344.075 KV: Natural Language Processing
Neural Networks – a Walkthrough

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Agenda*

- Artificial Neural Networks
- Forward pass and backpropagation
- Non-linearities, softmax, and loss
- Optimization and regularization

* The content of this lecture will NOT be a part of the final exam

Notation – recap

- $a \rightarrow$ scalar

- $\boldsymbol{b} \rightarrow$ vector
  - i^{th} element of $\boldsymbol{b}$ is the scalar b_i

- $\boldsymbol{C} \rightarrow$ matrix
  - i^{th} vector of $\boldsymbol{C}$ is $\boldsymbol{c}_i$
  - j^{th} element of the i^{th} vector of $\boldsymbol{C}$ is the scalar $c_{i,j}$

- Tensor: generalization of scalar, vector, matrix to any arbitrary dimension

Probability

- Conditional probability, given two random variables X and Y:

$$P(Y|X)$$

- Probability distribution
  - For a discrete random variable Y with K states (classes)
    - $0 \leq P(Y_i) \leq 1$
    - $\sum_{i=1}^{K} P(Y_i) = 1$
  - E.g. with $K = 4$ states: $[0.2 \quad 0.3 \quad 0.45 \quad 0.05]$

- Expected value over a set $\mathcal{D}$

$$\mathbb{E}_{\mathcal{D}}[f] = \frac{1}{|\mathcal{D}|} \sum_{x \in \mathcal{D}} f(x)$$

Note: The definition of expected value is not completely precise. Though, it suffices for our use in this lecture

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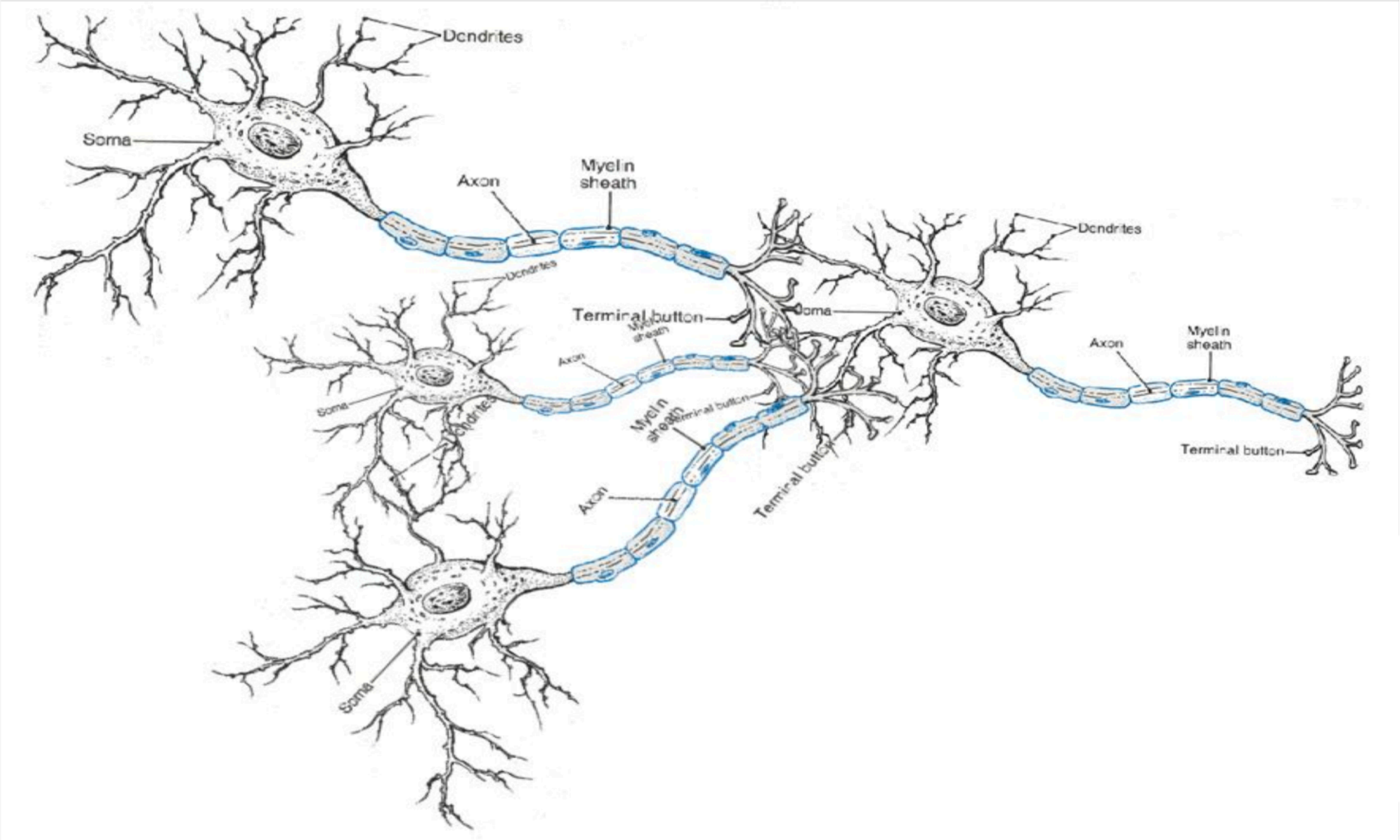
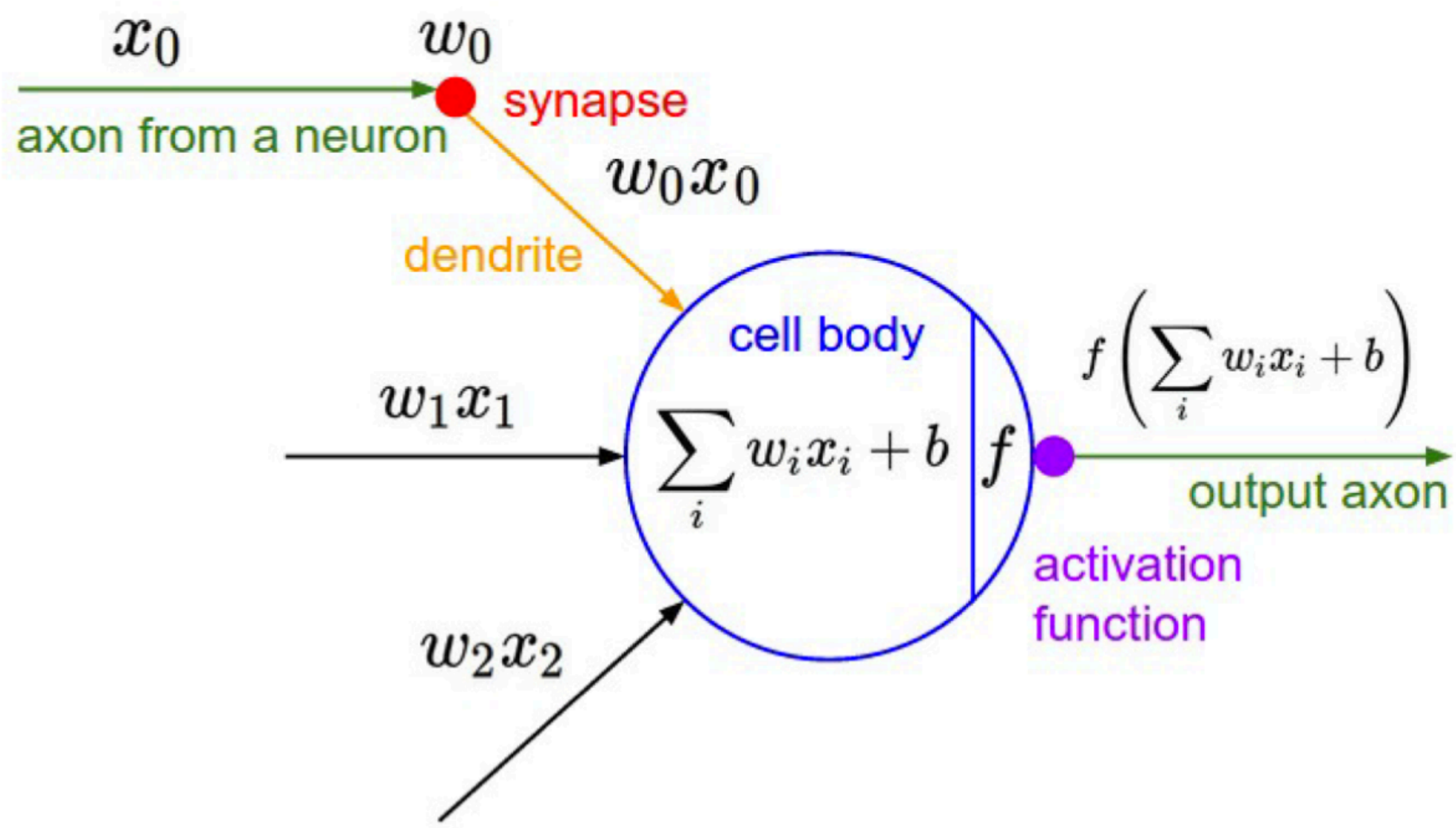
Neural Computation



An Artificial Neuron



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Artificial Neural Networks

- Neural Networks are non-linear functions and universal approximators

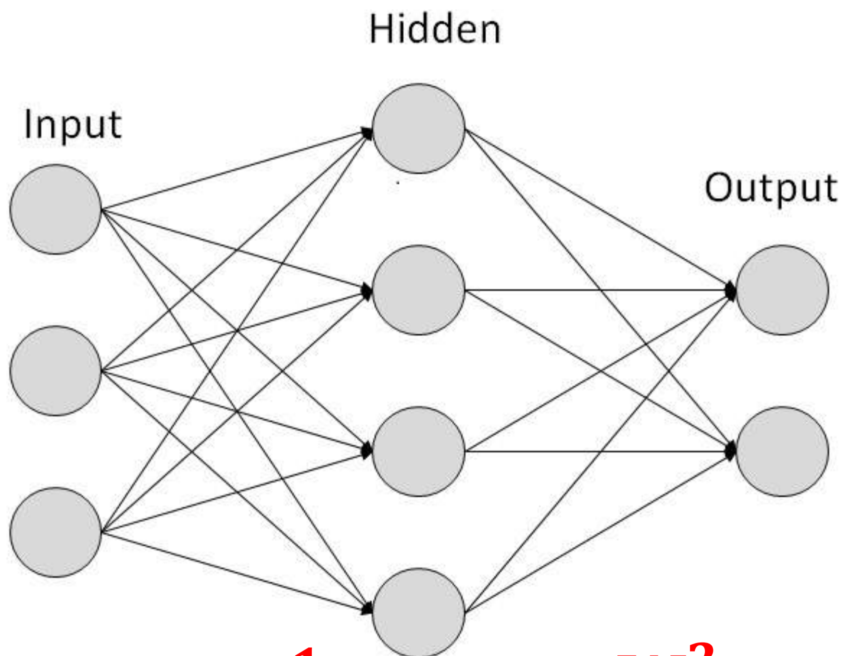
- Neural networks can readily be defined as probabilistic models which estimate $P(Y|X)$

