Deep Learning

CSCI 1470/2470
Spring 2023

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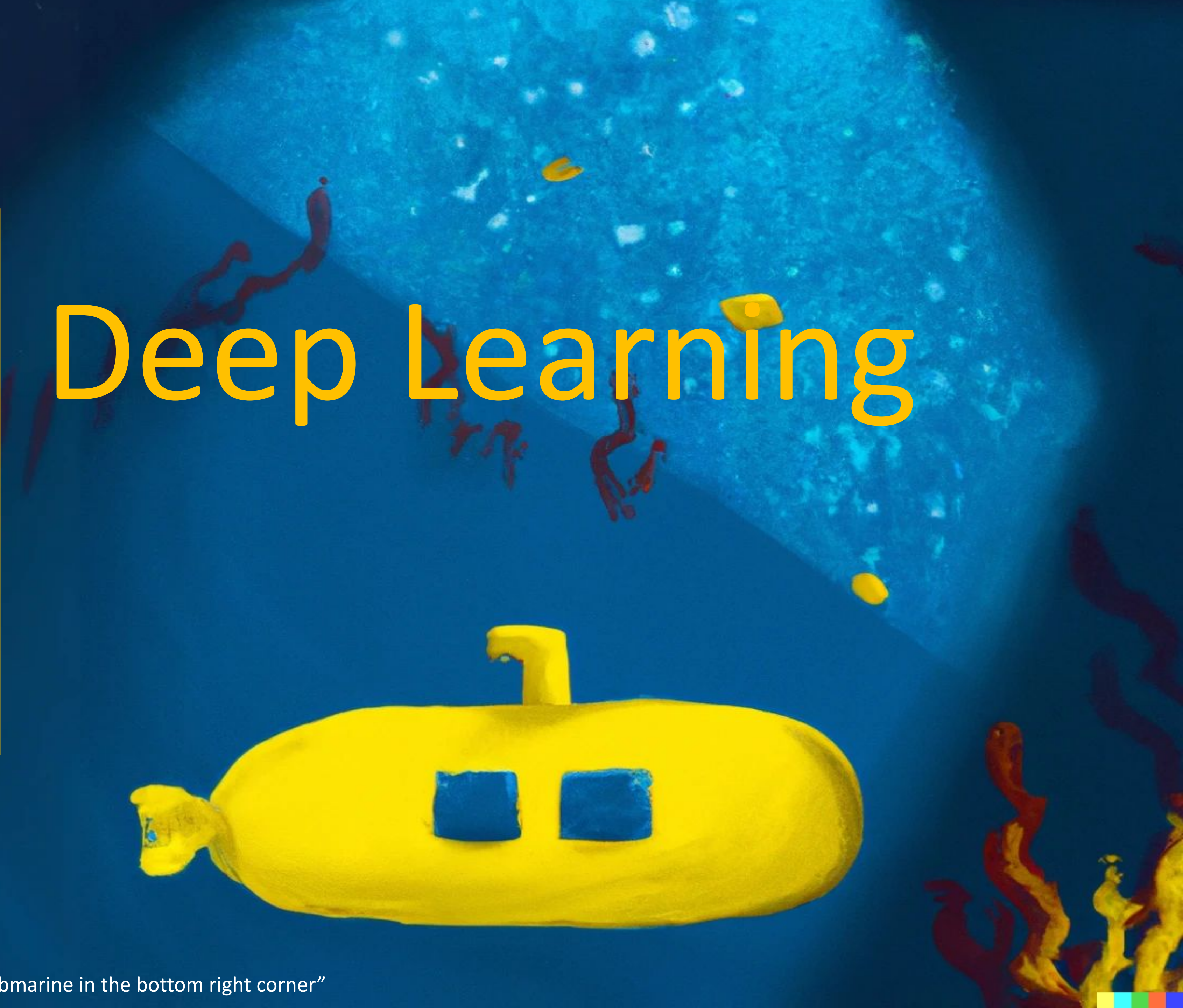
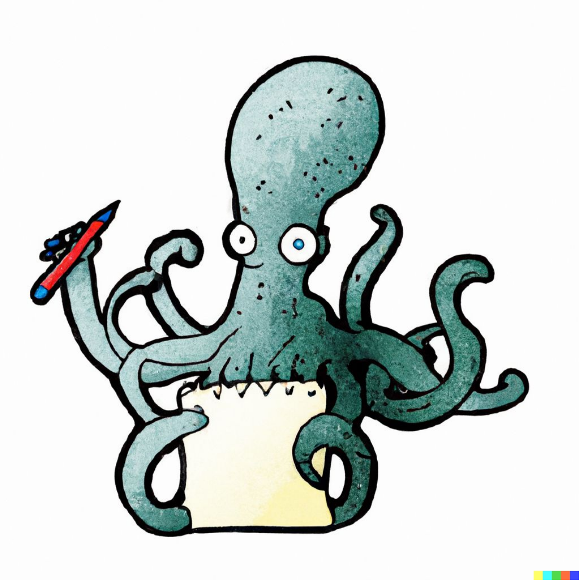
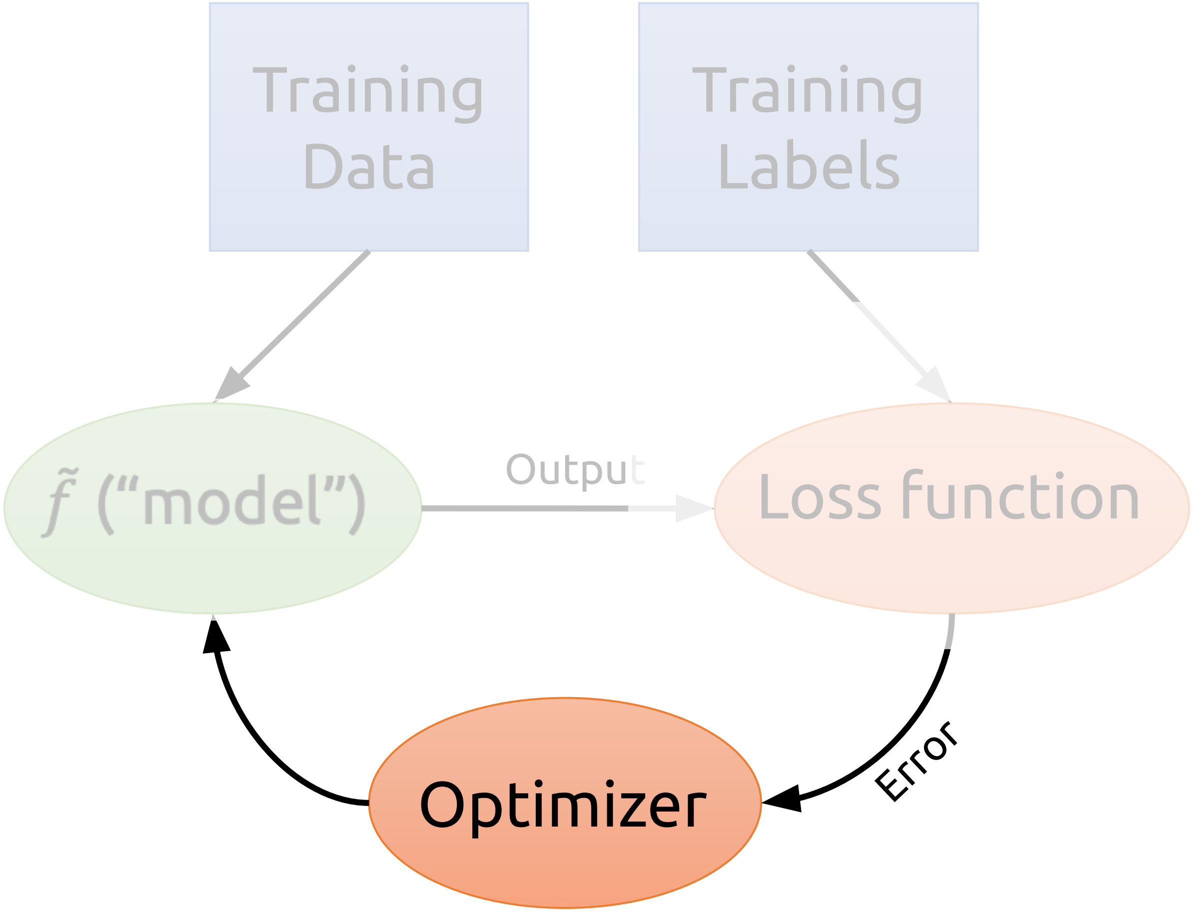
February 06, 2023
Monday



DALL-E 2 prompt “a painting of deep underwater with a yellow submarine in the bottom right corner”

Recap: **Optimizer**

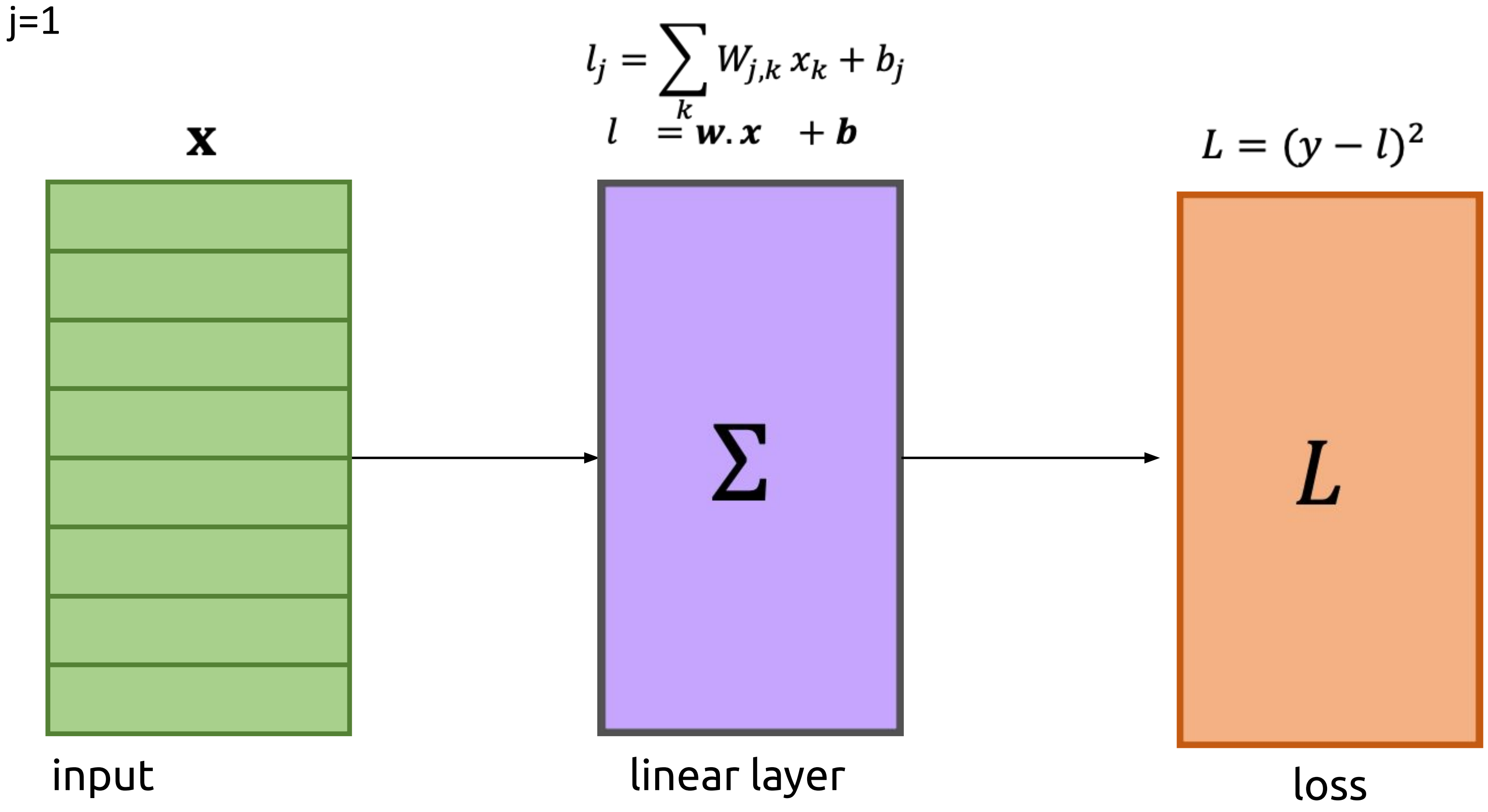




Recap: Gradient Descent

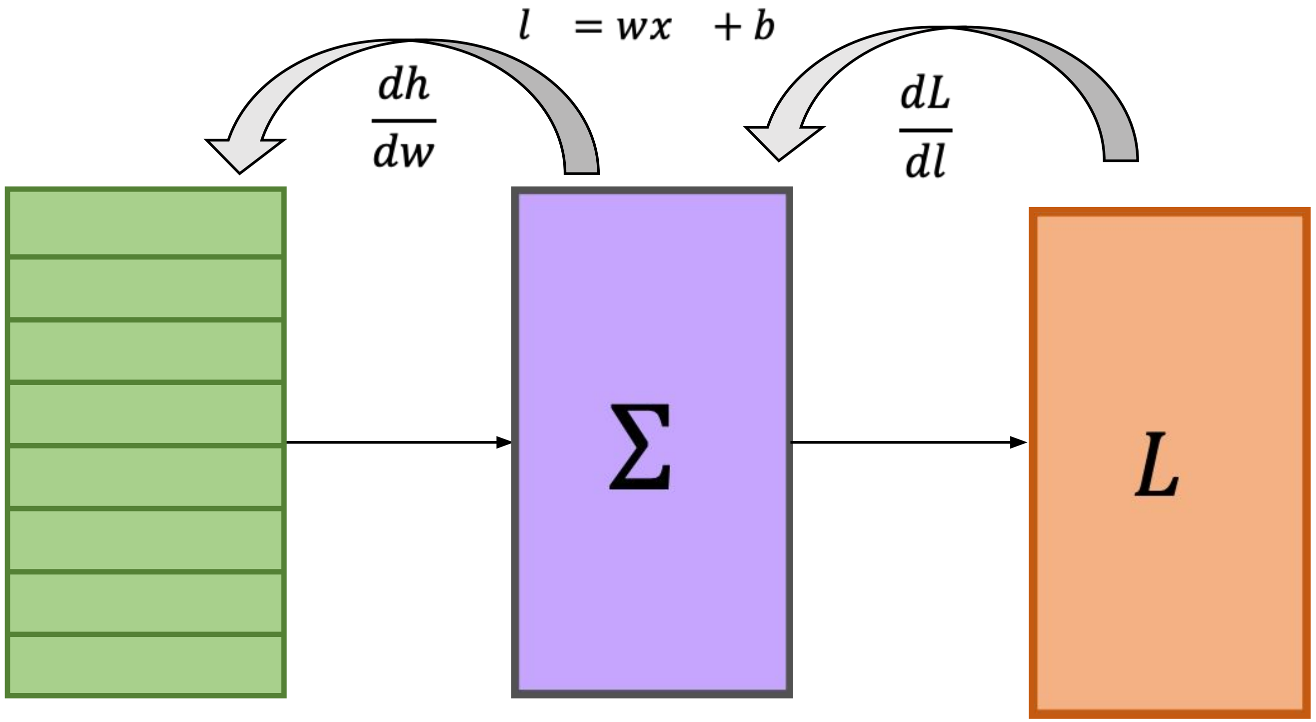
- Basic update rule: $\Delta w_{j,i} = -\alpha \cdot \frac{\partial L}{\partial w_{j,i}}$
  - $w_{j,i}$: one network parameter (or “weight”)
  - $\Delta w_{j,i}$: how we change this weight to decrease loss
  - α : a constant called the ***learning rate***
  - L : the loss value

Recap: Our simple regression model



Recap: Backpropagation

- $\frac{dL}{dw} = \frac{dL}{dl} \cdot \frac{dl}{dw} = -2(\mathrm{y} - \mathrm{l}).\mathrm{x} = -2\mathrm{x}(\mathrm{y} - \mathrm{wx} - \mathrm{b}) = 2\mathrm{x}(\mathrm{wx} + \mathrm{b} - \mathrm{y})$



Today's goal – continue learning about backpropagation

(1) Building a simple neural network for multi-class classification

(2) Backpropagation of our network (via Chain Rule)

(3) Computation graph for neural networks

Recap: Cross Entropy Loss (for Multi-class classification)

$$-\sum_{j=1}^{m} y_j \log(p_j)$$

$$= -\log(p_{a)}$$

p	Classes (m)	y
0.3	“0”	0
0.2	“1”	0
0.5	“2”	1

One hot encoding

0				a			m
0	0	0	0	1	0	0	0

y

Some examples:

$\log(0.9) = -0.04$

$\log(0.5) = -0.3$

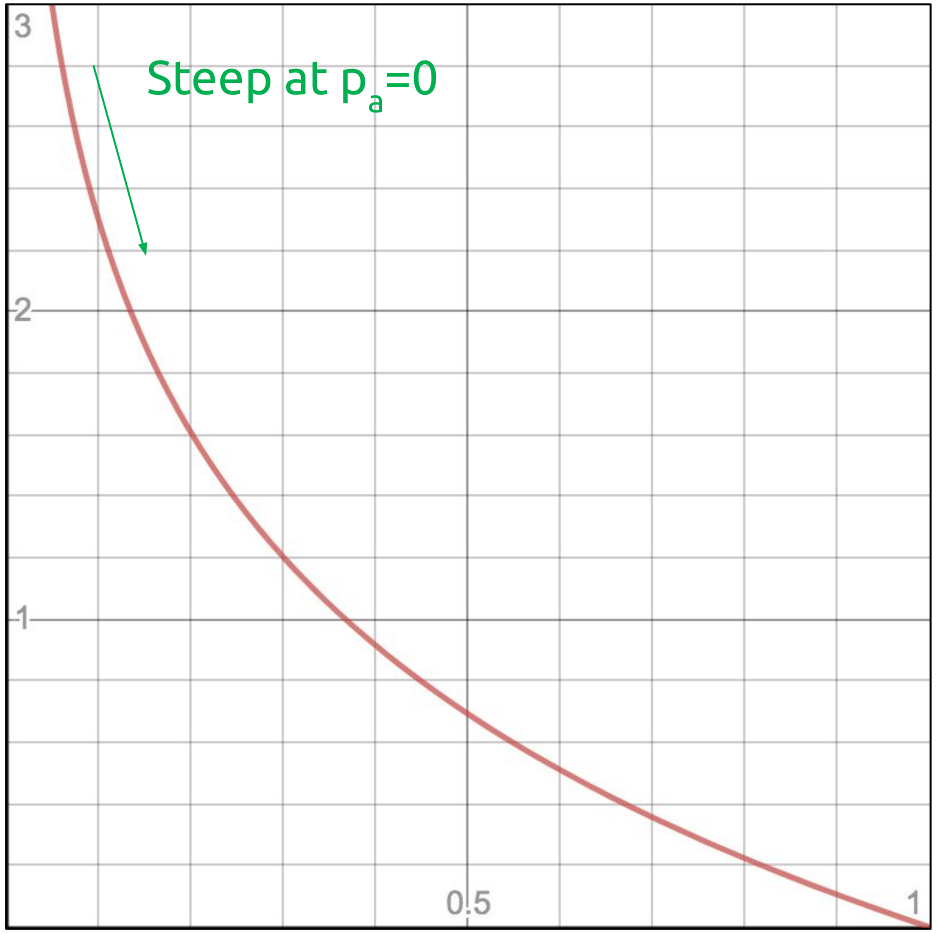
$\log(0.001) = -3$

We want model to assign high probability to the true class and low to others

A Better Loss: $-\log(p_a)$

Let p_a be the probab

No Maximum

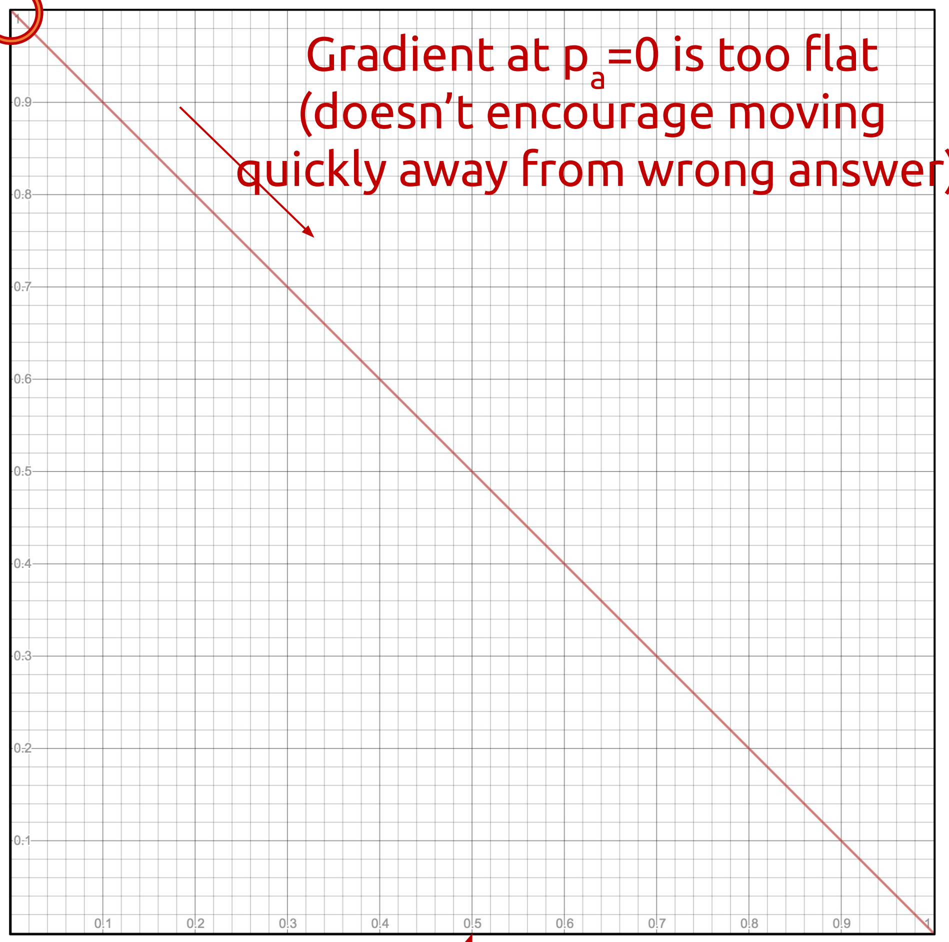


Operating in "log space" means that near-zero probabilities become large negative numbers □ no numerical underflow

Inverse Probability $1 - p_a$ as Loss

Maximum is 1 (insufficiently strong penalty)

Gradient at p_a=0 is too flat (doesn't encourage moving quickly away from wrong answer)



When probabilities get small, floating point numbers often fail to represent differences between them (i.e. numerical 'underflow')

Recap: Cross Entropy Loss (for Multi-class classification)

$$-\sum_{j=1}^{m} y_j \log(p_j)$$

$$= -\log(p_a)$$

p	Classes (m)	y
0.3	"0"	0
0.2	"1"	0
0.5	"2"	1

How do we get these probabilities?

We want model to assign high probability to the true class and low to others

Some examples:

$\log(0.9) = -0.04$

$\log(0.5) = -0.3$

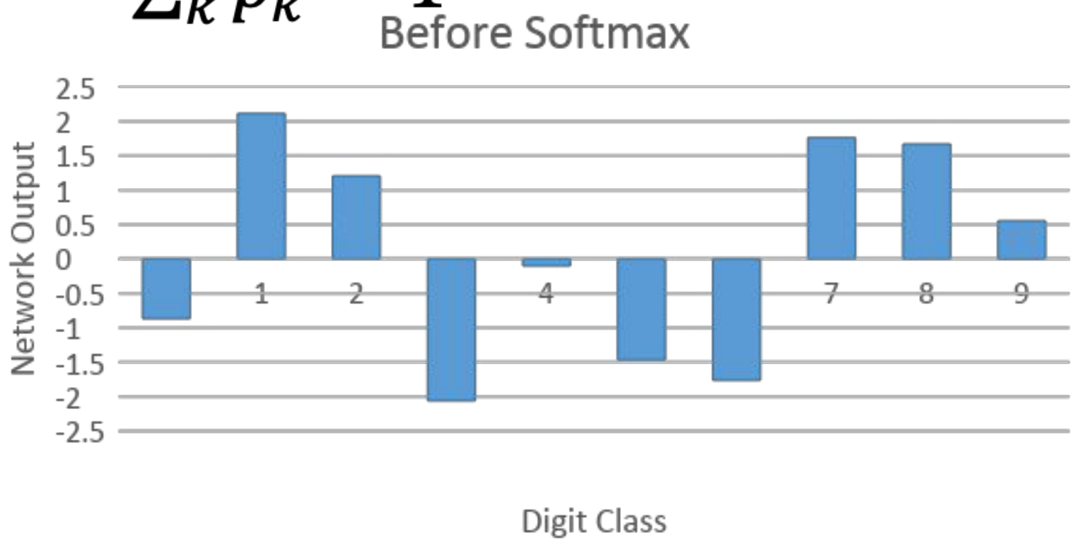
$\log(0.001) = -3$

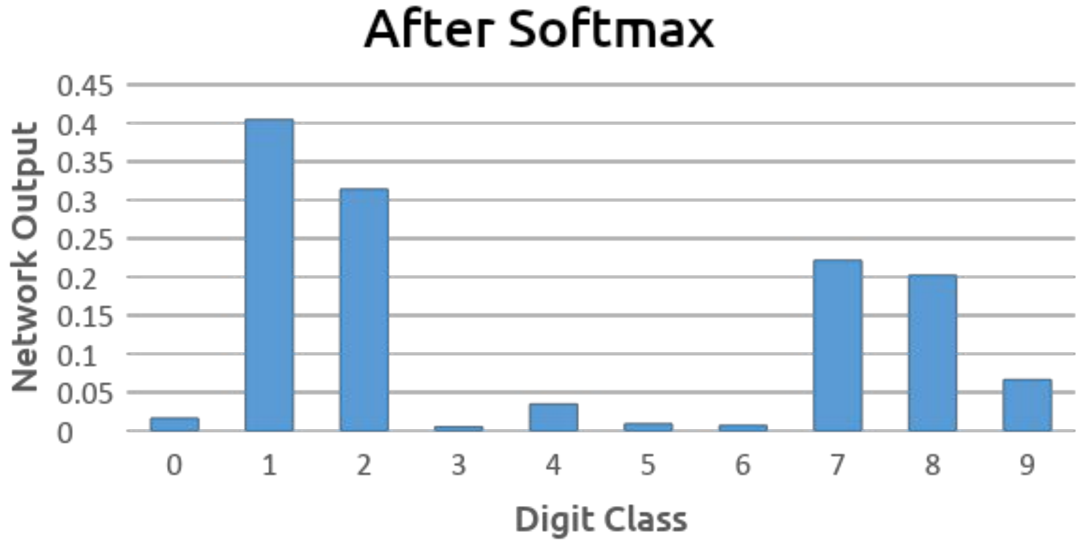
Our new probability layer

- What does a probability distribution, p look like?
  - For any digit j: $p_j \in [0,1]$
  - $\sum_k p_k = 1$
- Currently, our outputs l do not satisfy these properties
  - For any digit j: $l_j \in \mathbb{R}$
  - $\sum_k l_k = \mathbb{R}$
- How to make our network output satisfy these properties?

The Softmax Function

- The formula: $p_j = \dfrac{e^{l_j}}{\sum_k e^{l_k}}$
- Using exponents e^{l_j} means every number is positive
- Dividing by $\sum_k e^{l_k}$ means every p_j is between 0 and 1, and that $\sum_k p_k = 1$





We call these numbers ***logits*** (l notation)

Recap: Cross Entropy Loss (for Multi-class classification)

$$-\sum_{j=1}^{m} y_j \log(p_j)$$

$$= -\log(p_{a})$$

p	Classes (m)	y
0.3	"0"	0
0.2	"1"	0
0.5	"2"	1

We can get these probabilities by using a Softmax function

We want model to assign high probability to the true class and low to others

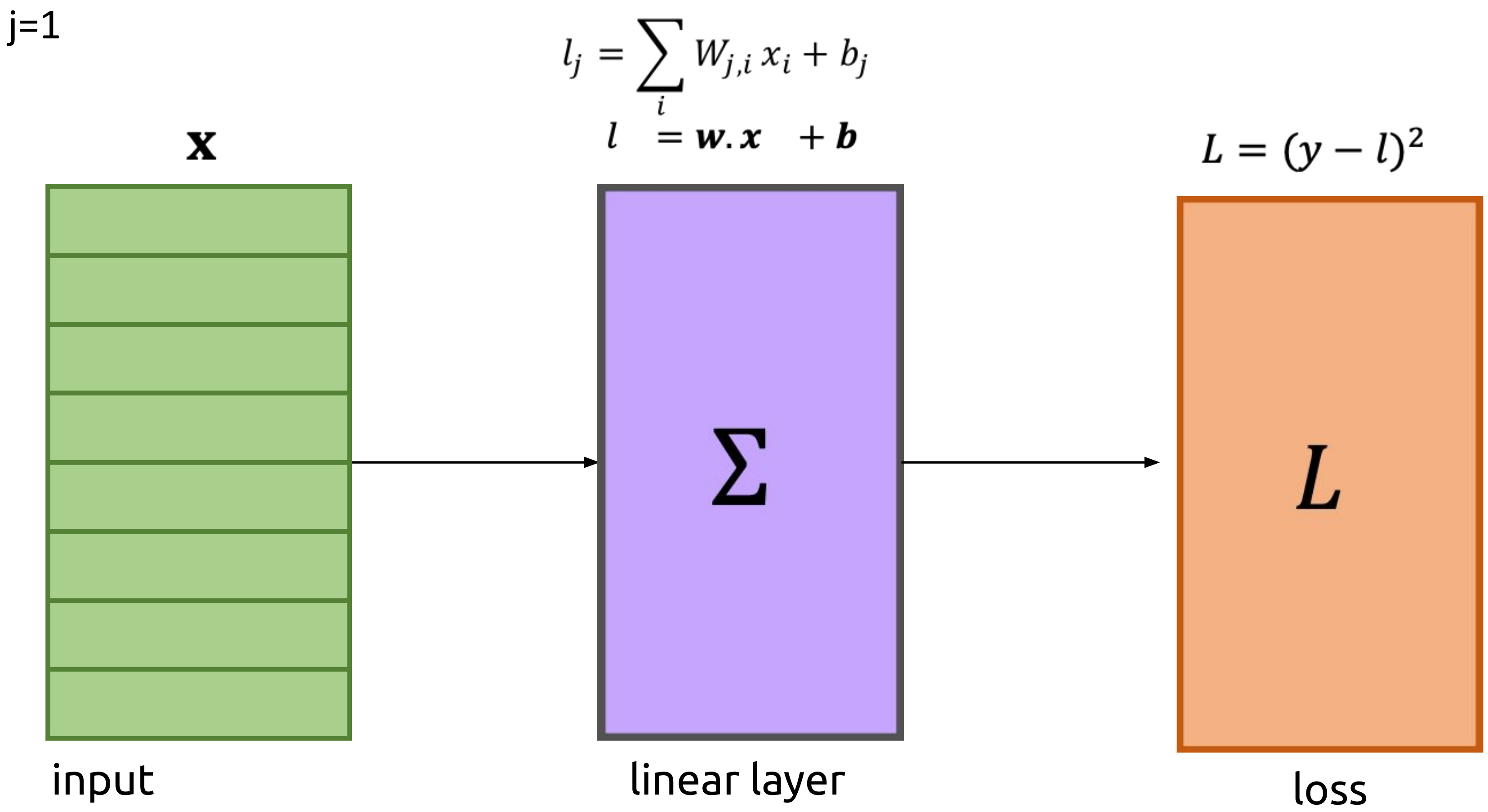
Some examples:

$\log(0.9) = -0.04$

$\log(0.5) = -0.3$

$\log(0.001) = -3$

What changes do we make for this task?



