Topics in Social Data Science

Week 3

Artificial Neural Networks 2

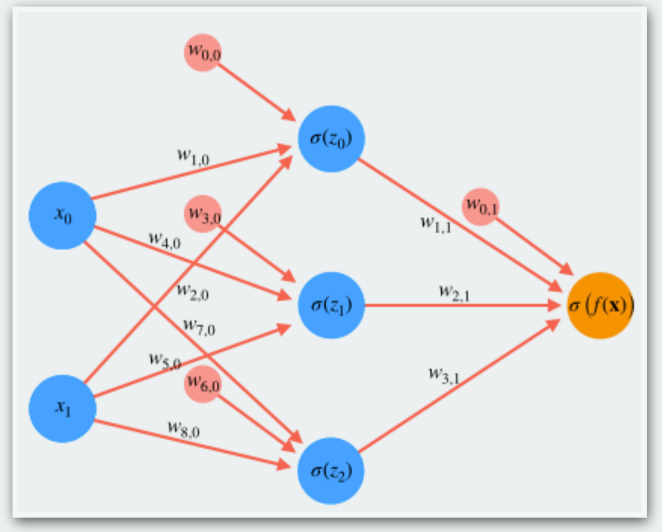
Backpropagation, regularization, vanishing gradients

Overview of today + tomorrow

- Watch 3BLUE1BROWN's chapter 3+4 on Neural Networks
- Read (or at least familiarize yourself with) Michael Nielsen's book up to and including Chapter 4
- My lecture (backprop, regul., vanishing grad.)
- Exercises in Python

Quick recap…

Find the gradients with **Backpropagation** … this week



(1) The model

Input ⟶ Neural network function ⟶ **Output**

Datapoints, **X**

Parameters: Weights, **W**

Prediction, $\tilde{\mathbf{y}}$

(2) Its performance

Input ⟶ Cost function ⟶ **Output**

Weights, **W**

Many training examples

One number, **the cost**

$$
\begin{aligned}
C(\mathbf{W}) &= \frac{1}{N}\sum_i (\tilde{y}_i - y_i)^2 \\
&= (0.96 - 1)^2 \\
&+ (0.10 - 0)^2 \\
&+ (0.04 - 0)^2 \\
&+ \ldots \\
&+ (0.70 - 1)^2 \\
&+ (0.02 - 0)^2 \\
&+ (0.99 - 1)^2
\end{aligned}
$$

(3) The cost function gradient in **W**

$$
-\nabla C(\mathbf{W}) = \begin{bmatrix} -0.23 \\ 1.32 \\ 0.20 \\ 0.38 \\ -1.23 \\ 0.01 \\ 1.20 \\ -2.12 \\ 0.73 \\ 2.17 \\ 0.54 \\ -0.23 \\ -0.93 \\ 0.45 \end{bmatrix}
$$

(4) Updating **W**

$$
\mathbf{W} = \mathbf{W}^{\mathbf{old}} + r\left(-\nabla C(\mathbf{W}^{\mathbf{old}})\right)
$$

(5) Repeat 3 and 4

r is usually called the *learning rate*

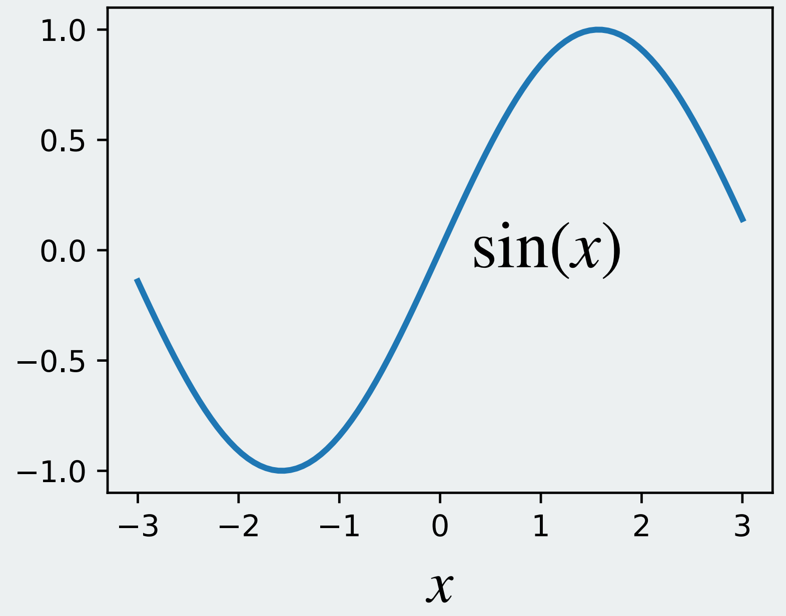
Backpropagation

THE algorithm for computing the analytical **gradient** of the cost function

Chain rule – Taking derivatives of *composite functions*

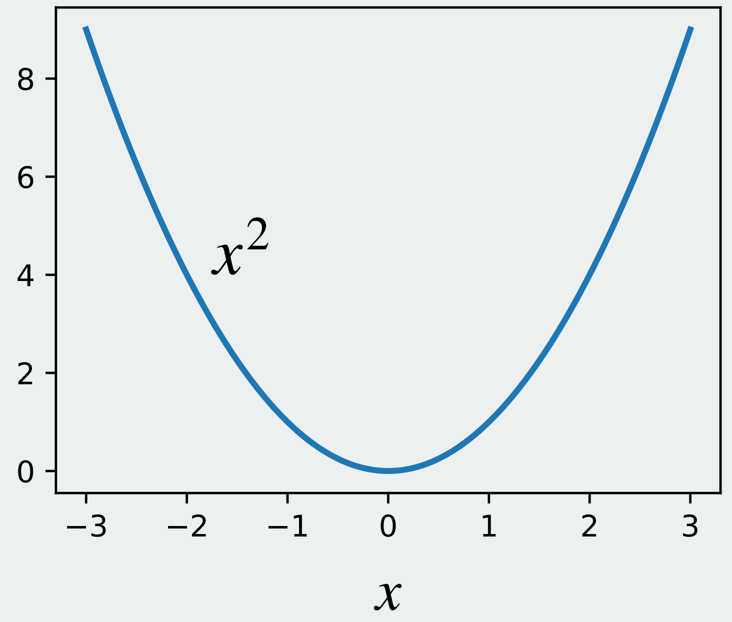
one function

$h(x)$



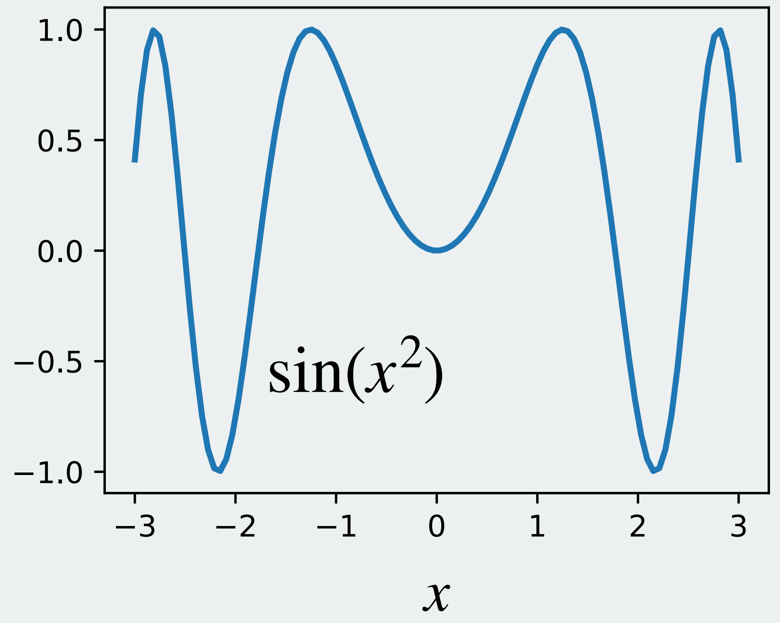
another function

$g(x)$



a *composite* of the two

$h\left(g(x)\right)$



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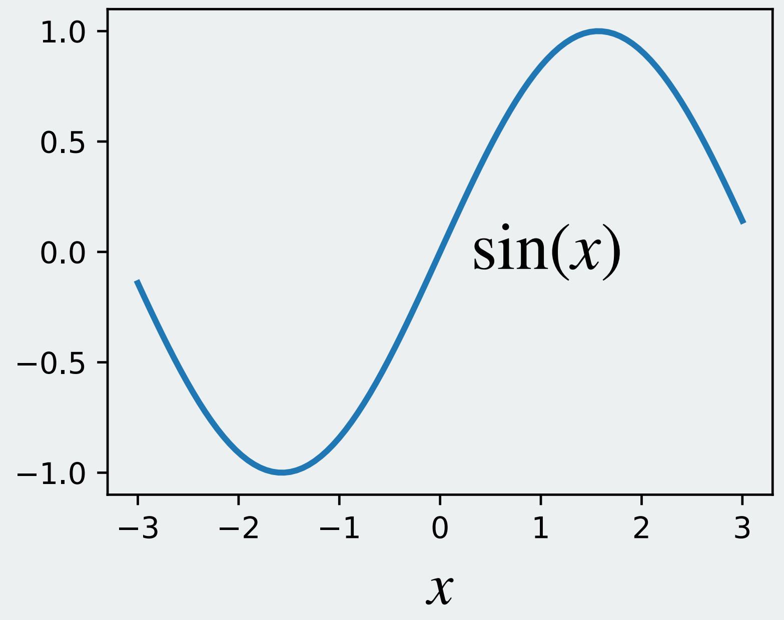

