

# Chapter ML:IV (continued)

## IV. Neural Networks

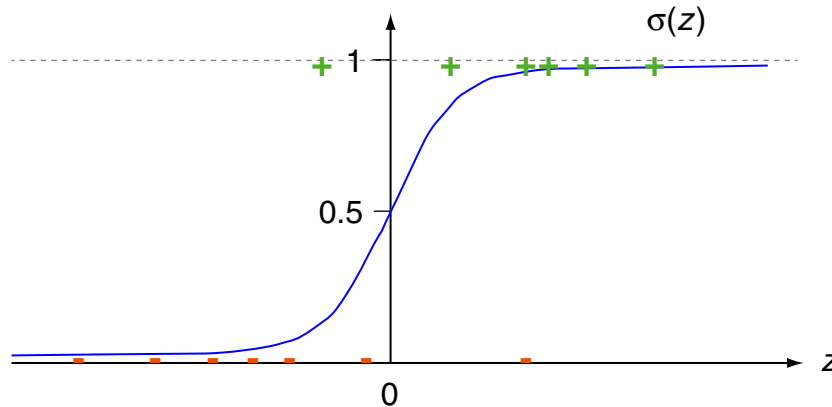
- ❑ Perceptron Learning
- ❑ Multilayer Perceptron Basics
- ❑ Multilayer Perceptron with Two Layers
- ❑ Multilayer Perceptron at Arbitrary Depth
- ❑ **Advanced MLPs**
- ❑ **Automatic Gradient Computation**

# Advanced MLPs

## Output Normalization: Softmax

For two classes ( $k = 2$ ), the scalar sigmoid output  $\sigma(z)$  determines both class probabilities for  $\mathbf{x}$ :  $p(1 \mid \mathbf{x}) := \sigma(z)$  and  $p(0 \mid \mathbf{x}) := 1 - \sigma(z)$ .

$z$  is the dot product of the final layer's weights with the previous layer's output. I.e., for networks with one active layer  $z = \mathbf{w}^T \mathbf{x}$ ; for  $d$  active layers  $z = \mathbf{w}_d^T \mathbf{y}^{h_{d-1}}$ .

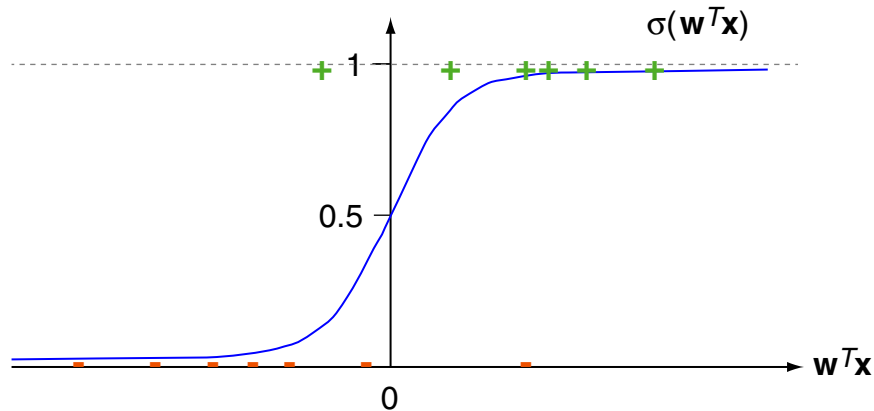


# Advanced MLPs

## Output Normalization: Softmax (continued)

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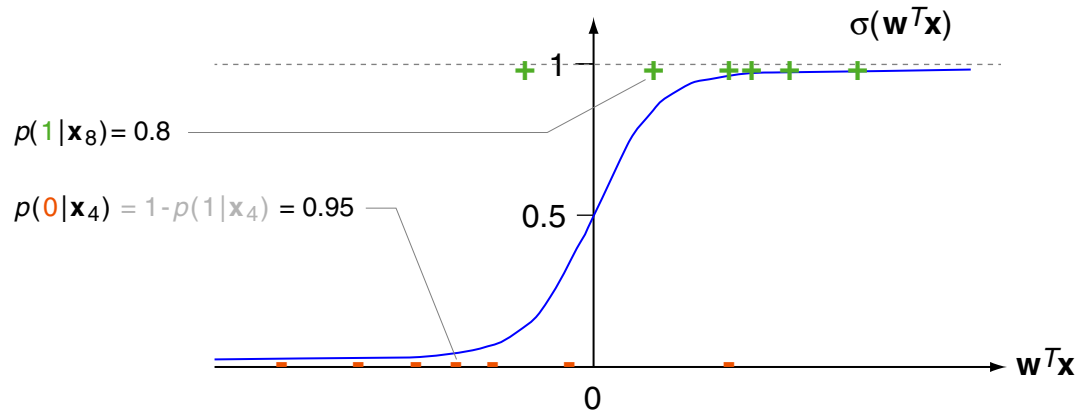


# Advanced MLPs

## Output Normalization: Softmax (continued)

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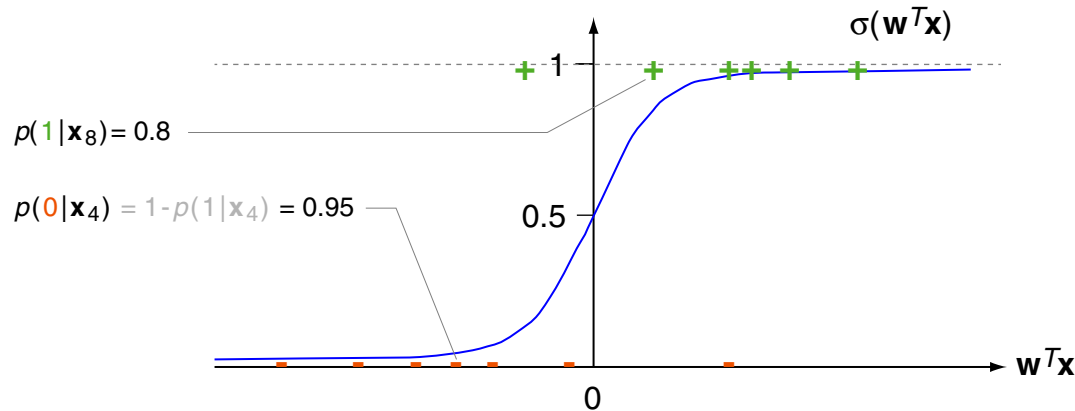


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The softmax function  $\sigma_1 : \mathbf{R}^k \rightarrow \underline{\Delta}^{k-1}$ ,  $\Delta^{k-1} \subset \mathbf{R}^k$ , generalizes the logistic (sigmoid) function to  $k$  dimensions (to  $k$  exclusive classes) [\[Wikipedia\]](#):

$$\sigma_1(\mathbf{z})|_i = \frac{e^{z_i}}{\sum_{j=1}^k e^{z_j}}$$

# Advanced MLPs

## Output Normalization: Softmax (continued)

The class probabilities for the two-class setting can be represented as an equivalent softmax vector:

$$\mathbf{x} \rightarrow \begin{bmatrix} p(0 \mid \mathbf{x}) \\ p(1 \mid \mathbf{x}) \end{bmatrix} = \begin{bmatrix} 1 - \sigma(z) \\ \sigma(z) \end{bmatrix} = \begin{bmatrix} \sigma(-z) \\ \frac{1}{1 + e^{-z}} \end{bmatrix} = \begin{bmatrix} \frac{1}{1 + e^z} \\ \frac{e^z}{1 + e^z} \end{bmatrix} = \begin{bmatrix} \frac{e^0}{e^0 + e^z} \\ \frac{e^z}{e^0 + e^z} \end{bmatrix} = \boldsymbol{\sigma}_1\left(\begin{pmatrix} 0 \\ z \end{pmatrix}\right)$$