Remove the MSE loss layer

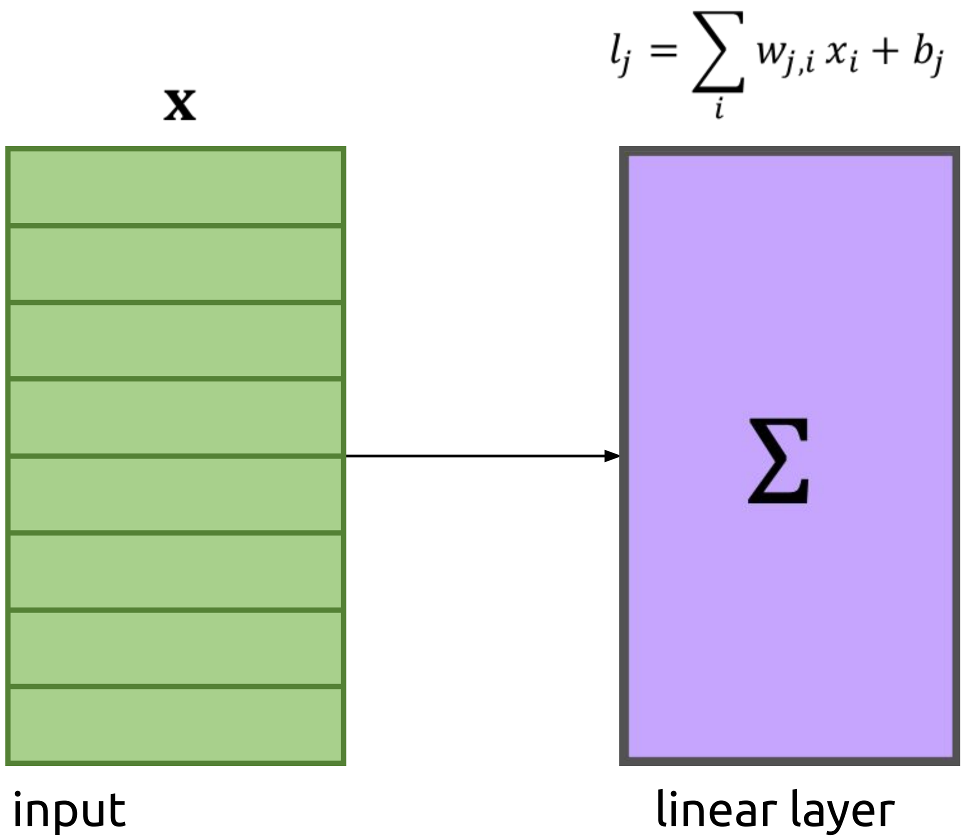
Increase the number of outputs to m classes

Add a softmax layer

Add a cross entropy loss layer

Our model before

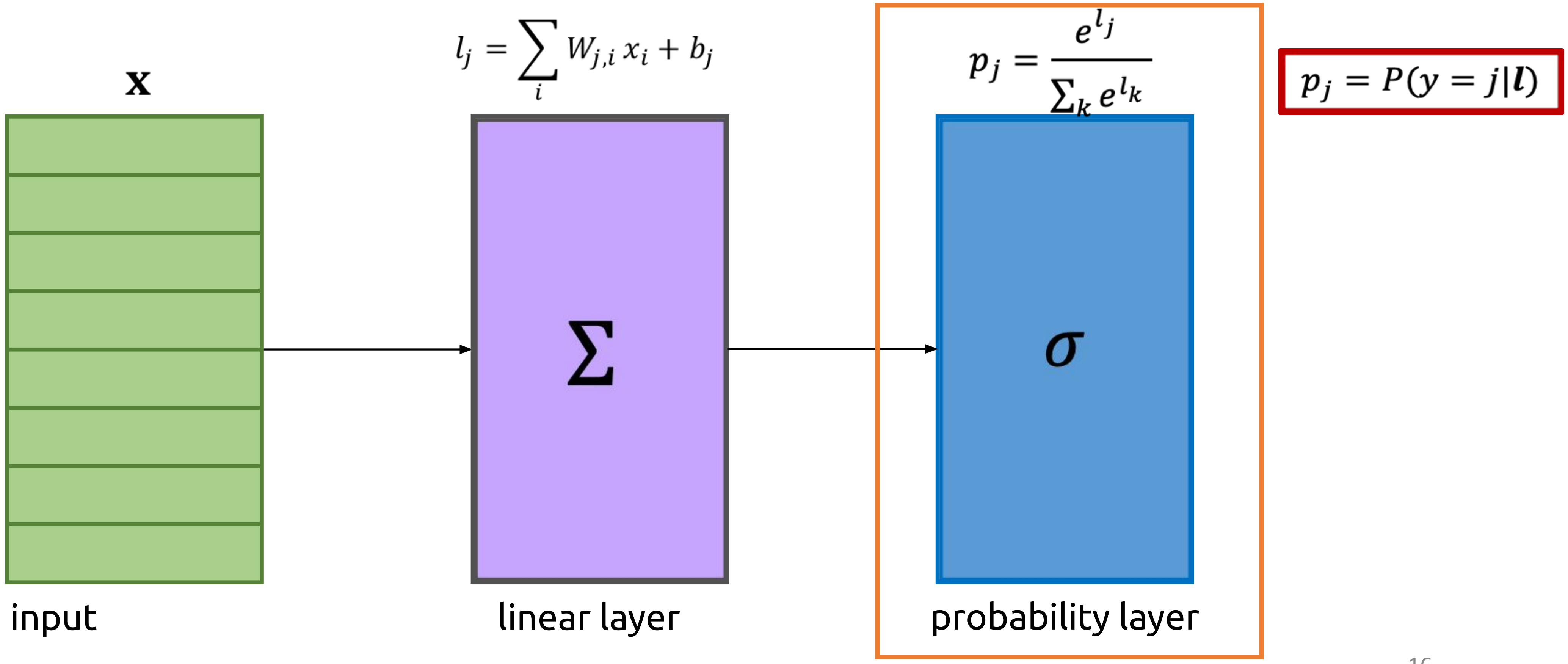
- This is a simplified view of our model with an input and a linear layer



Our model after

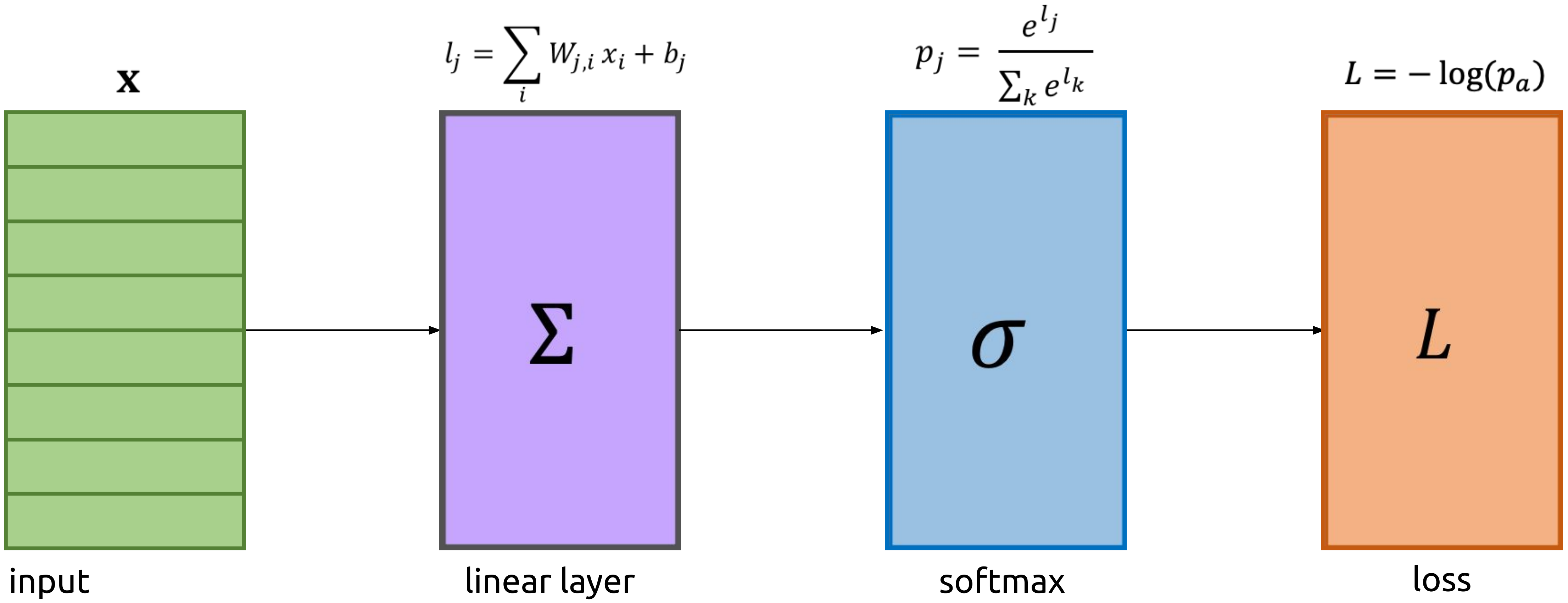
Our new layer

- This is our model with the new probability layer



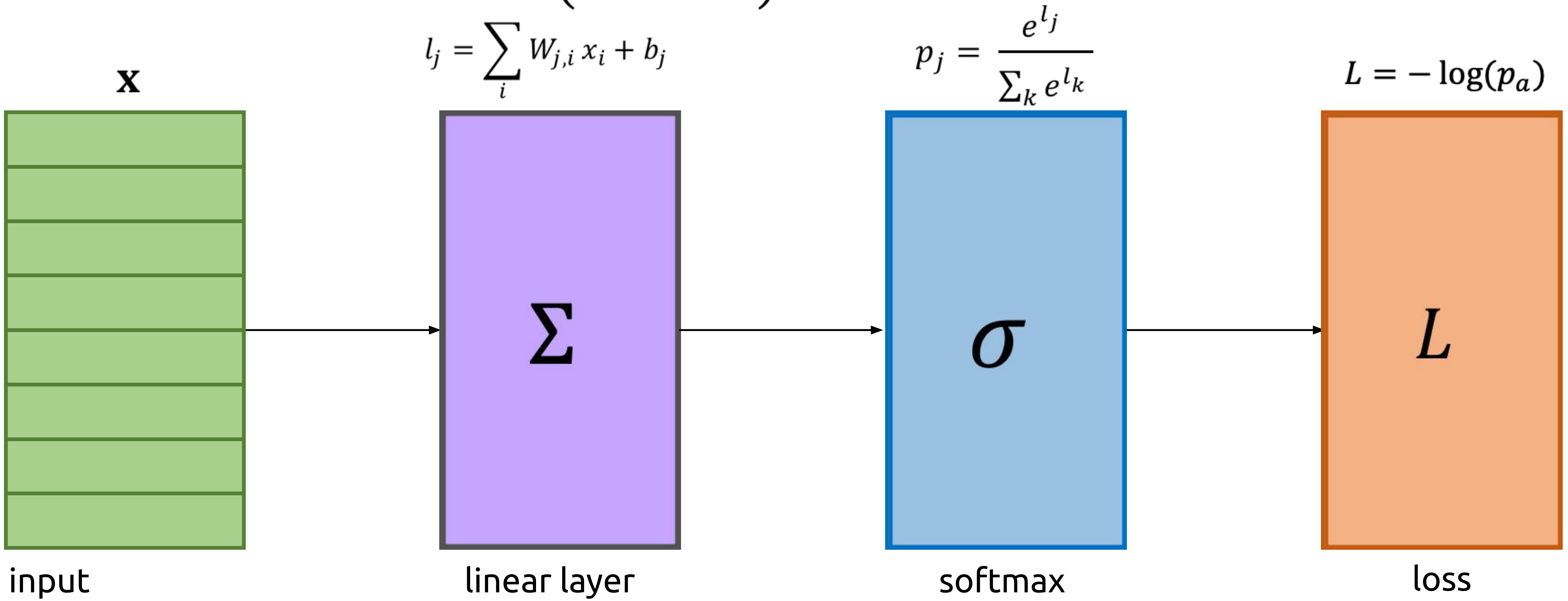
Adding Cross Entropy Loss to Our Network

Any questions?



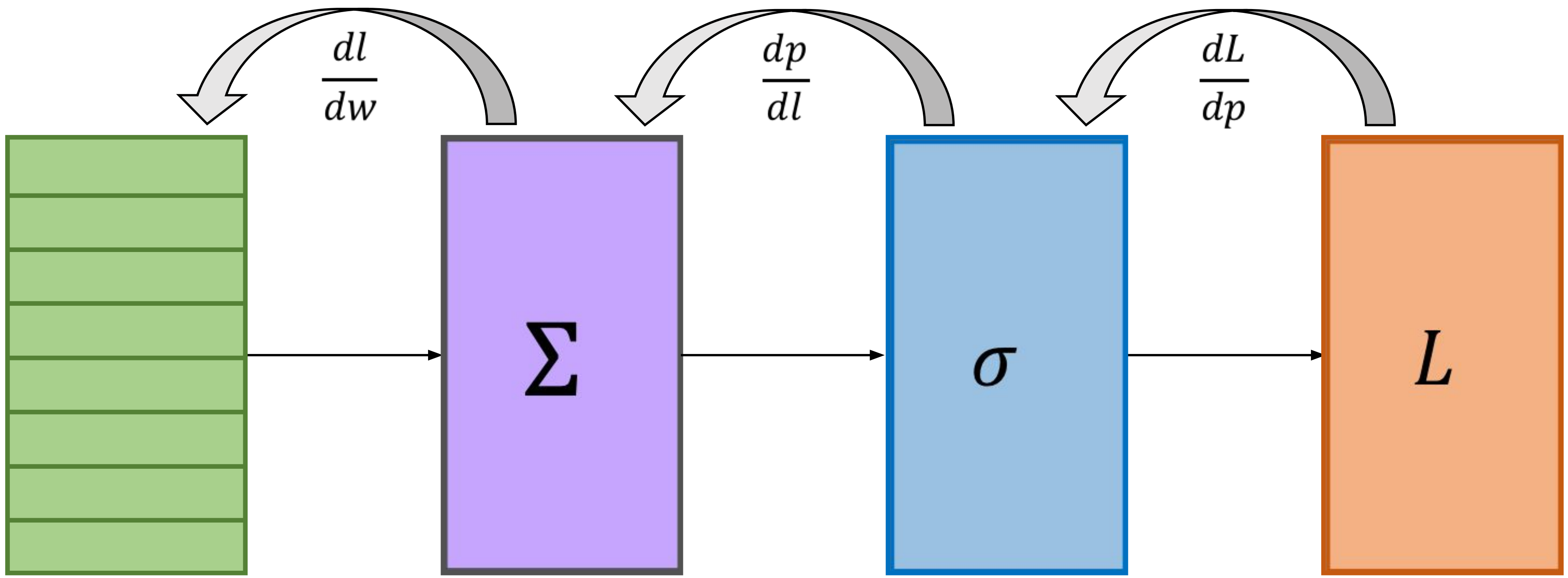
What is the Chain Rule in Our Network?

- Here's our function: $L\left(p\left(l(w)\right)\right) \Rightarrow$

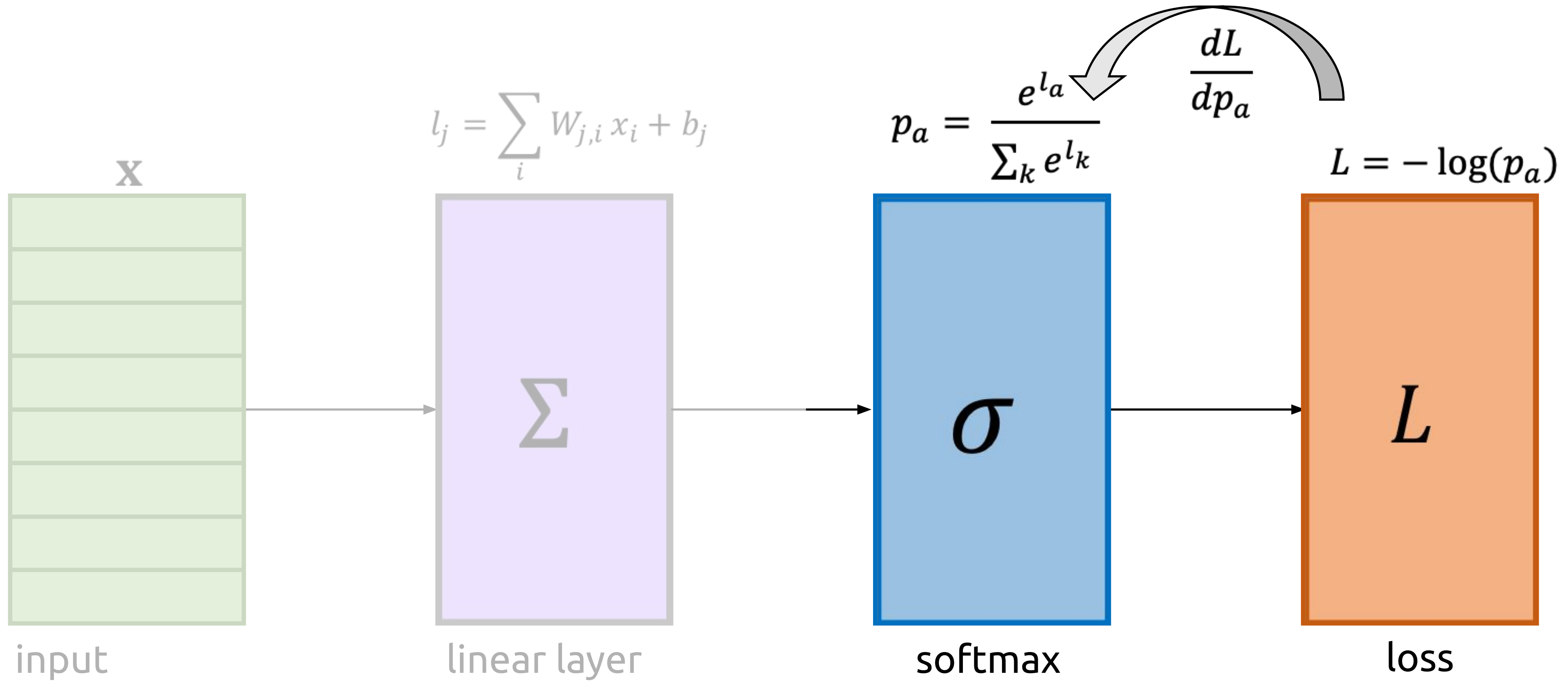


The Chain Rule in Our Network

- Here's our function: $L\left(p(l(w))\right) \Rightarrow \frac{dL}{dw} = \frac{dL}{dp} \cdot \frac{dp}{dl} \cdot \frac{dl}{dw}$

