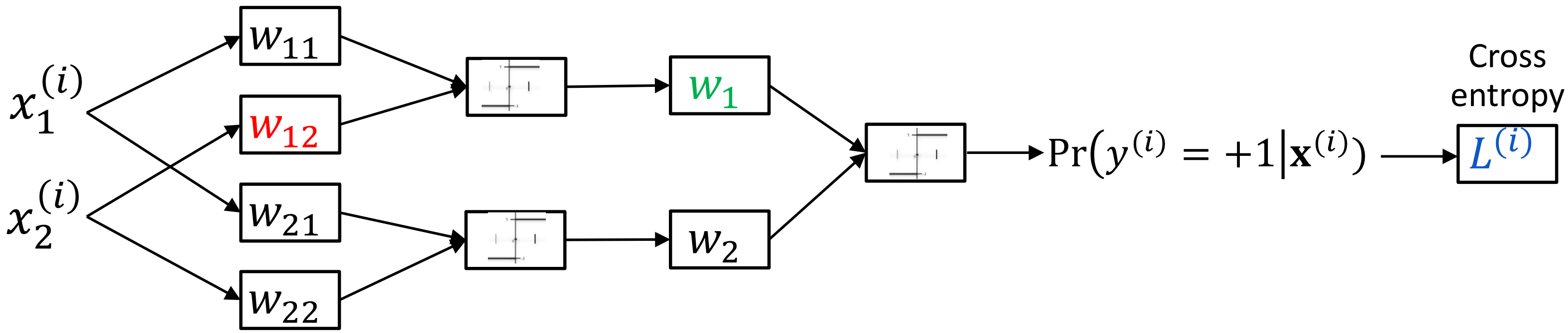


Parameter estimation for neural networks: Gradient is all you need

- The objective function for training a neural network is the same as that of logistic regression, i.e., the *cross entropy*:
  - When SGD is used, the cross entropy (only for the i-th instance) is

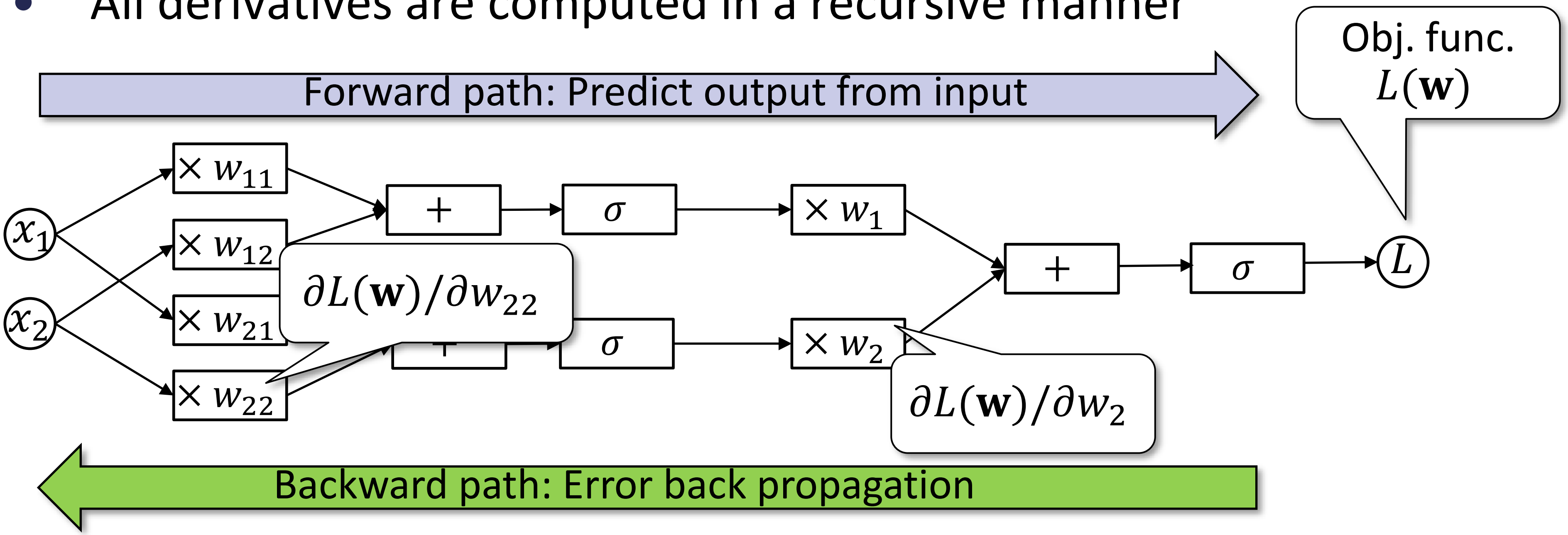
$$L^{(i)}(\mathbf{w}) = -\delta\left(y^{(i)} = 1\right)\log f_{\mathbf{w}}\left(y^{(i)} = +1 \middle| \mathbf{x}^{(i)}\right) - \delta\left(y^{(i)} = -1\right)\log f_{\mathbf{w}}\left(y^{(i)} = -1 \middle| \mathbf{x}^{(i)}\right)$$