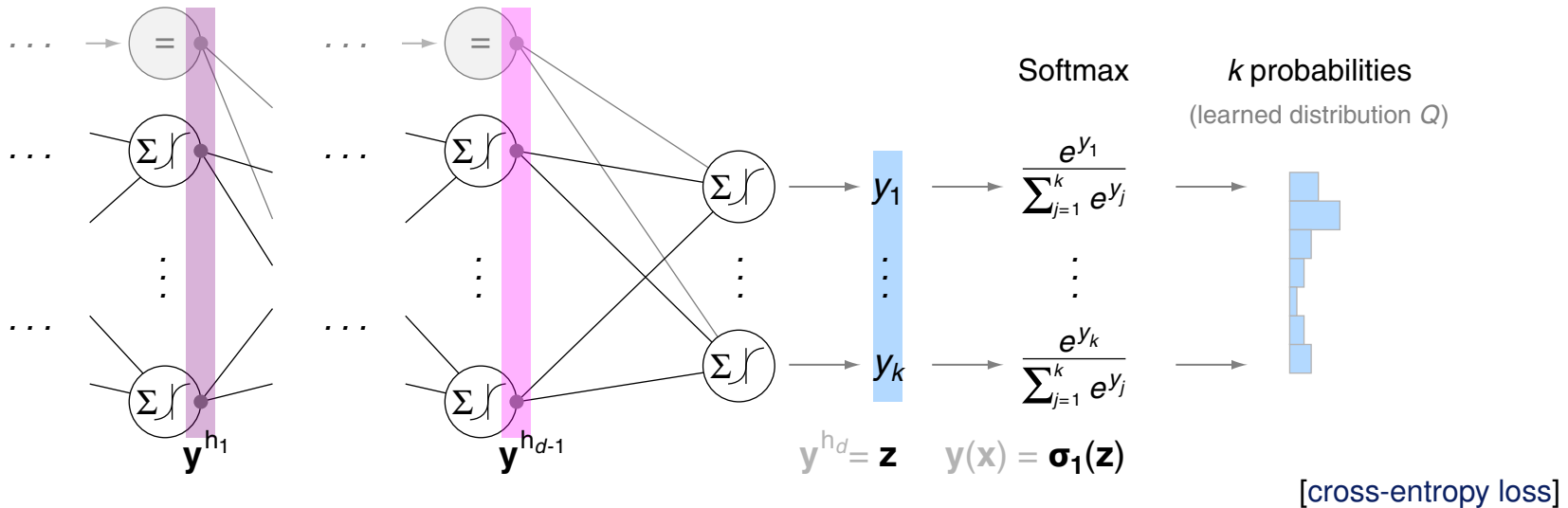
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General case for  $k$  classes:



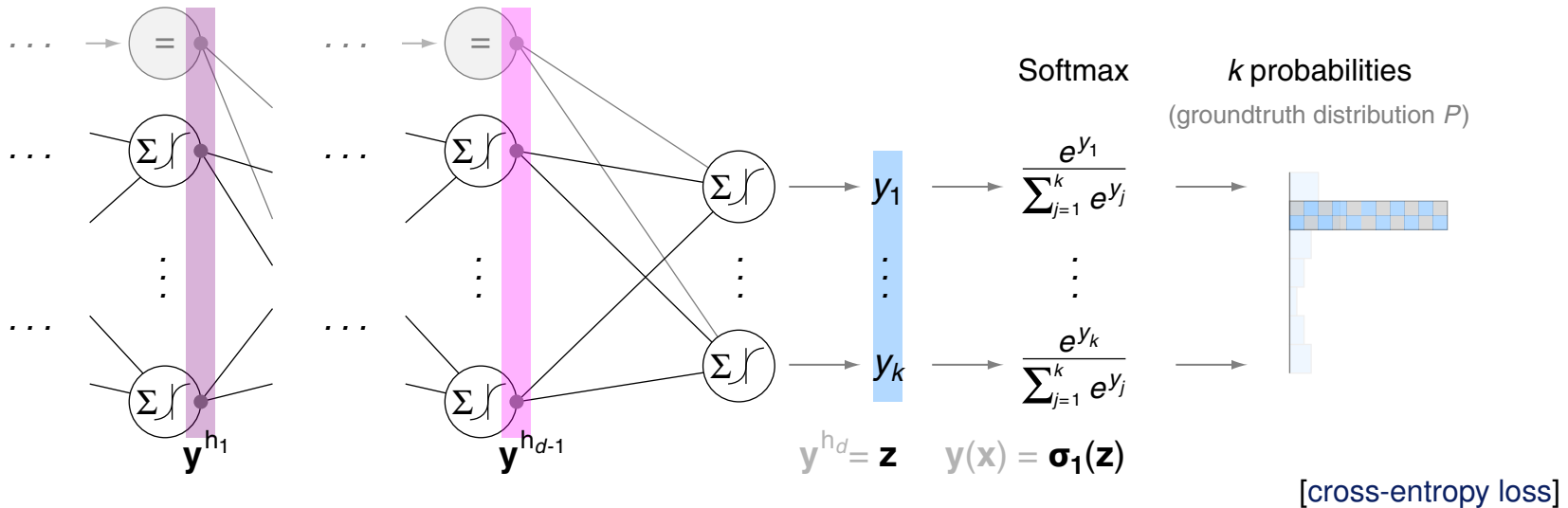
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General case for  $k$  classes:





## Remarks:

- The standard  $k-1$ -simplex contains all  $k$ -tuples with non-negative elements that sum to 1:

$$\Delta^{k-1} = \left\{ (p_1, \dots, p_k) \in \mathbf{R}^k : \sum_{i=1}^k p_i = 1 \text{ and } p_i \geq 0 \text{ for all } i \right\}$$

- The softmax function ensures Axiom I (positivity) and Axiom II (unitarity) of Kolmogorov.

# Advanced MLPs

## Loss Function: Cross-Entropy

### Definition 2 (Cross Entropy)

Let  $C$  be a random variable with distribution  $P$  and a finite number of realizations  $\mathcal{C}$ . Let  $Q$  be another distribution of  $C$ . Then, the cross entropy of distribution  $Q$  relative to the distribution  $P$ , denoted as  $H(P, Q)$ , is defined as follows:

$$H(P, Q) = - \sum_{c \in \mathcal{C}} P(\mathbf{C}=c) \cdot \log (Q(\mathbf{C}=c))$$

# Advanced MLPs

## Loss Function: Cross-Entropy (continued)

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- The cross entropy  $H(P, Q)$  is the average number of *total* bits to represent an event  $C=c$  under the distribution  $Q$  instead of under the distribution  $P$ .
- The relative entropy, also called Kullback-Leibler divergence, is the average number of *additional* bits to represent an event under  $Q$  instead of under  $P$ .