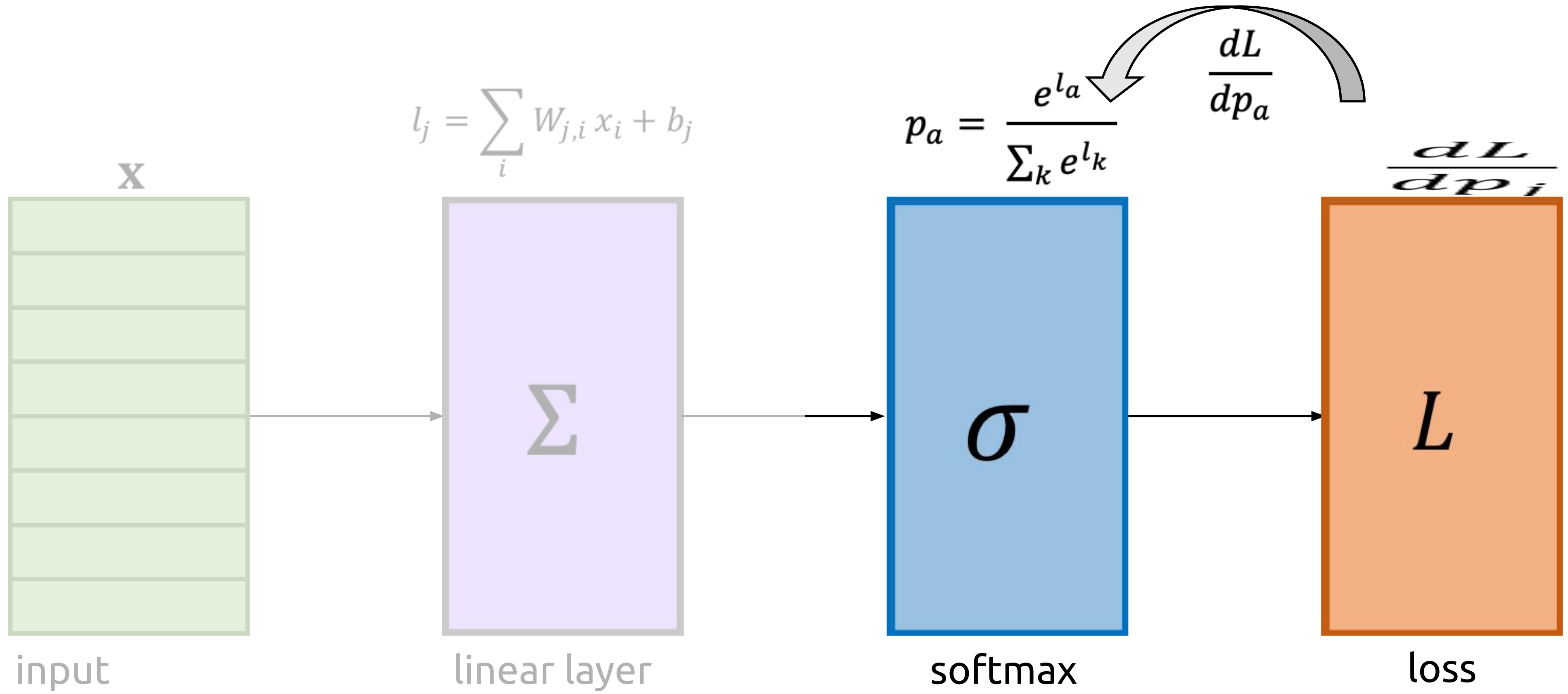


Derivative for Cross Entropy Loss Layer



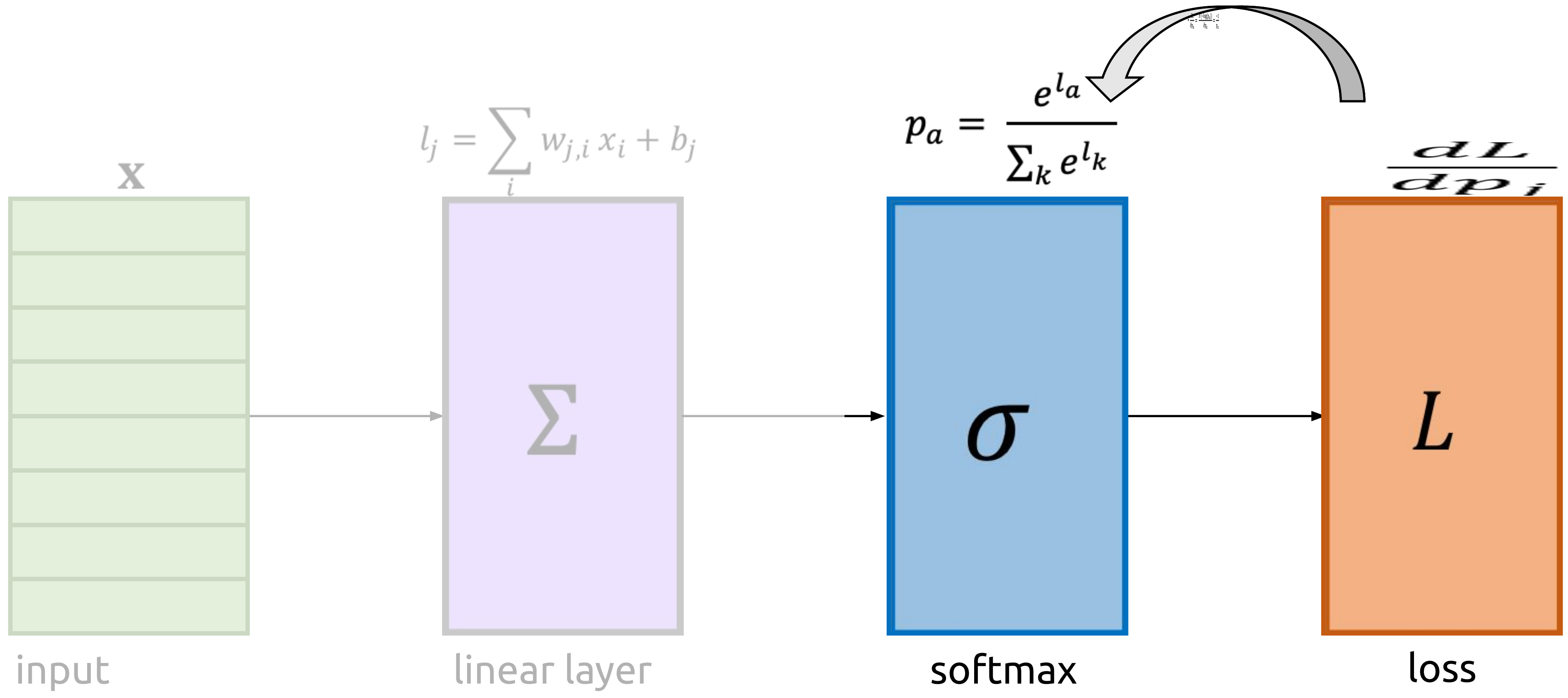
Derivative for Cross Entropy Loss Layer

- $\frac{\partial L}{\partial p_a} = \frac{\partial\,(-\log(p_a))}{\partial p_a} =$

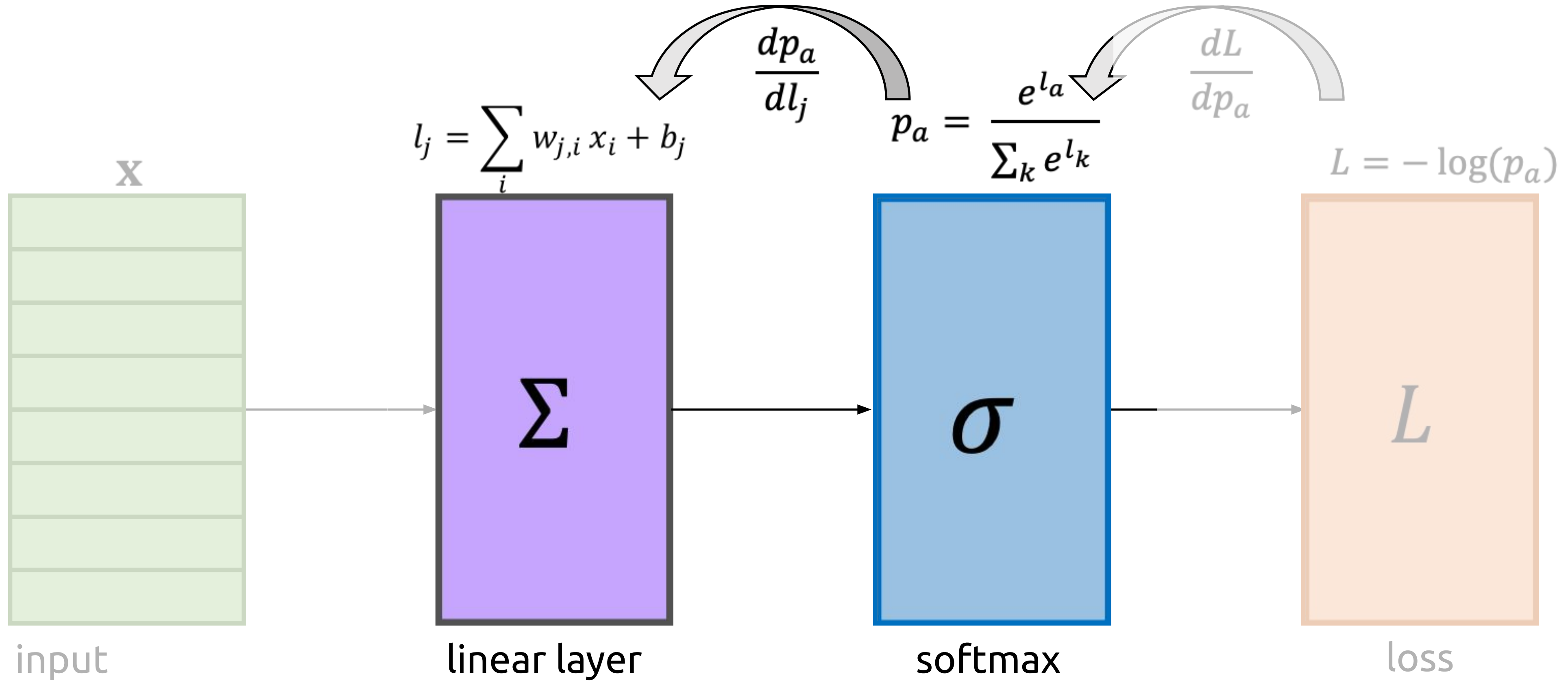


Derivative for Cross Entropy Loss Layer

- $\frac{\partial L}{\partial p_a} = \frac{\partial\left(-\log(p_a)\right)}{\partial p_a} = \frac{-1}{p_a}$

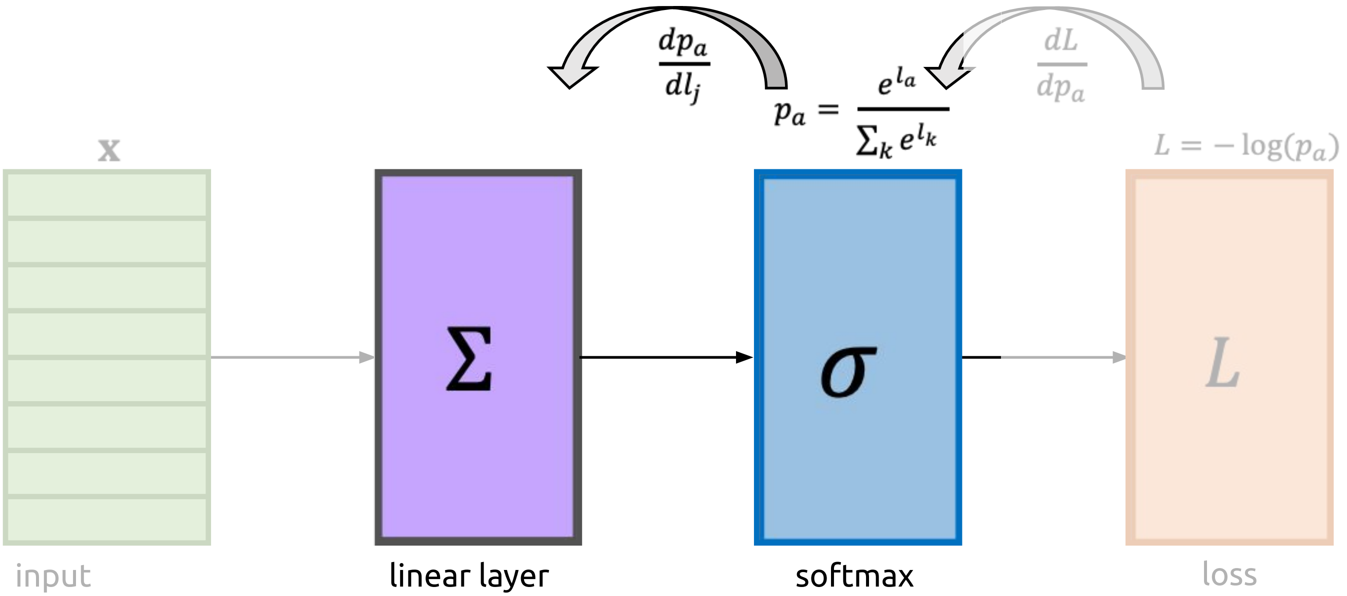


Chain Rule for Softmax Layer



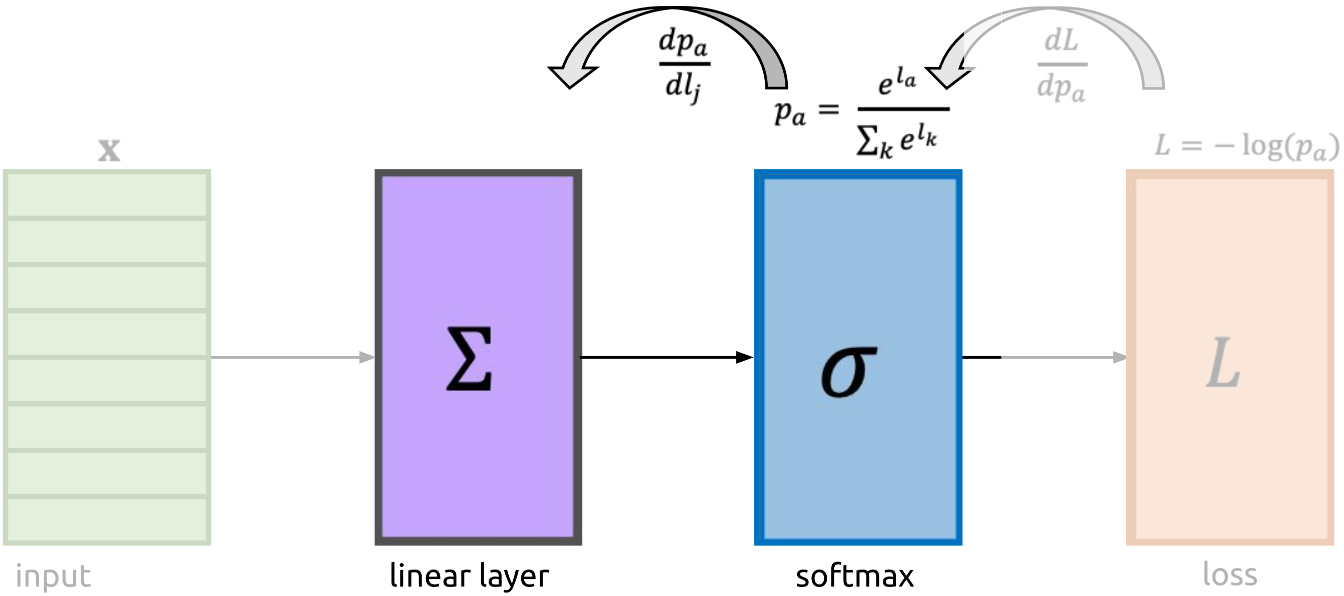
Chain Rule for Softmax Layer

$$\frac{\partial p_a}{\partial l_j} =$$



Chain Rule for Softmax Layer

$$\frac{\partial p_a}{\partial l_j} = \frac{\partial\left(\frac{e^{l_a}}{\sum_k e^{l_k}}\right)}{\partial l_j} =$$



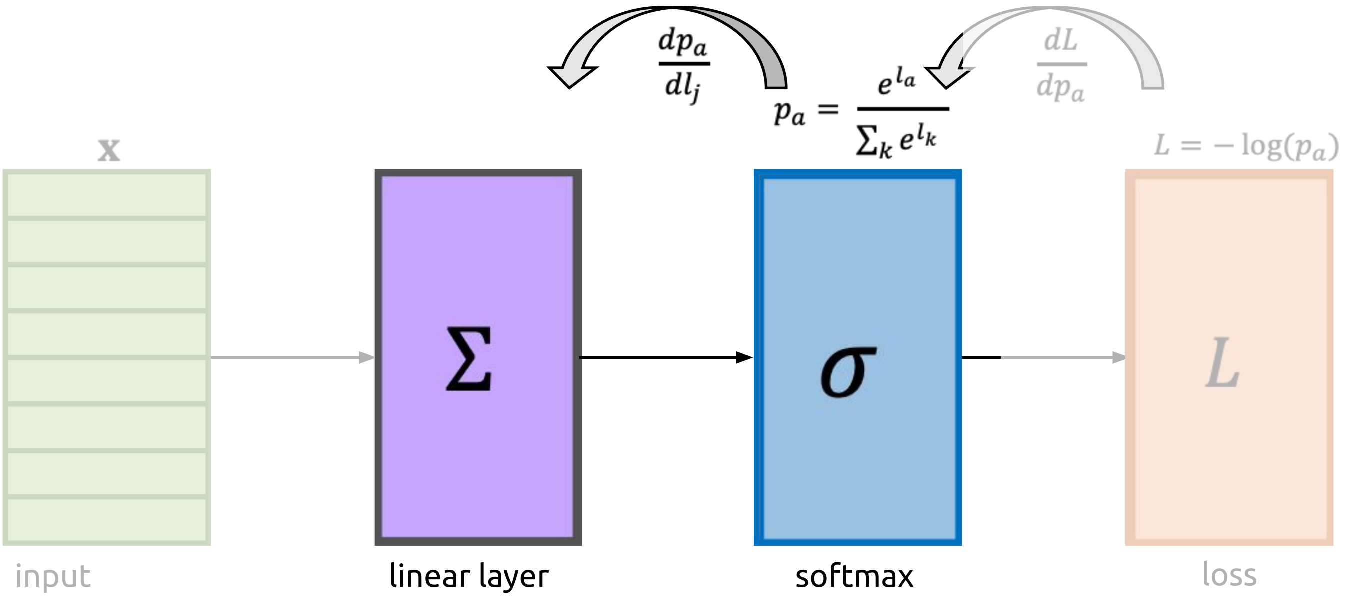
Chain Rule for Softmax Layer

Because of multiple inputs and outputs

Which component (output element) of softmax we're seeking to find the derivative of?

