Chapter ML:IV

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

Loss Function: Cross-Entropy

Definition 2 (Cross-Entropy)

Let *C* be a random variable with distribution P and a finite number of realizations 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:

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

Advanced MLPs

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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, $D_{\text{KL}}(P \,||\, Q)$, is the average number of *additional* bits to represent an event under Q instead of under P.

Advanced MLPs

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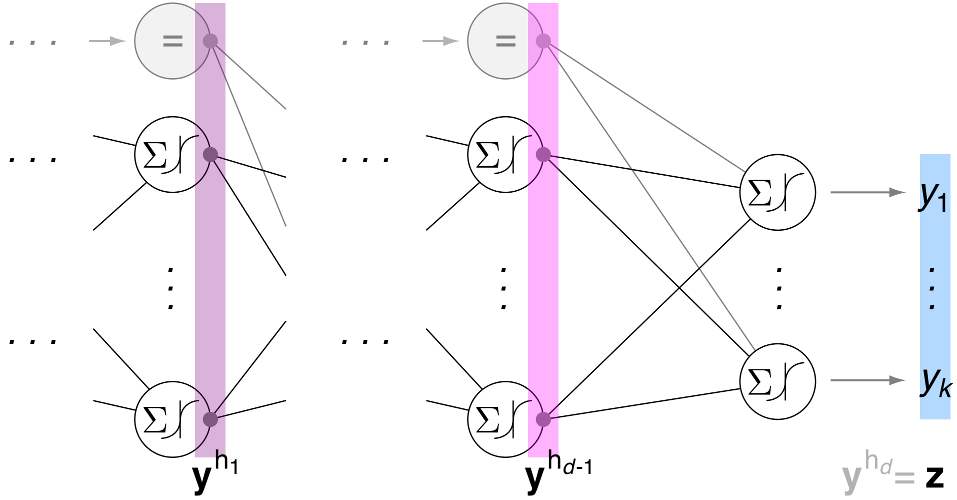
Multi-layer perceptron for k classes: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=
Σ∫
⋮
$\mathbf{y}^{\mathrm{h}_1}$
$\mathbf{y}^{\mathrm{h}_{d\text{-}1}}$
y_1
y_k
$\mathbf{y}^{\mathrm{h}_d} = \mathbf{z}$

Advanced MLPs

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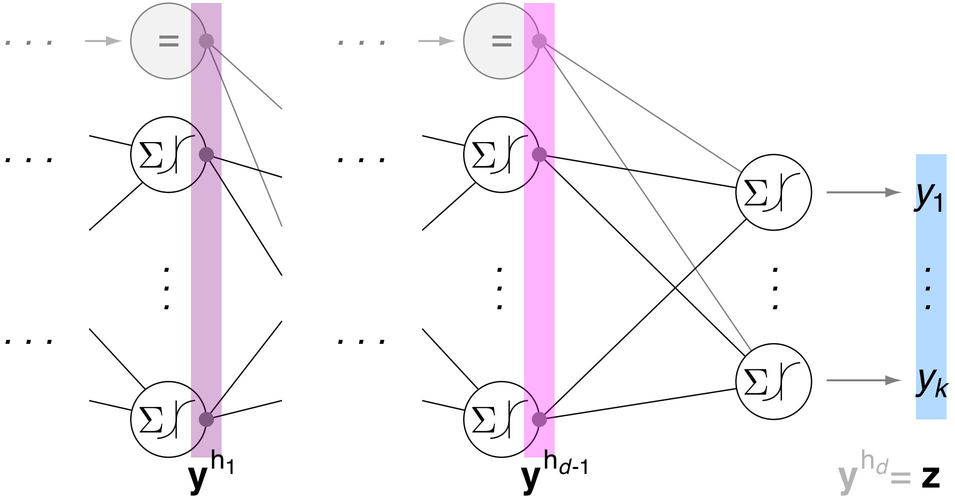
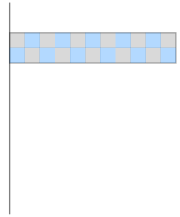


k probabilities

(groundtruth distribution P)



Advanced MLPs

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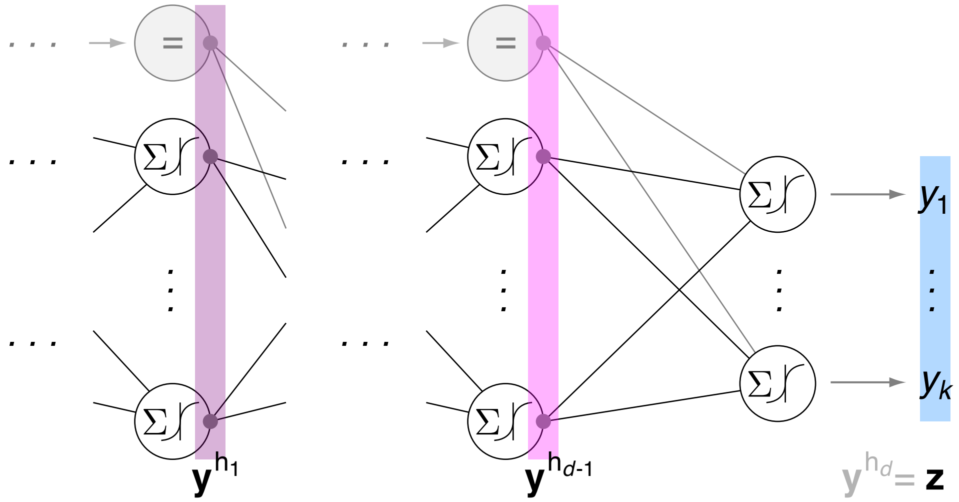
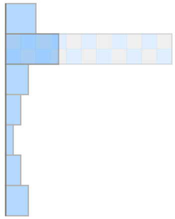
Multi-layer perceptron for k classes:



k probabilities

(learned distribution *Q*)