- Considering model parameter, $P(Y|X)$ can be written as $P(Y|\boldsymbol{x};\mathbb{W})$
  - $\boldsymbol{x}$ is an input vector and $\mathbb{W}$ is the set of model parameters
  - The model's predicted probability distribution is:

$$\hat{\boldsymbol{y}} = P(Y|\boldsymbol{x};\mathbb{W})$$

A sample neural network (Multi Layer Perceptron)

input vector
$\boldsymbol{x}$



Predicted output
probability distribution
$\widehat{\boldsymbol{y}} = P(Y|\boldsymbol{x}; \mathbb{W})$

$\boldsymbol{W^1}$
size 3x4

$\boldsymbol{W^2}$
size 4x2

parameter matrices

Learning with Neural Networks

- Design the network's architecture
  - Consider proper **regularization** methods
- Initialize parameters
- Loop until some **exit criteria** are met
  - Sample a **(mini)batch** from training data $\mathcal{D}$
  - For each data point in the minibatch
    - **Forward pass**: given input $\boldsymbol{x}$ predict output distribution $\hat{\boldsymbol{y}} = P(Y|\boldsymbol{x}; \mathbb{W})$
  - Calculate **loss** function of the (mini)batch
  - Calculate the **gradient** of each parameter regarding the loss function using the **backpropagation** algorithm
  - **Update** parameters using their gradients

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Forward pass

- Let's see how a neural network calculates the following function:

$$f(x; \mathbb{W}) = 2 * w_2{}^2 + 2 * x * w_1 + w_0$$

  - x is input and $\mathbb{W}$ is the tensor of parameters
  - Parameters are initialized with

$$w_0 = 1 \quad w_1 = 3 \quad w_2 = 2$$

- A neural network splits the function to subfunctions on each of basic operations, and rewrites it using new intermediary variables*:

$$a = 2 * x * w_1$$

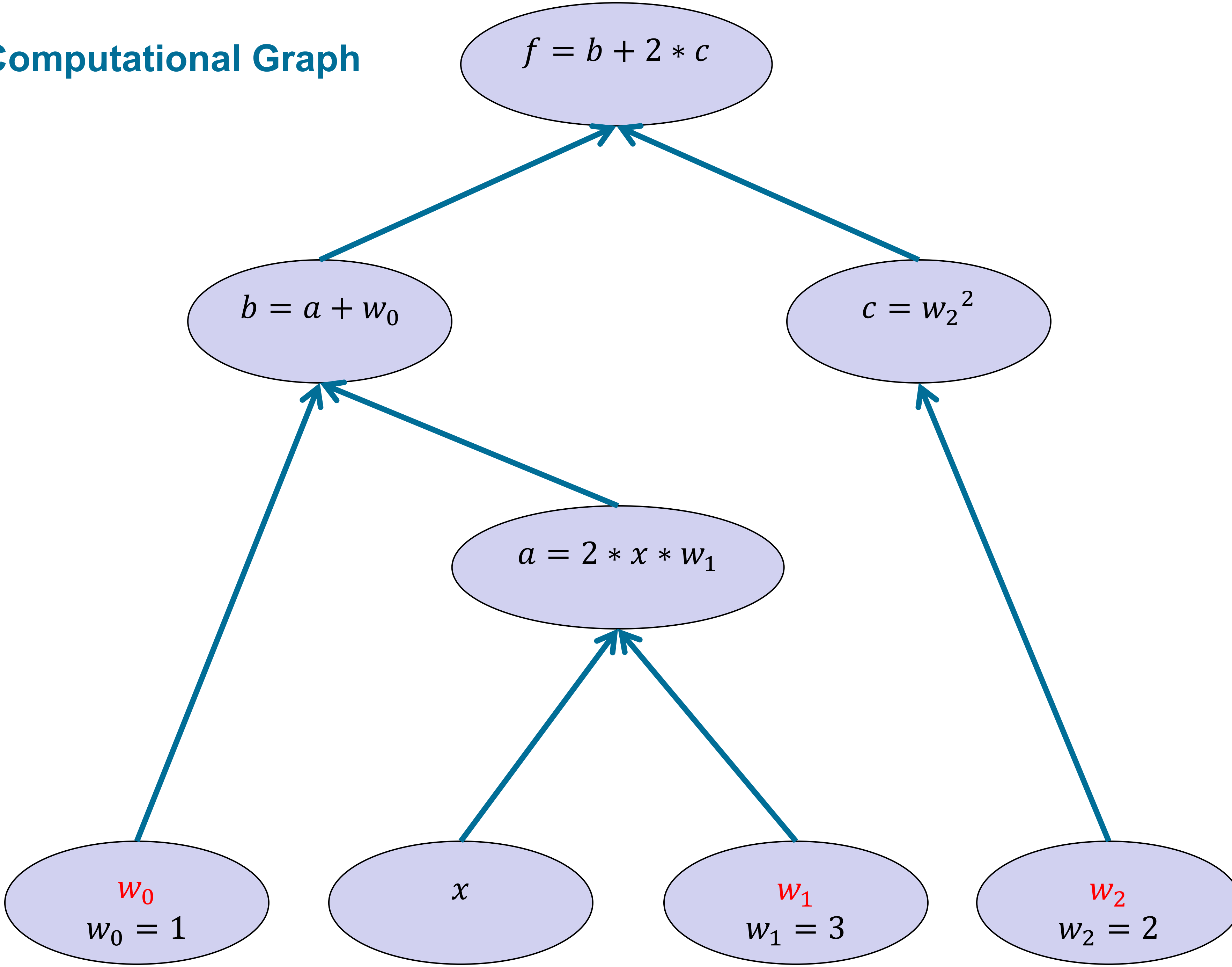
$$b = a + w_0$$

$$c = w_2{}^2$$

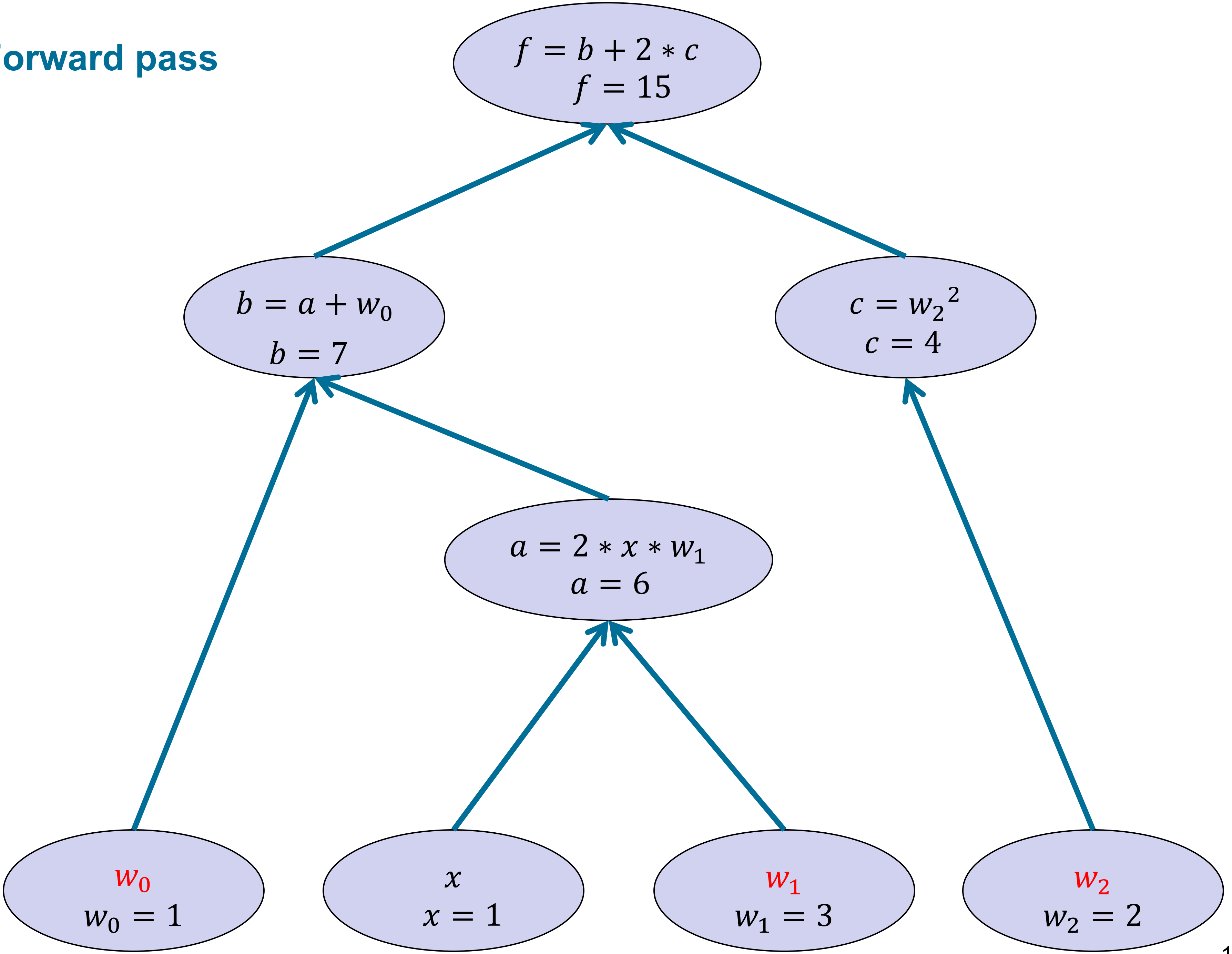
$$f = b + 2 * c$$

* To keep the example simple, the splitting is not applied to all basic operation

Computational Graph



Forward pass



Towards backpropagation – Gradient vector

- To optimize the model's parameters, we need to calculate the gradient vector of f regarding parameters $\boldsymbol{w}$:

$$\nabla_{\boldsymbol{w}} f = \left[\frac{\partial f}{\partial w_0} \quad \frac{\partial f}{\partial w_1} \quad \frac{\partial f}{\partial w_2}\right]$$