With respect to which input element the partial derivative is computed?

$$\frac{\partial p_a}{\partial l_j} = \frac{\partial \left(\frac{e^{l_a}}{\sum_k e^{l_k}} \right)}{\partial l_j} = ???$$



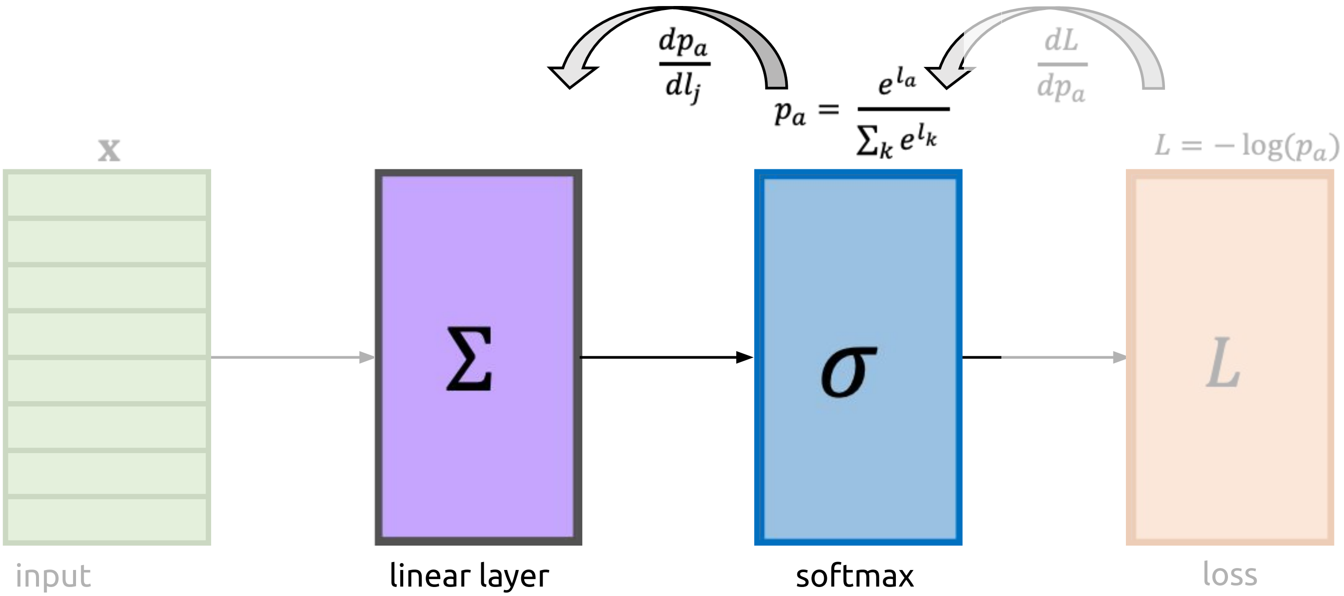
https://eli.thegreenplace.net/2016/the-softmax-function-and-its-derivative/

Chain Rule for Softmax Layer

$$\frac{\partial p_a}{\partial l_j} = \frac{\partial \left(\frac{e^{l_a}}{\sum_k e^{l_k}} \right)}{\partial l_j} = ???$$

Because of multiple inputs and outputs
Two cases to consider:

1. $j = a$ (i.e. the logit of the correct answer)
2. $j \neq a$



$$\frac{\partial p_a}{\partial l_j} = \frac{\partial \left(\frac{e^{l_a}}{\sum_k e^{l_k}} \right)}{\partial l_j}$$

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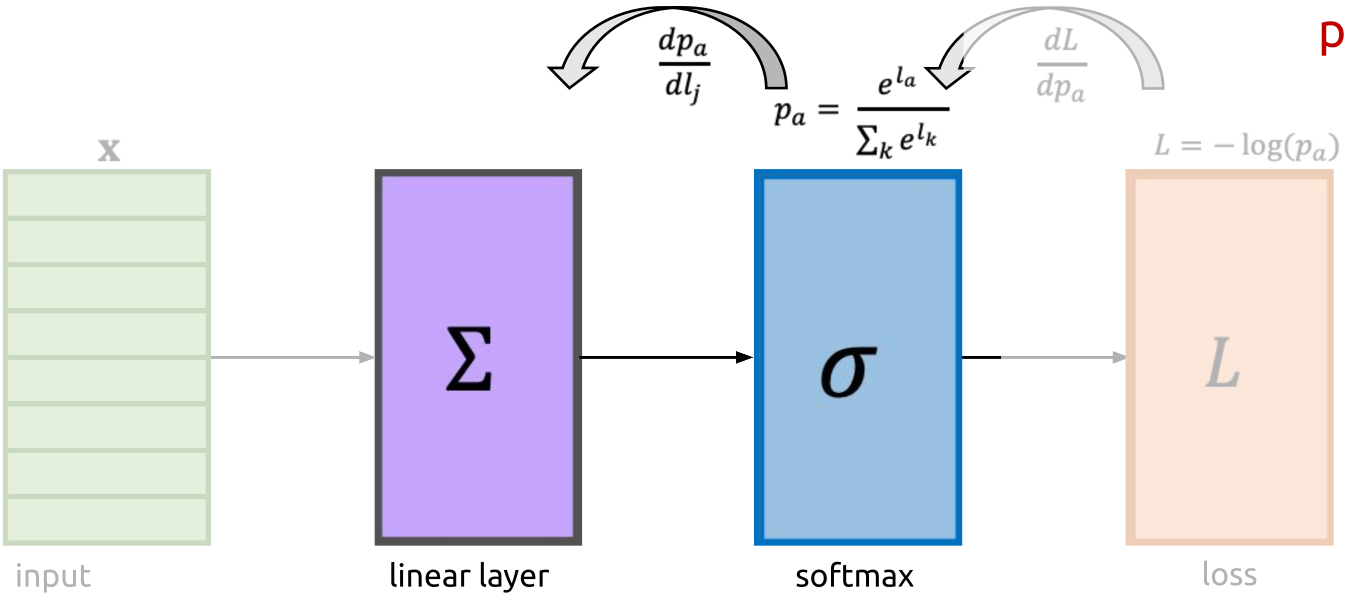
Chain Rule for Softmax Layer

$$\frac{\partial p_a}{\partial l_j} = \frac{\partial\left(\frac{e^{l_a}}{\sum_k e^{l_k}}\right)}{\partial l_j} = \begin{cases}(1-p_j)p_a & a=j\\ -p_j p_a & a\neq j\end{cases}$$

Derivative is positive (increasing the a^{th} logit will boost the probability of predicting the correct answer)

Derivative is negative (decreasing the probability of every other logit will boost the probability of predicting the correct answer)



Chain Rule for Softmax Layer

$$\frac{\partial p_a}{\partial l_j} = \begin{cases} (1 - p_j)p_a & a = j \\ -p_j p_a & a \neq j \end{cases}$$

A simpler way to write it:

The vector of all predicted probabilities

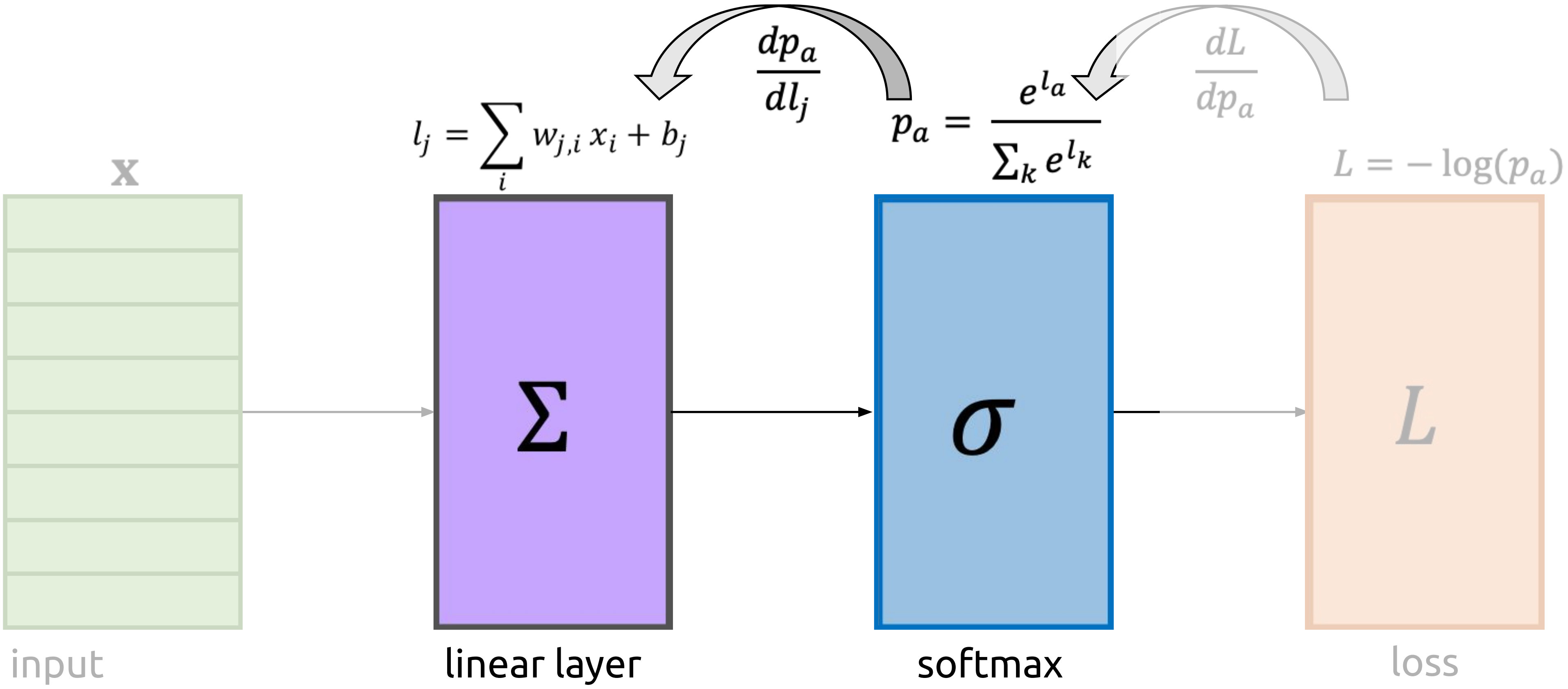
$$\nabla_{\mathbf{l}}\, p_a = (\mathbf{y} - \mathbf{p})p_a$$

The ***gradient*** of p_a with respect to the logit vector $\mathbf{l}$

A **one-hot** vector

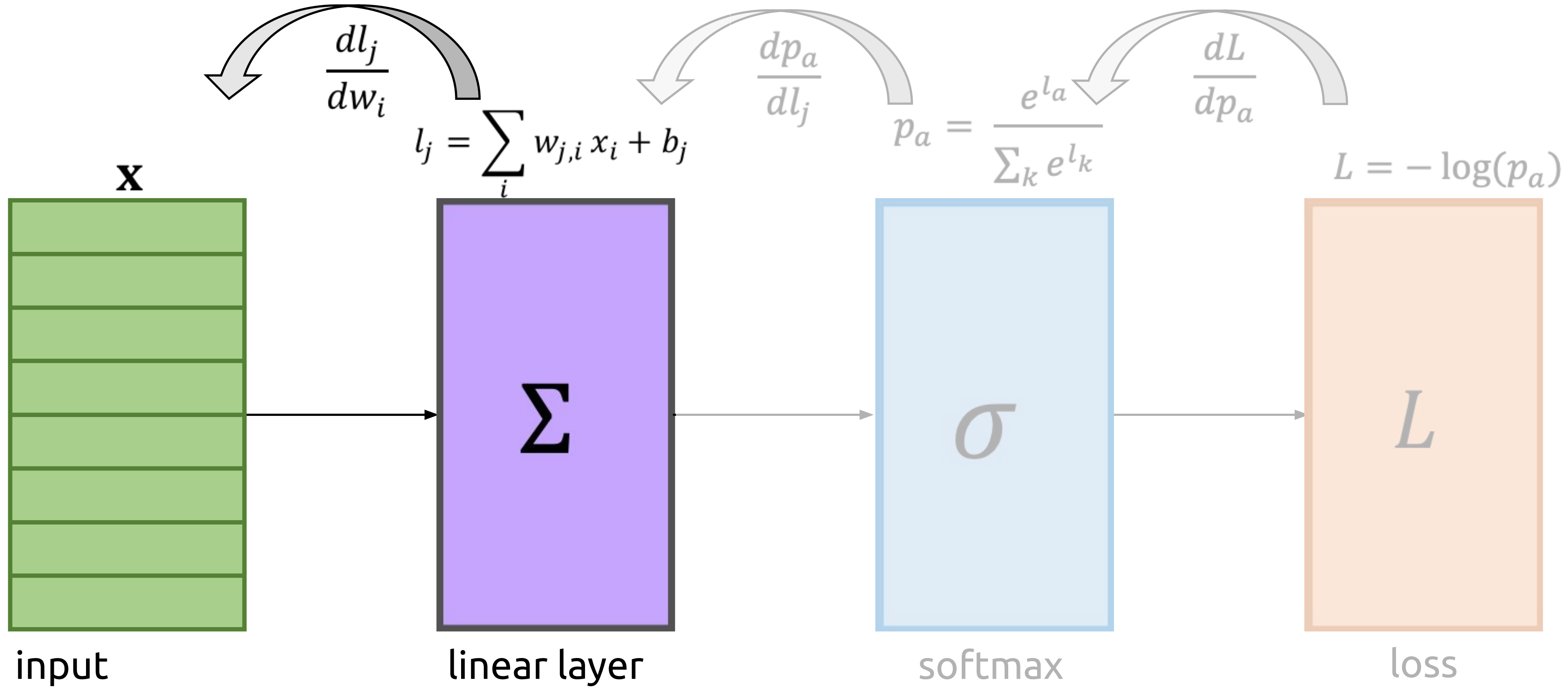
$$\begin{array}{cccccccc} 0 & & & & a & & & m \\ \boxed{0} & \boxed{0} & \boxed{0} & \boxed{0} & \boxed{1} & \boxed{0} & \boxed{0} & \boxed{0} \\ & & & & \mathbf{y} & & & \end{array}$$