- Gradient descent update: $\mathbf{w}^{\mathrm{NEW}} \leftarrow \mathbf{w} - \eta \nabla L^{(i)}(\mathbf{w})$
- How can we obtain the gradient $\nabla L^{(i)}(\mathbf{w}) = \partial L^{(i)} / \partial \mathbf{w}$?
  - E.g., how can we obtain $\partial L^{(i)} / \partial w_{12}$? (They are separated via w_1)



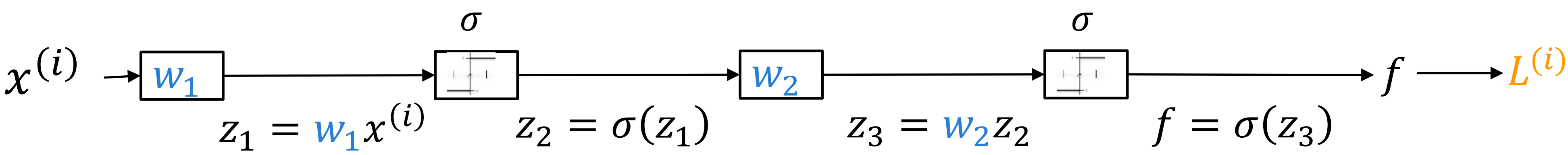
Error back propagation:
An efficient strategy to compute the gradient

- Once we differentiate the objective function, we can apply SGD
- *Error backpropagation* can compute the gradient
  - Forward path: computes output (objective func.) from the input
  - Backward path: computes derivatives from output to input
    - All derivatives are computed in a recursive manner



How error back propagation works:
Gradient computation using the chain rule of derivatives

- 1-dimensional case (of no practical use)



$$L^{(i)}(w_1, w_2) = -\delta\left(y^{(i)} = +1\right)\log f\left(x^{(i)}\right) - \delta\left(y^{(i)} = -1\right)\log\left(1 - f\left(x^{(i)}\right)\right)$$

- Chain rule of derivatives:
  - $\dfrac{\partial L^{(i)}}{\partial w_2} = \dfrac{\partial L^{(i)}}{\partial f} \cdot \dfrac{\partial f}{\partial z_3} \cdot \dfrac{\partial z_3}{\partial w_2}$
  - $\dfrac{\partial L^{(i)}}{\partial w_1} = \dfrac{\partial L^{(i)}}{\partial f} \cdot \dfrac{\partial f}{\partial z_3} \cdot \dfrac{\partial z_3}{\partial z_2} \cdot \dfrac{\partial z_2}{\partial z_1} \cdot \dfrac{\partial z_1}{\partial w_1}$

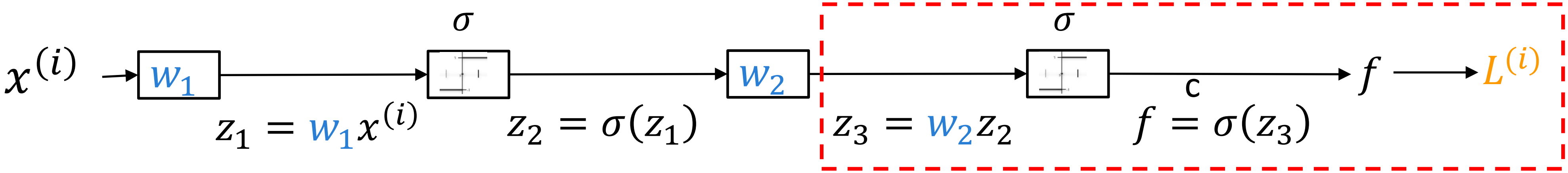
$$\left\{\begin{aligned}
\frac{\partial L^{(i)}}{\partial f} &= \frac{\delta\left(y^{(i)} = -1\right)}{1 - f\left(x^{(i)}\right)} - \frac{\delta\left(y^{(i)} = +1\right)}{f\left(x^{(i)}\right)} \\
\frac{\partial f}{\partial z_3} &= \sigma(z_3)\left(1 - \sigma(z_3)\right) \\
\frac{\partial z_3}{\partial w_2} &= z_2 \\
\frac{\partial z_3}{\partial z_2} &= w_2 \\
\frac{\partial z_2}{\partial z_1} &= \sigma(z_1)\left(1 - \sigma(z_1)\right) \\
\frac{\partial z_1}{\partial w_1} &= x^{(i)}
\end{aligned}\right.$$