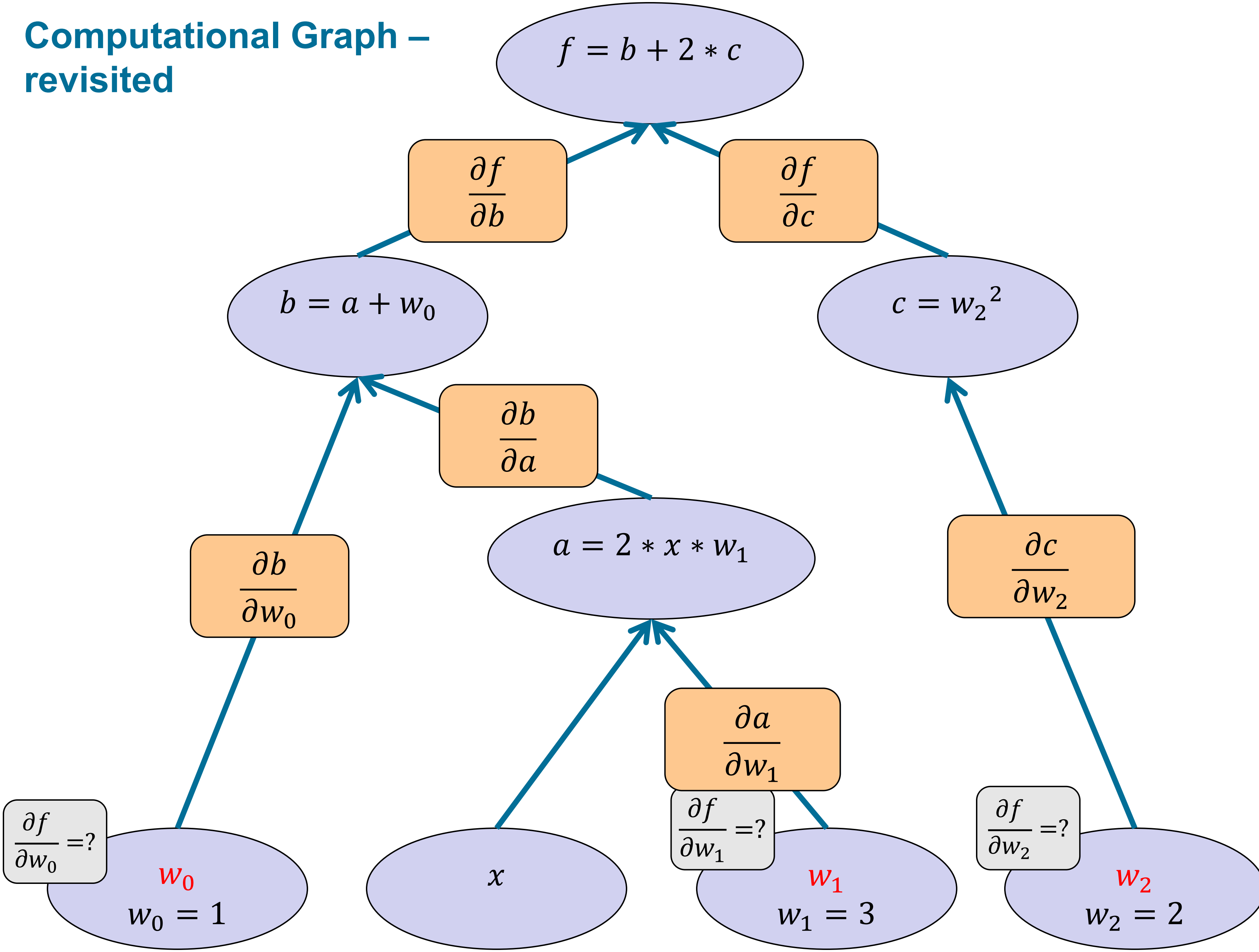
- The elements of the gradient vector are the partial derivatives of f to each parameter:

$$\frac{\partial f}{\partial w_0} = ?$$

$$\frac{\partial f}{\partial w_1} = ?$$

$$\frac{\partial f}{\partial w_2} = ?$$

Computational Graph – revisited



Chain rule

- Gradient vector: $\nabla_{\boldsymbol{w}} f = \left[\frac{\partial f}{\partial w_0} \quad \frac{\partial f}{\partial w_1} \quad \frac{\partial f}{\partial w_2}\right]$
- We can calculate partial derivatives using local derivates and chain rule:

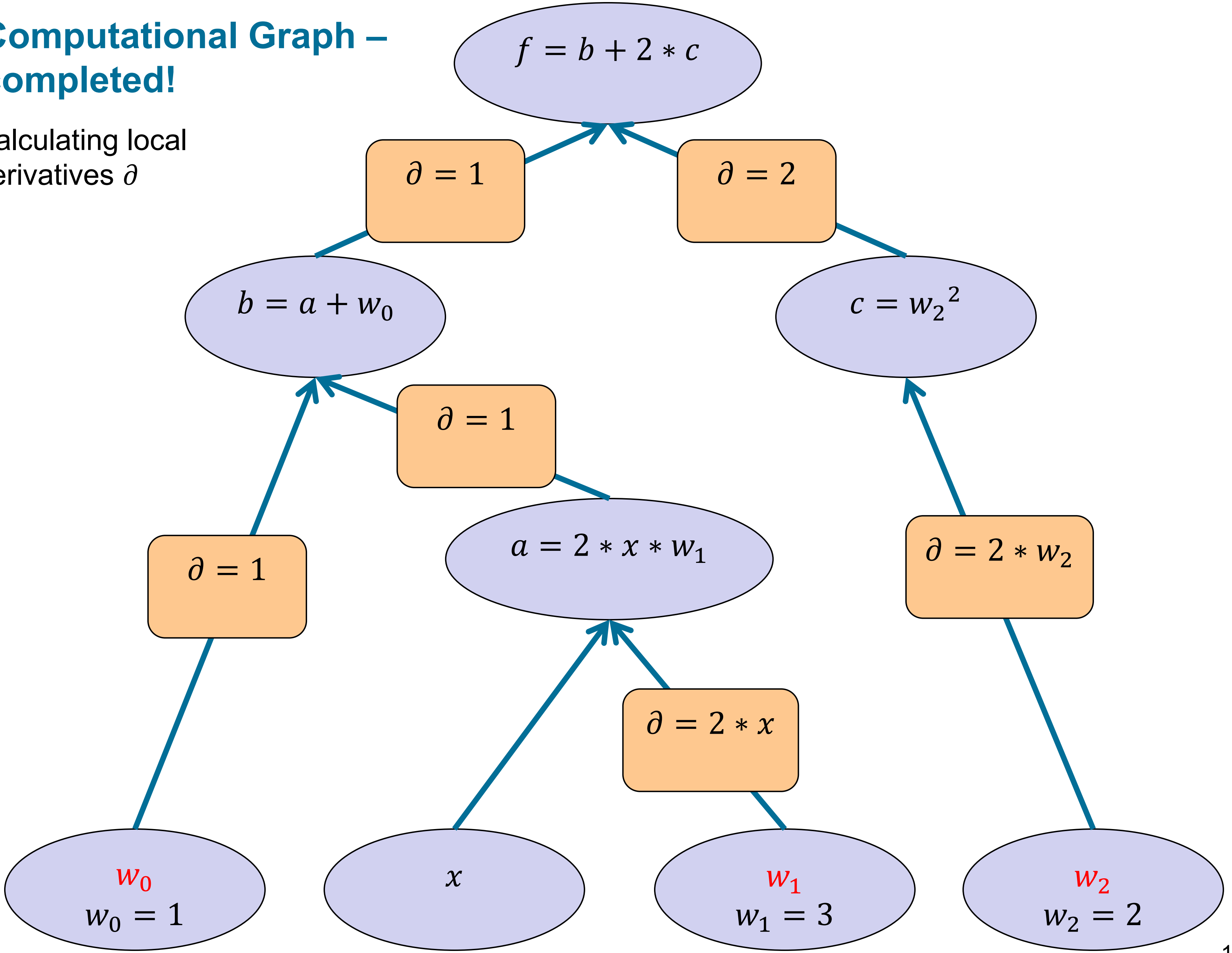
$$\frac{\partial f}{\partial w_0} = \frac{\partial f}{\partial b}\frac{\partial b}{\partial w_0}$$

$$\frac{\partial f}{\partial w_1} = \frac{\partial f}{\partial b}\frac{\partial b}{\partial a}\frac{\partial a}{\partial w_1}$$

$$\frac{\partial f}{\partial w_2} = \frac{\partial f}{\partial c}\frac{\partial c}{\partial w_2}$$