another function

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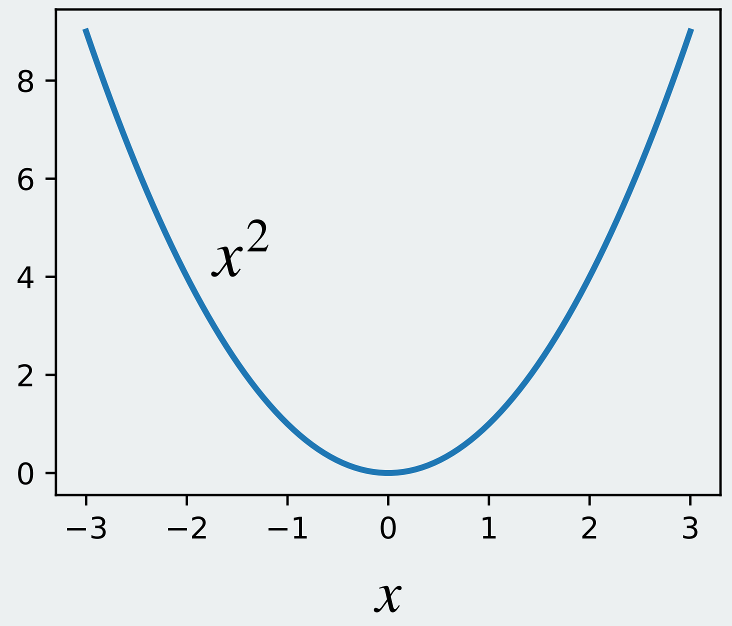

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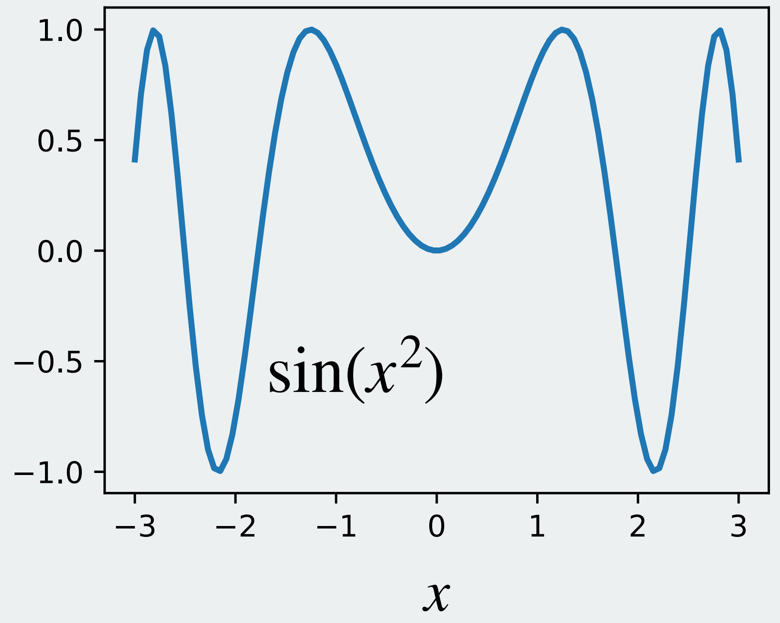

$$h\left(g(x)\right)$$

$$x \longrightarrow g \longrightarrow h$$

one function

another function

a *composite* of the two

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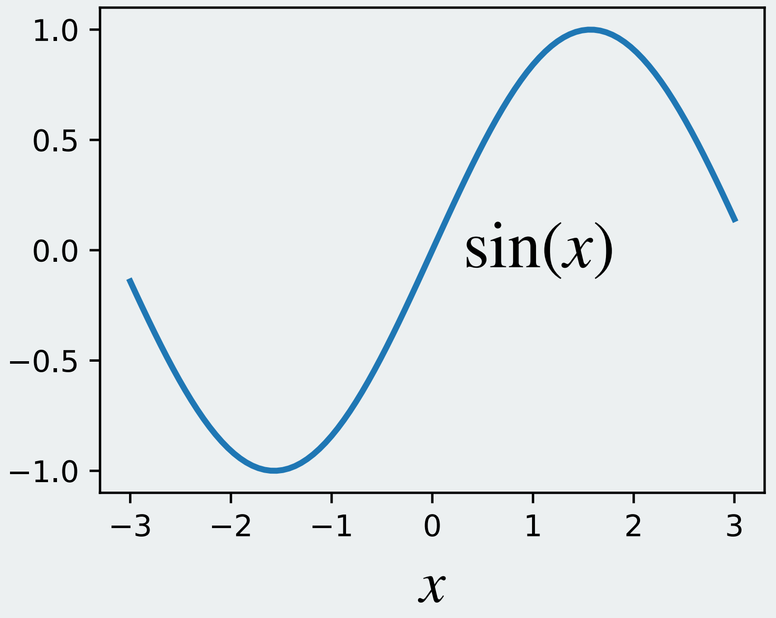

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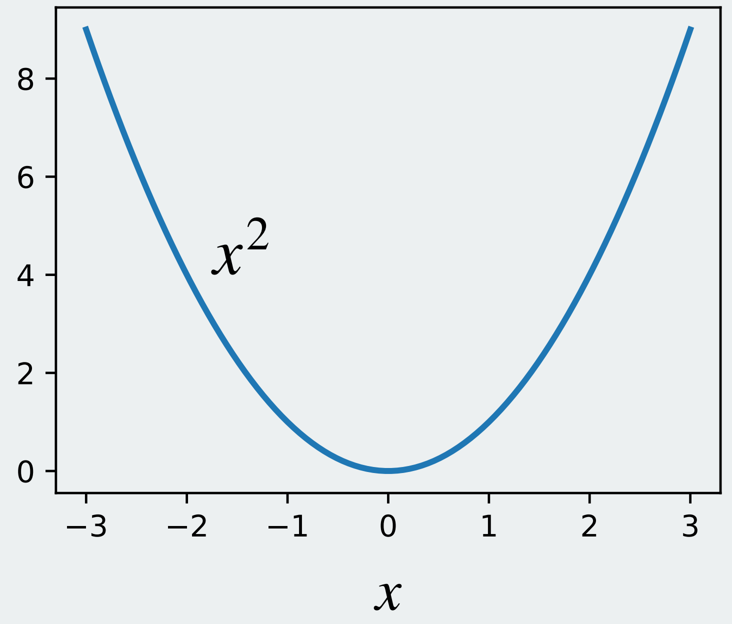

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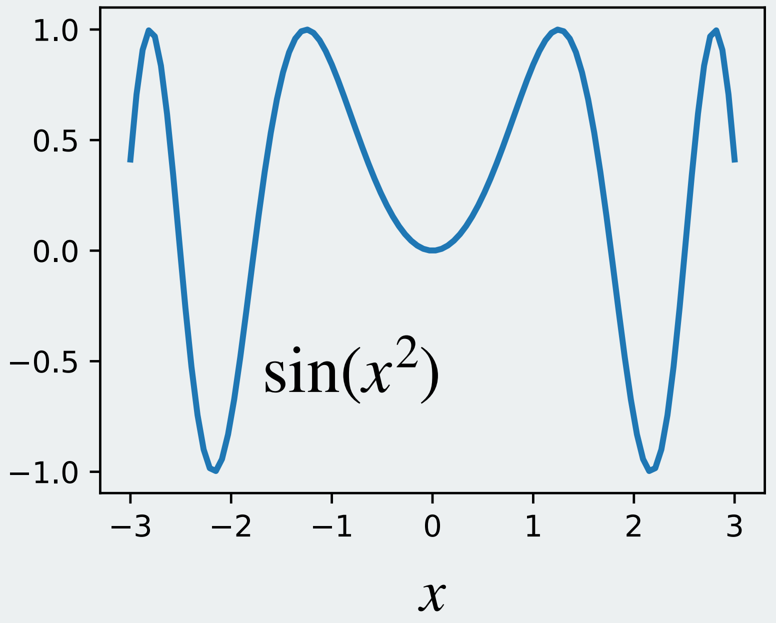