Advanced MLPs

Loss Function: Cross-Entropy

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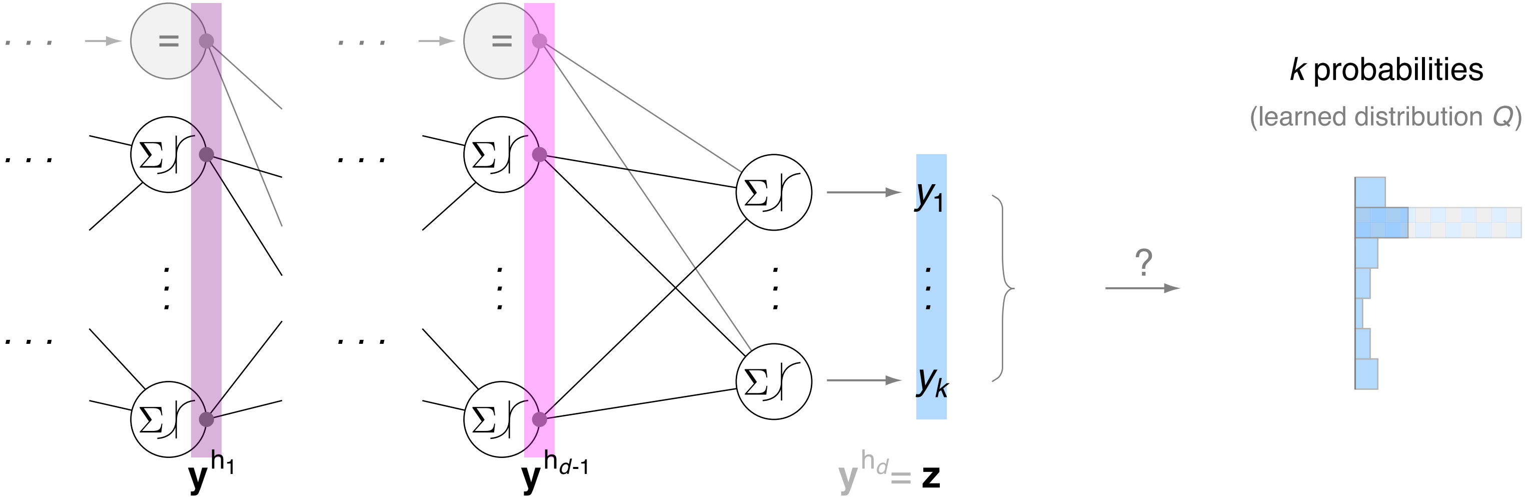
Multi-layer perceptron for k classes:



. . .
=
Σ
$\mathbf{y}^{\mathrm{h}_1}$
$\mathbf{y}^{\mathrm{h}_{d\text{-}1}}$
y_1
y_k
$\mathbf{y}^{\mathrm{h}_d} = \mathbf{z}$
?
k probabilities
(learned distribution *Q*)

Remarks (cross-entropy, Kullback-Leibler divergence) :

- Cross-entropy = (self-)entropy + Kullback-Leibler divergence

$$\underline{H(p, q)} = \underline{H(p)} + \underline{D_{\mathsf{KL}}(p \,||\, q)}$$

- Notation. The argument(s) of $H()$ and $D_{\mathsf{KL}}()$ vary in different definitions.

  We use large letters to denote probability distributions (probability measures), whose arguments in turn are events. For instance, $Q(\mathsf{C}{=}c)$ denotes the probability of the event $\mathsf{C}{=}c$, with random variable *C* and realization c; $q(c)$ denotes the related probability mass function. Both notations can be used interchangeably. See section Evaluating Effectiveness in part Machine Learning Basics.

  It is also common to use the random variable as argument of the entropy, i.e., *C* in our example. Hence, one will find the expressions $H(Q)$, $H(q)$, and $H(\mathsf{C})$ all of which denoting the same entropy.

Advanced MLPs

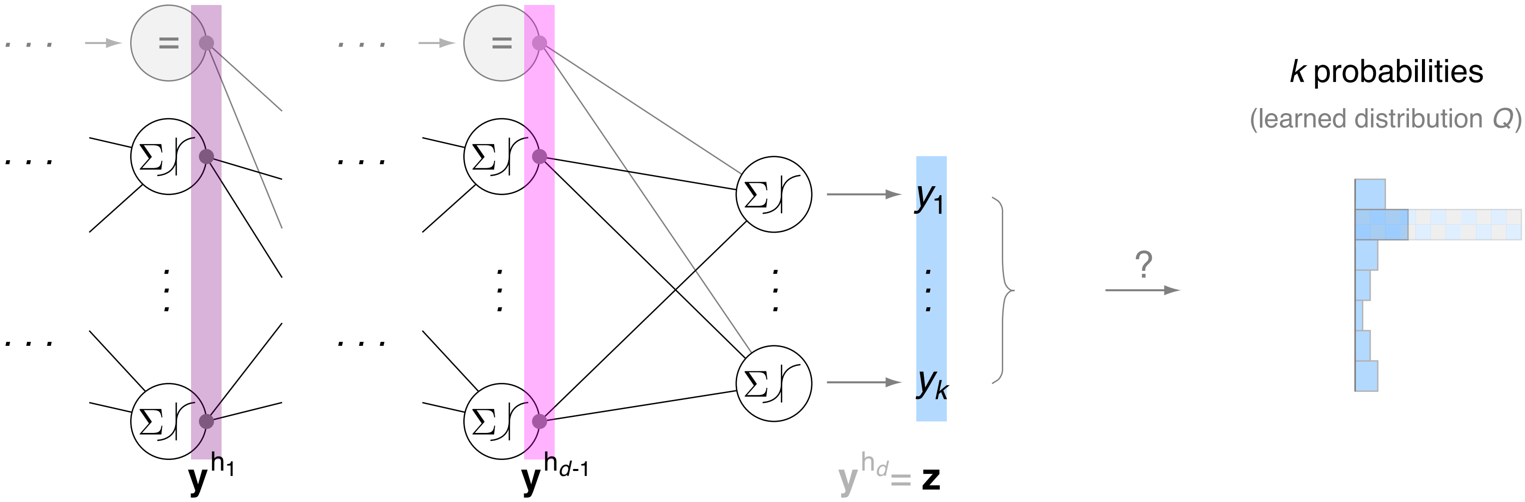
Output Normalization: Softmax [Wikipedia]

Definition 3 (Softmax)

The softmax function $\boldsymbol{\sigma}_\Delta : \mathbf{R}^k \to \Delta^{k-1}$, $\Delta^{k-1} \subset \mathbf{R}^k$, generalizes the logistic (sigmoid) function to k dimensions or k exclusive classes:

$$\boldsymbol{\sigma}_\Delta(\mathbf{z})\big|_i = \frac{e^{z_i}}{\sum_{j=1}^{k} e^{z_j}}$$

Multi-layer perceptron for k classes:



Advanced MLPs

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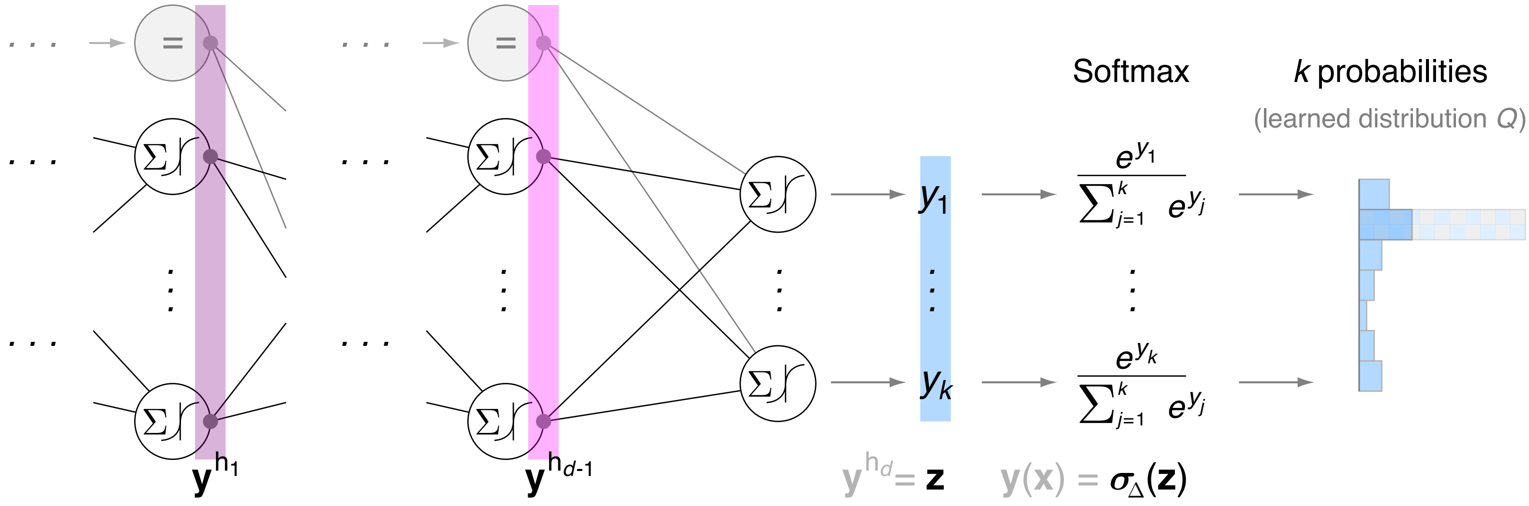

$\mathbf{y}^{\mathrm{h}_1}$
$\mathbf{y}^{\mathrm{h}_{d\text{-}1}}$
y_1
y_k
Softmax
$\frac{e^{y_1}}{\sum_{j=1}^k e^{y_j}}$
$\frac{e^{y_k}}{\sum_{j=1}^k e^{y_j}}$
k probabilities
(learned distribution *Q*)
$\mathbf{y}^{\mathrm{h}_d} = \mathbf{z}$
$\mathbf{y}(\mathbf{x}) = \boldsymbol{\sigma}_\Delta(\mathbf{z})$

Advanced MLPs

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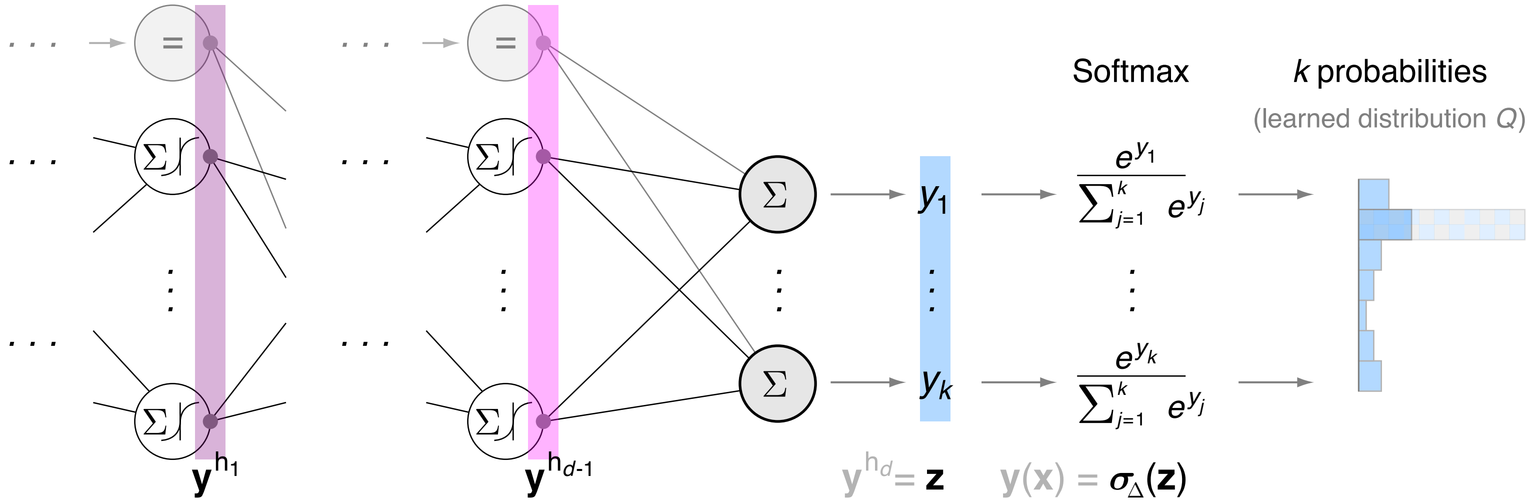

Softmax
k probabilities
(learned distribution Q)
=
Σ
$\mathbf{y}^{h_1}$
$\mathbf{y}^{h_{d-1}}$
y_1
y_k
$\frac{e^{y_1}}{\sum_{j=1}^{k} e^{y_j}}$
$\frac{e^{y_k}}{\sum_{j=1}^{k} e^{y_j}}$
$\mathbf{y}^{h_d} = \mathbf{z}$
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Advanced MLPs