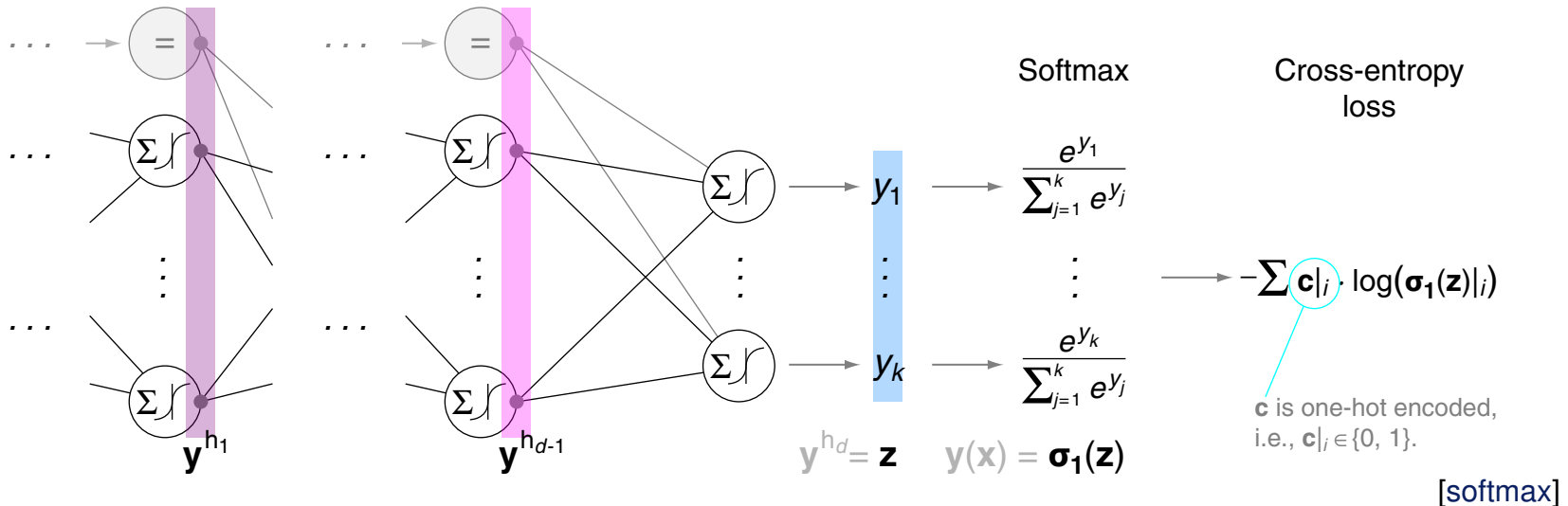
# Advanced MLPs

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# Advanced MLPs

## Cross-Entropy in Classification Settings

[logistic loss: definition, derivation]

$$H(P, Q) = - \sum_{c \in C} P(\mathbf{C}=c) \cdot \log(Q(\mathbf{C}=c))$$

- ❑ Random variable  $\mathbf{C}$  denotes a class.
- ❑ Realizations of  $\mathbf{C}$ :  $C = \{c_1, \dots, c_k\}$ .
- ❑  $P, Q$  define distributions of  $\mathbf{C}$ .

$$H(p, q) = - \sum_{c \in C} p(c) \cdot \log(q(c))$$

- ❑ Probability functions  $p, q$  related to  $P, Q$ .
- ❑ Class labels  $C = \{c_1, \dots, c_k\}$ .

$$l_{\sigma}(z) = -c \cdot \log(\sigma(z)) - (1-c) \cdot \log(1-\sigma(z))$$

- ❑ Two classes encoded as  $c, c \in \{0, 1\}$ .
- ❑ Example with groundtruth  $(\mathbf{x}, c) \in D$ .
- ❑ Classifier output  $\sigma(z), z = y(\mathbf{x})$ .

$$l_{\sigma_1}(\mathbf{z}) = - \sum_{i=1}^k \mathbf{c}|_i \cdot \log(\sigma_1(\mathbf{z})|_i)$$

- ❑  $k$  classes, hot-encoded as  $\mathbf{c}^T$ ,  
 $\mathbf{c}^T \in \{(1, 0, \dots, 0), \dots, (0, \dots, 0, 1)\}$ .
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# Advanced MLPs

## Cross-Entropy in Classification Settings (continued)

[logistic loss: [definition](#), [derivation](#)]

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## Remarks:

- ❑ If not stated otherwise,  $\log$  means  $\log_2$ .
- ❑ Synonyms: cross-entropy loss function, logarithmic loss, log loss, logistic loss.



# Advanced MLPs

Activation Function: Rectified Linear Unit (ReLU)

[*TODO*]

# Advanced MLPs

Regularization: Dropout

[*TODO*]

# Advanced MLPs

## Learning Rate Adaptation: Momentum

Momentum principle: a weight adaptation in iteration  $t$  considers the adaptation in iteration  $t-1$  :

$$\underline{\Delta W^o(t)} = \eta \cdot (\boldsymbol{\delta}^o \otimes \mathbf{y}^h(\mathbf{x})|_{1,\dots,l}) + \alpha \cdot \Delta W^o(t-1)$$

$$\underline{\Delta W^h(t)} = \eta \cdot (\boldsymbol{\delta}^h \otimes \mathbf{x}) + \alpha \cdot \Delta W^h(t-1)$$

$$\underline{\Delta W^{h_s}(t)} = \eta \cdot (\boldsymbol{\delta}^{h_s} \otimes \mathbf{y}^{h_{s-1}}(\mathbf{x})|_{1,\dots,l_{s-1}}) + \alpha \cdot \Delta W^{h_s}(t-1), \quad s = d, d-1, \dots, 2$$

$$\underline{\Delta W^{h_1}(t)} = \eta \cdot (\boldsymbol{\delta}^{h_1} \otimes \mathbf{x}) + \alpha \cdot \Delta W^{h_1}(t-1)$$

The term  $\alpha$ ,  $0 \leq \alpha < 1$ , is called “momentum”.

# Advanced MLPs

## Learning Rate Adaptation: Momentum (continued)

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Effects:

- Due the “adaptation inertia” local minima can be overcome.
- If the direction of the descent does not change, the adaptation increment and, as a consequence, the speed of convergence is increased.