Chain Rule for Softmax Layer



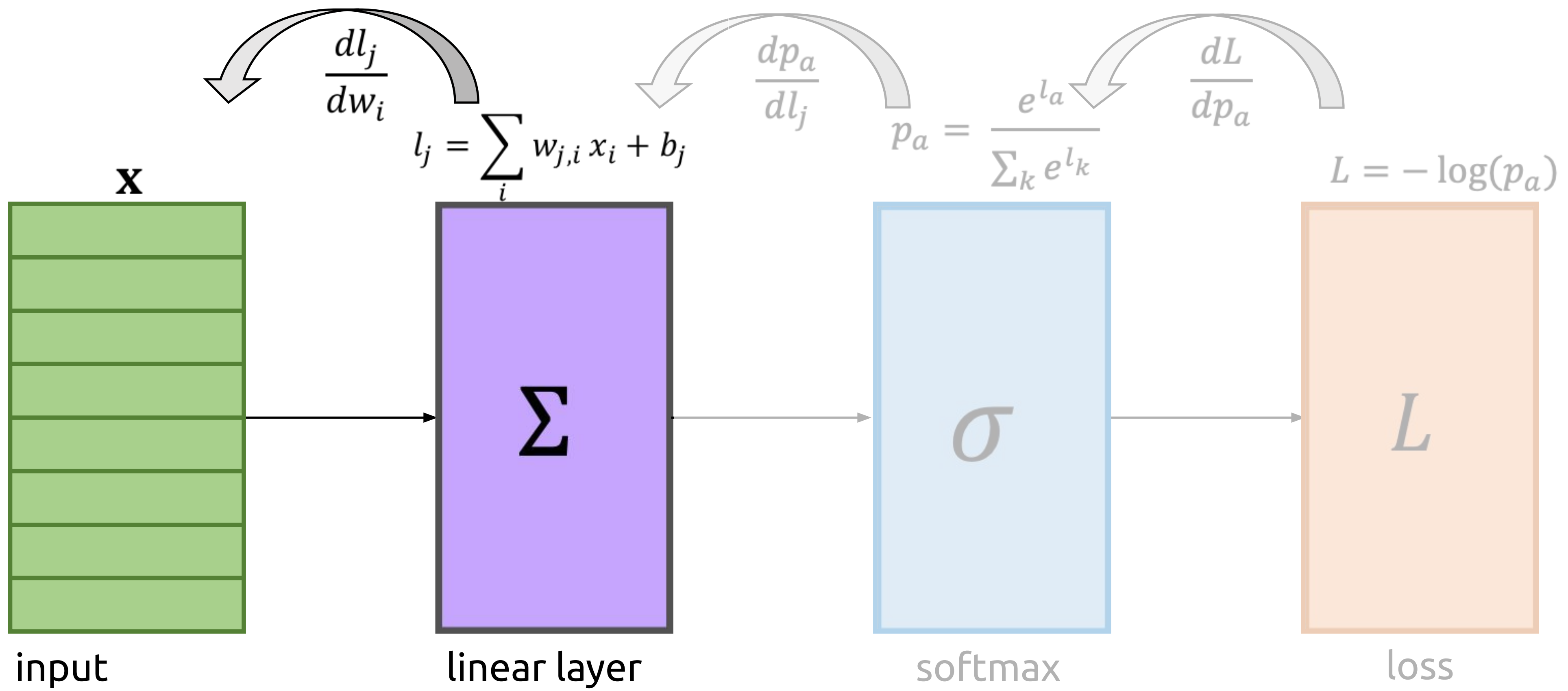
Chain Rule for Linear Layer

- $\frac{\partial l_j}{\partial w_{j,i}} =$



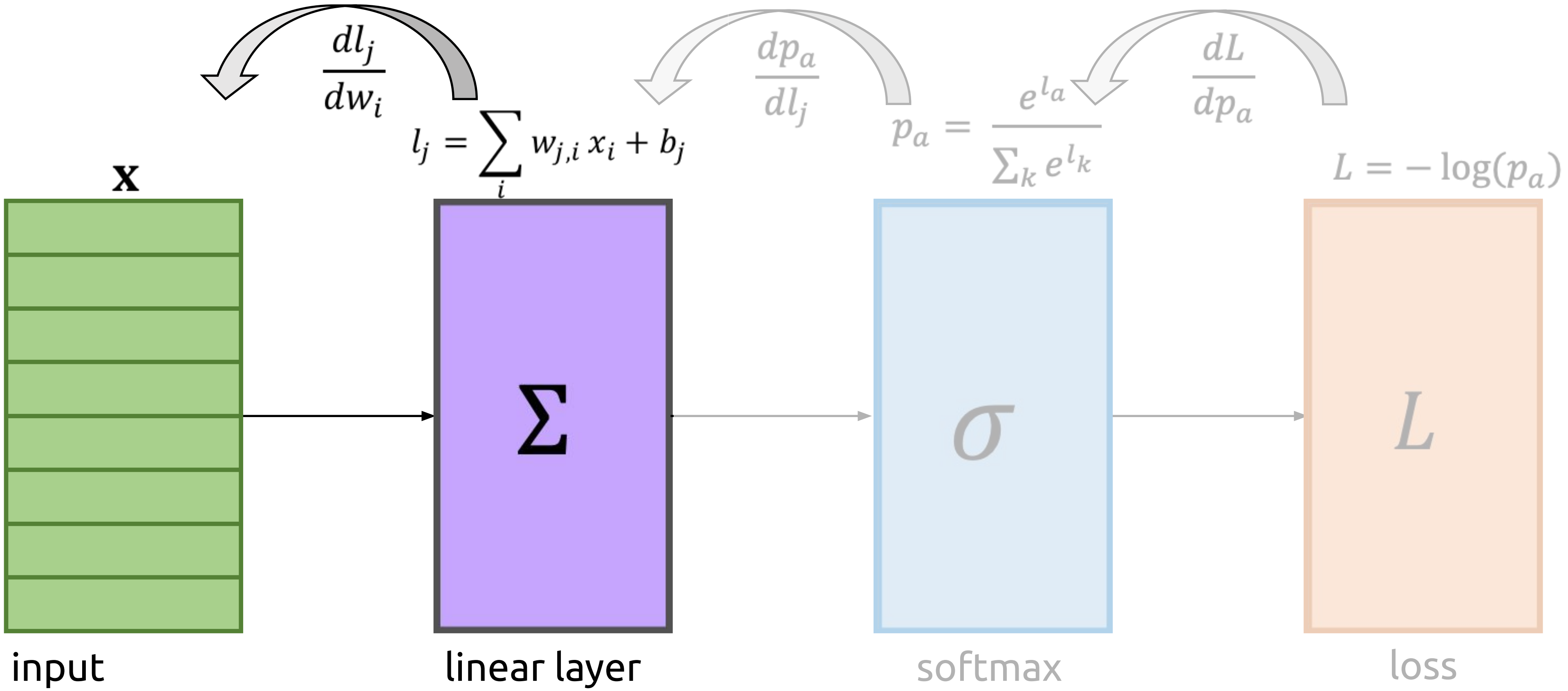
Chain Rule for Linear Layer

- $\dfrac{\partial l_j}{\partial w_{j,i}} = \dfrac{\partial(\sum_i w_{j,i} x_i)}{\partial w_{j,i}}$:



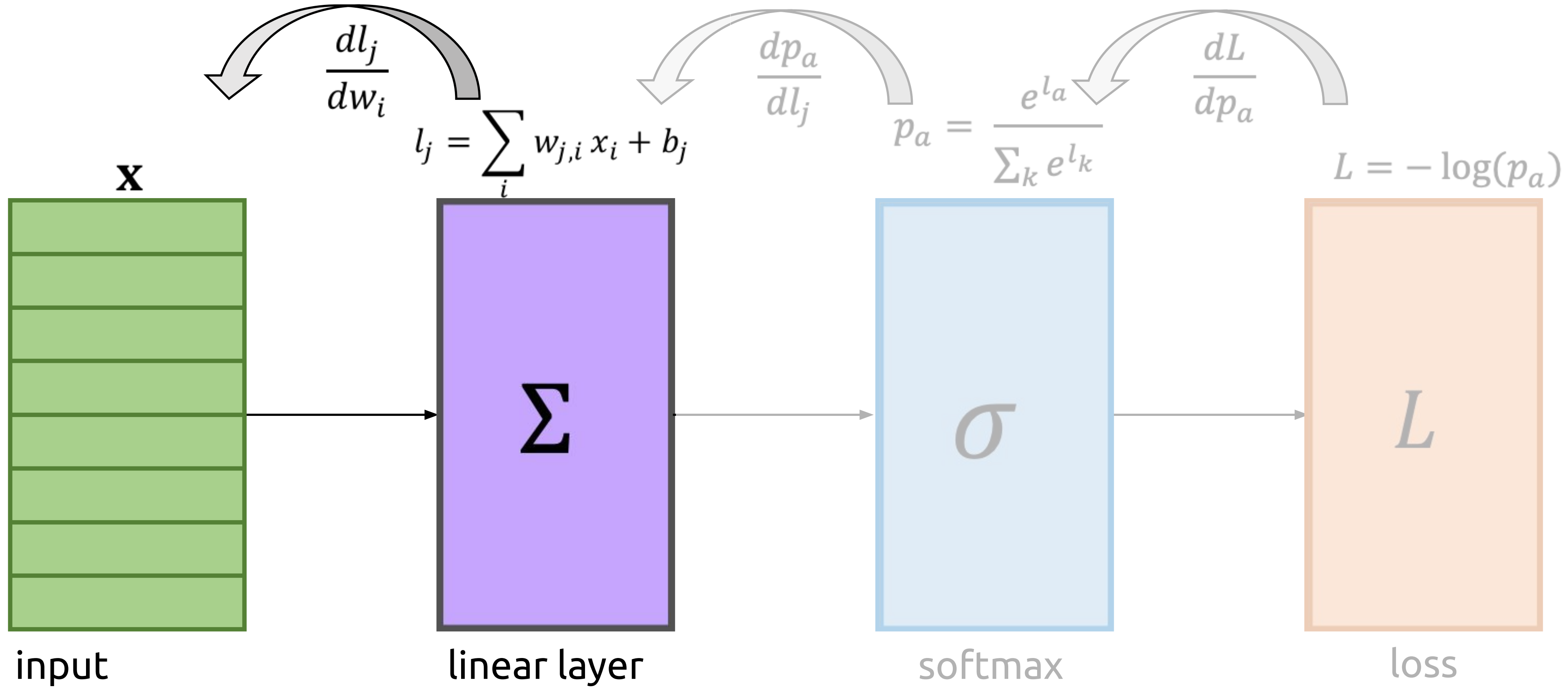
Chain Rule for Linear Layer

- $\frac{\partial l_j}{\partial w_{j,i}} = \frac{\partial(\sum_i w_{j,i}x_i)}{\partial w_{j,i}} = \frac{\partial(\ldots + w_{j,i}x_i + \cdots)}{\partial w_{j,i}}$



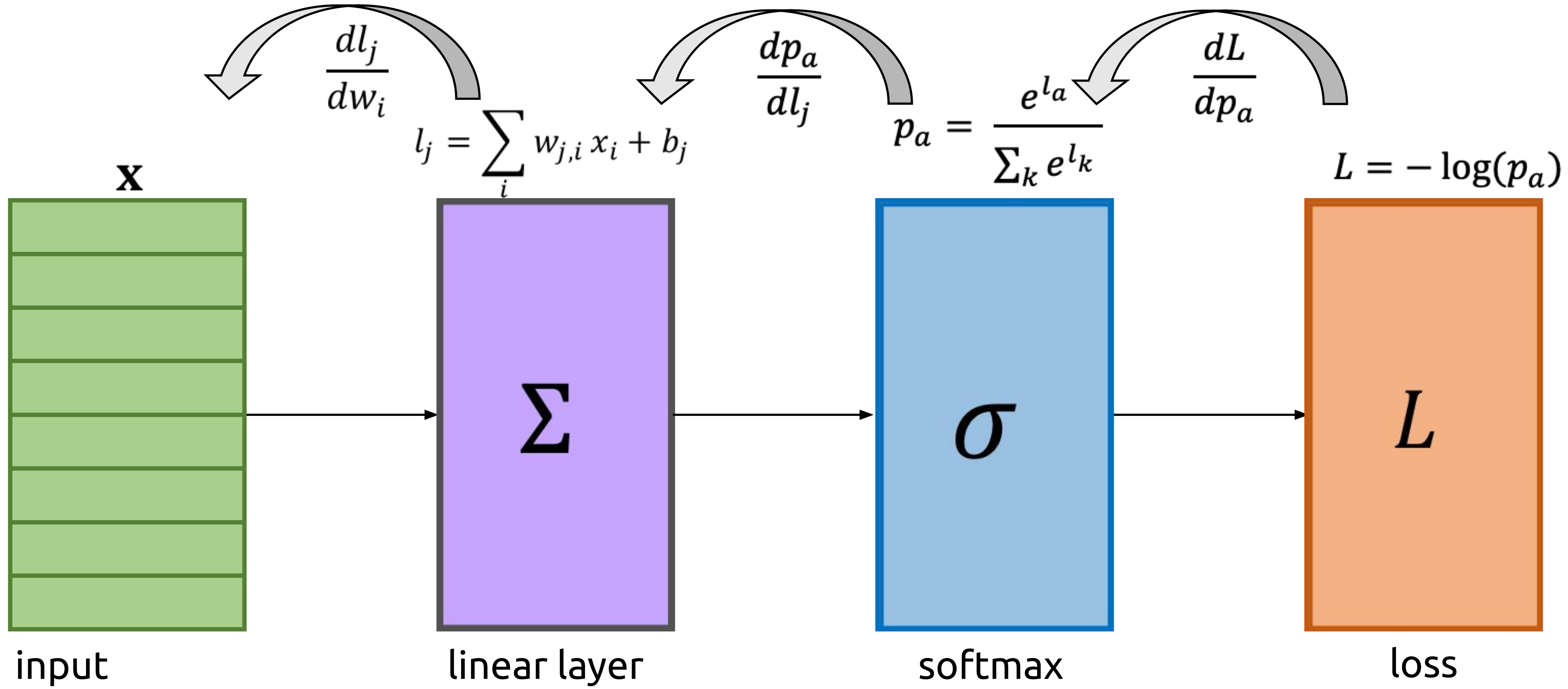
Chain Rule for Linear Layer

- $\frac{\partial l_j}{\partial w_{j,i}} = \frac{\partial(\sum_i w_{j,i}x_i)}{\partial w_{j,i}} = \frac{\partial(\ldots + w_{j,i}x_i + \cdots)}{\partial w_{j,i}} = x_i$