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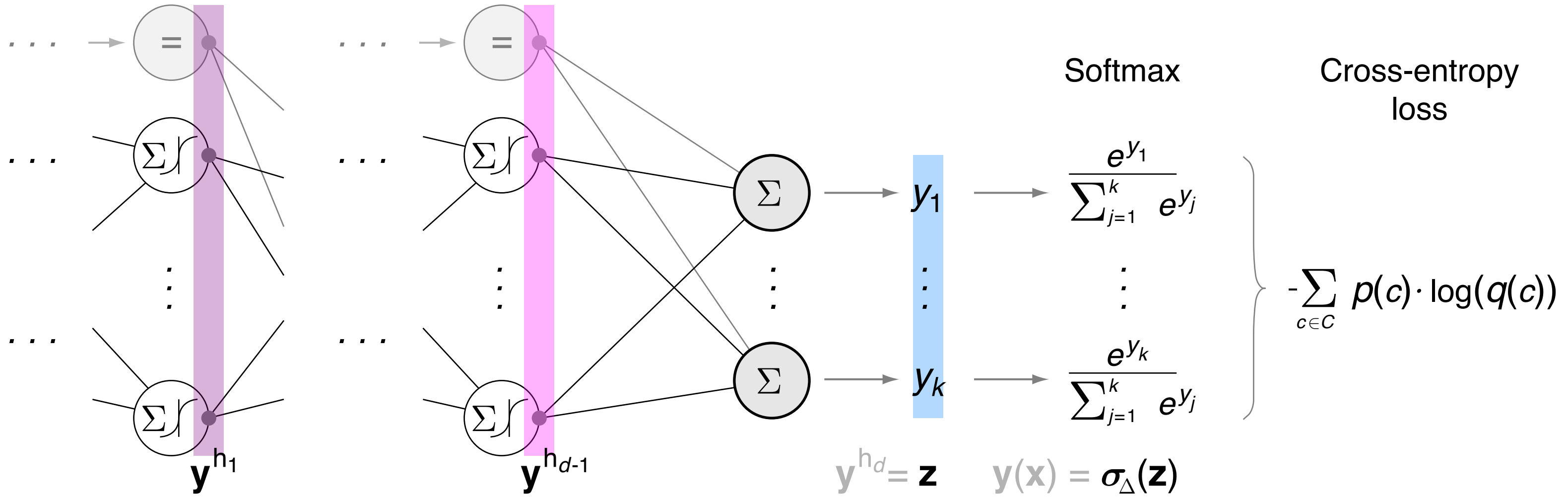
Softmax
Cross-entropy loss
$=$
Σ
y_1
y_k
$\frac{e^{y_1}}{\sum_{j=1}^{k} e^{y_j}}$
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$-\sum_{c \in C} p(c) \cdot \log(q(c))$
$\mathbf{y}^{h_1}$
$\mathbf{y}^{h_{d-1}}$
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Advanced MLPs

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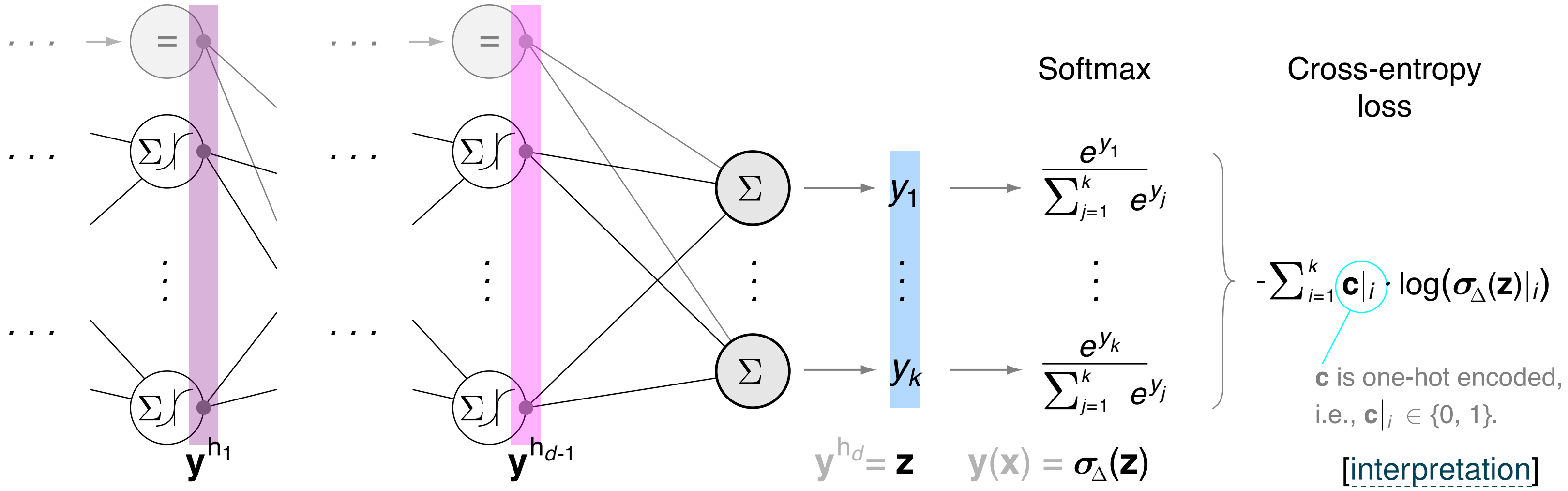
Multi-layer perceptron for k classes:



Softmax

$\dfrac{e^{y_1}}{\sum_{j=1}^{k} e^{y_j}}$

$\vdots$

$\dfrac{e^{y_k}}{\sum_{j=1}^{k} e^{y_j}}$

$\mathbf{y}(\mathbf{x}) = \boldsymbol{\sigma}_\Delta(\mathbf{z})$

Cross-entropy loss

$-\sum_{i=1}^{k} \mathbf{c}|_i \cdot \log(\boldsymbol{\sigma}_\Delta(\mathbf{z})|_i)$

c is one-hot encoded, i.e., $\mathbf{c}|_i \in \{0, 1\}$.

[interpretation]

Remarks (softmax) :

- The standard $k-1$-simplex, denoted as Δ^{k-1}, contains all k-tuples with non-negative elements that sum to 1:

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

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

- Note that the softmax operation increases the (relative) distances between the maximum value and all other values, forcing a clear class decision. Hence a softmax normalization is not suitable for multi-label classification where multiple nonexclusive labels may be assigned to an instance.

- If not stated otherwise, $\log$ means $\log_2$.

- $|_i$ (in $\mathbf{c}|_i$ as well as in $\boldsymbol{\sigma}_{\triangle}(\mathbf{z})|_i$) denotes the projection operator, which returns the ith vector component (dimension) of $\mathbf{c}$, $\mathbf{c} = (c_1, \ldots, c_k)$, or of $\boldsymbol{\sigma}_{\triangle}(\mathbf{z})$.

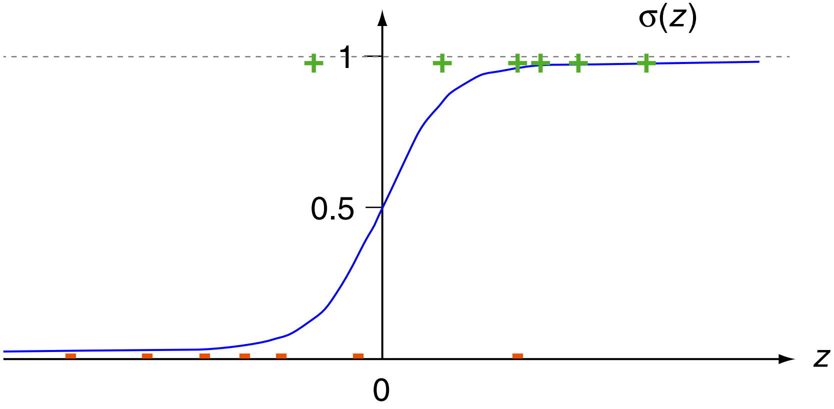
Advanced MLPs

Relation to Logistic Regression

For two classes ($k = 2$), the scalar sigmoid output $\sigma(z)$, determines both class probabilities for $\mathbf{x}$:

- $p(1 \mid \mathbf{x}) := \sigma(z)$
- $p(0 \mid \mathbf{x}) := 1 - \sigma(z)$

The variable z is the dot product of the final layer's weights with the previous layer's output; 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

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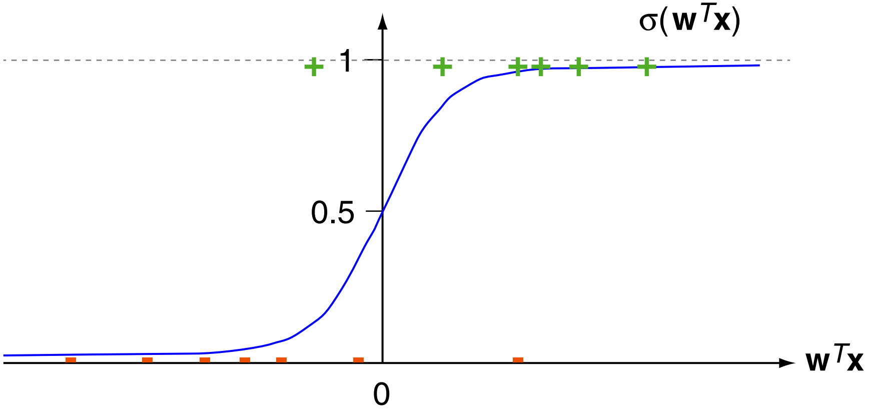

Advanced MLPs

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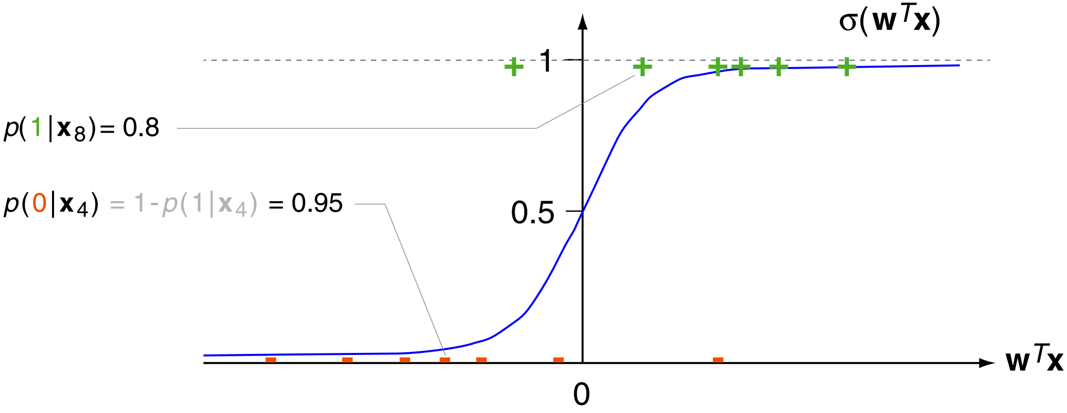

Remarks (softmax and logistic regression) :

- Compare (a) a single sigmoid output, which is interpreted as class 1 probability, and (b) two sigmoid outputs, which are normalized via softmax and interpreted as class 1 and class 2 probabilities.

- The single output in the two-class setting, the class 1 probability $\sigma(z)$, $z = \mathbf{w}^T\mathbf{x}$, can be rewritten as softmax vector that comprises both class probabilities:

$$\mathbf{x} \;\rightarrow\; \begin{bmatrix} \sigma(z) \\ 1-\sigma(z) \end{bmatrix} =: \begin{bmatrix} p(1 \mid \mathbf{x}) \\ p(0 \mid \mathbf{x}) \end{bmatrix} = \begin{bmatrix} \sigma(z) \\ \sigma(-z) \end{bmatrix} \overset{z = z_1 - z_2}{\overset{\downarrow}{=}} \begin{bmatrix} \frac{1}{1+e^{z_2-z_1}} \\ \frac{1}{1+e^{z_1-z_2}} \end{bmatrix} \overset{\text{expand by } e^{z_1},\, e^{z_2}}{\overset{\downarrow}{=}} \begin{bmatrix} \frac{e^{z_1}}{e^{z_1}+e^{z_2}} \\ \frac{e^{z_2}}{e^{z_2}+e^{z_1}} \end{bmatrix} = \boldsymbol{\sigma}_{\Delta}\left(\binom{z_1}{z_2}\right) =: \begin{bmatrix} p(1 \mid \mathbf{x}) \\ p(0 \mid \mathbf{x}) \end{bmatrix}$$

  The transformation shows the correspondence of the (a) logistic regression classifier and (b) a k-class architecture with $k = 2$ that is normalized with the softmax function.

Advanced MLPs

Cross-Entropy in Classification Settings

[logistic loss: definition, derivation]

The following expressions are per example $(\mathbf{x}, c) \in D$ and compute the same quantity: the point-wise cross-entropy loss.

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

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

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Advanced MLPs

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$$l_{\boldsymbol{\sigma}_\Delta}(\mathbf{c}, \mathbf{y}(\mathbf{x})) = -\sum_{i=1}^{k} \mathbf{c}|_i \cdot \log\big(\, \boldsymbol{\sigma}_\Delta(\mathbf{z})|_i \,\big)$$

- ❑ k classes, one-hot encoded as $\mathbf{c}^T$, $\mathbf{c}^T \in \{(1,0,\ldots,0), \ldots, (0,\ldots,0,1)\}$.
- ❑ Example with ground truth $(\mathbf{x}, \mathbf{c}) \in D$.
- ❑ Classifier output $\mathbf{y}(\mathbf{x}) = \boldsymbol{\sigma}_\Delta(\mathbf{z})$, $\mathbf{z} = \mathbf{y}^{h_d}$.

Advanced MLPs

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Advanced MLPs

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Advanced MLPs

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- ❑ Classifier output $\mathbf{y}(\mathbf{x}) = \boldsymbol{\sigma}_\Delta(\mathbf{z})$, $\mathbf{z} = \mathbf{y}^{h_d}$.

$$l_\sigma(c, y(\mathbf{x})) = -c \cdot \log\big(\sigma(z)\big) - (1-c) \cdot \log\big(1 - \sigma(z)\big)$$

- ❑ 2 classes encoded as c, $c \in \{0, 1\}$.
- ❑ Example with ground truth $(\mathbf{x}, c) \in D$.
- ❑ Classifier output $y(\mathbf{x}) = \sigma(z)$, $z = \mathbf{w}^T\mathbf{x}$.

Remarks (cross-entropy for classification) :

- In logistic regression, we derived the logistic loss (function) under the probabilistic framework of maximum likelihood estimation; in the derivation, the log likelihood function is inverted and becomes the negative log likelihood function (see Hint (3)).