Already obtained in forward path

How error back propagation works:

Efficient computation using the chain rule of derivatives

- Naïve application of the chain rules requires $O(|U|^2)$ computation



- Backward computation allows reuse of common parts
  $\Rightarrow$ results in $O(|U|^2)$ computation

$|U|$: number of operation units

- Chain rule of derivatives:

  - $$\frac{\partial L^{(i)}}{\partial w_2} = \boxed{\frac{\partial L^{(i)}}{\partial f} \cdot \frac{\partial f}{\partial z_3}} \cdot \frac{\partial z_3}{\partial w_2}$$

  - $$\frac{\partial L^{(i)}}{\partial w_1} = \boxed{\frac{\partial L^{(i)}}{\partial f} \cdot \frac{\partial f}{\partial z_3}} \cdot \frac{\partial z_3}{\partial z_2} \cdot \frac{\partial z_2}{\partial z_1} \cdot \frac{\partial z_1}{\partial w_1}$$

Reusable common part in backward path

Computational Graphs and Automatic Differentiation

Computational graph: General representation of NN structure as a DAG

- A neural net can be constructed by stacking logistic regression models
  - Parameter estimation requires differentiating the output (the objective function) by parameters in the middle of the NN
  - This can be computed by applying the chain rule on this graph

⇒ Let us generalize them for other neural networks!

- Computational graph:
  A directed acyclic graph representing computational process from input to output (NN decision process) using simple computational units:
  - Addition and multiplication (matrix multiplication)
  - Sigmoid transformation (simple nonlinear transformation)

⇒ Can we also use other types of units?

Requirements for computational unit in NN: Output and its derivatives w.r.t. inputs and parameters

- Q: What computational units are allowed to be used in NN?

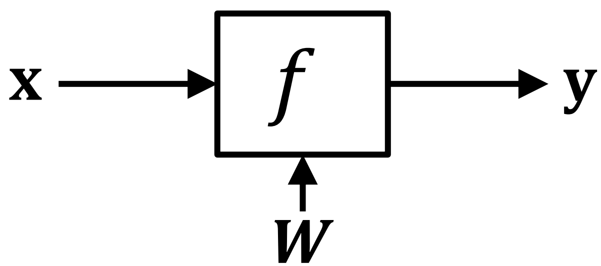
  A: Required to have its output is differentiable w.r.t its

  1. Inputs
  2. Parameters

- In other words, we can use arbitrary units that offer

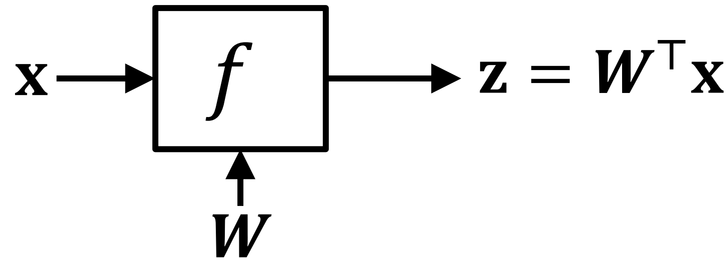
  1. Output (for its input) : $\mathbf{y} = f(\mathbf{x}; \boldsymbol{W})$ — Used in forward path
  2. Derivative of the output w.r.t its *inputs*: $\partial\mathbf{y}/\partial\mathbf{x}$
  3. Derivative of the output w.r.t its *parameters* : $\partial\mathbf{y}/\partial\boldsymbol{W}$

  Used in backward path (2, 3)

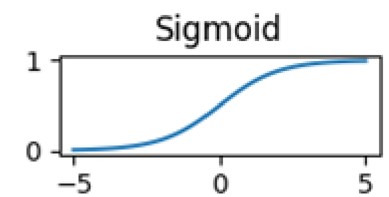


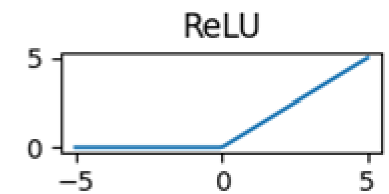
Examples of computational units in NN: Output and its derivatives w.r.t. inputs and parameters