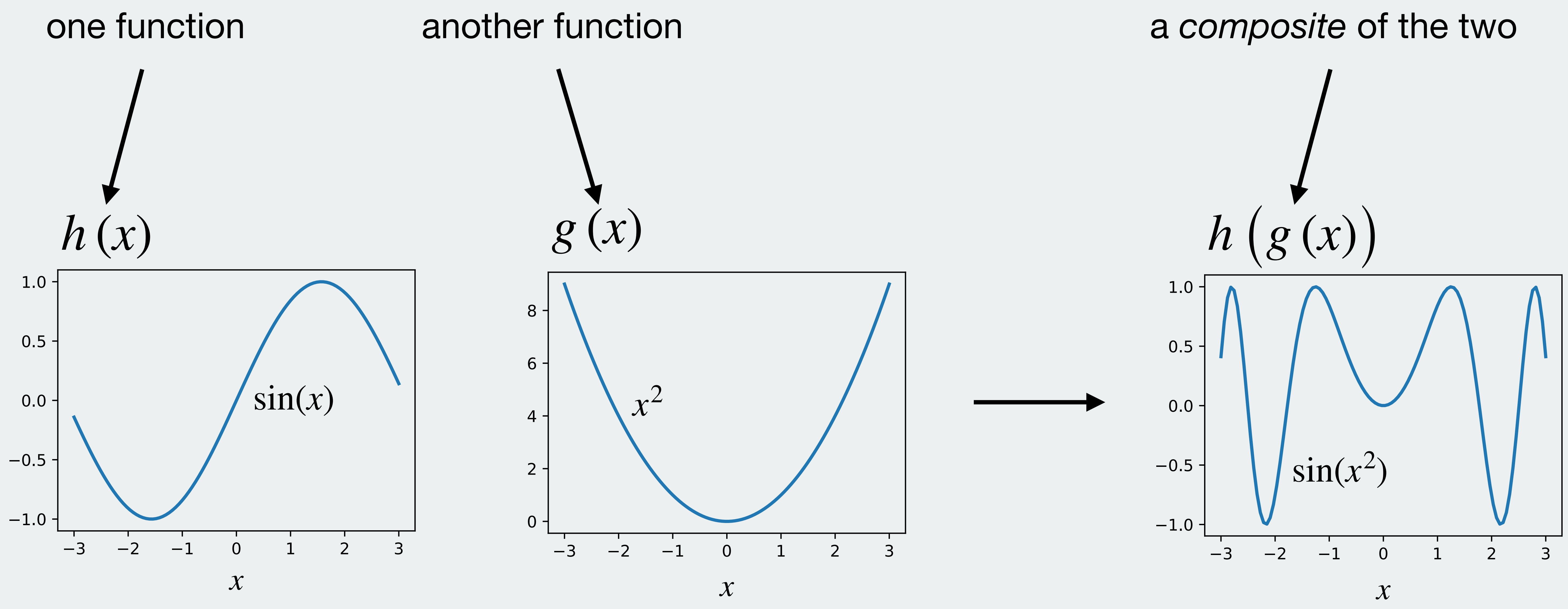
$h\left(g(x)\right)$

$$x \longrightarrow g \longrightarrow h$$

Chain rule says:

$$\frac{dh}{dx} = \frac{dh}{dg}\frac{dg}{dx}$$

Chain rule – Taking derivatives of *composite functions*



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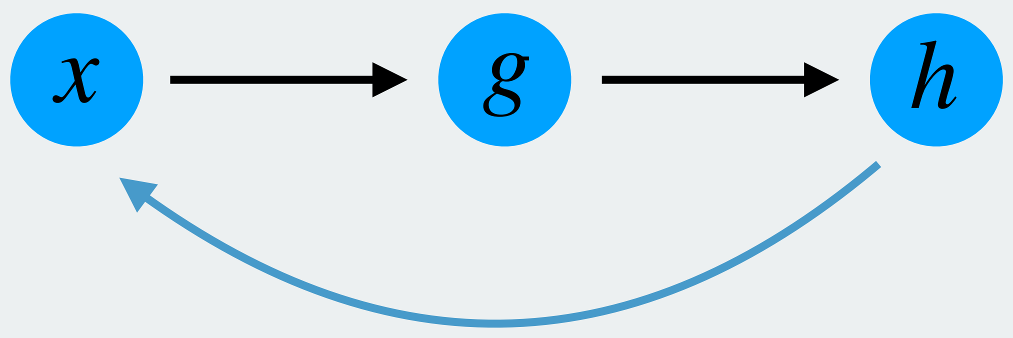

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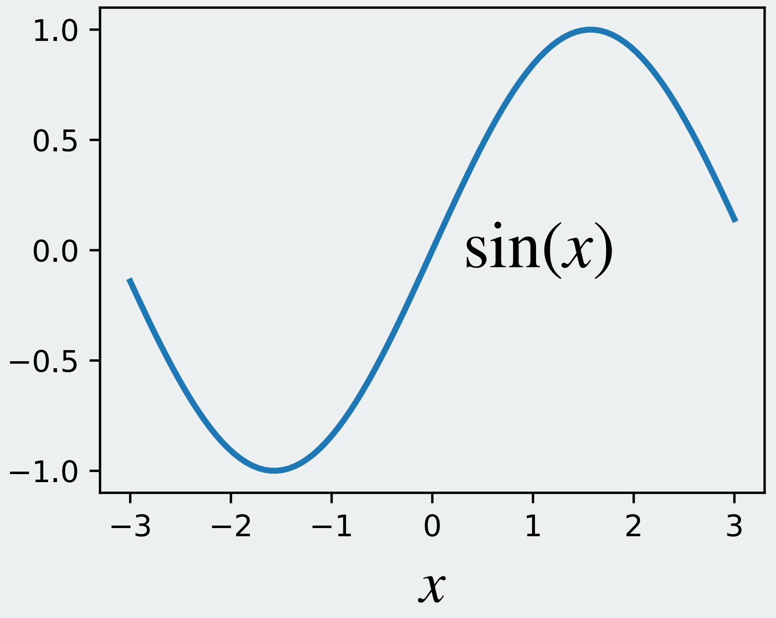

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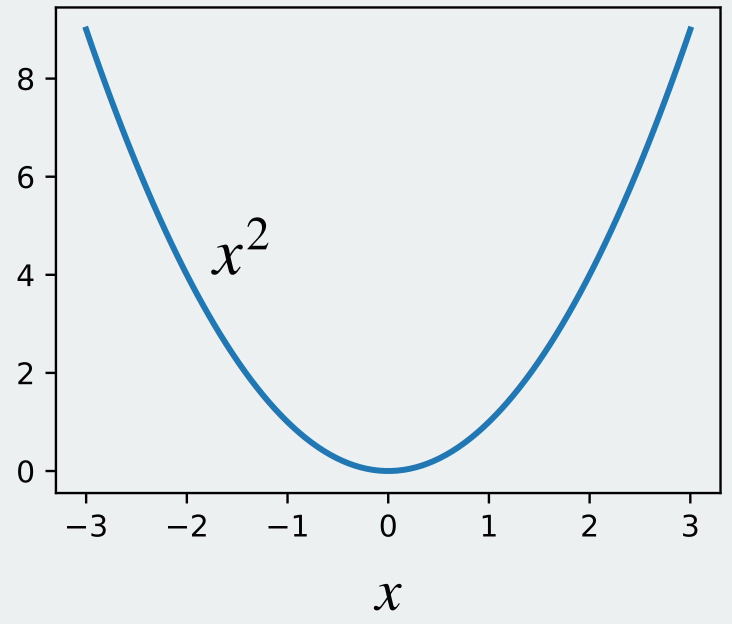