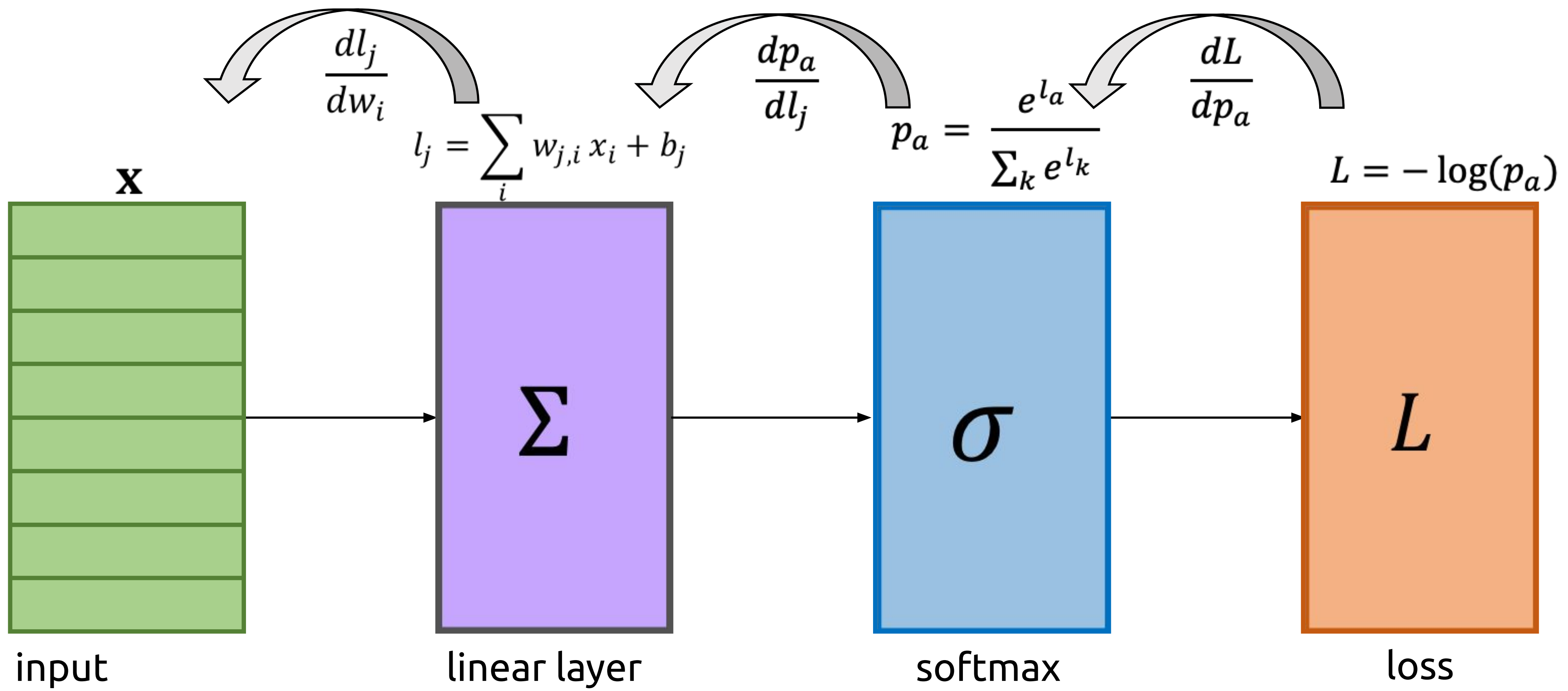
Chain Rule Put Together

$\Delta w_{j,i} =$



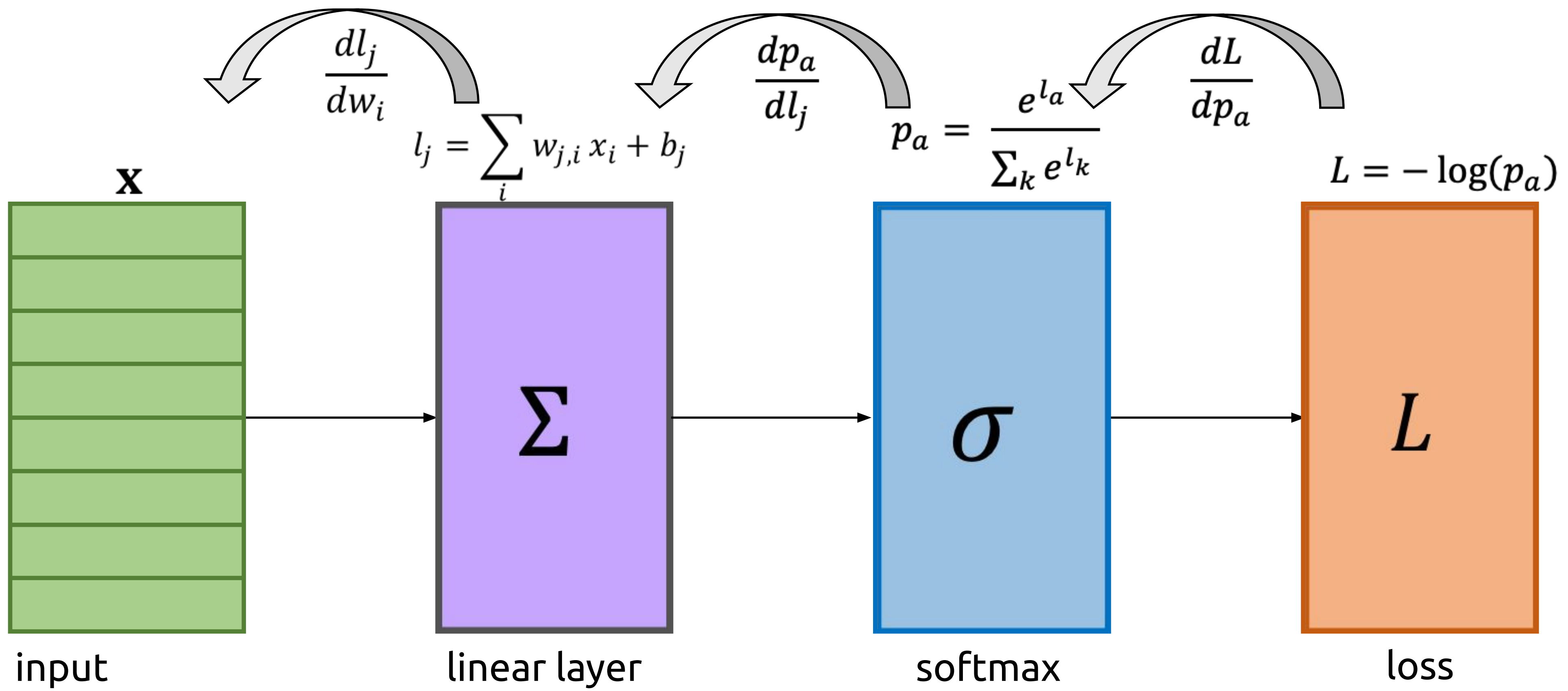
Chain Rule Put Together

- $\Delta w_{j,i} = -\alpha \dfrac{\partial L}{\partial w_{j,i}} =$



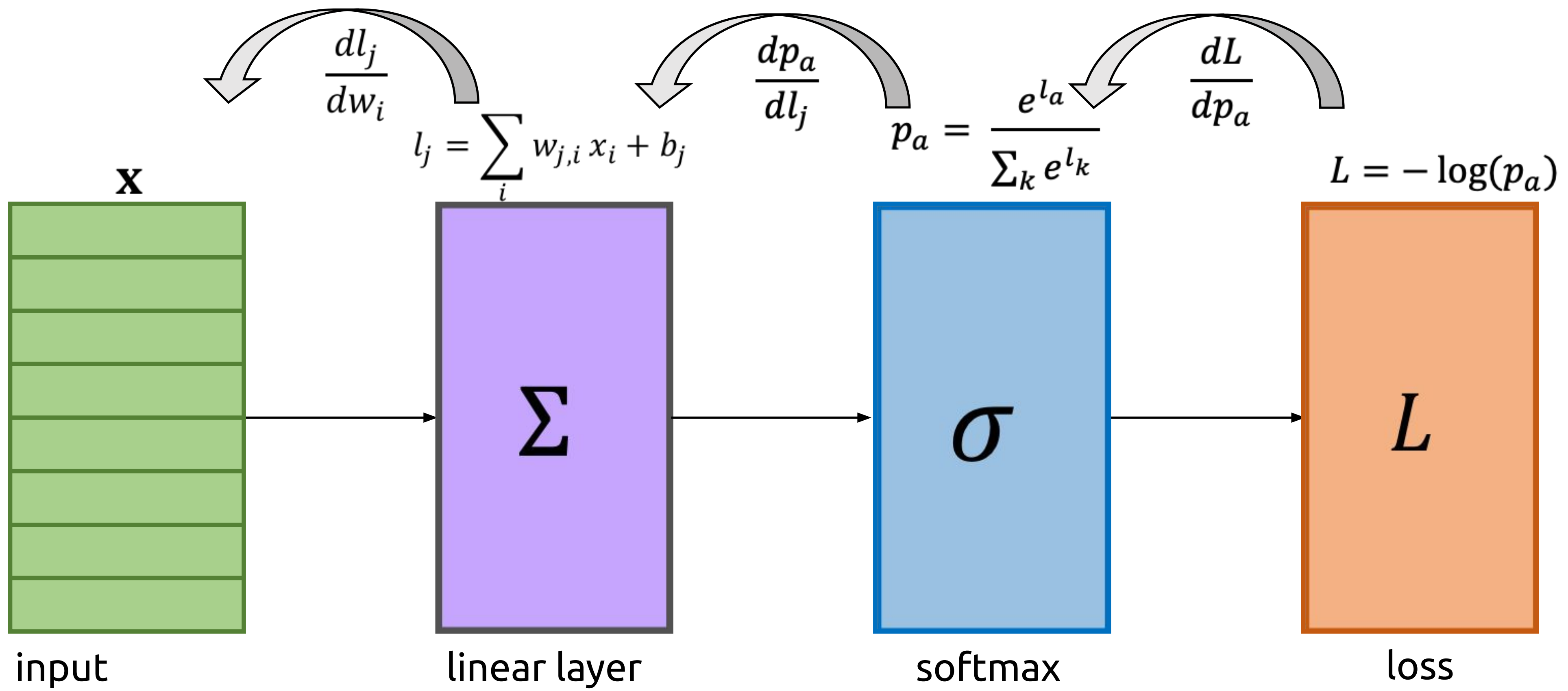
Chain Rule Put Together

$$\Delta w_{j,i} = -\alpha \frac{\partial L}{\partial w_{j,i}} = -\alpha \cdot \frac{\partial L}{\partial p_a} \cdot \frac{\partial p_a}{\partial l_j} \cdot \frac{\partial l_j}{\partial w_{j,i}} =$$



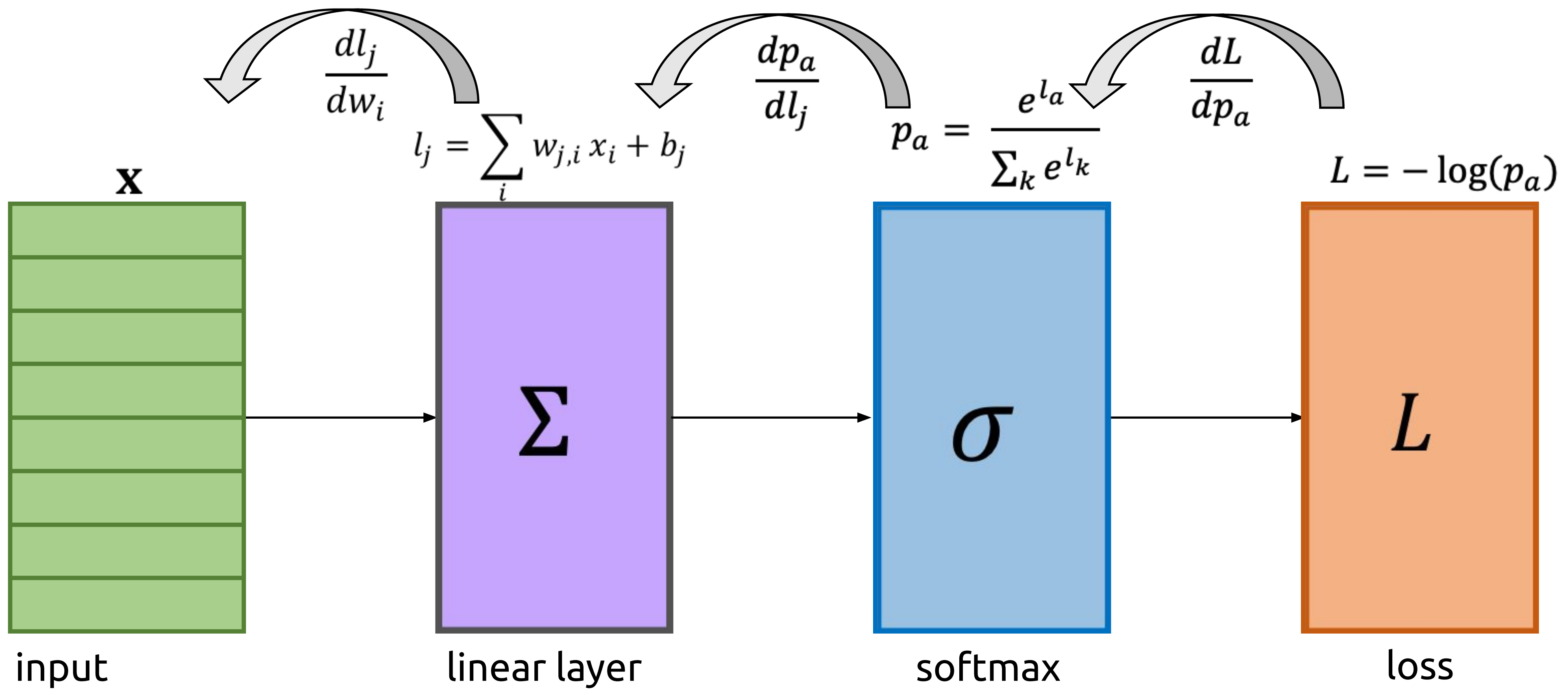
Chain Rule Put Together

- $$\Delta w_{j,i} = -\alpha \frac{\partial L}{\partial w_{j,i}} = -\alpha \cdot \frac{\partial L}{\partial p_a} \cdot \frac{\partial p_a}{\partial l_j} \cdot \frac{\partial l_j}{\partial w_{j,i}} = -\alpha \cdot \left(\frac{-1}{p_a}\right) \cdot \left(p_a\left(y_j - p_j\right)\right) \cdot (x_i) =$$



Chain Rule Put Together

$$\Delta w_{j,i} = -\alpha \frac{\partial L}{\partial w_{j,i}} = -\alpha \cdot \frac{\partial L}{\partial p_a} \cdot \frac{\partial p_a}{\partial l_j} \cdot \frac{\partial l_j}{\partial w_{j,i}} = -\alpha \cdot \left(\frac{-1}{p_a}\right) \cdot \left(p_a(y_j - p_j)\right) \cdot (x_i) = -\alpha \cdot (p_j - y_j) \cdot x_i$$



Gradient Descent: Conclusion

- Update rule: $\Delta w_{j,i} = -\alpha \cdot (p_j - y_j) \cdot x_i = \alpha \cdot (y_j - p_j) \cdot x_i$

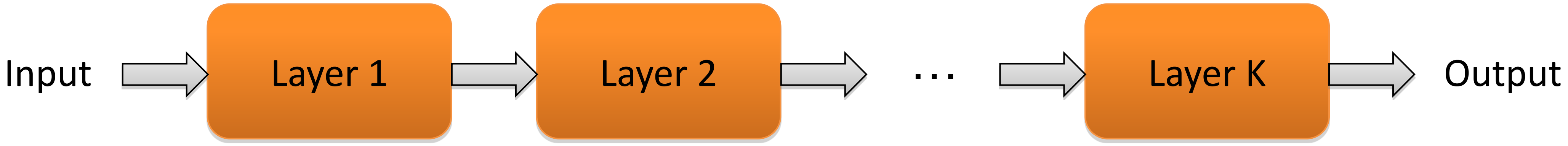
- We use this to descend along the gradient toward the minimum loss value

- We used chain rule to propagate backwards through the entire network while doing the derivative - ***backpropagation***

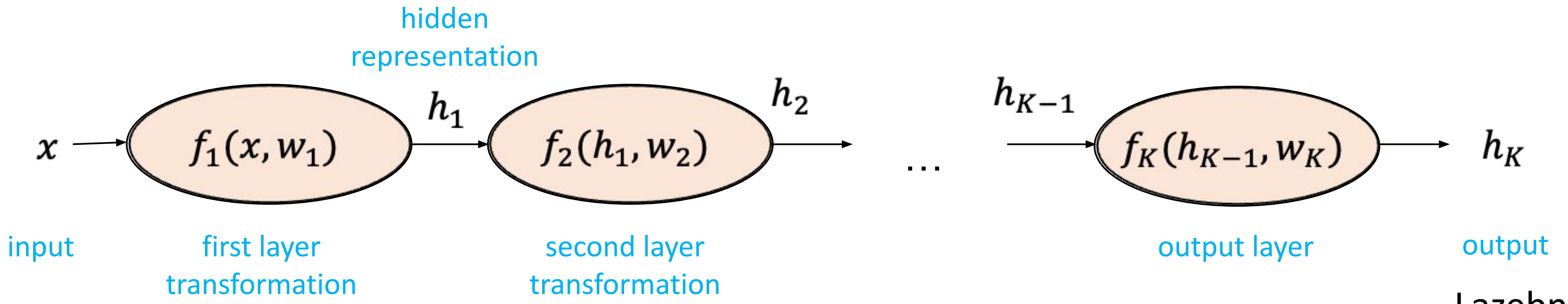
Any questions?

Backpropagation for Deeper Networks

- The function computed by the network is a composition of the functions computed by individual layers (e.g., linear layers and nonlinearities):



- More precisely:



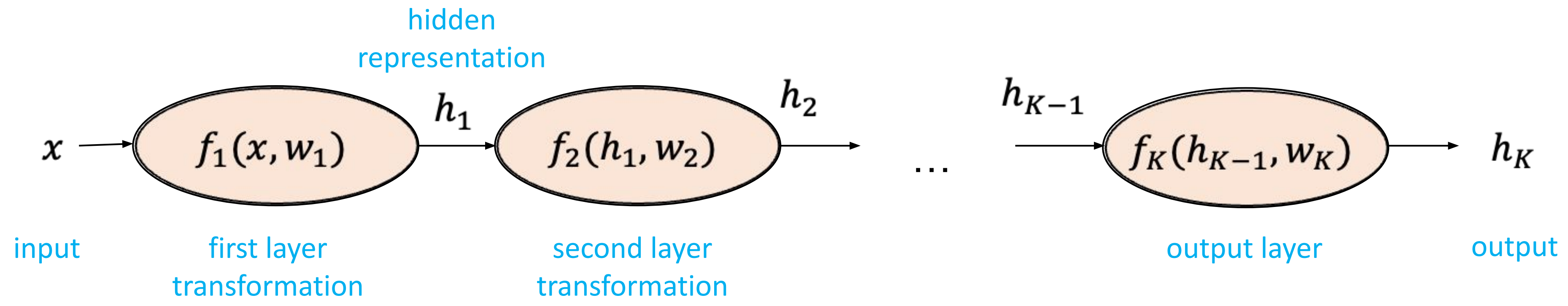
Lazebnik

Computation Graph

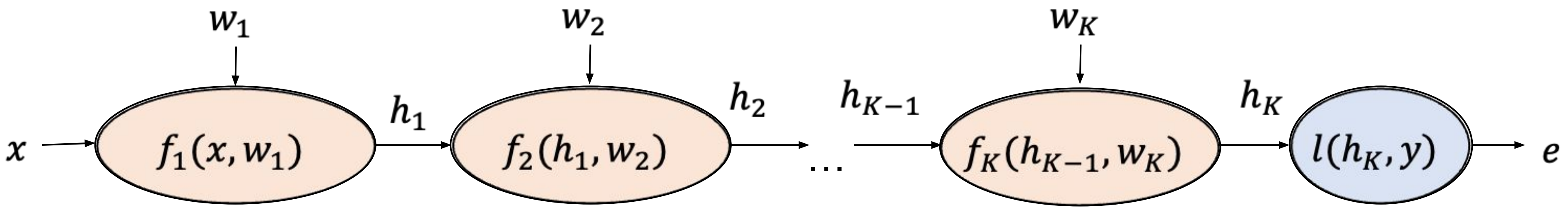
- A directed acyclic graph (DAG) that is used to specify mathematical computations:
  - Each edge represents a data dependency (i.e. feed a variable as input to the function)
  - Each node represents a function, or a variable (scalars, vectors, matrices, tensors)
- Recall that neural networks are compositions of functions
- A computation graph can be used to specify a general neural network