- Linear unit:
  - Output: $\mathbf{z} = \boldsymbol{W}^\top \mathbf{x}$
  - Derivatives: $\partial \mathbf{z} / \partial \mathbf{x} = \boldsymbol{W}, \quad \partial \mathbf{z} / \partial \boldsymbol{W} = \mathbf{x}$



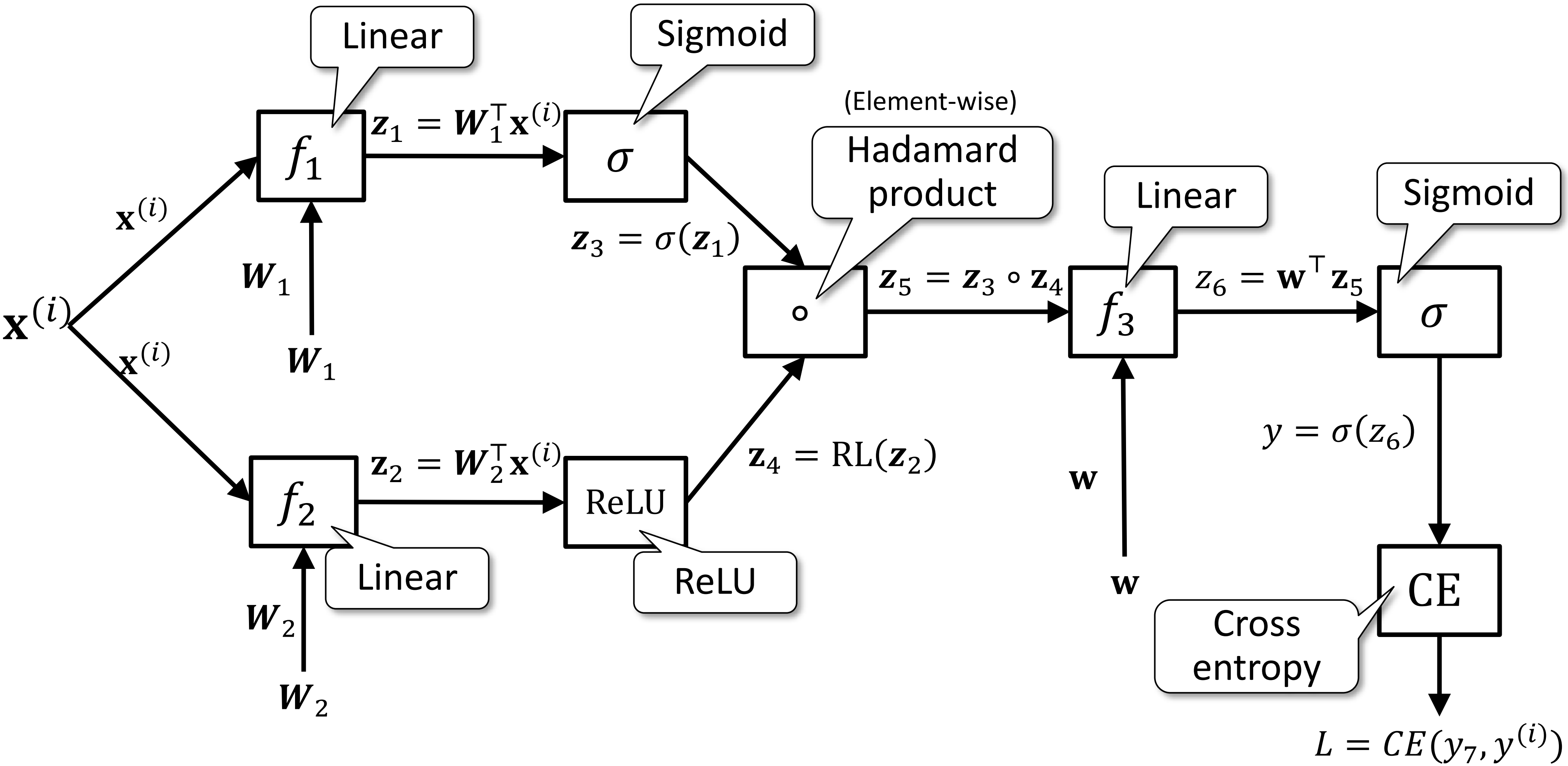
- Sigmoid unit (Logistic unit):
  - Output: $\mathbf{z} = \sigma(\mathbf{x})$ (σ is element-wise application of sigmoid function)
  - Derivatives: $\frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \sigma(\mathbf{x})(1 - \sigma(\mathbf{x}))$ (No parameter derivative)
- ReLU unit (Rectangular Linear Unit):
  - Output: $\mathbf{z} = \max\{\mathbf{0}, \mathbf{x}\}$ (element-wise max)
  - Derivatives: $\frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \min\{\mathbf{0}, \mathbf{1}\}$ (No parameter derivative)