  Synonyms for the logistic loss function are logarithmic loss, log loss, and negative log likelihood.

- Cross-entropy is not logistic loss, but both functions calculate the same quantity when used as loss functions for classification problems.

  Note that c (in the two-class setting) or $\mathbf{c}|_i$ (in the general case) is either 0 or 1, which can be interpreted as occurrence probability of the respective class (if no label noise is given); a similar argument applies to the functions $\sigma(z)$ and the elements of $\boldsymbol{\sigma}_{\Delta}(\mathbf{z})$, which are interpreted as class probabilities as well.

  Under this interpretation, the logistic loss can be rewritten as cross-entropy (and vice versa):

$$
\begin{aligned}
l_\sigma(c, y(\mathbf{x})) = l_\sigma(c, \sigma(z)) &= -c \cdot \log(\sigma(z)) - (1-c) \cdot \log(1-\sigma(z)) \\
&= -(c \cdot \log(\sigma(z)) + (1-c) \cdot \log(1-\sigma(z))) \\
&= -(p(c_1) \cdot \log(q(c_1)) + p(c_2) \cdot \log(q(c_2))) \\
&= -\textstyle\sum_{c \in C} p(c) \cdot \log(q(c)) \;=\; H(p, q)
\end{aligned}
$$

  Hence, the cross-entropy loss in the MLP illustration can be (and is here) noted as logistic loss.

Advanced MLPs

Activation Function: Rectified Linear Unit (ReLU)

$\rightsquigarrow$ *BOARD*

Advanced MLPs

Regularization: Dropout

$\leadsto$ *BOARD*

Advanced MLPs

Learning Rate Adaptation: Momentum

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

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

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

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

$$\underline{\Delta W^{\mathsf{h}_1}(t)} = \eta \cdot (\boldsymbol{\delta}^{\mathsf{h}_1} \otimes \mathbf{x}) + \alpha \cdot \Delta W^{\mathsf{h}_1}(t{-}1)$$

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

Advanced MLPs

Learning Rate Adaptation: Momentum

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

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

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

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

$$\underline{\Delta W^{\mathsf{h}_1}(t)} = \eta \cdot (\boldsymbol{\delta}^{\mathsf{h}_1} \otimes \mathbf{x}) + \alpha \cdot \Delta W^{\mathsf{h}_1}(t{-}1)$$

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

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 »$\otimes$« 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: $\mathbf{v} \otimes \mathbf{w} \equiv \mathbf{v}\mathbf{w}^T$. [Wikipedia]

Chapter ML:IV

IV. Neural Networks

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

Automatic Gradient Computation

The IGD Algorithm

Algorithm: 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 $\mathbf{x} \in \mathbf{R}^p$, $\mathbf{c} \in \{0,1\}^k$.
η, $l()$, $R()$, λ Learning rate, loss and regularization functions and parameters.
Output: $W^{\mathsf{h}_1}, \ldots, W^{\mathsf{h}_d}$ Weight matrices of the d layers. (= hypothesis)

```
 1.  FOR $s = 1$ TO $d$ DO *initialize_random_weights*$(W^{\mathsf{h}_s})$ ENDDO, $t = 0$
 2.  REPEAT
 3.    $t = t + 1$
 4.    FOREACH $(\mathbf{x}, \mathbf{c}) \in D$ DO
 5.      $\mathbf{y}^{\mathsf{h}_1}(\mathbf{x}) = \begin{pmatrix} 1 \\ \mathbf{tanh}(W^{\mathsf{h}_1}\mathbf{x}) \end{pmatrix}$ // forward propagation; $\mathbf{x}$ is extended by $x_0 = 1$
         FOR $s = 2$ TO $d{-}1$ DO $\mathbf{y}^{\mathsf{h}_s}(\mathbf{x}) = \begin{pmatrix} 1 \\ \mathbf{ReLU}(W^{\mathsf{h}_s}\mathbf{y}^{\mathsf{h}_{s-1}}(\mathbf{x})) \end{pmatrix}$ ENDDO
         $\mathbf{y}(\mathbf{x}) = \boldsymbol{\sigma}_\Delta(W^{\mathsf{h}_d}\mathbf{y}^{\mathsf{h}_{d-1}}(\mathbf{x}))$
 6.      $\boldsymbol{\delta} = \mathbf{c} - \mathbf{y}(\mathbf{x})$
7a.      $\ell(\mathbf{w}) = l(\boldsymbol{\delta}) + \frac{\lambda}{n} R(\mathbf{w})$ // backpropagation (Steps 7a+7b)
         $\nabla \ell(\mathbf{w}) = \text{autodiff}(\ell(), \mathbf{w})$
7b.      FOR $s = 1$ TO $d$ DO $_\Delta W^{\mathsf{h}_s} = \eta \cdot \nabla^{\mathsf{h}_s} \ell(\mathbf{w})$ ENDDO
 8.      FOR $s = 1$ TO $d$ DO $W^{\mathsf{h}_s} = W^{\mathsf{h}_s} + {_\Delta}W^{\mathsf{h}_s}$ ENDDO
 9.    ENDDO
10.  UNTIL(*convergence*$(D, \mathbf{y}(\cdot), t)$)
11.  *return*$(W^{\mathsf{h}_1}, \ldots, W^{\mathsf{h}_d})$
```

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 $\mathbf{x} \in \mathbf{R}^p$, $\mathbf{c} \in \{0,1\}^k$.

η, $l()$, $R()$, λ Learning rate, loss and regularization functions and parameters.