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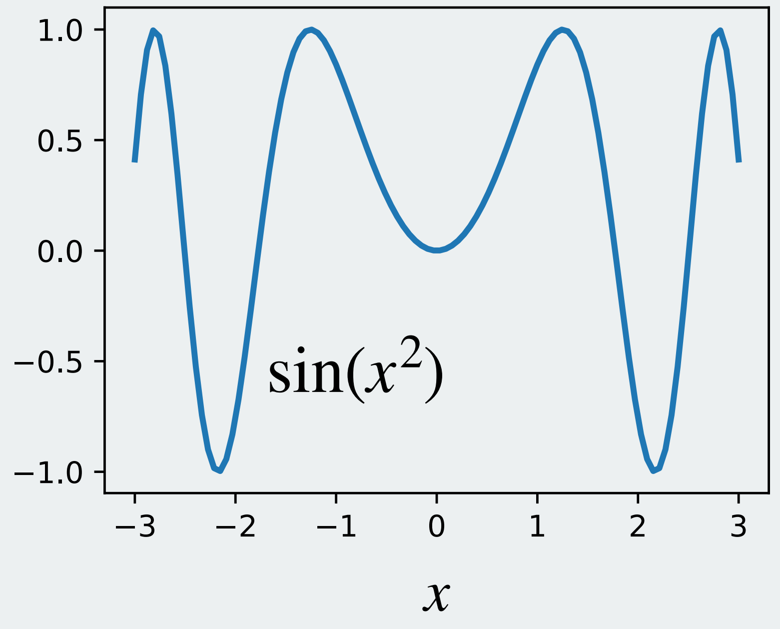

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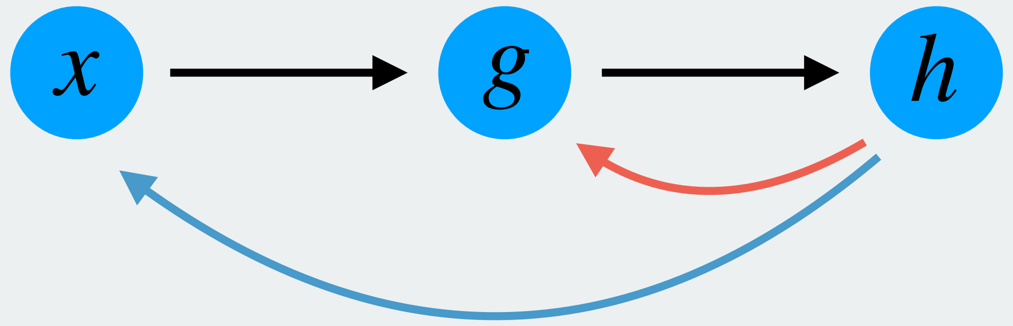

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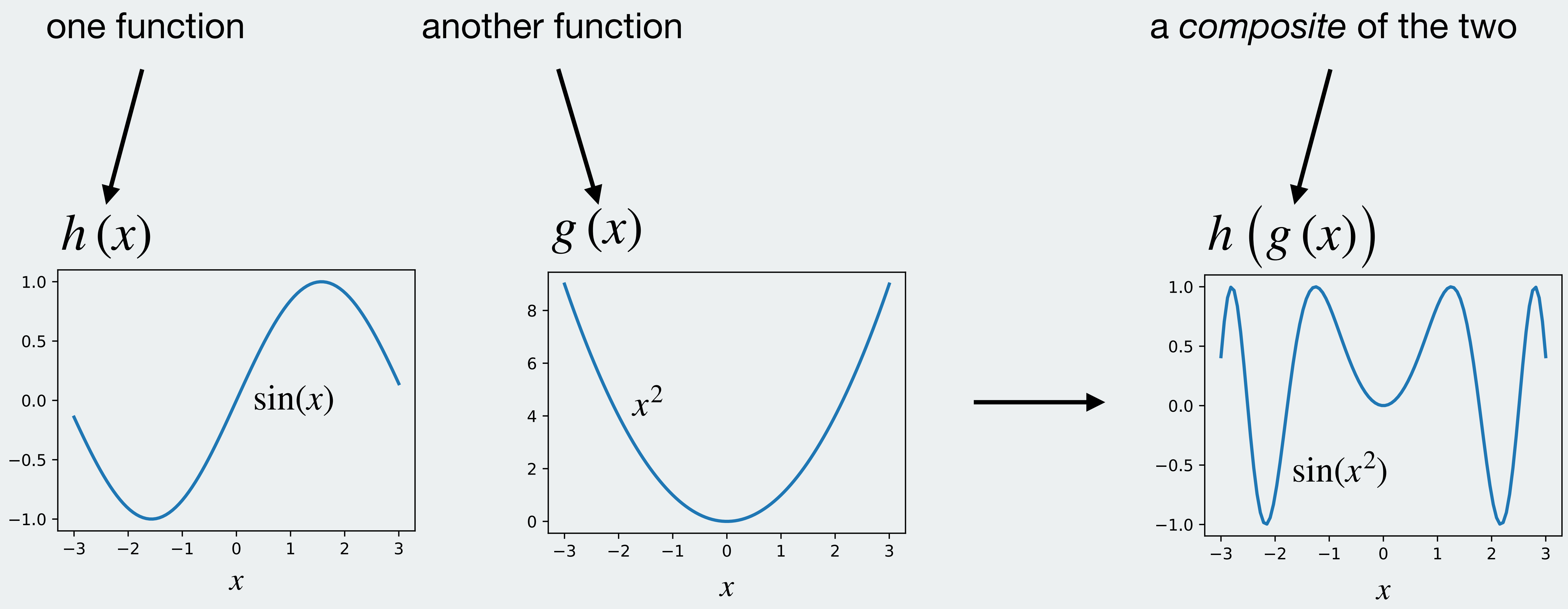

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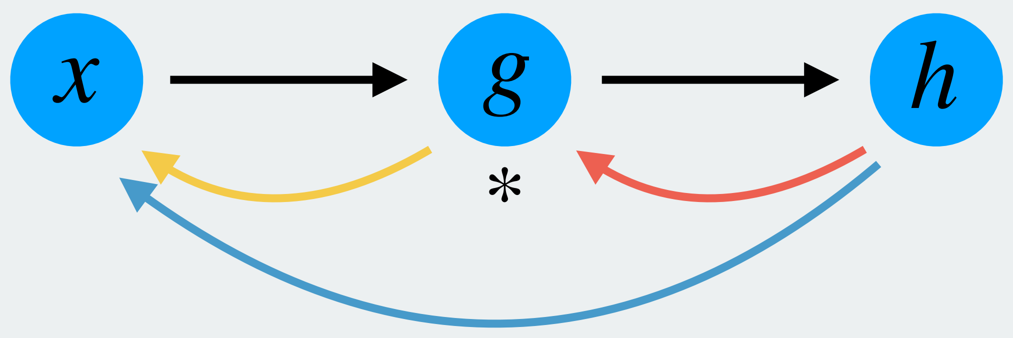

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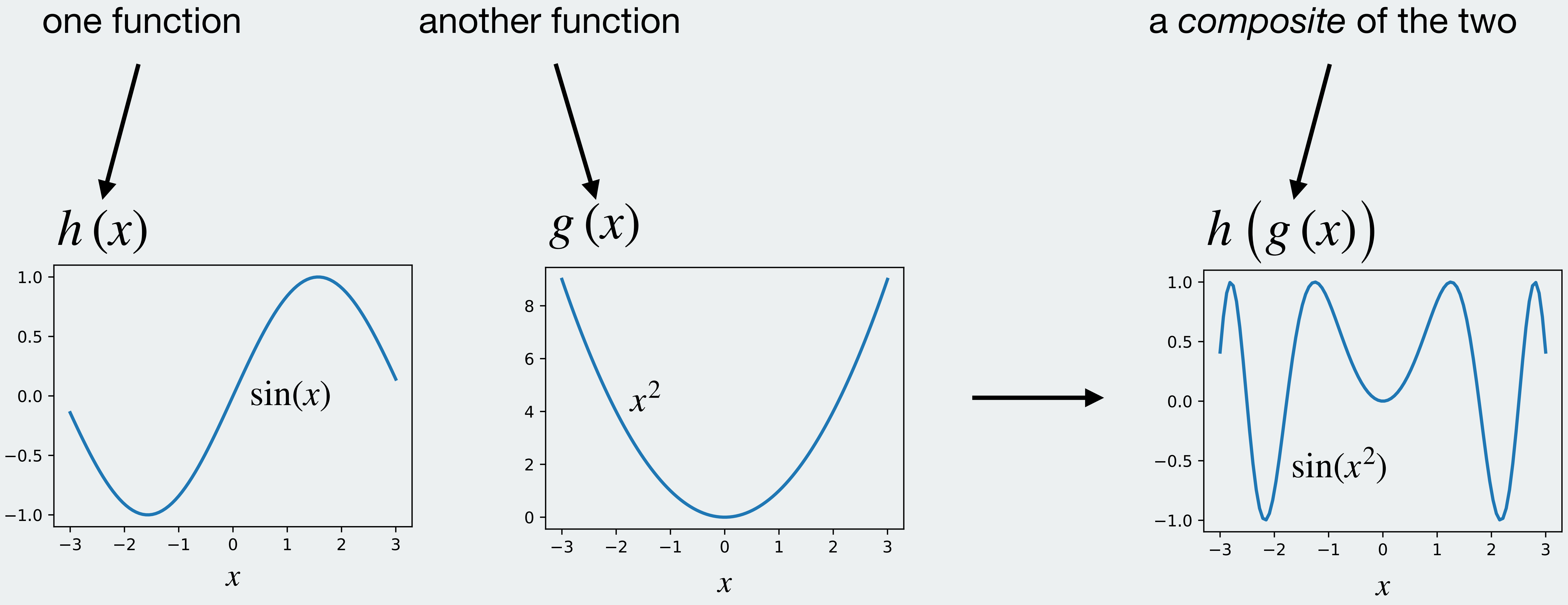