## Remarks:

- Recap. The symbol  $\gg \otimes \ll$  denotes the dyadic product, also called outer product or tensor product. The dyadic product takes two vectors and returns a second order tensor, called a dyadic in this context:  $\mathbf{v} \otimes \mathbf{w} \equiv \mathbf{vw}^T$ . [\[Wikipedia\]](#)

# Chapter ML:IV (continued)

## IV. Neural Networks

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- ❑ Advanced MLPs
- ❑ Automatic Gradient Computation

# Automatic Gradient Computation

## The IGD Algorithm

Algorithm:  $\text{IGD}_{\text{MLP}^*}$  IGD for the  $d$ -layer MLP with arbitrary model and objective functions.  
Input:  $D$  Multiset of examples  $(\mathbf{x}, \mathbf{c})$  with  $\mathbf{x} \in \mathbf{R}^p$ ,  $\mathbf{c} \in \{0, 1\}^k$ .  
 $\eta, l(), R(), \lambda$  Learning rate, loss and regularization functions and parameters.  
Output:  $W^{h_1}, \dots, W^{h_d}$  Weight matrices of the  $d$  layers. (= hypothesis)

```
1. FOR  $s = 1$  TO  $d$  DO initialize_random_weights( $W^{h_s}$ ) ENDDO,  $t = 0$ 
2. REPEAT
3.    $t = t + 1$ 
4.   FOREACH  $(\mathbf{x}, \mathbf{c}) \in D$  DO
5.      $\mathbf{y}^{h_1}(\mathbf{x}) = (\tanh^1_{(W^{h_1} \mathbf{x})})$  // forward propagation;  $\mathbf{x}$  is extended by  $x_0 = 1$ 
     FOR  $s = 2$  TO  $d-1$  DO  $\mathbf{y}^{h_s}(\mathbf{x}) = (\text{ReLU}^1_{(W^{h_s} \mathbf{y}^{h_{s-1}}(\mathbf{x}))})$  ENDDO
      $\mathbf{y}(\mathbf{x}) = \sigma_1(W^{h_d} \mathbf{y}^{h_{d-1}}(\mathbf{x}))$ 
6.      $\delta = \mathbf{c} - \mathbf{y}(\mathbf{x})$ 
7a.     $\ell(\mathbf{w}) = l(\delta) + \frac{\lambda}{n} R(\mathbf{w})$  // backpropagation (Steps 7a+7b)
         $\nabla \ell(\mathbf{w}) = \text{autodiff}(\ell(), \mathbf{w})$ 
7b.    FOR  $s = 1$  TO  $d$  DO  $\Delta W^{h_s} = \eta \cdot \nabla^{h_s} \ell(\mathbf{w})$  ENDDO
8.    FOR  $s = 1$  TO  $d$  DO  $W^{h_s} = W^{h_s} + \Delta W^{h_s}$  ENDDO
9.   ENDDO
10. UNTIL(convergence( $D, \mathbf{y}(\cdot), t$ ))
11. return( $W^{h_1}, \dots, W^{h_d}$ )
```

# Automatic Gradient Computation

## The IGD Algorithm (continued)

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7b.    FOR  $s = 1$  TO  $d$  DO  $\Delta W^{h_s} = \eta \cdot \nabla^{h_s} \ell(\mathbf{w})$  ENDDO
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9.   ENDDO
10. UNTIL(convergence( $D, \mathbf{y}(\cdot), t$ ))
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# Automatic Gradient Computation