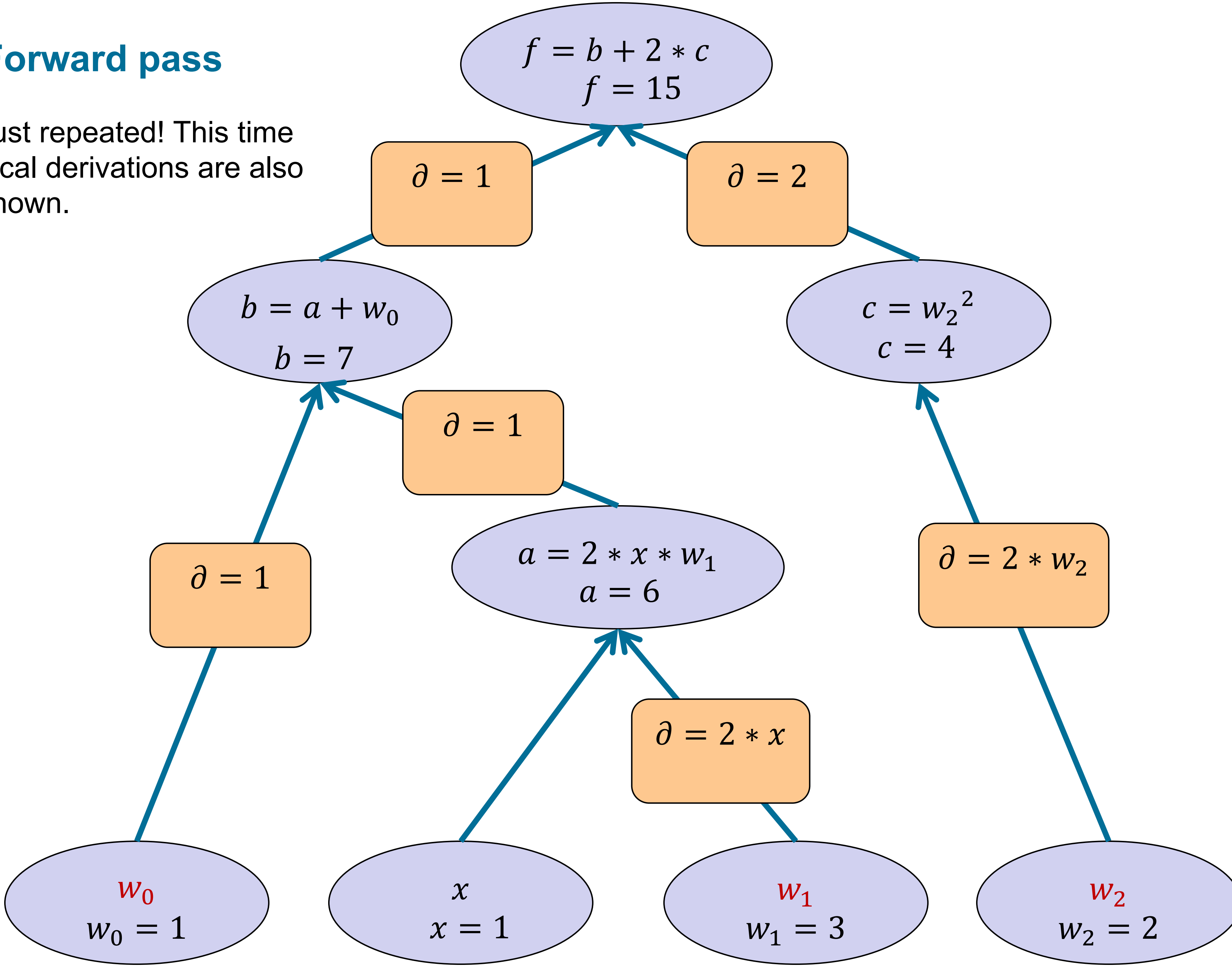
Computational Graph – completed!

Calculating local derivatives ∂



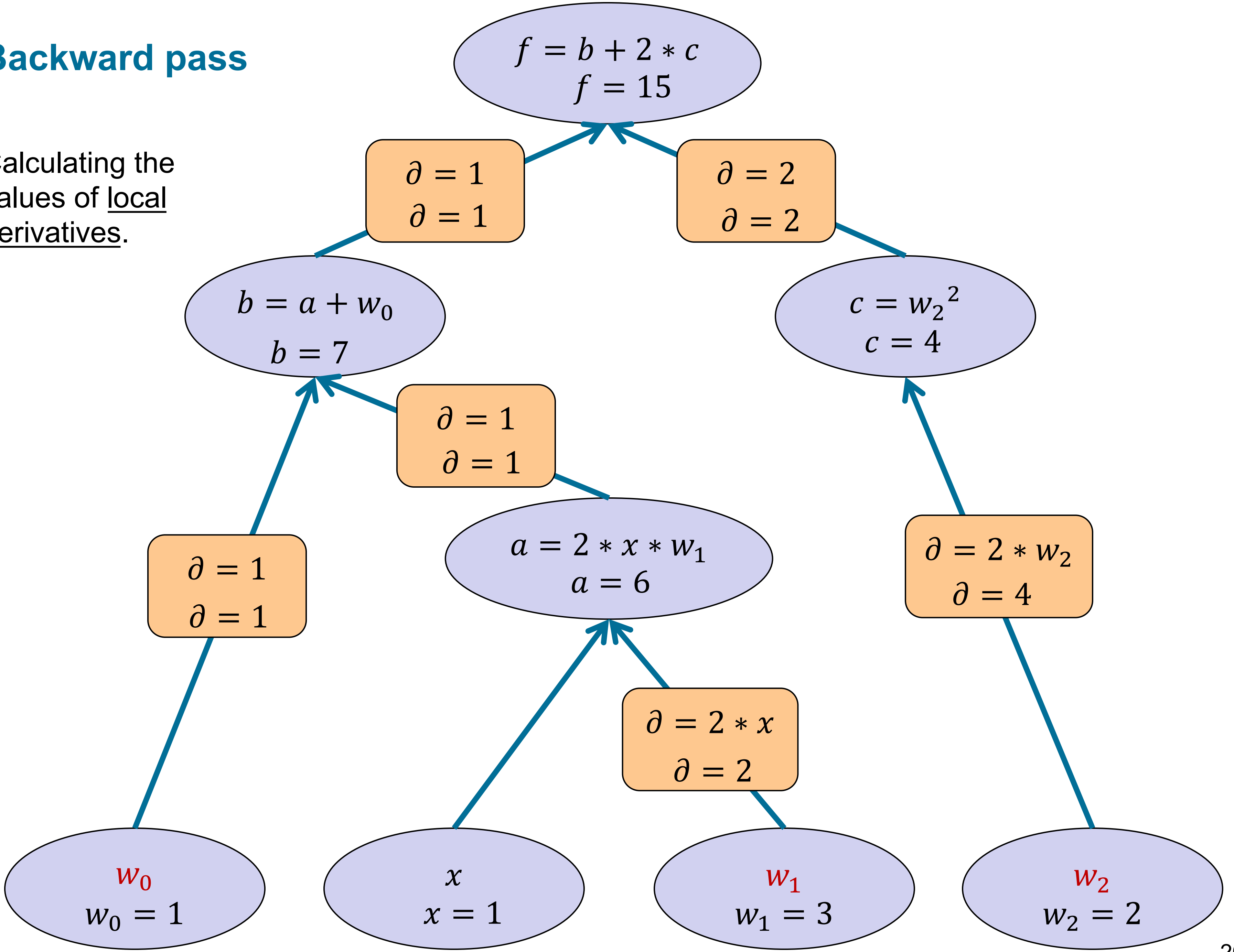
Forward pass

Just repeated! This time local derivations are also shown.



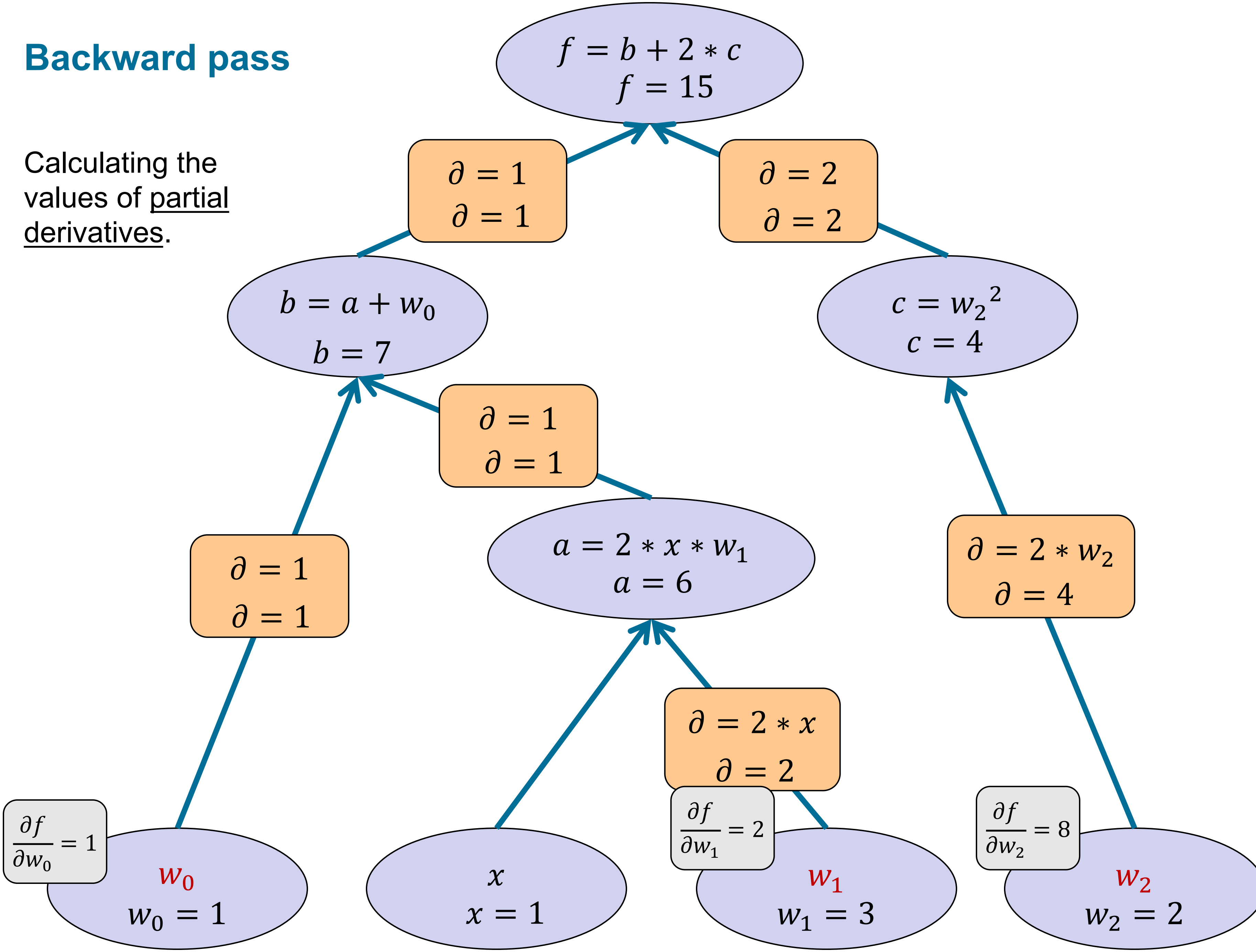
Backward pass

Calculating the values of local derivatives.



Backward pass

Calculating the values of partial derivatives.