$$f\Big(h\big(g(x)\big)\Big)$$

$$\begin{tikzcd} x \arrow[r] & g \arrow[r] & h \arrow[r] & f \arrow[lll, bend left] \end{tikzcd}$$

Chain rule says:

$$\frac{df}{dx} = ?$$

Chain rule – Taking derivatives of *composite functions*

one function

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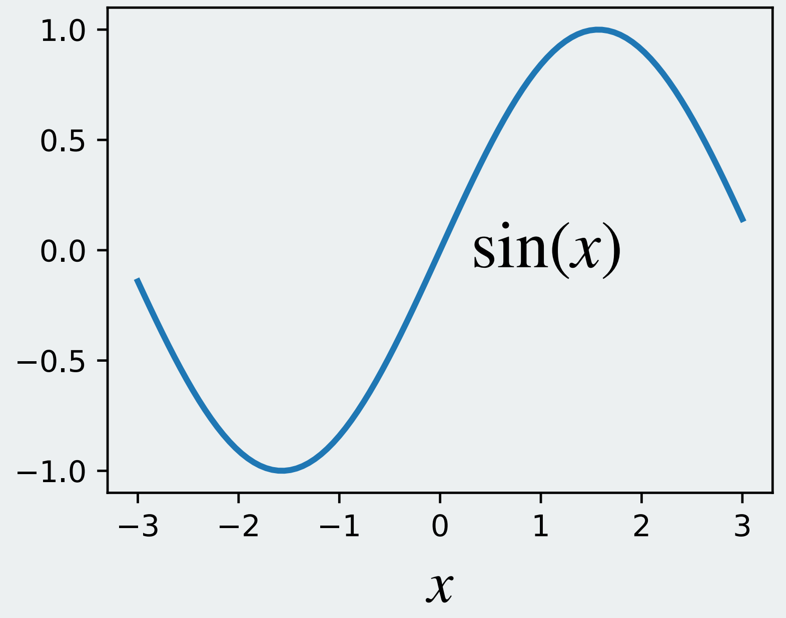

another function

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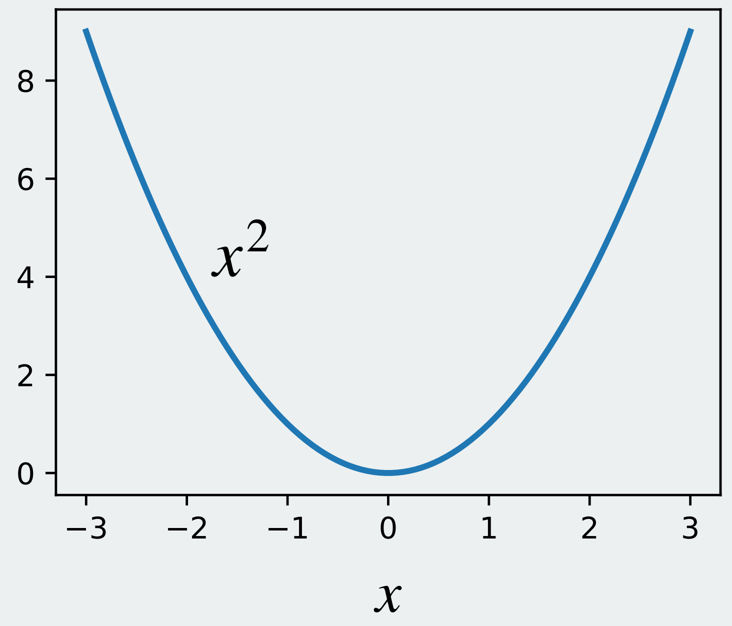

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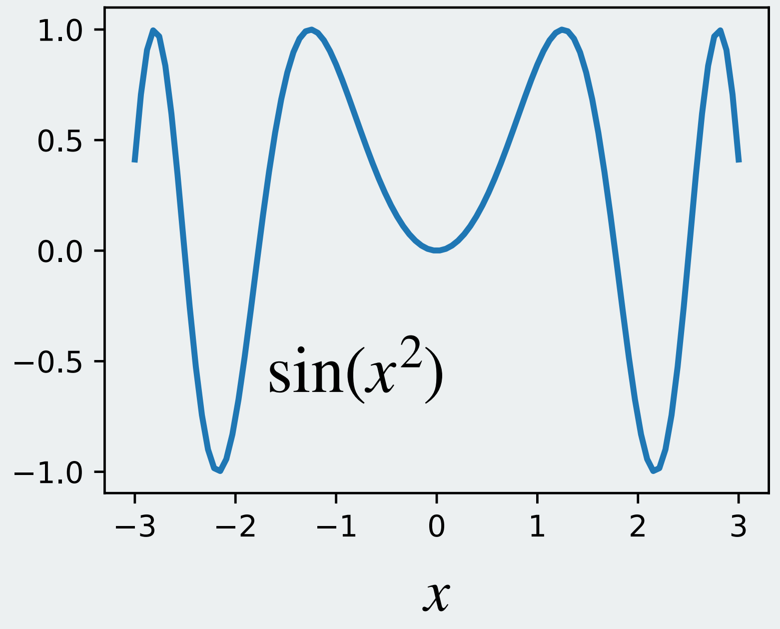