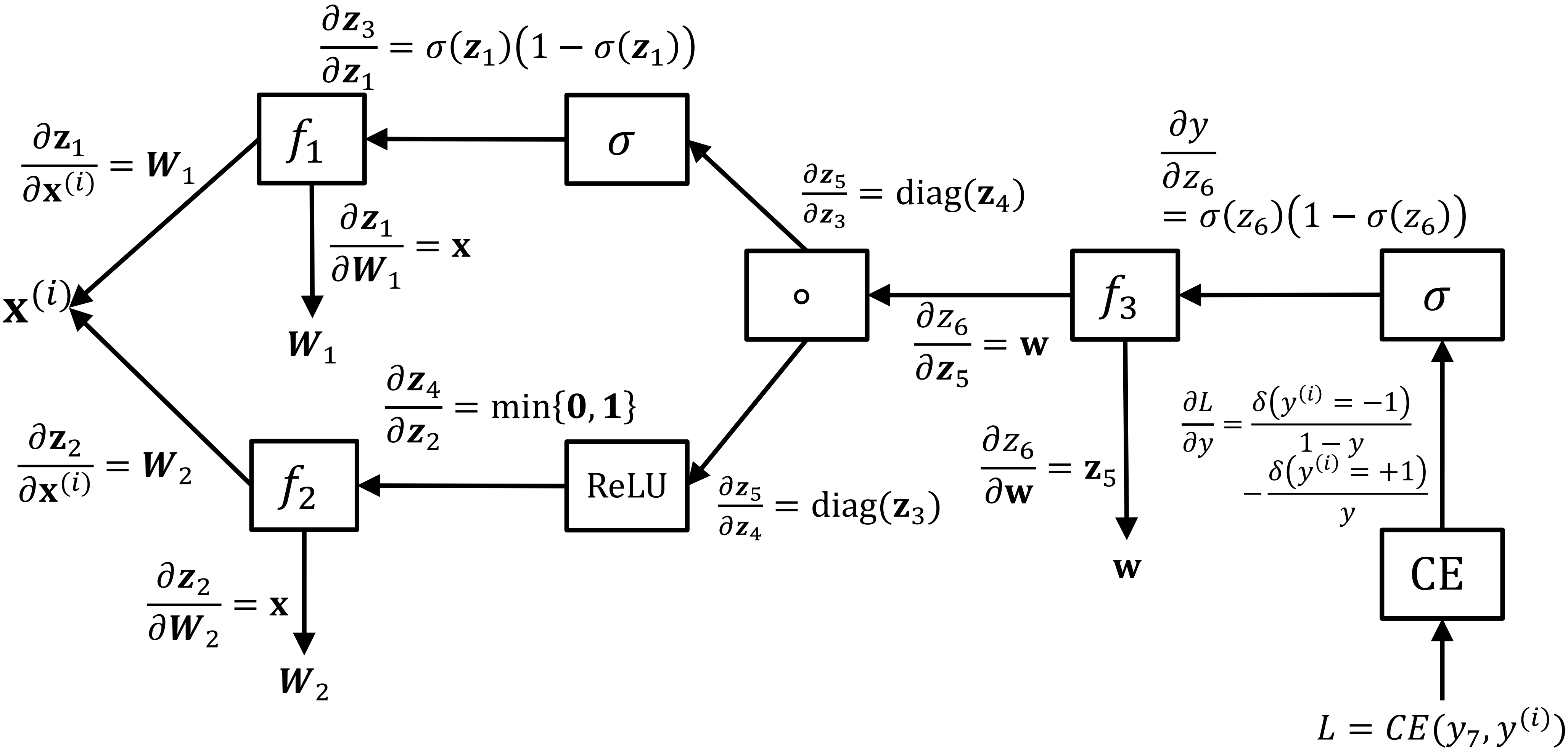
Automatic differentiation over computational graph: Forward path