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2. REPEAT
3.    $t = t + 1$ 
4.   FOREACH  $(\mathbf{x}, \mathbf{c}) \in D$  DO
5.      Model function evaluation.
6.      Calculation of residual vector.
7a.     Calculation of derivative of the loss.
7b.     Parameter vector update  $\hat{=}$  one gradient step down.
8.   ENDDO
9. UNTIL(convergence( $D, \mathbf{y}(\cdot), t$ ))
11. return( $W^{h_1}, \dots, W^{h_d}$ )
```

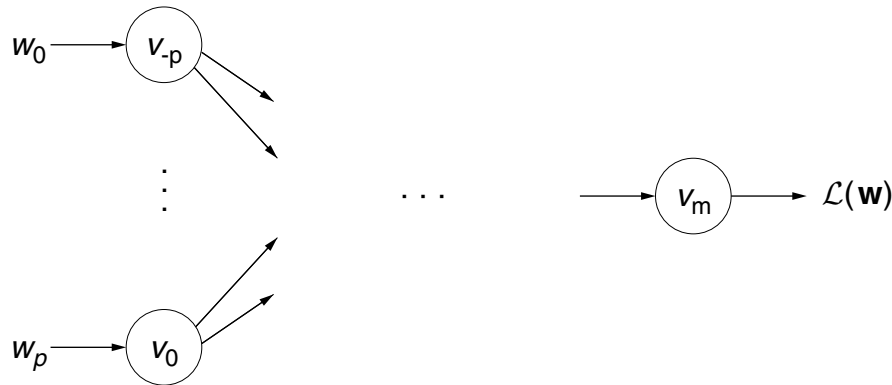
# Automatic Gradient Computation

## Reverse-Mode Automatic Differentiation in Computational Graphs

Reverse-mode AD corresponds to a generalized backpropagation algorithm.

Let  $\mathcal{L}(w_1, \dots, w_p)$  be the function to be differentiated.

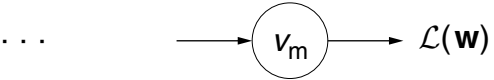
- Consider  $\mathcal{L}$  as a computational graph of elementary operations, assigning each intermediate result to a variable  $v_i$  with  $-p \leq i \leq m$   
(naming convention:  $v_{-p \dots 0}$  for inputs,  $v_{1 \dots m-1}$  for intermediate variables,  $v_m \equiv \mathcal{L}$  for the output)

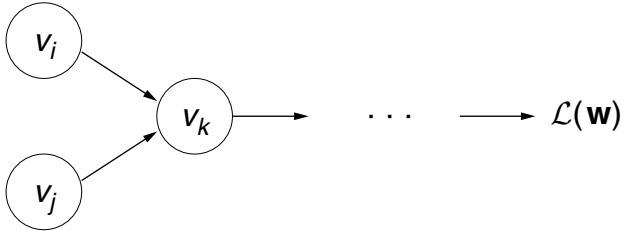


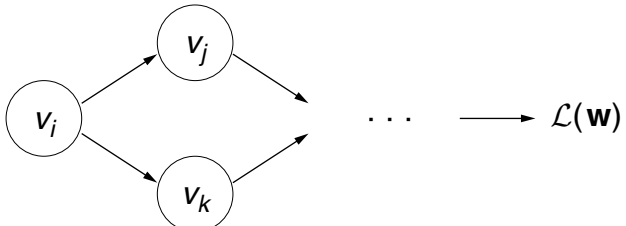
# Automatic Gradient Computation

## Reverse-Mode Automatic Differentiation in Computational Graphs (continued)

For each intermediate variable  $v_i$ , an adjoint value  $\nabla^{v_i} \mathcal{L} \equiv \frac{\partial \mathcal{L}}{\partial v_i}$  is computed based on its descendants in the computation graph.

(1)   $\nabla^{v_m} \mathcal{L} \equiv \frac{\partial \mathcal{L}}{\partial v_m} = \frac{\partial v_m}{\partial v_m} = 1$

(2)  
$$\nabla^{v_i} \mathcal{L} \equiv \frac{\partial \mathcal{L}}{\partial v_i} = \frac{\partial \mathcal{L}}{\partial v_k} \cdot \frac{\partial v_k}{\partial v_i} = \nabla^{v_k} \mathcal{L} \cdot \frac{\partial v_k}{\partial v_i}$$
$$\nabla^{v_j} \mathcal{L} \equiv \frac{\partial \mathcal{L}}{\partial v_j} = \frac{\partial \mathcal{L}}{\partial v_k} \cdot \frac{\partial v_k}{\partial v_j} = \nabla^{v_k} \mathcal{L} \cdot \frac{\partial v_k}{\partial v_j}$$

(3)  
$$\nabla^{v_i} \mathcal{L} = \nabla^{v_j} \mathcal{L} \cdot \frac{\partial v_j}{\partial v_i} + \nabla^{v_k} \mathcal{L} \cdot \frac{\partial v_k}{\partial v_i}$$

## Remarks:

- Adjoints are computed in reverse, starting from  $\nabla^{v_m} \mathcal{L}$ .
- For any step  $v_j = g(\dots, v_i, \dots)$  in the graph, the local gradients  $\frac{\partial g}{\partial v_i}$  must be computable.

# Automatic Gradient Computation

## Autodiff Example: Setting

Consider the RSS loss for a simple logistic regression model and a very small dataset.

Dataset:  $D = \{((1, 1.5)^T, 0), ((1.5, -1)^T, 1)\}$

Model function:  $y(x) = \sigma(\mathbf{w}^T \mathbf{x})$

Loss function:  $\mathcal{L}(\mathbf{w}) = L_2(\mathbf{w}) = \sum_{(\mathbf{x}, c) \in D} (c - y(\mathbf{x}))^2$

$\mathcal{L}(\mathbf{w})$  is the objective function to be minimized, and hence what we want to compute the derivative of; everything except  $\mathbf{w}$  is held constant.

Given the setting above, we can rewrite  $\mathcal{L}$  as:

$$\begin{aligned}\mathcal{L}(\mathbf{w}) &= (c_1 - \sigma(\mathbf{w}^T \mathbf{x}_1))^2 + (c_2 - \sigma(\mathbf{w}^T \mathbf{x}_2))^2 \\ &= (-\sigma(w_0 + w_1 + 1.5w_2))^2 + (1 - \sigma(w_0 + 1.5w_1 - w_2))^2\end{aligned}$$

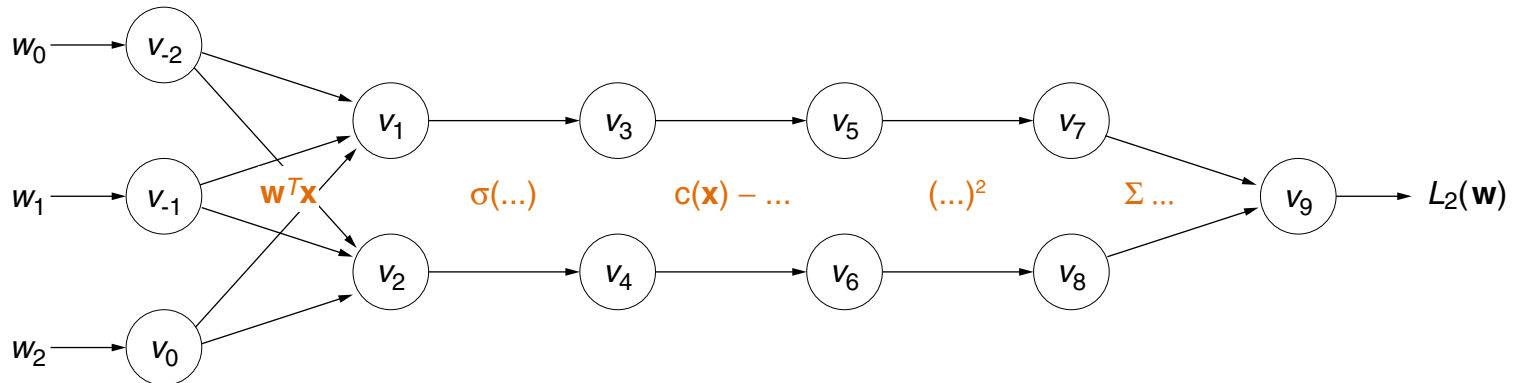
Using reverse-mode automatic differentiation, we'll simultaneously evaluate the loss and its derivative at  $\mathbf{w} = (-1, 1.5, 0.5)^T$ .

# Automatic Gradient Computation

## Autodiff Example: Computational Graph

$$\mathcal{L}(\mathbf{w}) = \underbrace{\underbrace{\underbrace{\underbrace{v_7}_{v_3}}_{v_1}}_{v_5}}_{v_9}^2 + \underbrace{\underbrace{\underbrace{\underbrace{v_8}_{v_4}}_{v_2}}_{v_6}}_{v_9}^2$$

$$\mathcal{L}(\mathbf{w}) = (-\sigma(\underbrace{w_0 + w_1 + 1.5w_2}_{v_1}))^2 + (1 - \sigma(\underbrace{w_0 + 1.5w_1 - w_2}_{v_2}))^2$$



# Automatic Gradient Computation

## Autodiff Example: Forward and Reverse Trace

$$\mathcal{L}(\mathbf{w}) = \underbrace{\underbrace{\underbrace{\underbrace{w_0 + w_1 + 1.5w_2}_{v_1}}_{v_3}}_{v_5}}_{v_7}^2 + \underbrace{\underbrace{\underbrace{\underbrace{w_0 + 1.5w_1 - w_2}_{v_2}}_{v_4}}_{v_6}}_{v_8}^2$$

at

$\mathbf{w} = (-1, 1.5, 0.5)^T$

| Forward primal trace                    |           | Reverse adjoint trace |
|---|-----------|-----------------------|
| $v_0 = w_0$                             | $= -1$    |                       |
| $v_{-1} = w_1$                          | $= 1.5$   |                       |
| $v_{-2} = w_2$                          | $= 0.5$   |                       |
| $v_1 = v_0 + v_{-1} + 1.5 \cdot v_{-2}$ | $= 1.25$  |                       |
| $v_2 = v_0 + 1.5 \cdot v_{-1} - v_{-2}$ | $= 0.75$  |                       |
| $v_3 = \sigma(v_1)$                     | $= 0.78$  |                       |
| $v_4 = \sigma(v_2)$                     | $= 0.68$  |                       |
| $v_5 = 0 - v_3$                         | $= -0.78$ |                       |
| $v_6 = 1 - v_4$                         | $= 0.32$  |                       |
| $v_7 = v_5^2$                           | $= 0.61$  |                       |
| $v_8 = v_6^2$                           | $= 0.1$   |                       |
| $v_9 = v_7 + v_8$                       | $= 0.71$  |                       |
| $\mathcal{L} = v_9$                     | $= 0.71$  |                       |

# Automatic Gradient Computation

## Autodiff Example: Forward and Reverse Trace (continued)

$$\mathcal{L}(\mathbf{w}) = \underbrace{\underbrace{\underbrace{\underbrace{w_0 + w_1 + 1.5w_2}_{v_1}}_{v_3}}_{v_5}}_{v_7}^2 + \underbrace{\underbrace{\underbrace{\underbrace{w_0 + 1.5w_1 - w_2}_{v_2}}_{v_4}}_{v_6}}_{v_8}^2$$

at  $\mathbf{w} = (-1, 1.5, 0.5)^T$

| Forward primal trace                    |           | Reverse adjoint trace  |       |
|---|-----------|--|-------|
| $v_0 = w_0$                             | $= -1$    |  |       |
| $v_{-1} = w_1$                          | $= 1.5$   |  |       |
| $v_{-2} = w_2$                          | $= 0.5$   |  |       |
| $v_1 = v_0 + v_{-1} + 1.5 \cdot v_{-2}$ | $= 1.25$  |  |       |
| $v_2 = v_0 + 1.5 \cdot v_{-1} - v_{-2}$ | $= 0.75$  |  |       |
| $v_3 = \sigma(v_1)$                     | $= 0.78$  |  |       |
| $v_4 = \sigma(v_2)$                     | $= 0.68$  |  |       |
| $v_5 = 0 - v_3$                         | $= -0.78$ |  |       |
| $v_6 = 1 - v_4$                         | $= 0.32$  |  |       |
| $v_7 = v_5^2$                           | $= 0.61$  |  |       |
| $v_8 = v_6^2$                           | $= 0.1$   |  |       |
| $v_9 = v_7 + v_8$                       | $= 0.71$  |  |       |
| $\mathcal{L} = v_9$                     | $= 0.71$  | $\nabla^{v_9} \mathcal{L} = \frac{\partial \mathcal{L}}{\partial v_9}$ | $= 1$ |



# Automatic Gradient Computation

## Autodiff Example: Forward and Reverse Trace (continued)

$$\mathcal{L}(\mathbf{w}) = \underbrace{\underbrace{\underbrace{\underbrace{w_0 + w_1 + 1.5w_2}_{v_1}}_{v_3}}_{v_5}}_{v_7}^2 + \underbrace{\underbrace{\underbrace{w_0 + 1.5w_1 - w_2}_{v_2}}_{v_4}}_{v_6}^2$$