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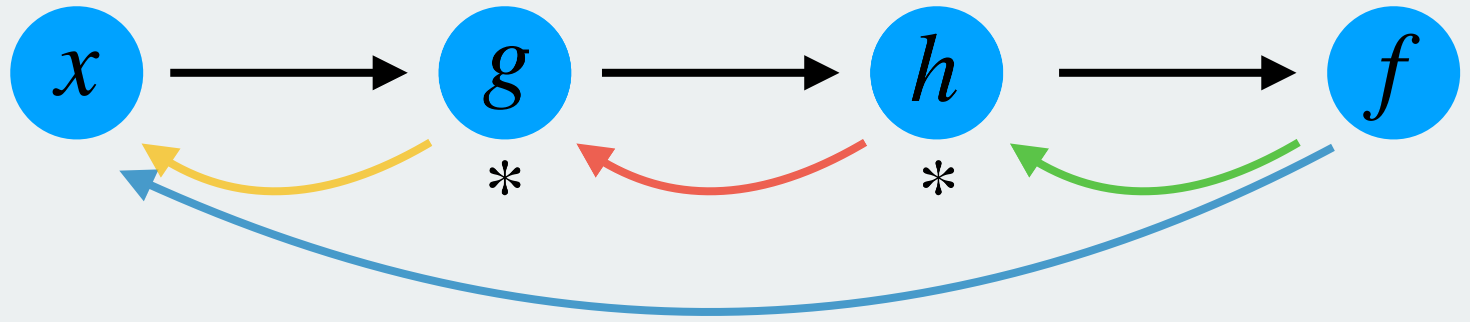
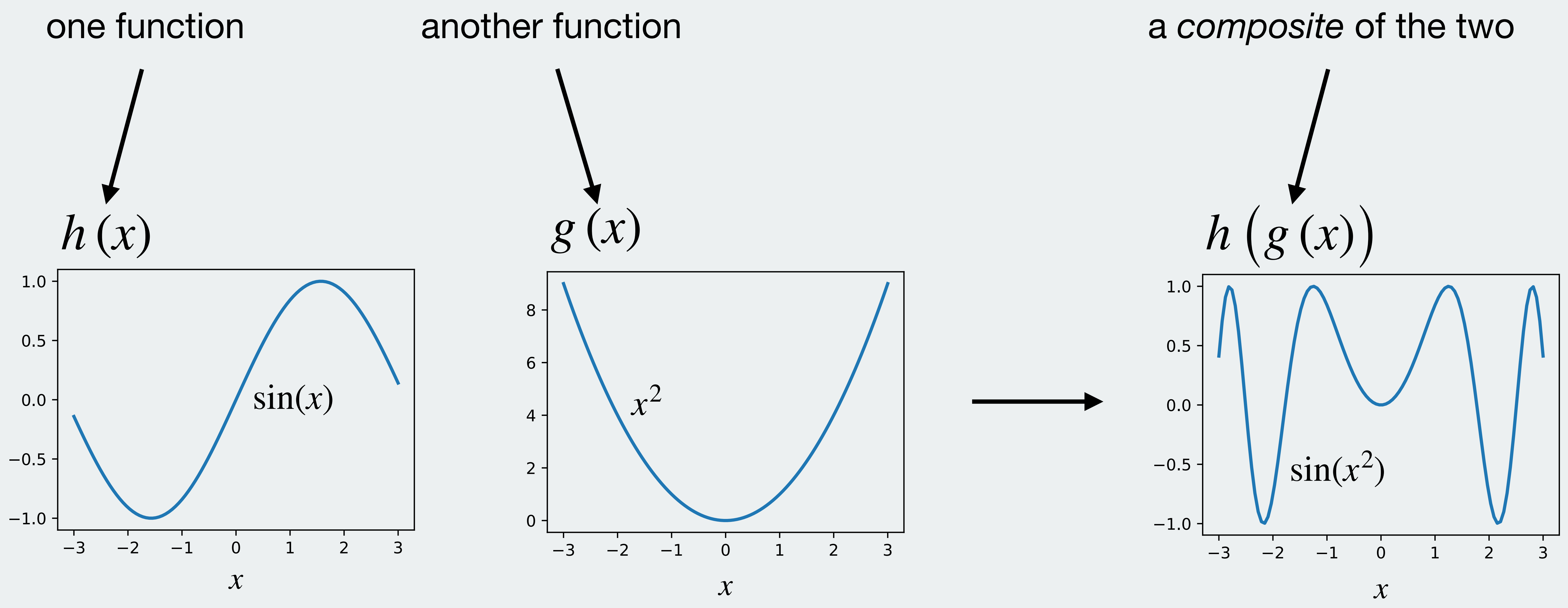


Chain rule says:

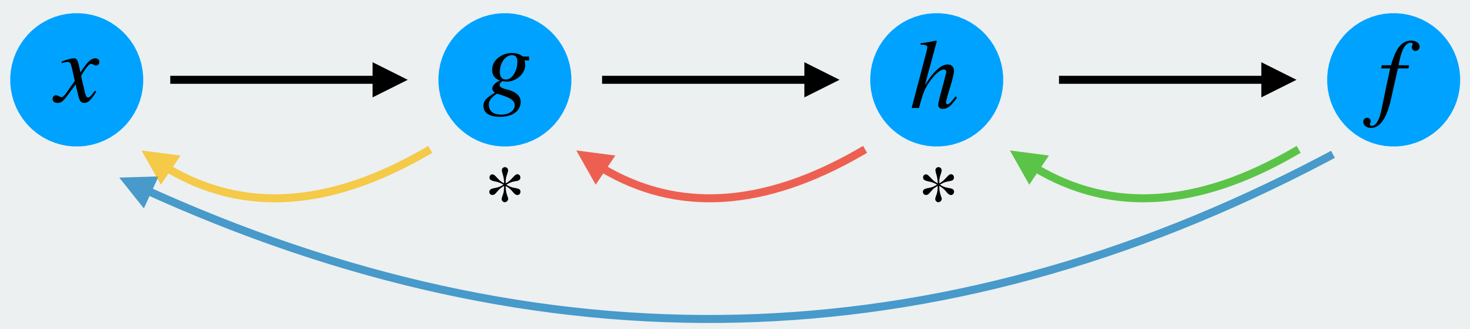
$$\frac{df}{dx} = \boxed{\frac{df}{dh}}\frac{dh}{dg}\frac{dg}{dx}$$

3Blue1Brown Chain Rule video

Chain rule – Taking derivatives of *composite functions*



$$f\left(h\left(g\left(x\right)\right)\right)$$



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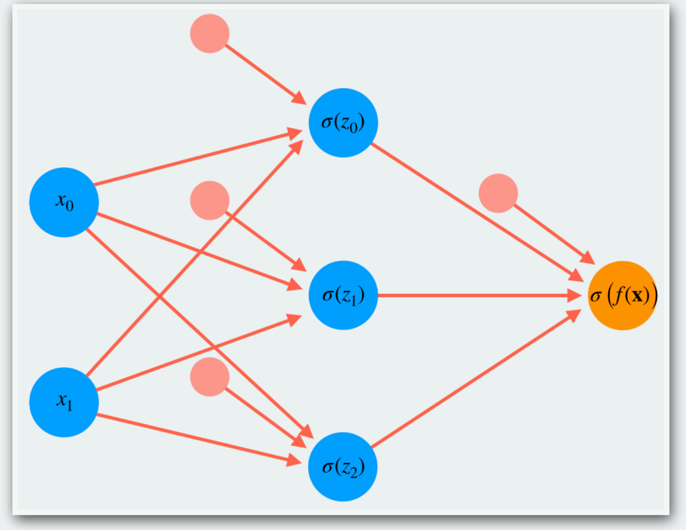

$$\sigma\left(w_{0,1} + \sigma(w_{0,0} + x_0 w_{1,0} + x_1 w_{2,0}) w_{1,1} + \sigma(w_{3,0} + x_0 w_{4,0} + x_1 w_{5,0}) w_{2,1} + \sigma(w_{6,0} + x_0 w_{7,0} + x_1 w_{8,0}) w_{3,1}\right) = \sigma\left(f(x)\right)$$

3Blue1Brown Chain Rule video

Backpropagation – simple example

Model:

$$m(z) = -z$$

$$g(z) = \exp(z)$$

$$h(z) = z + 1$$

$$f(z) = \frac{1}{z}$$

Data:

$$x_0 = 1$$

$$x_1 = 1.1$$

$$m \longrightarrow g \longrightarrow h \longrightarrow f \longrightarrow$$

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Data:

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$$x \xrightarrow{1} m \xrightarrow{-1} g \xrightarrow{0.37} h \xrightarrow{1.37} f \xrightarrow{0.73}$$

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$$x \xrightarrow{1.1} m \xrightarrow{-1.1} g \xrightarrow{0.33} h \xrightarrow{1.33} f \xrightarrow{0.75}$$

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Q: How does a small nudge in *x* influence *f*(*h*(*g*(*m*(*x*))))?

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Model derivatives:

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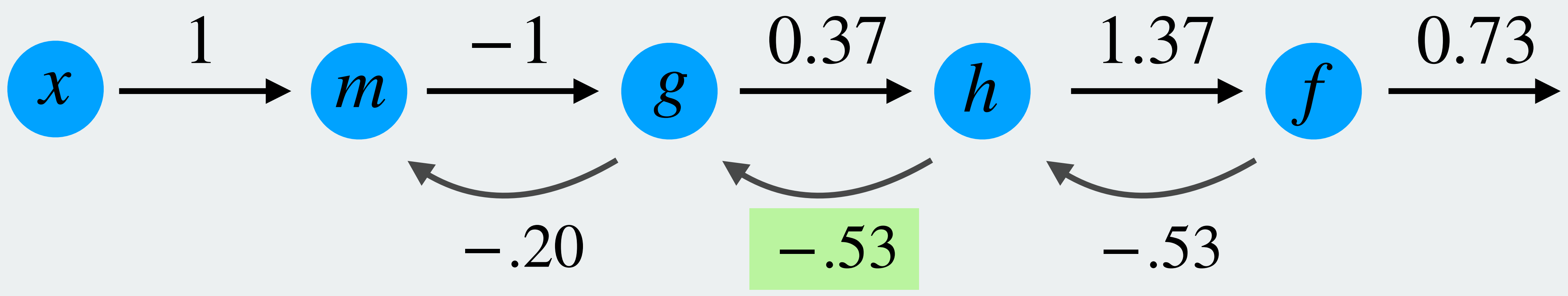