Backpropagation

Calculating partial derivatives:

$$\frac{\partial f}{\partial w_0} = \frac{\partial f}{\partial b} \frac{\partial b}{\partial w_0} = 1 * 1 = 1$$

$$\frac{\partial f}{\partial w_1} = \frac{\partial f}{\partial b} \frac{\partial b}{\partial a} \frac{\partial a}{\partial w_1} = 1 * 1 * 2 = 2$$

$$\frac{\partial f}{\partial w_2} = \frac{\partial f}{\partial c} \frac{\partial c}{\partial w_2} = 2 * 4 = 8$$

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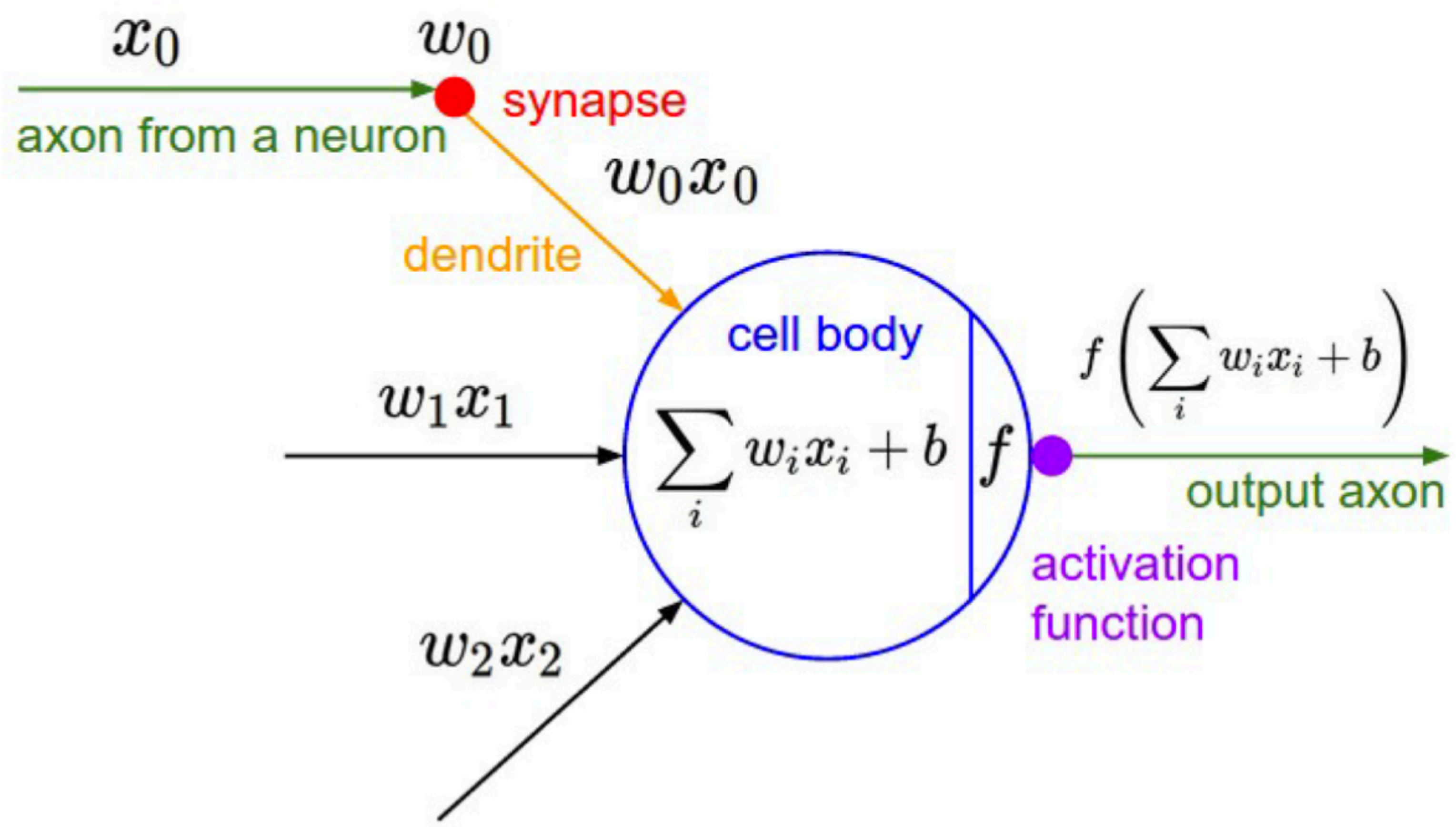
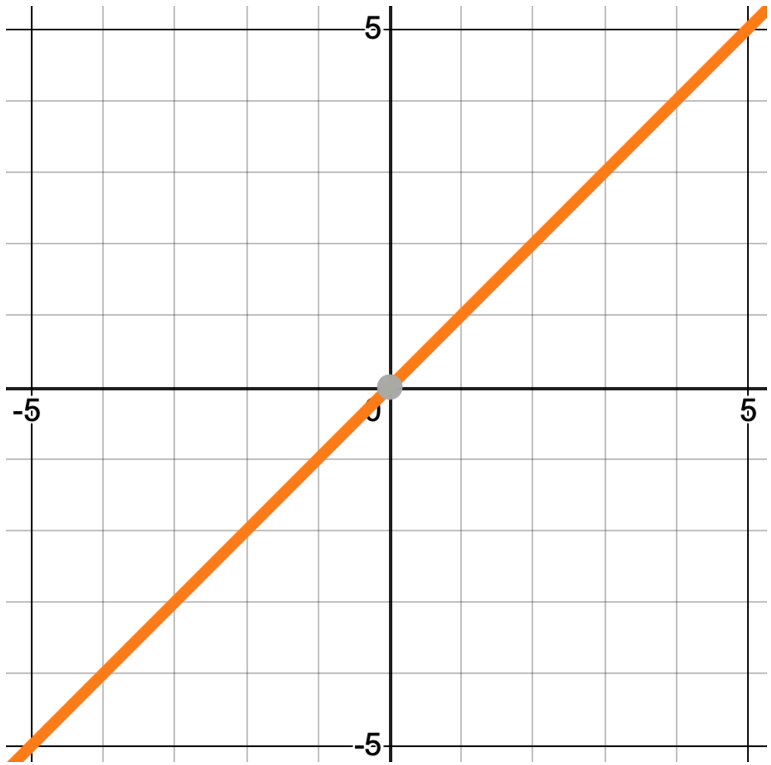
An Artificial Neuron



Linear

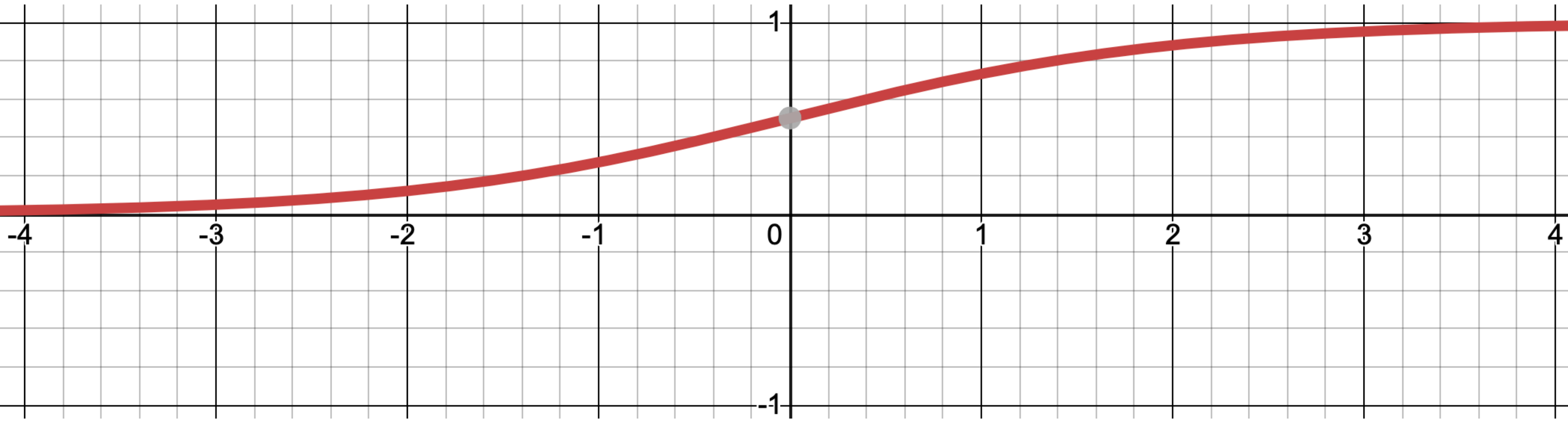
$$f(x) = x$$



Sigmoid

$$f(x) = \sigma(x) = \frac{1}{1 + e^{-x}}$$

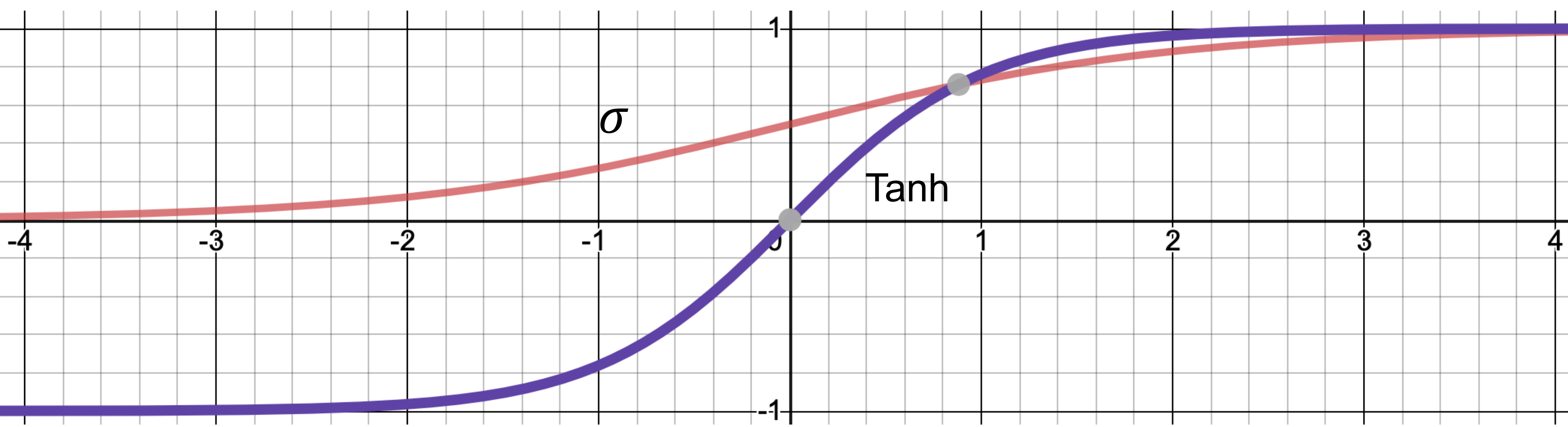
- squashes input between 0 and 1
- Output becomes like a probability value