at

$\mathbf{w} = (-1, 1.5, 0.5)^T$

| Forward primal trace                    |           | Reverse adjoint trace   |       |
|---|-----------|---|-------|
| $v_0 = w_0$                             | $= -1$    |   |       |
| $v_{-1} = w_1$                          | $= 1.5$   |   |       |
| $v_{-2} = w_2$                          | $= 0.5$   |   |       |
| $v_1 = v_0 + v_{-1} + 1.5 \cdot v_{-2}$ | $= 1.25$  |   |       |
| $v_2 = v_0 + 1.5 \cdot v_{-1} - v_{-2}$ | $= 0.75$  |   |       |
| $v_3 = \sigma(v_1)$                     | $= 0.78$  |   |       |
| $v_4 = \sigma(v_2)$                     | $= 0.68$  |   |       |
| $v_5 = 0 - v_3$                         | $= -0.78$ |   |       |
| $v_6 = 1 - v_4$                         | $= 0.32$  |   |       |
| $v_7 = v_5^2$                           | $= 0.61$  |   |       |
| $v_8 = v_6^2$                           | $= 0.1$   |   |       |
| $v_9 = v_7 + v_8$                       | $= 0.71$  | $\nabla^{v_8} \mathcal{L} = \nabla^{v_9} \mathcal{L} \cdot \frac{\partial v_9}{\partial v_8} = 1 \cdot 1$ | $= 1$ |
|   |           | $\nabla^{v_7} \mathcal{L} = \nabla^{v_9} \mathcal{L} \cdot \frac{\partial v_9}{\partial v_7} = 1 \cdot 1$ | $= 1$ |
| $\mathcal{L} = v_9$                     | $= 0.71$  | $\nabla^{v_9} \mathcal{L} = \frac{\partial \mathcal{L}}{\partial v_9}$                                    | $= 1$ |

# Automatic Gradient Computation

## Autodiff Example: Forward and Reverse Trace (continued)

$$\mathcal{L}(\mathbf{w}) = \underbrace{\underbrace{\underbrace{\underbrace{v_7}_{w_0 + w_1 + 1.5w_2}}_{v_3}}_{v_1}}_{v_5}^2 + \underbrace{\underbrace{\underbrace{\underbrace{v_8}_{w_0 + 1.5w_1 - w_2}}_{v_4}}_{v_2}}_{v_6}^2$$

at  $\mathbf{w} = (-1, 1.5, 0.5)^T$

| Forward primal trace                    |           | Reverse adjoint trace   |           |
|---|-----------|---|-----------|
| $v_0 = w_0$                             | $= -1$    |   |           |
| $v_{-1} = w_1$                          | $= 1.5$   |   |           |
| $v_{-2} = w_2$                          | $= 0.5$   |   |           |
| $v_1 = v_0 + v_{-1} + 1.5 \cdot v_{-2}$ | $= 1.25$  |   |           |
| $v_2 = v_0 + 1.5 \cdot v_{-1} - v_{-2}$ | $= 0.75$  |   |           |
| $v_3 = \sigma(v_1)$                     | $= 0.78$  |   |           |
| $v_4 = \sigma(v_2)$                     | $= 0.68$  |   |           |
| $v_5 = 0 - v_3$                         | $= -0.78$ | $\nabla^{v_3} \mathcal{L} = \nabla^{v_5} \mathcal{L} \cdot (-1)$  | $= 1.55$  |
| $v_6 = 1 - v_4$                         | $= 0.32$  | $\nabla^{v_4} \mathcal{L} = \nabla^{v_6} \mathcal{L} \cdot (-1)$  | $= -0.64$ |
| $v_7 = v_5^2$                           | $= 0.61$  | $\nabla^{v_5} \mathcal{L} = \nabla^{v_7} \mathcal{L} \cdot \frac{\partial v_7}{\partial v_5} = \nabla^{v_7} \mathcal{L} \cdot 2v_5$ | $= -1.55$ |
| $v_8 = v_6^2$                           | $= 0.1$   | $\nabla^{v_6} \mathcal{L} = \nabla^{v_8} \mathcal{L} \cdot \frac{\partial v_8}{\partial v_6} = \nabla^{v_8} \mathcal{L} \cdot 2v_6$ | $= 0.64$  |
| $v_9 = v_7 + v_8$                       | $= 0.71$  | $\nabla^{v_8} \mathcal{L} = \nabla^{v_9} \mathcal{L} \cdot \frac{\partial v_9}{\partial v_8} = 1 \cdot 1$                           | $= 1$     |
|   |           | $\nabla^{v_7} \mathcal{L} = \nabla^{v_9} \mathcal{L} \cdot \frac{\partial v_9}{\partial v_7} = 1 \cdot 1$                           | $= 1$     |
| $\mathcal{L} = v_9$                     | $= 0.71$  | $\nabla^{v_9} \mathcal{L} = \frac{\partial \mathcal{L}}{\partial v_9}$  | $= 1$     |

# Automatic Gradient Computation

## Autodiff Example: Forward and Reverse Trace (continued)

$$\mathcal{L}(\mathbf{w}) = \underbrace{\underbrace{\underbrace{\underbrace{w_0 + w_1 + 1.5w_2}_{v_1}}_{v_3}}_{v_7}}_{v_5}^2 + \underbrace{\underbrace{\underbrace{w_0 + 1.5w_1 - w_2}_{v_2}}_{v_4}}_{v_6}^2$$

at  $\mathbf{w} = (-1, 1.5, 0.5)^T$

| Forward primal trace                           |           | Reverse adjoint trace   |           |
|--|-----------|---|-----------|
| $v_0 = w_0$                                    | $= -1$    |   |           |
| $v_{-1} = w_1$                                 | $= 1.5$   |   |           |
| $v_{-2} = w_2$                                 | $= 0.5$   |   |           |
| $v_1 = v_0 + v_{-1} + 1.5 \cdot v_{-2} = 1.25$ |           |   |           |
| $v_2 = v_0 + 1.5 \cdot v_{-1} - v_{-2} = 0.75$ |           |   |           |
| $v_3 = \sigma(v_1)$                            | $= 0.78$  | $\nabla^{v_1} \mathcal{L} = \nabla^{v_3} \mathcal{L} \cdot \sigma(v_1) \cdot (1 - \sigma(v_1))$                                     | $= 0.27$  |
| $v_4 = \sigma(v_2)$                            | $= 0.68$  | $\nabla^{v_2} \mathcal{L} = \nabla^{v_4} \mathcal{L} \cdot \sigma(v_2) \cdot (1 - \sigma(v_2))$                                     | $= -0.14$ |
| $v_5 = 0 - v_3$                                | $= -0.78$ | $\nabla^{v_3} \mathcal{L} = \nabla^{v_5} \mathcal{L} \cdot (-1)$  | $= 1.55$  |
| $v_6 = 1 - v_4$                                | $= 0.32$  | $\nabla^{v_4} \mathcal{L} = \nabla^{v_6} \mathcal{L} \cdot (-1)$  | $= -0.64$ |
| $v_7 = v_5^2$                                  | $= 0.61$  | $\nabla^{v_5} \mathcal{L} = \nabla^{v_7} \mathcal{L} \cdot \frac{\partial v_7}{\partial v_5} = \nabla^{v_7} \mathcal{L} \cdot 2v_5$ | $= -1.55$ |
| $v_8 = v_6^2$                                  | $= 0.1$   | $\nabla^{v_6} \mathcal{L} = \nabla^{v_8} \mathcal{L} \cdot \frac{\partial v_8}{\partial v_6} = \nabla^{v_8} \mathcal{L} \cdot 2v_6$ | $= 0.64$  |
| $v_9 = v_7 + v_8$                              | $= 0.71$  | $\nabla^{v_8} \mathcal{L} = \nabla^{v_9} \mathcal{L} \cdot \frac{\partial v_9}{\partial v_8} = 1 \cdot 1$                           | $= 1$     |
|  |           | $\nabla^{v_7} \mathcal{L} = \nabla^{v_9} \mathcal{L} \cdot \frac{\partial v_9}{\partial v_7} = 1 \cdot 1$                           | $= 1$     |
| $\mathcal{L} = v_9$                            | $= 0.71$  | $\nabla^{v_9} \mathcal{L} = \frac{\partial \mathcal{L}}{\partial v_9}$  | $= 1$     |

# Automatic Gradient Computation

## Autodiff Example: Forward and Reverse Trace (continued)

$$\mathcal{L}(\mathbf{w}) = \underbrace{\underbrace{\underbrace{\underbrace{v_7}_{v_3}}_{v_1}}_{v_5}}_{v_9}^2 + \underbrace{\underbrace{\underbrace{\underbrace{v_8}_{v_4}}_{v_2}}_{v_6}}_{v_9}^2 \quad \text{at} \quad \mathbf{w} = (-1, 1.5, 0.5)^T$$

| Forward primal trace                    |           | Reverse adjoint trace   |           |
|---|-----------|---|-----------|
| $v_0 = w_0$                             | $= -1$    |   |           |
| $v_{-1} = w_1$                          | $= 1.5$   |   |           |
| $v_{-2} = w_2$                          | $= 0.5$   |   |           |