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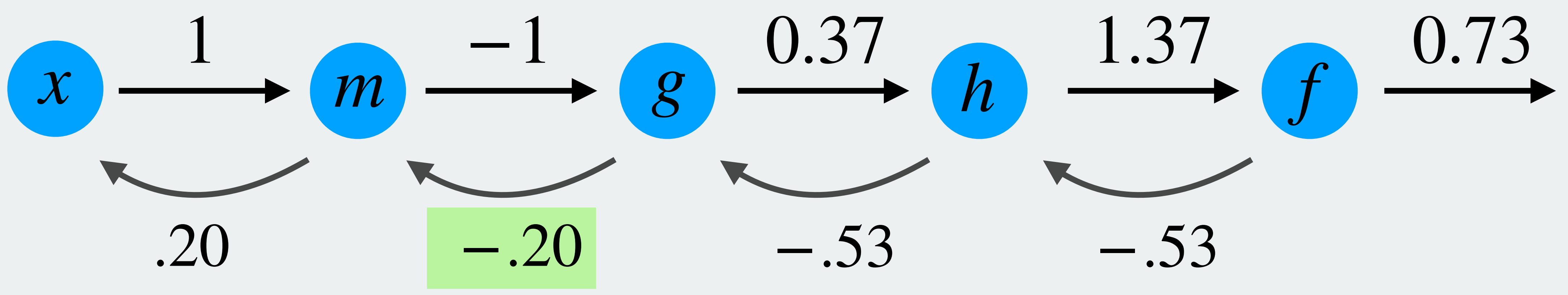

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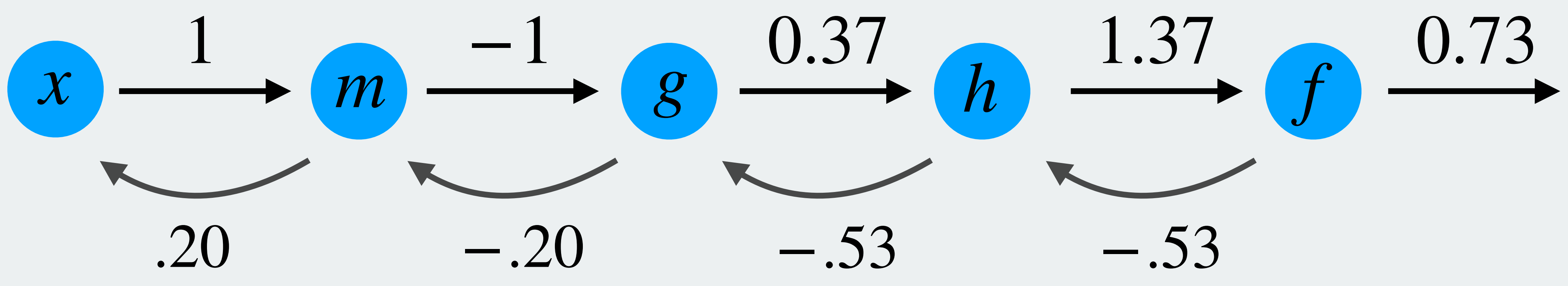

Sigmoid function:

$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$

Sigmoid derivative:

$$\sigma'(z) = \sigma(z)(1 - \sigma(z))$$

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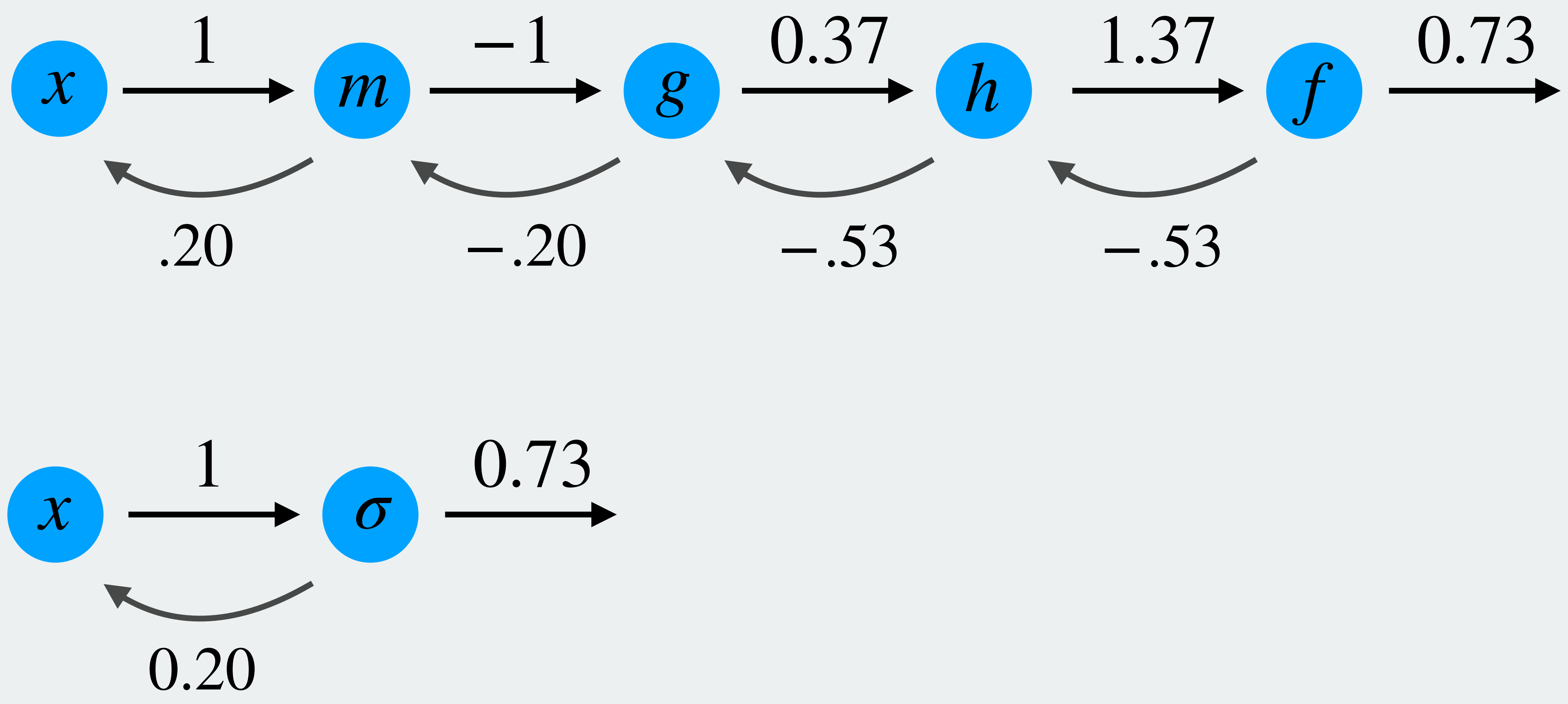

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$$f(z) = \frac{1}{z}$$

Data:

$$\boxed{x_0 = 1}$$

$$x_1 = 1.1$$

Q: How does a small nudge in *x* influence *f*(*h*(*g*(*m*(*x*))))?

A: Propagate gradients backwards using the chain rule!