- All units are differentiable w.r.t. inputs & parameters



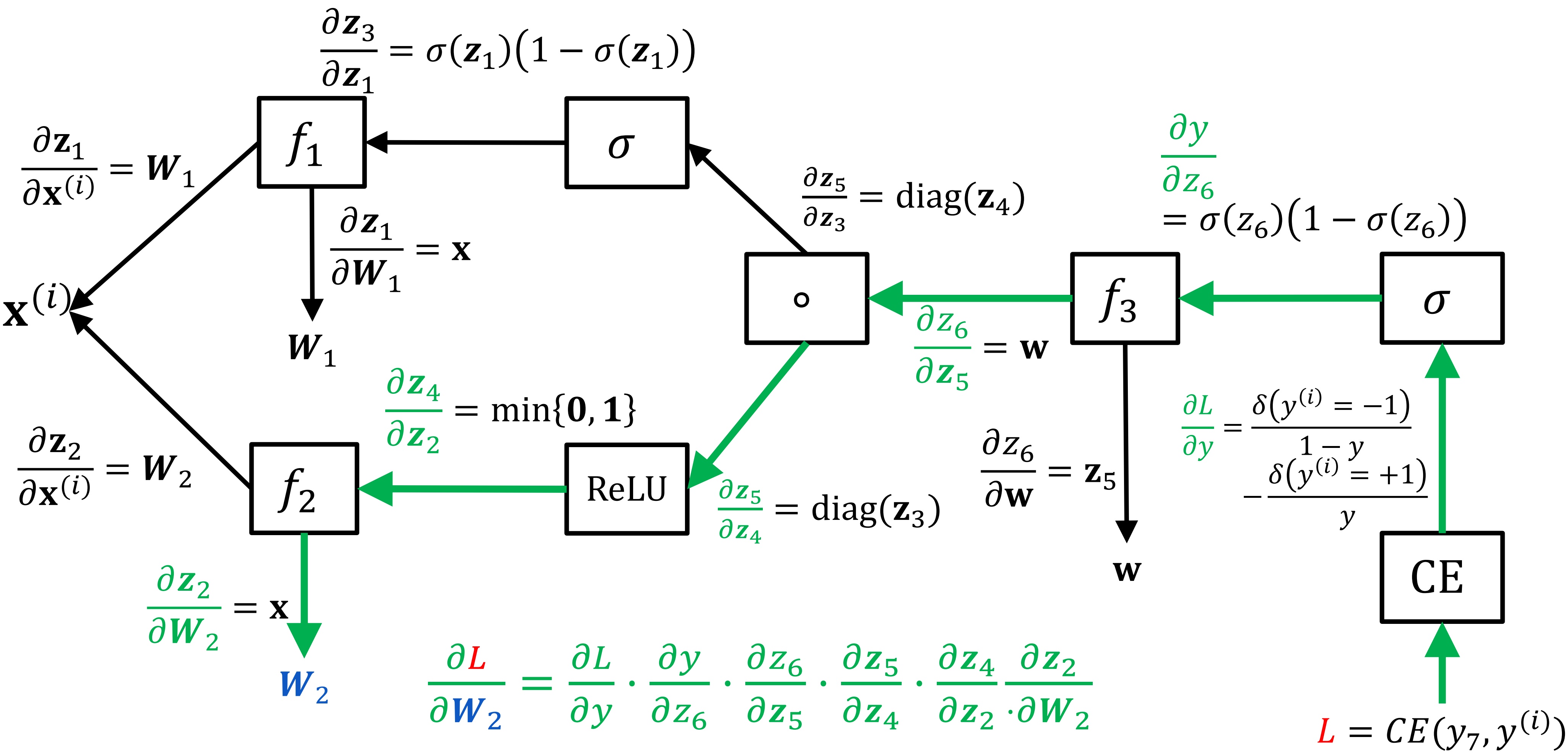
Automatic differentiation over computational graph: Backward path

- Traversals on backward paths give arbitrary derivatives



Automatic differentiation over computational graph: Backward path

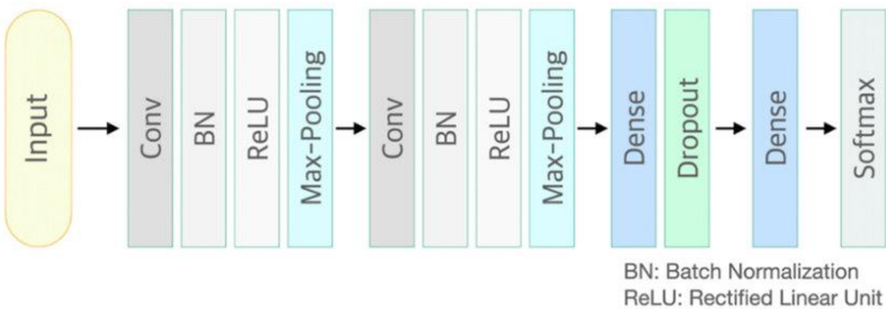
- Traversals on backward paths give arbitrary derivatives