Output: $W^{\mathsf{h}_1}, \ldots, W^{\mathsf{h}_d}$ Weight matrices of the d layers. (= hypothesis)

```
 1.  FOR $s = 1$ TO $d$ DO *initialize_random_weights*$(W^{\mathsf{h}_s})$ ENDDO, $t = 0$
 2.  REPEAT
 3.    $t = t + 1$
 4.    FOREACH $(\mathbf{x}, \mathbf{c}) \in D$ DO
 5.      $\mathbf{y}^{\mathsf{h}_1}(\mathbf{x}) = \left(\begin{smallmatrix} 1 \\ \tanh(W^{\mathsf{h}_1}\mathbf{x}) \end{smallmatrix}\right)$ // forward propagation; $\mathbf{x}$ is extended by $x_0 = 1$
         FOR $s = 2$ TO $d{-}1$ DO $\mathbf{y}^{\mathsf{h}_s}(\mathbf{x}) = \left(\begin{smallmatrix} 1 \\ \text{ReLU}(W^{\mathsf{h}_s}\mathbf{y}^{\mathsf{h}_{s-1}}(\mathbf{x})) \end{smallmatrix}\right)$ ENDDO
         $\mathbf{y}(\mathbf{x}) = \boldsymbol{\sigma}_{\Delta}(W^{\mathsf{h}_d}\,\mathbf{y}^{\mathsf{h}_{d-1}}(\mathbf{x}))$
 6.      $\boldsymbol{\delta} = \mathbf{c} - \mathbf{y}(\mathbf{x})$
7a.      $\ell(\mathbf{w}) = l(\boldsymbol{\delta}) + \frac{\lambda}{n} R(\mathbf{w})$ // backpropagation (Steps 7a+7b)
         $\nabla\ell(\mathbf{w}) = \text{autodiff}(\ell(), \mathbf{w})$
7b.      FOR $s = 1$ TO $d$ DO $_{\Delta}W^{\mathsf{h}_s} = \eta \cdot \nabla^{\mathsf{h}_s}\ell(\mathbf{w})$ ENDDO
 8.      FOR $s = 1$ TO $d$ DO $W^{\mathsf{h}_s} = W^{\mathsf{h}_s} + {_{\Delta}W^{\mathsf{h}_s}}$ ENDDO
 9.    ENDDO
10.  UNTIL(*convergence*$(D, \mathbf{y}(\,\cdot\,), t)$)
11.  *return*$(W^{\mathsf{h}_1}, \ldots, W^{\mathsf{h}_d})$
```

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 $\mathbf{x} \in \mathbf{R}^p$, $\mathbf{c} \in \{0,1\}^k$.
	η, $l()$, $R()$, λ	Learning rate, loss and regularization functions and parameters.
Output:	$W^{\mathsf{h}_1}, \ldots, W^{\mathsf{h}_d}$	Weight matrices of the d layers. (= hypothesis)

```
FOR $s = 1$ TO $d$ DO initialize_random_weights($W^{\mathsf{h}_s}$) ENDDO, $t = 0$
REPEAT
  $t = t + 1$
  FOREACH $(\mathbf{x}, \mathbf{c}) \in D$ DO
                Model function evaluation.
                Calculation of residual vector.
                Calculation of derivative of the loss.
                Parameter vector update $\widehat{=}$ one gradient step down.
  ENDDO
UNTIL(convergence($D, \mathbf{y}(\cdot), t$))
return($W^{\mathsf{h}_1}, \ldots, W^{\mathsf{h}_d}$)
```

Automatic Gradient Computation

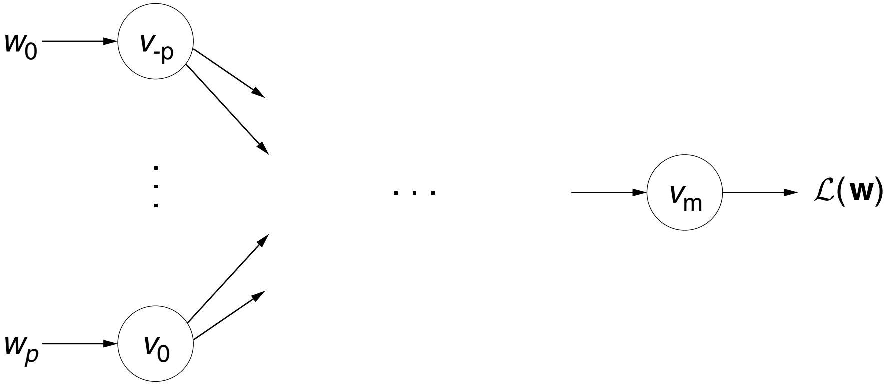
Reverse-Mode Automatic Differentiation in Computational Graphs

Reverse-mode AD corresponds to a generalized backpropagation algorithm.

Let $\mathcal{L}(w_1, \ldots, w_p)$ 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: $v_{-p \ldots 0}$ for inputs, $v_{1 \ldots m-1}$ for intermediate variables, $v_m \equiv \mathcal{L}$ for the output)

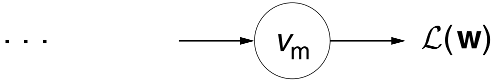


Automatic Gradient Computation

Reverse-Mode Automatic Differentiation in Computational Graphs (continued)

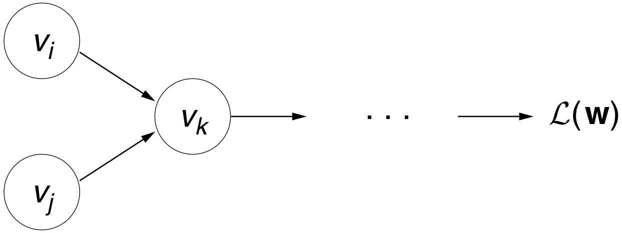
For each intermediate variable v_i, an adjoint value $\nabla^{v_i}\mathcal{L} \equiv \frac{\partial \mathcal{L}}{\partial v_i}$ is computed based on its descendants in the computation graph.

(1)



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

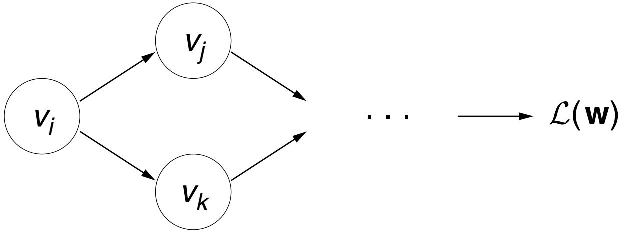
(2)



$$\nabla^{v_i}\mathcal{L} \equiv \frac{\partial \mathcal{L}}{\partial v_i} = \frac{\partial \mathcal{L}}{\partial v_k} \cdot \frac{\partial v_k}{\partial v_i} = \nabla^{v_k}\mathcal{L} \cdot \frac{\partial v_k}{\partial v_i}$$

$$\nabla^{v_j}\mathcal{L} \equiv \frac{\partial \mathcal{L}}{\partial v_j} = \frac{\partial \mathcal{L}}{\partial v_k} \cdot \frac{\partial v_k}{\partial v_j} = \nabla^{v_k}\mathcal{L} \cdot \frac{\partial v_k}{\partial v_j}$$

(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 $v_j = g(\ldots, v_i, \ldots)$ 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:

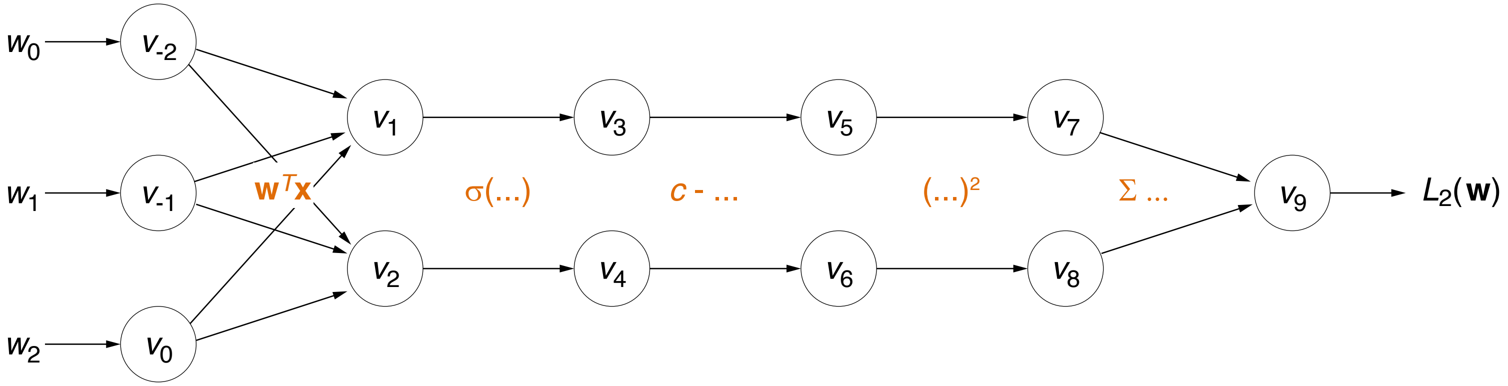
$$\begin{aligned} \mathcal{L}(\mathbf{w}) &= (c_1 - \sigma(\mathbf{w}^T\mathbf{x}_1))^2 + (c_2 - \sigma(\mathbf{w}^T\mathbf{x}_2))^2 \\ &= (-\sigma(w_0 + w_1 + 1.5w_2))^2 + (1 - \sigma(w_0 + 1.5w_1 - w_2))^2 \end{aligned}$$

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

$$\mathcal{L}(\mathbf{w}) = \underbrace{\overbrace{(\underbrace{-\,\overbrace{\sigma(\underbrace{w_0 + w_1 + 1.5w_2}_{v_1})}^{v_3})}_{v_5})^2}^{v_7} + \overbrace{(\underbrace{1 - \overbrace{\sigma(\underbrace{w_0 + 1.5w_1 - w_2}_{v_2})}^{v_4})}_{v_6})^2}^{v_8}}_{v_9}$$



Automatic Gradient Computation

Autodiff Example: Forward and Reverse Trace

$$\mathcal{L}(\mathbf{w}) = \underbrace{\overbrace{(\underbrace{-\overbrace{\sigma(\underbrace{w_0 + w_1 + 1.5w_2}_{v_1})}^{v_3}}_{v_5})^2}^{v_7} + \overbrace{(\underbrace{1 - \overbrace{\sigma(\underbrace{w_0 + 1.5w_1 - w_2}_{v_2})}^{v_4}}_{v_6})^2}^{v_8}}_{v_9}$$

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

$$\mathcal{L}(\mathbf{w}) = \underbrace{\overbrace{(\underbrace{-\overbrace{\sigma(\underbrace{w_0+w_1+1.5w_2}_{v_1})}^{v_3}}_{v_5})^2}^{v_7} + \overbrace{(\underbrace{1-\overbrace{\sigma(\underbrace{w_0+1.5w_1-w_2}_{v_2})}^{v_4}}_{v_6})^2}^{v_8}}_{v_9} \qquad \text{at} \qquad \mathbf{w} = (-1, 1.5, 0.5)^T$$

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

$$\mathcal{L}(\mathbf{w}) = \underbrace{\overbrace{(\underbrace{-\overbrace{\sigma(\underbrace{w_0+w_1+1.5w_2}_{v_1})}^{v_3}}_{v_5})^2}^{v_7} + \overbrace{(\underbrace{1-\overbrace{\sigma(\underbrace{w_0+1.5w_1-w_2}_{v_2})}^{v_4}}_{v_6})^2}^{v_8}}_{v_9} \qquad \text{at} \qquad \mathbf{w} = (-1, 1.5, 0.5)^T$$

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

$$\mathcal{L}(\mathbf{w}) = \underbrace{\overbrace{(\underbrace{-\overbrace{\sigma(\underbrace{w_0 + w_1 + 1.5w_2}_{v_1})}^{v_3}}_{v_5})^2}^{v_7} + \overbrace{(\underbrace{1 - \overbrace{\sigma(\underbrace{w_0 + 1.5w_1 - w_2}_{v_2})}^{v_4}}_{v_6})^2}^{v_8}}_{v_9} \qquad \text{at} \qquad \mathbf{w} = (-1, 1.5, 0.5)^T$$

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

$$\mathcal{L}(\mathbf{w}) = \underbrace{\overbrace{(\underbrace{-\overbrace{\sigma(\underbrace{w_0 + w_1 + 1.5w_2}_{v_1})}^{v_3}}_{v_5})^2}^{v_7} + \overbrace{(\underbrace{1 - \overbrace{\sigma(\underbrace{w_0 + 1.5w_1 - w_2}_{v_2})}^{v_4}}_{v_6})^2}^{v_8}}_{v_9} \qquad \text{at} \qquad \mathbf{w} = (-1, 1.5, 0.5)^T$$

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

$$\mathcal{L}(\mathbf{w}) = \underbrace{\overbrace{(\underbrace{-\overbrace{\sigma(\underbrace{w_0 + w_1 + 1.5w_2}_{v_1})}^{v_3}}_{v_5})^2}^{v_7} + \overbrace{(\underbrace{1 - \overbrace{\sigma(\underbrace{w_0 + 1.5w_1 - w_2}_{v_2})}^{v_4}}_{v_6})^2}^{v_8}}_{v_9} \qquad \text{at} \qquad \mathbf{w} = (-1, 1.5, 0.5)^T$$

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

$$\mathcal{L}(\mathbf{w}) = \underbrace{\overbrace{(\underbrace{-\overbrace{\sigma(\underbrace{w_0+w_1+1.5w_2}_{v_1})}^{v_3}}_{v_5})^2}^{v_7} + \overbrace{(\underbrace{1-\overbrace{\sigma(\underbrace{w_0+1.5w_1-w_2}_{v_2})}^{v_4}}_{v_6})^2}^{v_8}}_{v_9} \qquad \text{at} \qquad \mathbf{w} = (-1, 1.5, 0.5)^T$$

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:	$f : \mathbf{R}^p \to \mathbf{R}$	Function to differentiate.
	$(w_1, \ldots, w_p)^T$	Point at which the gradient should be evaluated
Output:	$(\bar{w}_1, \ldots, \bar{w}_p)^T$	Gradient of f at the point $(w_1, \ldots, w_p)^T$.

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

Remarks:

- There exists also a forward mode of automatic differentiation. One key difference is in the runtime complexity; for a function $f : \mathbf{R}^n \to \mathbf{R}^m$, 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].