Lazebnik

Computation Graph

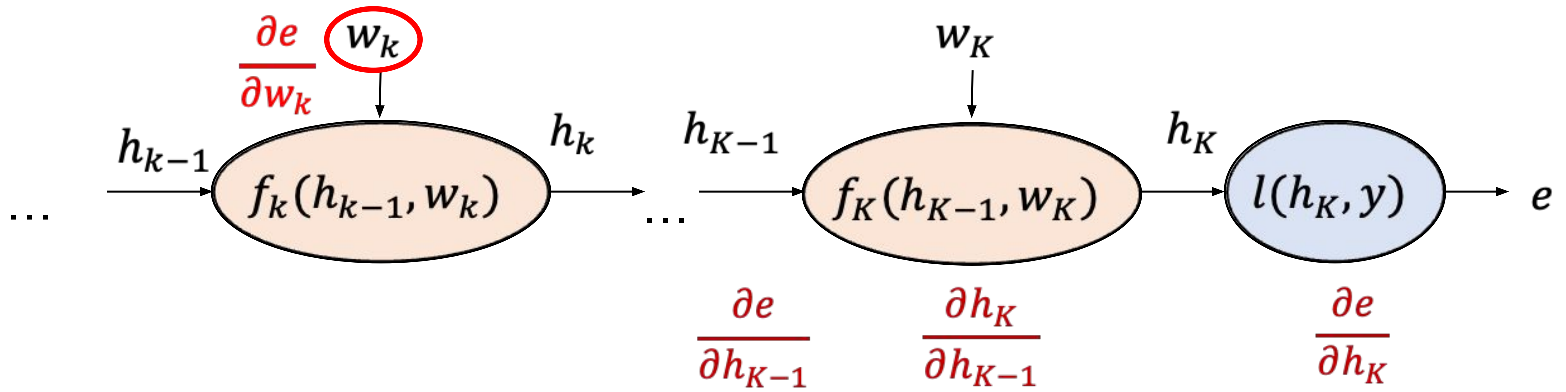


Example Computation Graph for a Neural Network with a Loss Layer:



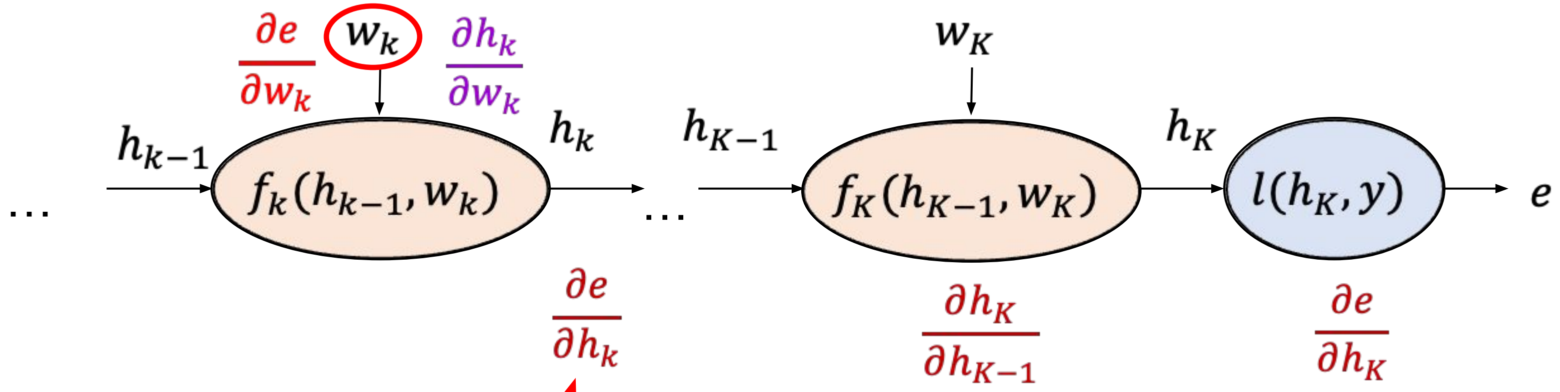
Lazebnik

Chain Rule on a Deeper Neural Network



- General case:
- $\frac{\partial e}{\partial w_k} = \boxed{\frac{\partial e}{\partial h_K} \frac{\partial h_K}{\partial h_{K-1}}}$

Chain Rule on a Deeper Neural Network



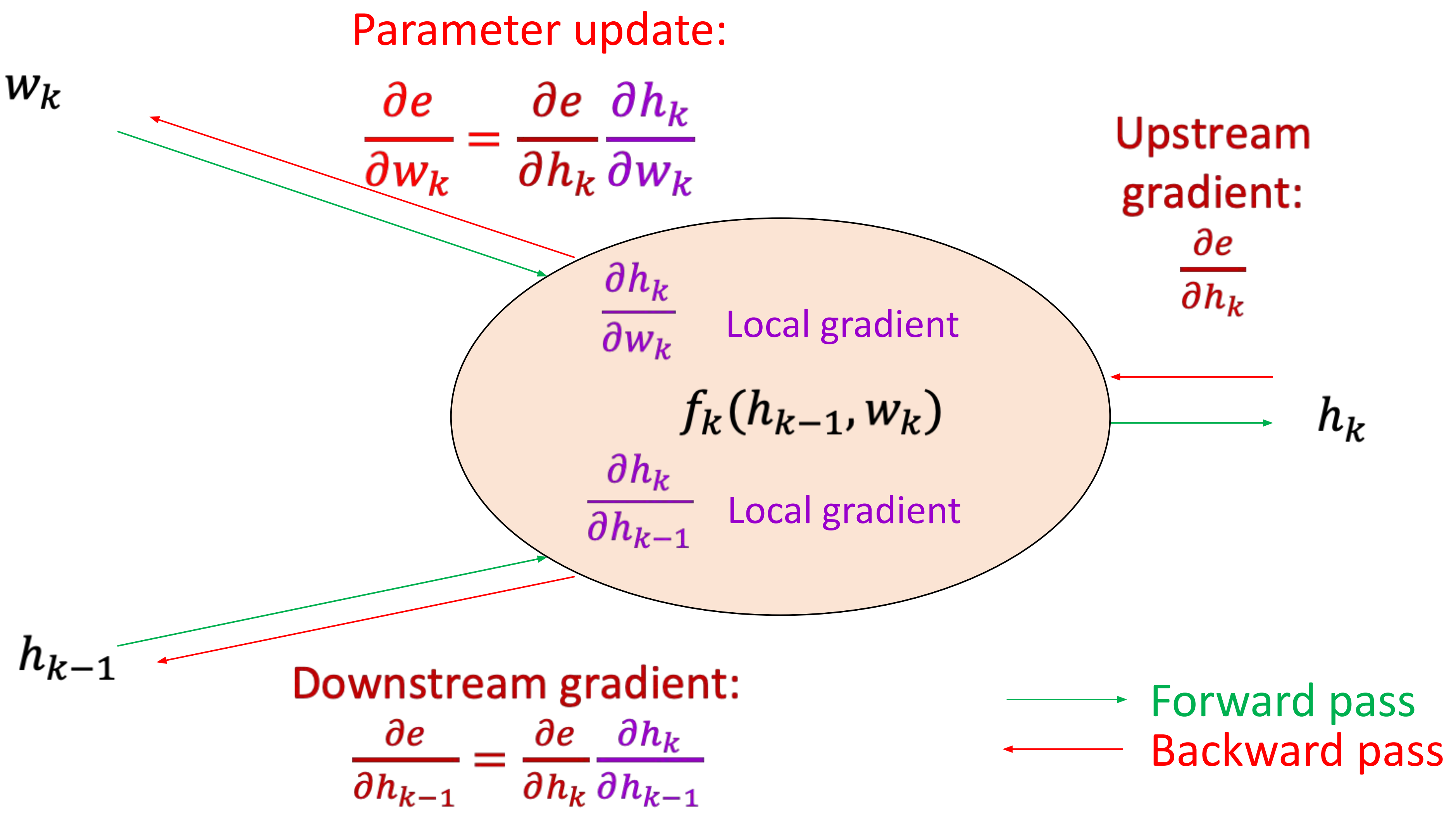
- General case:
- $$\frac{\partial e}{\partial w_k} = \boxed{\frac{\partial e}{\partial h_K} \frac{\partial h_K}{\partial h_{K-1}} \cdots \frac{\partial h_{k+1}}{\partial h_k}} \frac{\partial h_k}{\partial w_k}$$

Local gradient

Upstream gradient $\frac{\partial e}{\partial h_k}$

Lazebnik

Backpropagation: Summary



Lazebnik

Backpropagation: Layer Abstraction

$\frac{\partial h_k}{\partial w_k}$ Local gradient

$f_k(h_{k-1}, w_k)$

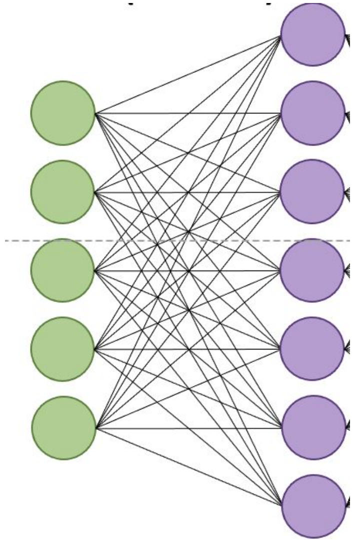
$\frac{\partial h_k}{\partial h_{k-1}}$ Local gradient

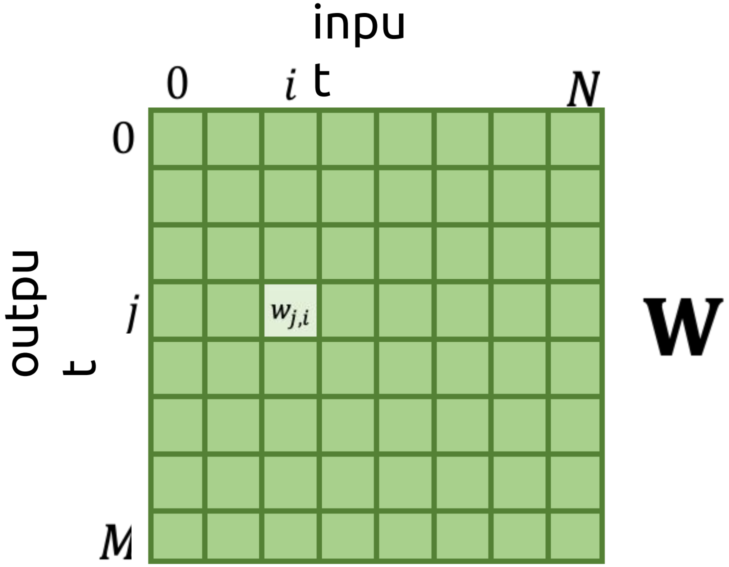
Any questions?

- Layer is an abstraction of a function (linear layer, softmax layer, ReLU layer)
- Forward pass: Just need to implement the function itself $f_k(h_{k-1}, w_k)$
- Backward pass requires two functions to compute local gradients: $\frac{\partial h_k}{\partial h_{k-1}}$ and also $\frac{\partial h_k}{\partial w_k}$ (if the function has parameters)

Recap: Our Weight Matrix

- We have an input vector of size N and an output vector of size M, so our weights matrix $\mathbf{W}$ is of dimensionality $M \times N$





Dealing with Vectors

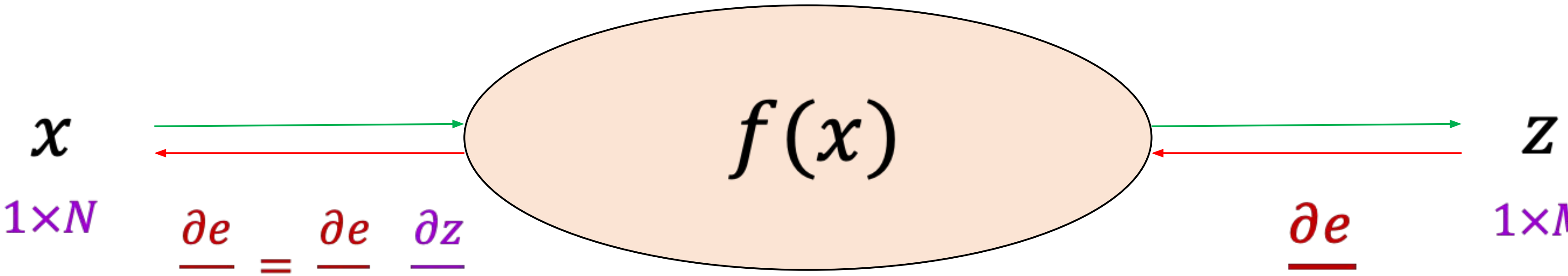
Jacobian: rows correspond to outputs, columns correspond to inputs.

The j, i th element of the Jacobian is the partial derivative of the jth output w.r.t. ith input

$$\frac{\partial z}{\partial x} = \begin{pmatrix} \frac{\partial z^{(1)}}{\partial x^{(1)}} & \cdots & \frac{\partial z^{(1)}}{\partial x^{(N)}} \\ \vdots & \ddots & \vdots \\ \frac{\partial z^{(M)}}{\partial x^{(1)}} & \cdots & \frac{\partial z^{(M)}}{\partial x^{(N)}} \end{pmatrix}$$

$M \times N$

Jacobian



$1 \times N$

$1 \times M$

$$\frac{\partial e}{\partial x} = \frac{\partial e}{\partial z} \frac{\partial z}{\partial x}$$

$1 \times N$ $\quad$ $1 \times M$ $\quad$ $M \times N$

$$\frac{\partial e}{\partial z}$$

$1 \times M$

Dealing with Vectors

Jacobian: rows correspond to outputs, columns correspond to inputs.

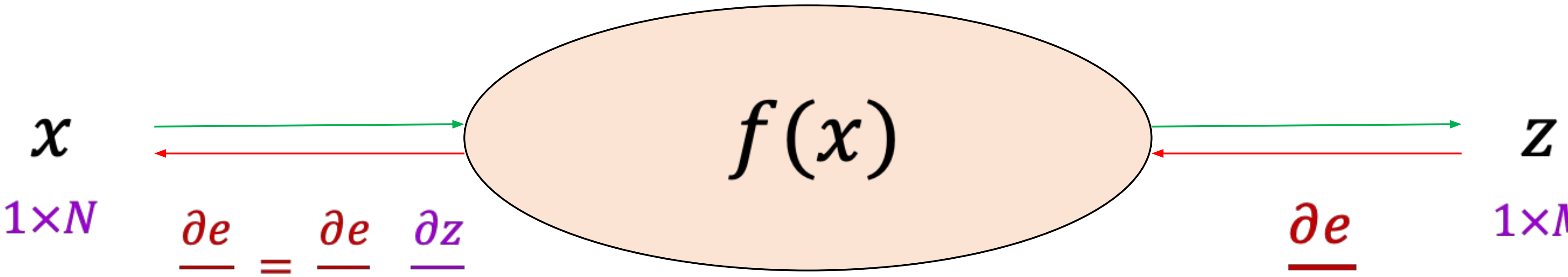
The j, i th element of the Jacobian is the partial derivative of the jth output w.r.t. ith input

$$\frac{\partial e}{\partial x^{(1)}} = \sum_{i=1}^{M} \frac{\partial e}{\partial z^{(i)}} \frac{\partial z^{(i)}}{\partial x^{(1)}}$$

$$\frac{\partial e}{\partial x^{(N)}} = \sum_{i=1}^{M} \frac{\partial e}{\partial z^{(i)}} \frac{\partial z^{(i)}}{\partial x^{(N)}}$$

$$\frac{\partial z}{\partial x} = \begin{pmatrix} \frac{\partial z^{(1)}}{\partial x^{(1)}} & \cdots & \frac{\partial z^{(1)}}{\partial x^{(N)}} \\ \vdots & \ddots & \vdots \\ \frac{\partial z^{(M)}}{\partial x^{(1)}} & \cdots & \frac{\partial z^{(M)}}{\partial x^{(N)}} \end{pmatrix}$$

$M \times N$
Jacobian



$1 \times N$

$1 \times M$

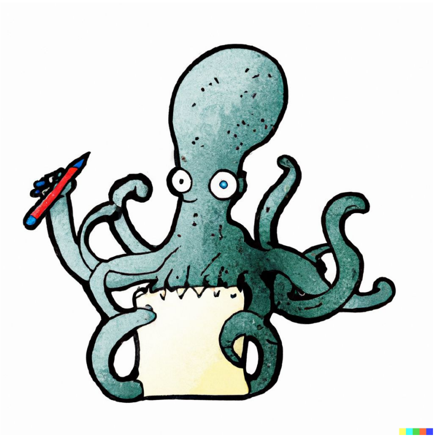
$$\frac{\partial e}{\partial x} = \frac{\partial e}{\partial z} \frac{\partial z}{\partial x}$$

$1 \times N$ $\quad 1 \times M$ $\quad M \times N$

$$\frac{\partial e}{\partial z}$$

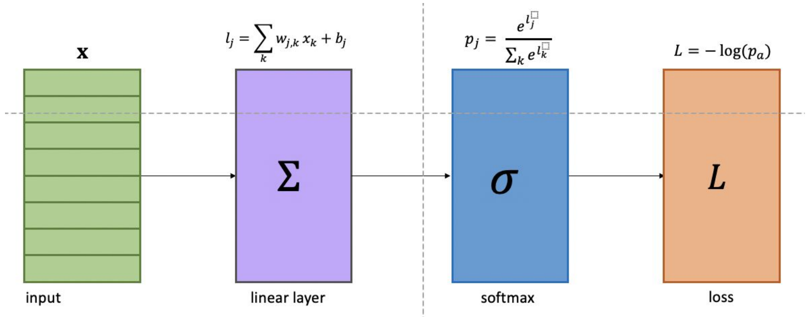
$1 \times M$

Recap



Multi-class classification neural network

- Cross entropy loss revisited
- Softmax function
- Building a simple model with new layers



Backpropagation and computation

- Chain rule for multi-class classification
- Computation graph
- Dealing with vectors