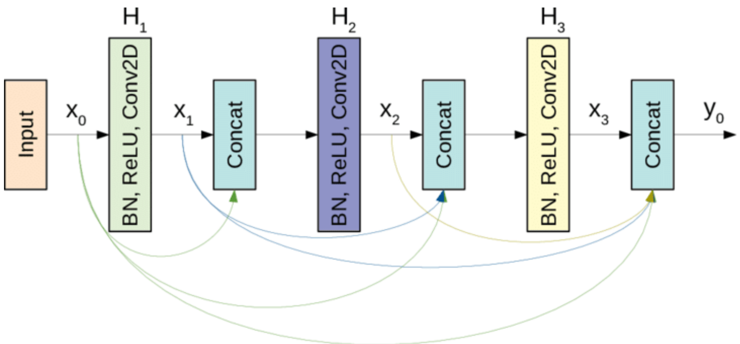


$$\frac{\partial L}{\partial \boldsymbol{W}_2} = \frac{\partial L}{\partial y} \cdot \frac{\partial y}{\partial z_6} \cdot \frac{\partial z_6}{\partial \mathbf{z}_5} \cdot \frac{\partial \mathbf{z}_5}{\partial \mathbf{z}_4} \cdot \frac{\partial \mathbf{z}_4}{\partial \mathbf{z}_2} \frac{\partial \mathbf{z}_2}{\cdot \partial \boldsymbol{W}_2}$$

Various deep neural network structure:
Flexible modeling by combining units

- NN allows intuitive and flexible modeling by combining various types of units like “*LEGO®*” blocks to form complex networks





  - Error back propagation can be left to DL frameworks such as PyTorch

- Various task dependent neural networks have been proposed:
  - Images: Convolutional Neural Network (CNN); Vision Transformer (ViT)
  - Languages: Recurrent Neural Network (RNN), Transformer,
  - Graphs: Graph neural networks (GNN)

Training Deep Networks

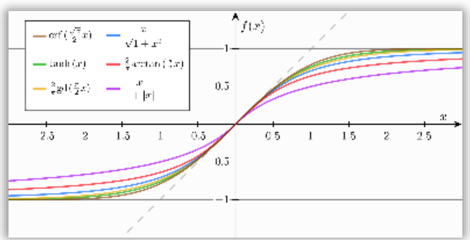
Gradient vanishing problem:
A major obstacle in training deep networks

- You can design and train arbitrary large networks, but in practice, we face the problem that training does not go well..
- Gradient vanishing problem: the derivative becomes weaker and weaker in the process of error back propagation
  - In the previous example, $\frac{\partial L}{\partial \boldsymbol{W}_2} = \frac{\partial L}{\partial y} \cdot \frac{\partial y}{\partial z_6} \cdot \frac{\partial z_6}{\partial \boldsymbol{z}_5} \cdot \frac{\partial \boldsymbol{z}_5}{\partial \boldsymbol{z}_4} \cdot \frac{\partial \boldsymbol{z}_4}{\partial \boldsymbol{z}_2} \frac{\partial \boldsymbol{z}_2}{\cdot \partial \boldsymbol{W}_2}$
  - Repeated multiplication of small derivative values results in progressively smaller overall derivative values
- In deep networks, the gradient tends to be small,
and hence gradient descent optimization does not proceed

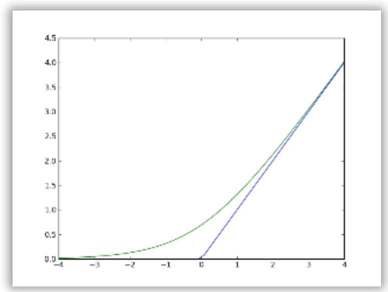
How to deal with gradient vanishing problem: ReLU and skip connection

- Gradient of logistic function becomes small away from the origin

- Activation functions other than logistic function
  - Rectangular linear unit: $\max(0, x)$
    - Its derivative is 1 (or 0)