Hyperbolic Tangent (Tanh)

$$f(x) = \tanh(x) = \frac{e^{2x} - 1}{e^{2x} + 1}$$

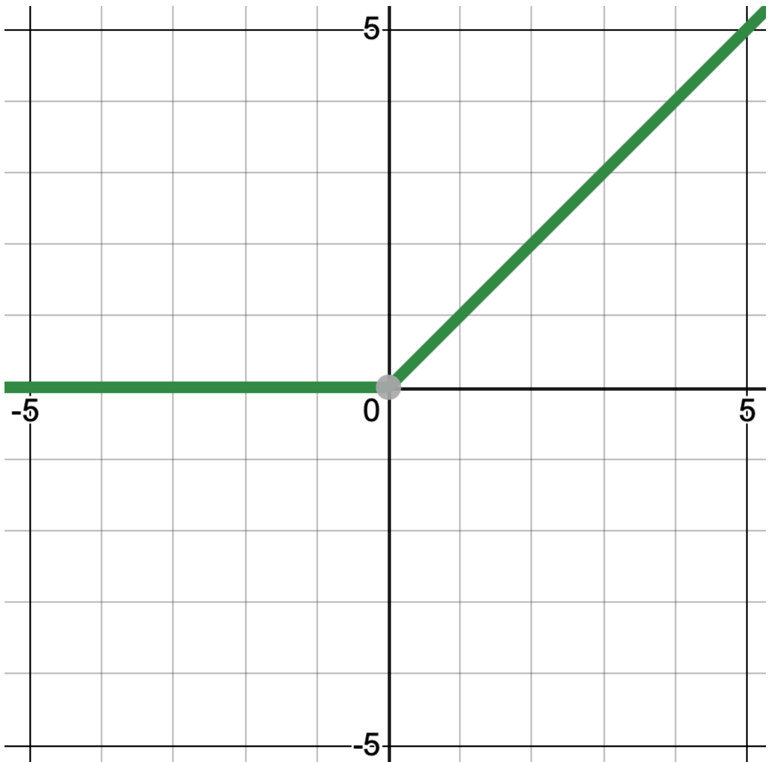
- squashes input between -1 and 1



Rectified Linear Unit (ReLU)

$$f(x) = \max(0, x)$$

- fits to deep architectures, as it prevents vanishing gradient



Examples

$$\boldsymbol{x} = \begin{bmatrix} 1 & 3 \end{bmatrix} \quad \boldsymbol{W} = \begin{bmatrix} 0.5 & -0.5 & 2 & 0 & 0 \\ 0 & 0 & 0 & 4 & -1 \end{bmatrix}$$

- Linear transformation $\boldsymbol{xW}$:

$$\boldsymbol{xW} = \begin{bmatrix} 1 & 3 \end{bmatrix} \begin{bmatrix} 0.5 & -0.5 & 2 & 0 & -1 \\ 0 & 0 & 0 & 4 & -1 \end{bmatrix} = \begin{bmatrix} \mathbf{0.5} & \mathbf{-0.5} & \mathbf{2} & \mathbf{12} & \mathbf{-4} \end{bmatrix}$$

- Non-linear transformation $\mathrm{ReLU}(\boldsymbol{xW})$:

$$\mathrm{ReLU}(\begin{bmatrix} 0.5 & -0.5 & 2 & 12 & -3 \end{bmatrix}) = \begin{bmatrix} \mathbf{0.5} & \mathbf{0.0} & \mathbf{2} & \mathbf{12} & \mathbf{0.0} \end{bmatrix}$$

- Non-linear transformation $\sigma(\boldsymbol{xW})$:

$$\sigma(\begin{bmatrix} 0.5 & -0.5 & 2 & 12 & -3 \end{bmatrix}) = \begin{bmatrix} \mathbf{0.62} & \mathbf{0.37} & \mathbf{0.88} & \mathbf{0.99} & \mathbf{0.018} \end{bmatrix}$$

- Non-linear transformation $\tanh(\boldsymbol{xW})$:

$$\tanh(\begin{bmatrix} 0.5 & -0.5 & 2 & 12 & -3 \end{bmatrix}) = \begin{bmatrix} \mathbf{0.46} & \mathbf{-0.46} & \mathbf{0.96} & \mathbf{0.99} & \mathbf{-0.99} \end{bmatrix}$$

Softmax

- As discussed, neural networks can readily turn to probabilistic models

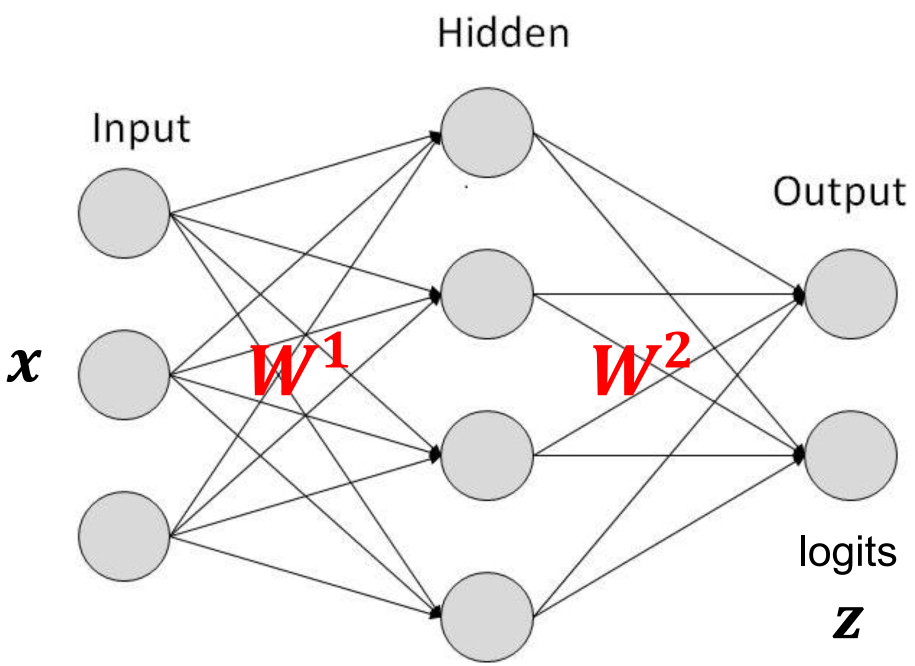
- To do it, we need to transform the output vector $\boldsymbol{z}$ of a neural network with K output classes to a probability distribution
  - In the context of neural networks, $\boldsymbol{z}$ is usually called **logits**

- softmax turns a vector to a probability distribution
  - $\boldsymbol{z}$ could be the output vector of a neural network

$$\text{softmax}(\boldsymbol{z})_l = \frac{e^{z_l}}{\sum_{i=1}^{K} e^{z_i}}$$

normalization term

A sample neural network



Predicted output probability distribution

$$\hat{\boldsymbol{y}} = P(Y|\boldsymbol{x}; \mathbb{W})$$
$$= \text{softmax}(\boldsymbol{z})$$

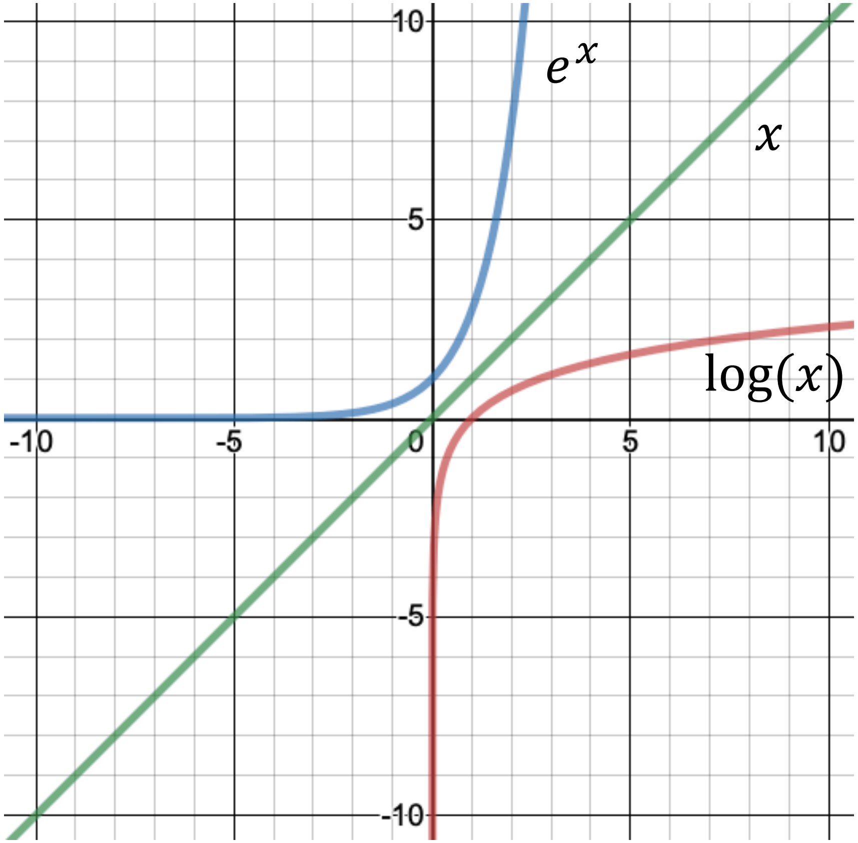
Softmax – example

$K = 4$ classes

$$\text{softmax}(\boldsymbol{z})_l = \frac{e^{z_l}}{\sum_{i=1}^{K} e^{z_i}}$$

$$\boldsymbol{z} = \begin{bmatrix} 1 \\ 2 \\ 5 \\ 6 \end{bmatrix}$$

$$\text{softmax}(\boldsymbol{z}) = \begin{bmatrix} 0.004 \\ 0.013 \\ 0.264 \\ 0.717 \end{bmatrix}$$



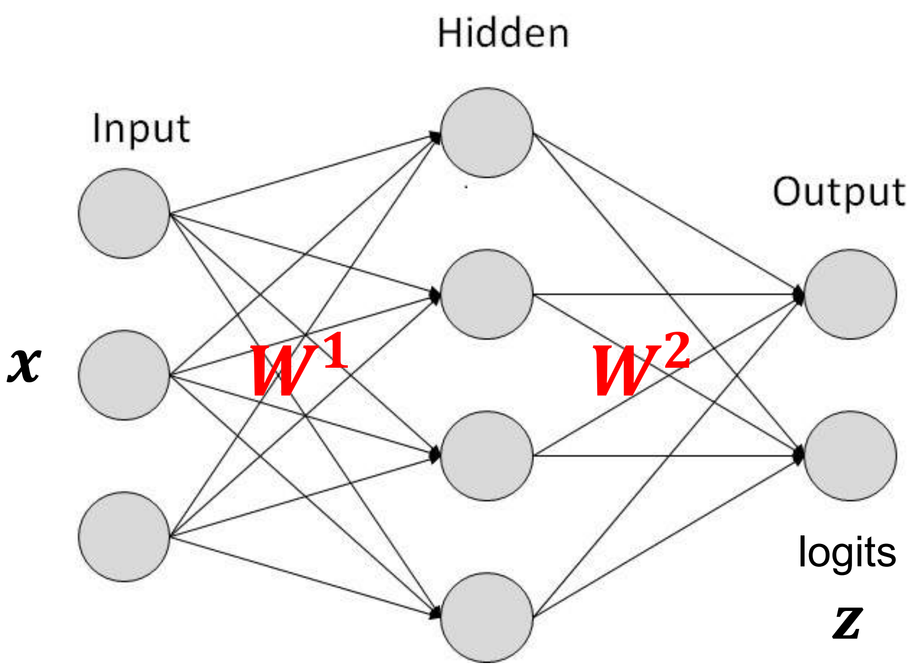
Softmax characteristics

- The exponential function in softmax makes the maximum becomes much higher than the others

- Softmax identifies the "*max*" but in a "*soft*" way!