| $v_1 = v_0 + v_{-1} + 1.5 \cdot v_{-2}$ | $= 1.25$  | $\nabla^{v_{-2}} \mathcal{L} = \nabla^{v_{-2}} \mathcal{L} + \nabla^{v_1} \mathcal{L} \cdot 1.5$                                    | $= 0.54$  |
|   |           | $\nabla^{v_{-1}} \mathcal{L} = \nabla^{v_{-1}} \mathcal{L} + \nabla^{v_1} \mathcal{L}$  | $= 0.06$  |
|   |           | $\nabla^{v_0} \mathcal{L} = \nabla^{v_0} \mathcal{L} + \nabla^{v_1} \mathcal{L}$  | $= 0.13$  |
| $v_2 = v_0 + 1.5 \cdot v_{-1} - v_{-2}$ | $= 0.75$  | $\nabla^{v_{-2}} \mathcal{L} = \nabla^{v_2} \mathcal{L} \cdot (-1)$   | $= 0.14$  |
|   |           | $\nabla^{v_{-1}} \mathcal{L} = \nabla^{v_2} \mathcal{L} \cdot 1.5$  | $= -0.28$ |
|   |           | $\nabla^{v_0} \mathcal{L} = \nabla^{v_2} \mathcal{L}$   | $= -0.14$ |
| $v_3 = \sigma(v_1)$                     | $= 0.78$  | $\nabla^{v_1} \mathcal{L} = \nabla^{v_3} \mathcal{L} \cdot \sigma(v_1) \cdot (1 - \sigma(v_1))$                                     | $= 0.27$  |
| $v_4 = \sigma(v_2)$                     | $= 0.68$  | $\nabla^{v_2} \mathcal{L} = \nabla^{v_4} \mathcal{L} \cdot \sigma(v_2) \cdot (1 - \sigma(v_2))$                                     | $= -0.14$ |
| $v_5 = 0 - v_3$                         | $= -0.78$ | $\nabla^{v_3} \mathcal{L} = \nabla^{v_5} \mathcal{L} \cdot (-1)$  | $= 1.55$  |
| $v_6 = 1 - v_4$                         | $= 0.32$  | $\nabla^{v_4} \mathcal{L} = \nabla^{v_6} \mathcal{L} \cdot (-1)$  | $= -0.64$ |
| $v_7 = v_5^2$                           | $= 0.61$  | $\nabla^{v_5} \mathcal{L} = \nabla^{v_7} \mathcal{L} \cdot \frac{\partial v_7}{\partial v_5} = \nabla^{v_7} \mathcal{L} \cdot 2v_5$ | $= -1.55$ |
| $v_8 = v_6^2$                           | $= 0.1$   | $\nabla^{v_6} \mathcal{L} = \nabla^{v_8} \mathcal{L} \cdot \frac{\partial v_8}{\partial v_6} = \nabla^{v_8} \mathcal{L} \cdot 2v_6$ | $= 0.64$  |
| $v_9 = v_7 + v_8$                       | $= 0.71$  | $\nabla^{v_8} \mathcal{L} = \nabla^{v_9} \mathcal{L} \cdot \frac{\partial v_9}{\partial v_8} = 1 \cdot 1$                           | $= 1$     |
|   |           | $\nabla^{v_7} \mathcal{L} = \nabla^{v_9} \mathcal{L} \cdot \frac{\partial v_9}{\partial v_7} = 1 \cdot 1$                           | $= 1$     |
| $\mathcal{L} = v_9$                     | $= 0.71$  | $\nabla^{v_9} \mathcal{L} = \frac{\partial \mathcal{L}}{\partial v_9}$  | $= 1$     |

# Automatic Gradient Computation

## Autodiff Example: Forward and Reverse Trace (continued)

$$\mathcal{L}(\mathbf{w}) = \underbrace{\underbrace{\underbrace{\underbrace{v_7}_{v_3}}_{v_1}}_{v_5}}_{v_9}^2 + \underbrace{\underbrace{\underbrace{\underbrace{v_8}_{v_4}}_{v_2}}_{v_6}}_{v_9}^2 \quad \text{at} \quad \mathbf{w} = (-1, 1.5, 0.5)^T$$

| Forward primal trace                    |           | Reverse adjoint trace   |                   |
|---|-----------|---|-------------------|
| $v_0 = w_0$                             | $= -1$    | $\nabla^{w_0} \mathcal{L} = \frac{\partial \mathcal{L}}{\partial w_0} = \nabla^{v_0} \mathcal{L}$                                   | $= \mathbf{0.13}$ |
| $v_{-1} = w_1$                          | $= 1.5$   | $\nabla^{w_1} \mathcal{L} = \frac{\partial \mathcal{L}}{\partial w_1} = \nabla^{v_{-1}} \mathcal{L}$                                | $= \mathbf{0.06}$ |
| $v_{-2} = w_2$                          | $= 0.5$   | $\nabla^{w_2} \mathcal{L} = \frac{\partial \mathcal{L}}{\partial w_2} = \nabla^{v_{-2}} \mathcal{L}$                                | $= \mathbf{0.54}$ |
| $v_1 = v_0 + v_{-1} + 1.5 \cdot v_{-2}$ | $= 1.25$  | $\nabla^{v_{-2}} \mathcal{L} = \nabla^{v_{-2}} \mathcal{L} + \nabla^{v_1} \mathcal{L} \cdot 1.5$                                    | $= 0.54$          |
|   |           | $\nabla^{v_{-1}} \mathcal{L} = \nabla^{v_{-1}} \mathcal{L} + \nabla^{v_1} \mathcal{L}$  | $= 0.06$          |
|   |           | $\nabla^{v_0} \mathcal{L} = \nabla^{v_0} \mathcal{L} + \nabla^{v_1} \mathcal{L}$  | $= 0.13$          |
| $v_2 = v_0 + 1.5 \cdot v_{-1} - v_{-2}$ | $= 0.75$  | $\nabla^{v_{-2}} \mathcal{L} = \nabla^{v_2} \mathcal{L} \cdot (-1)$   | $= 0.14$          |
|   |           | $\nabla^{v_{-1}} \mathcal{L} = \nabla^{v_2} \mathcal{L} \cdot 1.5$  | $= -0.28$         |
|   |           | $\nabla^{v_0} \mathcal{L} = \nabla^{v_2} \mathcal{L}$   | $= -0.14$         |
| $v_3 = \sigma(v_1)$                     | $= 0.78$  | $\nabla^{v_1} \mathcal{L} = \nabla^{v_3} \mathcal{L} \cdot \sigma(v_1) \cdot (1 - \sigma(v_1))$                                     | $= 0.27$          |
| $v_4 = \sigma(v_2)$                     | $= 0.68$  | $\nabla^{v_2} \mathcal{L} = \nabla^{v_4} \mathcal{L} \cdot \sigma(v_2) \cdot (1 - \sigma(v_2))$                                     | $= -0.14$         |
| $v_5 = 0 - v_3$                         | $= -0.78$ | $\nabla^{v_3} \mathcal{L} = \nabla^{v_5} \mathcal{L} \cdot (-1)$  | $= 1.55$          |
| $v_6 = 1 - v_4$                         | $= 0.32$  | $\nabla^{v_4} \mathcal{L} = \nabla^{v_6} \mathcal{L} \cdot (-1)$  | $= -0.64$         |
| $v_7 = v_5^2$                           | $= 0.61$  | $\nabla^{v_5} \mathcal{L} = \nabla^{v_7} \mathcal{L} \cdot \frac{\partial v_7}{\partial v_5} = \nabla^{v_7} \mathcal{L} \cdot 2v_5$ | $= -1.55$         |
| $v_8 = v_6^2$                           | $= 0.1$   | $\nabla^{v_6} \mathcal{L} = \nabla^{v_8} \mathcal{L} \cdot \frac{\partial v_8}{\partial v_6} = \nabla^{v_8} \mathcal{L} \cdot 2v_6$ | $= 0.64$          |
| $v_9 = v_7 + v_8$                       | $= 0.71$  | $\nabla^{v_8} \mathcal{L} = \nabla^{v_9} \mathcal{L} \cdot \frac{\partial v_9}{\partial v_8} = 1 \cdot 1$                           | $= 1$             |
|   |           | $\nabla^{v_7} \mathcal{L} = \nabla^{v_9} \mathcal{L} \cdot \frac{\partial v_9}{\partial v_7} = 1 \cdot 1$                           | $= 1$             |
| $\mathcal{L} = v_9$                     | $= 0.71$  | $\nabla^{v_9} \mathcal{L} = \frac{\partial \mathcal{L}}{\partial v_9}$  | $= 1$             |

## Remarks:

- For brevity, in the example, we assumed that the derivative  $\frac{\partial}{\partial z}\sigma(z) = \sigma(z) \cdot (1 - \sigma(z))$  is already known. We could also have decomposed  $\sigma(z) = \frac{1}{1+\exp(-z)}$  into e.g.,  $v_1 = -z$ ,  $v_2 = \exp(v_1)$ ,  $v_3 = 1 + v_2$ ,  $v_4 = \frac{1}{v_3}$ . In this case, only the four atomic derivatives would need to be known.
- The function to be automatically differentiated need not have a closed-form representation; it only has to be composed of computable and differentiable atomic steps. Thus, AD can also compute derivatives for various algorithms that may take different branches depending on the input.

# Automatic Gradient Computation

## Reverse-mode Autodiff Algorithm for Scalar-valued Functions

Algorithm: autodiff      Reverse-mode automatic differentiation

Input:  $f : \mathbf{R}^p \rightarrow \mathbf{R}$       Function to differentiate.  
 $(w_1, \dots, w_p)^T$       Point at which the gradient should be evaluated

Output:  $(\bar{w}_1, \dots, \bar{w}_p)^T$       Gradient of  $f$  at the point  $(w_1, \dots, w_p)^T$ .