Logistic function

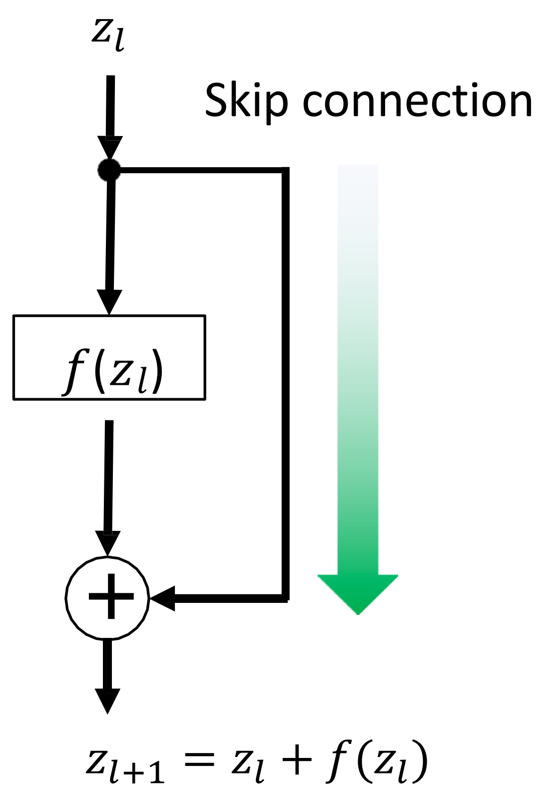


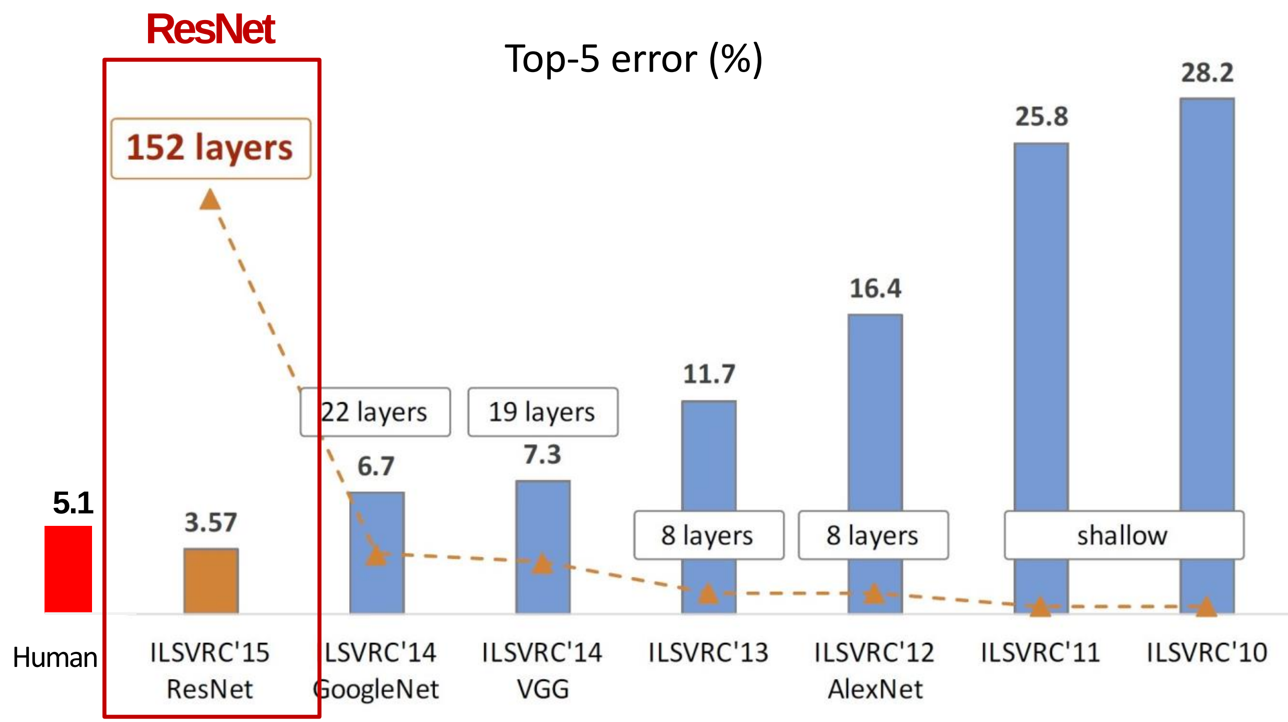
ReLU

    - Softplus: $\ln(1 + e^x)$, LeakyReLU, ... and others

How to deal with gradient vanishing problem:
ReLU and skip connection

- Skip connection: $z_{l+1} = z_l + f(z_l)$
- Gradient is propagated directly without decay





Summary:
Neural networks

1. Neural network: (Very roughly speaking) stacked logistic regression

2. Training neural networks: gradient method (SGD, mini-batch, …)

3. Computational graphs and automatic differentiation (error back propagation): gradients can be computed efficiently and systematically on a computational graph consisting of simple differentiable units

4. Training deep learning models: Dealing with the Gradient vanishing problem with ReLU, skip connection, …