- Softmax imposes competition between the predicted output values, as in fact "*winner takes (almost) all!*"
  - Winner-takes-all is the case when one value is 1 and the rest are 0
  - Softmax provides a soft distribution of winner-takes-all
  - This resembles the competition between nearby neurons in the cortex

Sample neural network



Predicted output probability distribution

$$\hat{\boldsymbol{y}} = P(Y|\boldsymbol{x};\mathbb{W})$$

$$= \text{softmax}(\boldsymbol{z})$$

$\longleftrightarrow$ $\mathcal{L}$

Labels

$\boldsymbol{y}$

Cross Entropy Loss

- Given a classification task with K classes
  - known as multi-class classification
- $\hat{\boldsymbol{y}} \rightarrow$ predicted probability distribution of the classes
- $\boldsymbol{y} \rightarrow$ actual probability distribution of the classes (labels)
- Cross Entropy loss is defined as:

$$\mathcal{L} = -\mathbb{E}_{\mathcal{D}} \sum_{i=1}^{K} y_i \log \hat{y}_i$$

  - $\mathcal{D} \rightarrow$ the set of training data
- In neural networks, we can write it as:

$$\mathcal{L}(\mathbb{W}) = -\mathbb{E}_{\mathcal{D}} \sum_{i=1}^{K} y_i \log P(Y_i | \boldsymbol{x}; \mathbb{W})$$

Cross Entropy Loss – example 1

- A multi-label scenario:

$$\hat{\boldsymbol{y}} = \begin{bmatrix} 0.004 \\ 0.013 \\ 0.264 \\ 0.717 \end{bmatrix} \qquad \boldsymbol{y} = \begin{bmatrix} 0 \\ 0.25 \\ 0 \\ 0.75 \end{bmatrix}$$

$$\mathcal{L} = -\sum_{i=1}^{K} y_i \log \hat{y}_i$$

$$\mathcal{L} = -(0 \times \log 0.004 + 0.25 \times \log 0.013 + 0 \times \log 0.264 + 0.75 \times \log 0.717)$$

$$\mathcal{L} = -(0 - 0.471 + 0 - 0.108)$$

$$\mathcal{L} = 0.579$$

Cross Entropy Loss – example 2

- A single-label scenario:

$$\hat{\boldsymbol{y}} = \begin{bmatrix} 0.004 \\ 0.013 \\ 0.264 \\ 0.717 \end{bmatrix} \qquad \boldsymbol{y} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\mathcal{L} = -\sum_{i=1}^{K} y_i \log \hat{y}_i$$

$$\mathcal{L} = -(0 \times \log 0.004 + 0 \times \log 0.013 + 0 \times \log 0.264 + 1 \times \log 0.717)$$

$$\mathcal{L} = -(0 + 0 + 0 - 0.144)$$

$$\mathcal{L} = 0.144$$

Negative Log Likelihood (NLL) Loss

- Single-label classification is the most common scenario
- In this case, we can simplify Cross Entropy formulation to

$$\mathcal{L}(\mathbb{W}) = -\mathbb{E}_{\mathcal{D}} \sum_{i=1}^{K} y_i \log P(Y_i | \boldsymbol{x}; \mathbb{W}) = -\mathbb{E}_{\mathcal{D}} \log P(Y_l | \boldsymbol{x}; \mathbb{W})$$

  - where l is the index of the correct class

- This loss function is known as Negative Log Likelihood (NLL)
  - NLL is a special case of Cross Entropy

NLL + softmax

- What happens when we use NLL and softmax in the output layer of a neural network?

$$\mathcal{L}(\mathbb{W}) = -\mathbb{E}_{\mathcal{D}} \log P(Y_l | \boldsymbol{x}; \mathbb{W}) = -\mathbb{E}_{\mathcal{D}} \log \operatorname{softmax}(\boldsymbol{z})_l$$

$\boldsymbol{z} \rightarrow$ output vector before softmax (logits)

$$\mathcal{L}(\mathbb{W}) = -\mathbb{E}_{\mathcal{D}} \log \frac{e^{z_l}}{\sum_{i=1}^{K} e^{z_i}} = -\mathbb{E}_{\mathcal{D}} \left[\log e^{z_l} - \log \sum_{i=1}^{K} e^{z_i} \right]$$

$$\mathcal{L}(\mathbb{W}) = -\mathbb{E}_{\mathcal{D}} \left[z_l - \log \sum_{i=1}^{K} e^{z_i} \right]$$

This term is (almost) equal to $\max(\boldsymbol{z})$

NLL + softmax – example 1

$$\mathcal{L} = -\left[z_l - \log \sum_{i=1}^{K} e^{z_i}\right]$$

$$\boldsymbol{z} = [1 \quad 2 \quad 0.5 \quad 6]$$

- If the correct class is the first one, $l = 1$:

$$\mathcal{L} = -[1 - \log(e^1 + e^2 + e^{0.5} + e^6)] = -1 + 6.02 = \mathbf{5.02}$$

- If the correct class is the third one, $l = 3$:

$$\mathcal{L} = -[0.5 - \log(e^1 + e^2 + e^{0.5} + e^6)] = -0.5 + 6.02 = \mathbf{5.52}$$

- If the correct class is the fourth one, $l = 4$:

$$\mathcal{L} = -[6 - \log(e^1 + e^2 + e^{0.5} + e^6)] = -6 + 6.02 = \mathbf{0.02}$$

NLL + softmax – example 2

$$\mathcal{L} = -\left[z_l - \log \sum_{i=1}^{K} e^{z_i}\right]$$

$$\boldsymbol{z} = [1 \quad 2 \quad 5 \quad 6]$$

- If the correct class is the first one, $l = 1$:

$$\mathcal{L} = -[1 - \log(e^1 + e^2 + e^5 + e^6)] = -1 + 6.33 = \mathbf{5.33}$$

- If the correct class is the third one, $l = 3$:

$$\mathcal{L} = -[5 - \log(e^1 + e^2 + e^5 + e^6)] = -5 + 6.33 = \mathbf{1.33}$$

- If the correct class is the fourth one, $l = 4$:

$$\mathcal{L} = -[6 - \log(e^1 + e^2 + e^5 + e^6)] = -6 + 6.33 = \mathbf{0.33}$$

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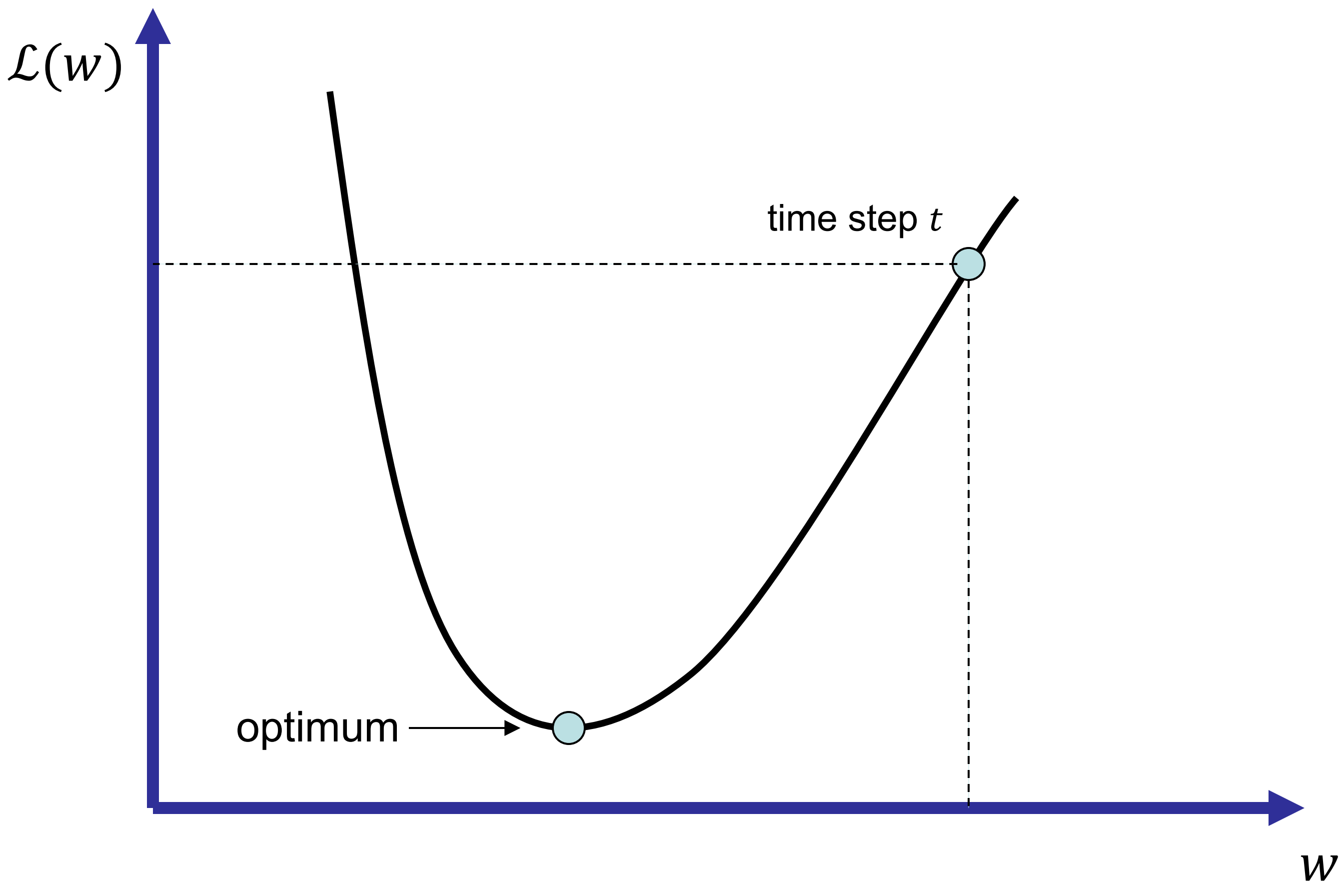
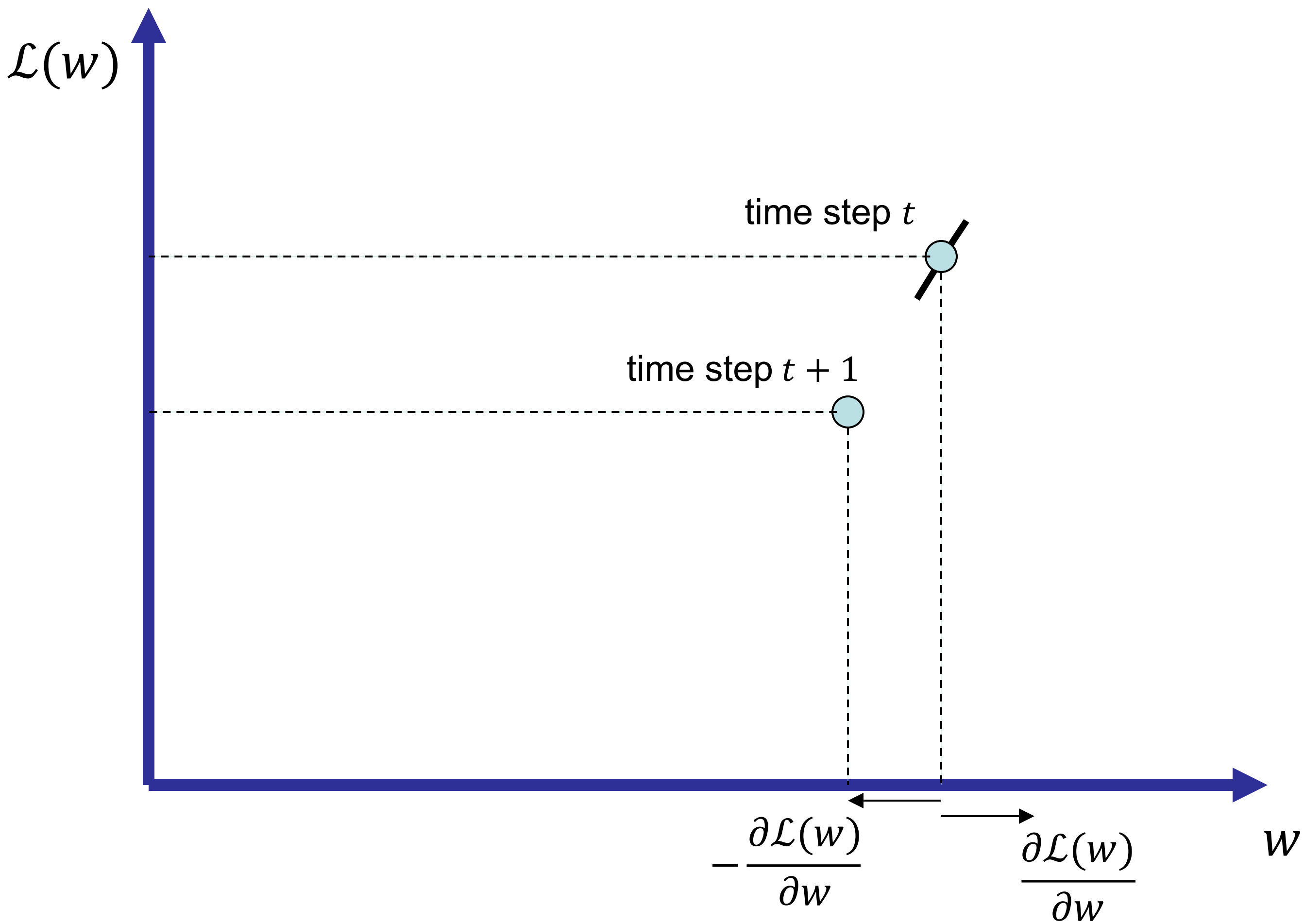
Stochastic Gradient Descent (SGD)

- For every $w \in \mathbb{W}$ and after calculating loss of one/some/all of data points …



Stochastic Gradient Descent (SGD)

- For every $w \in \mathbb{W}$ and after calculating loss of one/some/all of data points …



Stochastic Gradient Descent algorithm

- A model with a set of parameters $\mathbb{W}$ at time step $t \rightarrow \mathbb{W}^{(t)}$
- A **learning rate** η
- Loop until some exit criteria are met
  - $\widehat{\mathcal{D}}$ is a **minibatch** containing S data points, sampled from $\mathcal{D}$
  - Compute gradient tensor of parameters $\mathbb{G}$:

$$\mathbb{G} \leftarrow \frac{1}{S} \nabla_{\mathbb{W}} \sum_{(\boldsymbol{x}, y) \in \widehat{\mathcal{D}}} \mathcal{L}(\boldsymbol{x}, y; \mathbb{W})$$

  - Update the parameters by taking a step in the opposite direction of the corresponding gradients:

$$\mathbb{W}^{(t+1)} \leftarrow \mathbb{W}^{(t)} - \eta \mathbb{G}$$

  - Reduce learning rate (**annealing**) if some criteria are met or based on a schedule

Sampling (batch) size in (Stochastic) Gradient Descent

- If only one data point is used in every step; $S = 1$
  - Fast
  - learns **online**
  - Training can become unstable with a lot of fluctuations

- If all data points are used in every step; $S = N$
  - Also called **Batch Gradient Descent**
  - Training can take very long time

- If S is between these
  - Also called **Mini-Batch (Stochastic) Gradient Descent**
  - Typical setting for training deep learning models

Other gradient-based optimizations

- Some limitations of the mentioned SGD algorithms
  - Choosing learning rate is hard
  - Choosing annealing method/rate is hard
  - Same learning rate is applied to all parameters
  - Can get trapped in non-optimal local minima and saddle points

- Some other commonly used algorithms:
  - Nestrov accelerated gradient
  - Adagrad
  - Adam

Regularization techniques for neural networks and deep learning

- **Parameter norm penalty**
- **Early stopping**
- Dropout
- Batch normalization
- Transfer learning
- Multitask learning
- Unsupervised / Semi-supervised pre-training
- Noise robustness
- Dataset augmentation
- Ensemble
- Adversarial training

Parameter norm penalty

- Adds the norm of parameters to the loss function
- For instance, the squared L2 norm of parameters: $||\mathbb{W}||_2{}^2$

$$||\mathbb{W}||_2{}^2 = \left(\sqrt{\sum_{w \in \mathbb{W}} w^2}\right)^2 = \sum_{w \in \mathbb{W}} w^2$$

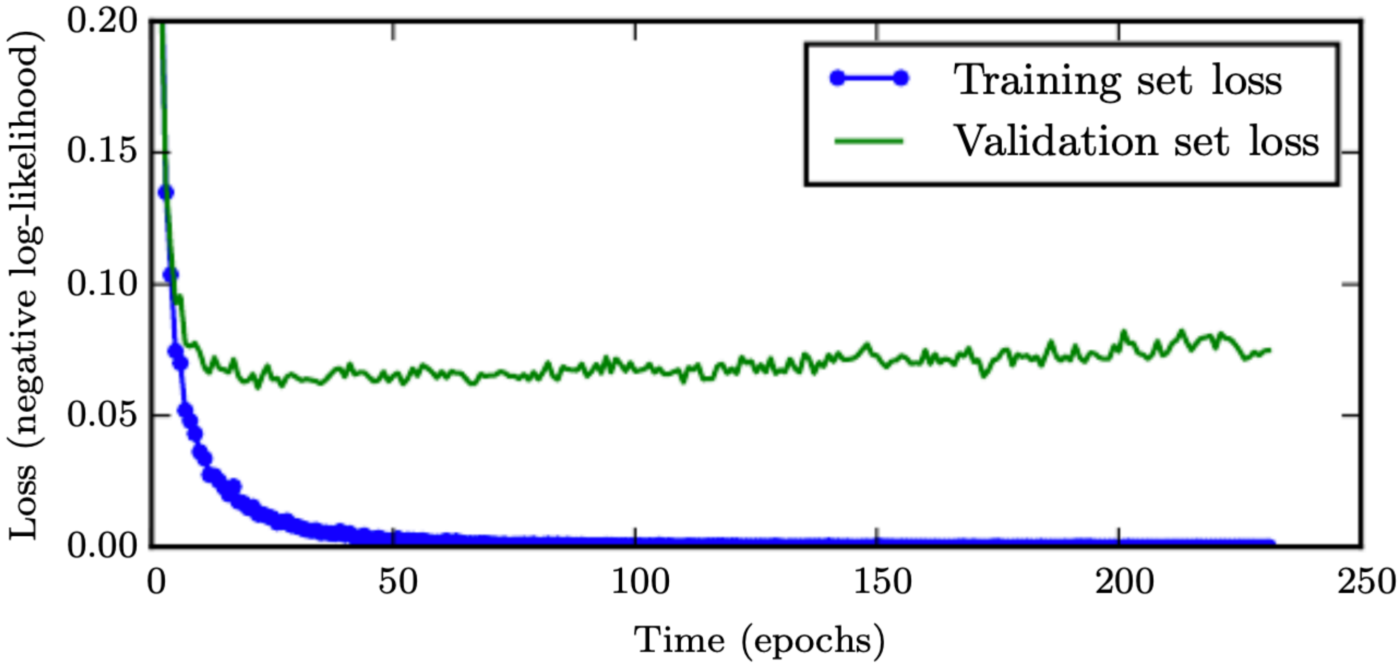
- Norm penalty in NLL loss:

$$\mathcal{L}(\mathbb{W}) = -\log P(Y_l|\boldsymbol{x};\mathbb{W}) + ||\mathbb{W}||_2{}^2$$

- This constraint forces the model to punish (decrease the values of) parameters with high values
  - Read more about L1, L2 norms here section 2.5

Early Stopping

- Run the model for several steps (epochs), and in each step evaluate the model on the validation set
- Store the model if the evaluation results improve
- At the end, take the stored model (with best validation results) as the final model



https://www.deeplearningbook.org/contents/regularization.html