```
1.  $\bar{w}_i = 0$  for  $i$  in  $1 \dots p$                                 // initialize gradients
2.  $v_1, \dots, v_k = \text{operands}(f)$ 
3.  $\frac{\partial f}{\partial v_1}, \dots, \frac{\partial f}{\partial v_k} = \text{gradients}(f)$     // gradient of  $f$  wrt. its immediate operands
4. FOREACH  $j = 1, \dots, k$  DO
5.     IF  $v_j \in \{w_1, \dots, w_p\}$  THEN
6.          $\bar{v}_j += \frac{\partial f}{\partial v_j}$ 
7.     ELSE
8.          $(\bar{w}_1, \dots, \bar{w}_p)^T += \frac{\partial f}{\partial v_j} \cdot \text{autodiff}(v_j, (w_1, \dots, w_p)^T)$ 
9. RETURN  $(\bar{w}_1, \dots, \bar{w}_p)^T$ 
```

## Remarks:

- There exists also a forward mode of automatic differentiation. One key difference is in the runtime complexity; for a function  $f : \mathbf{R}^n \rightarrow \mathbf{R}^m$ , to compute all  $n \cdot m$  partial derivatives in the Jacobian matrix requires  $O(n)$  iterations in forward mode and  $O(m)$  iterations in reverse mode. Reverse mode is usually preferred in machine learning, where we typically have  $m = 1$  (a scalar loss), and  $n$  arbitrarily large (e.g., billions of parameters of a deep neural network). See also [\[Baydin et al., 2018\]](#).