Chain rule:

$$\frac{df}{dx} = \frac{df}{dh}\frac{dh}{dg}\frac{dg}{dm}\frac{dm}{dx}$$

Model derivatives:

$$m'(z) = -1$$

$$g'(z) = \exp(z)$$

$$h'(z) = 1$$

$$f'(z) = -\frac{1}{z^2}$$

$$x \xrightarrow{1} m \xrightarrow{-1} g \xrightarrow{0.37} h \xrightarrow{1.37} f \xrightarrow{0.73}$$

$$x \xleftarrow{.20} m \xleftarrow{-.20} g \xleftarrow{-.53} h \xleftarrow{-.53} f$$

Sigmoid function:

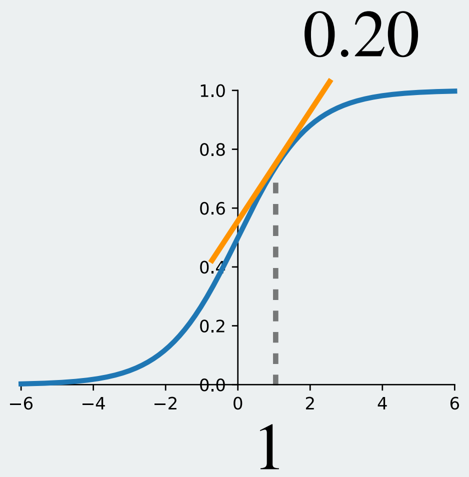
$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$

Sigmoid derivative:

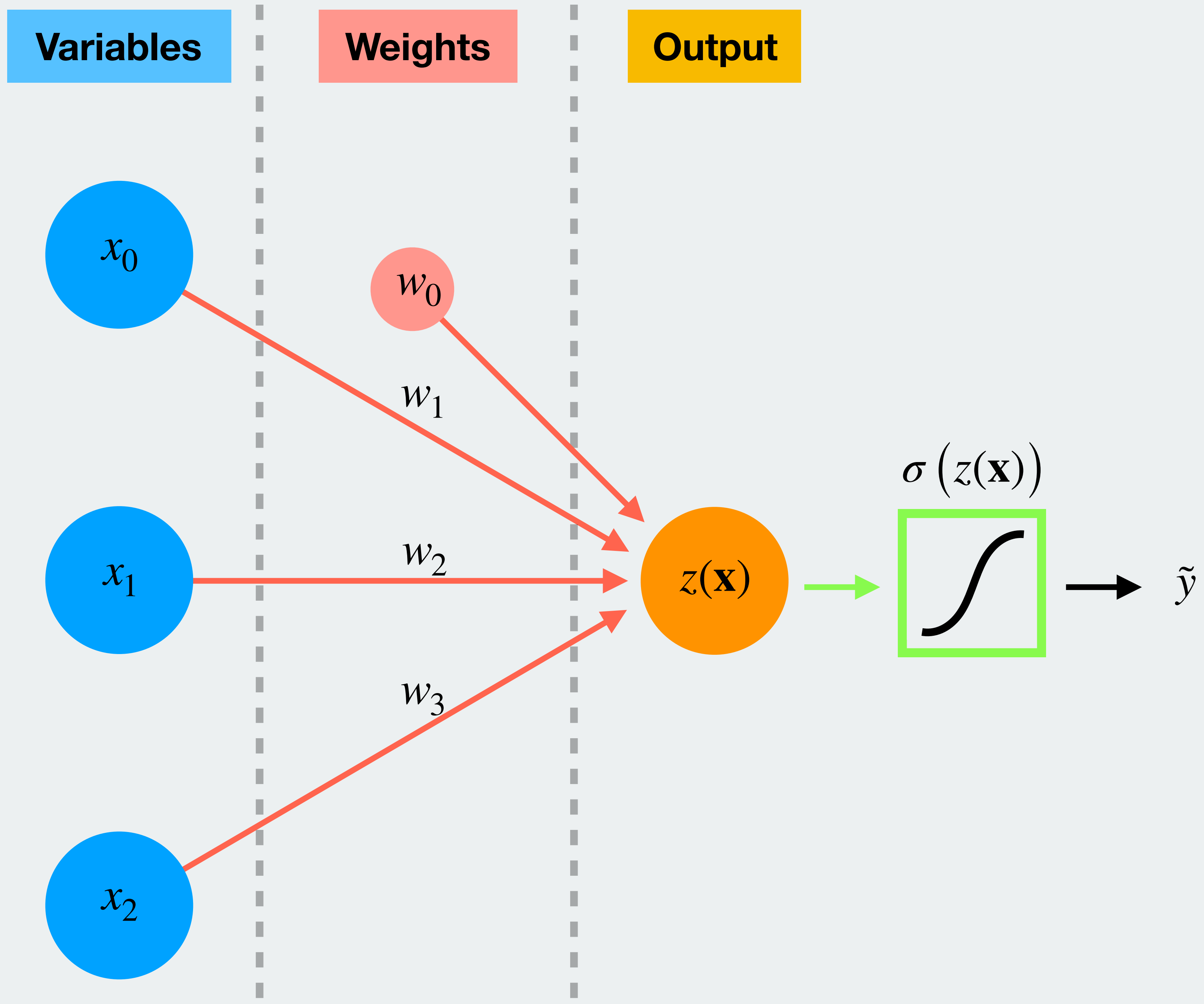
$$\sigma'(z) = \sigma(z)(1 - \sigma(z))$$

$$x \xrightarrow{1} \sigma \xrightarrow{0.73}$$

$$x \xleftarrow{0.20} \sigma$$



Backpropagation – on a neural network



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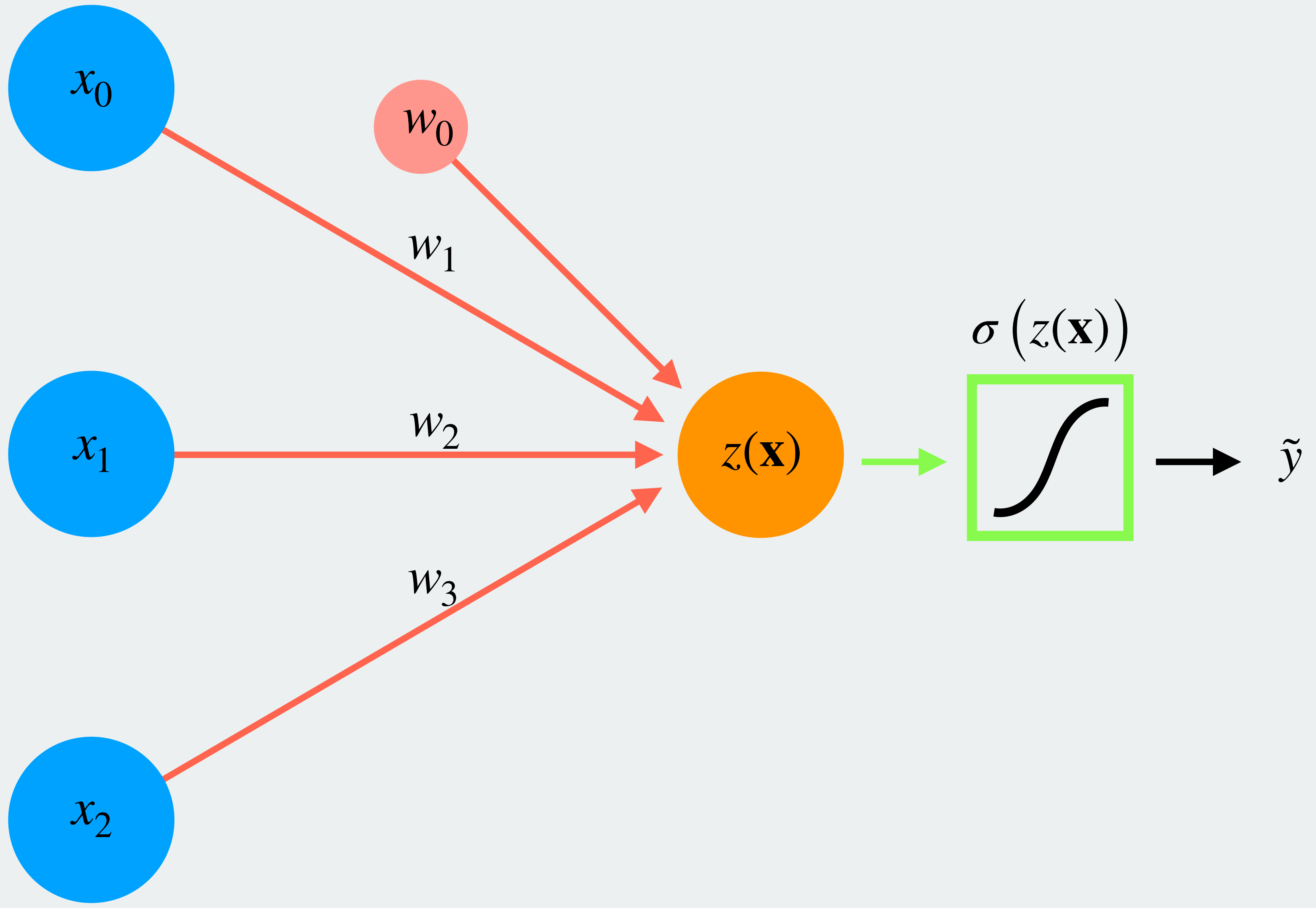

Model:

$$w_0 + x_0 w_1 + x_1 w_2 + x_2 w_3 = z(\mathbf{x})$$

$$\sigma(x) = \frac{1}{1 + \exp(-x)}$$

$$C(\tilde{y}, y) = \left(\tilde{y} - y\right)^2$$

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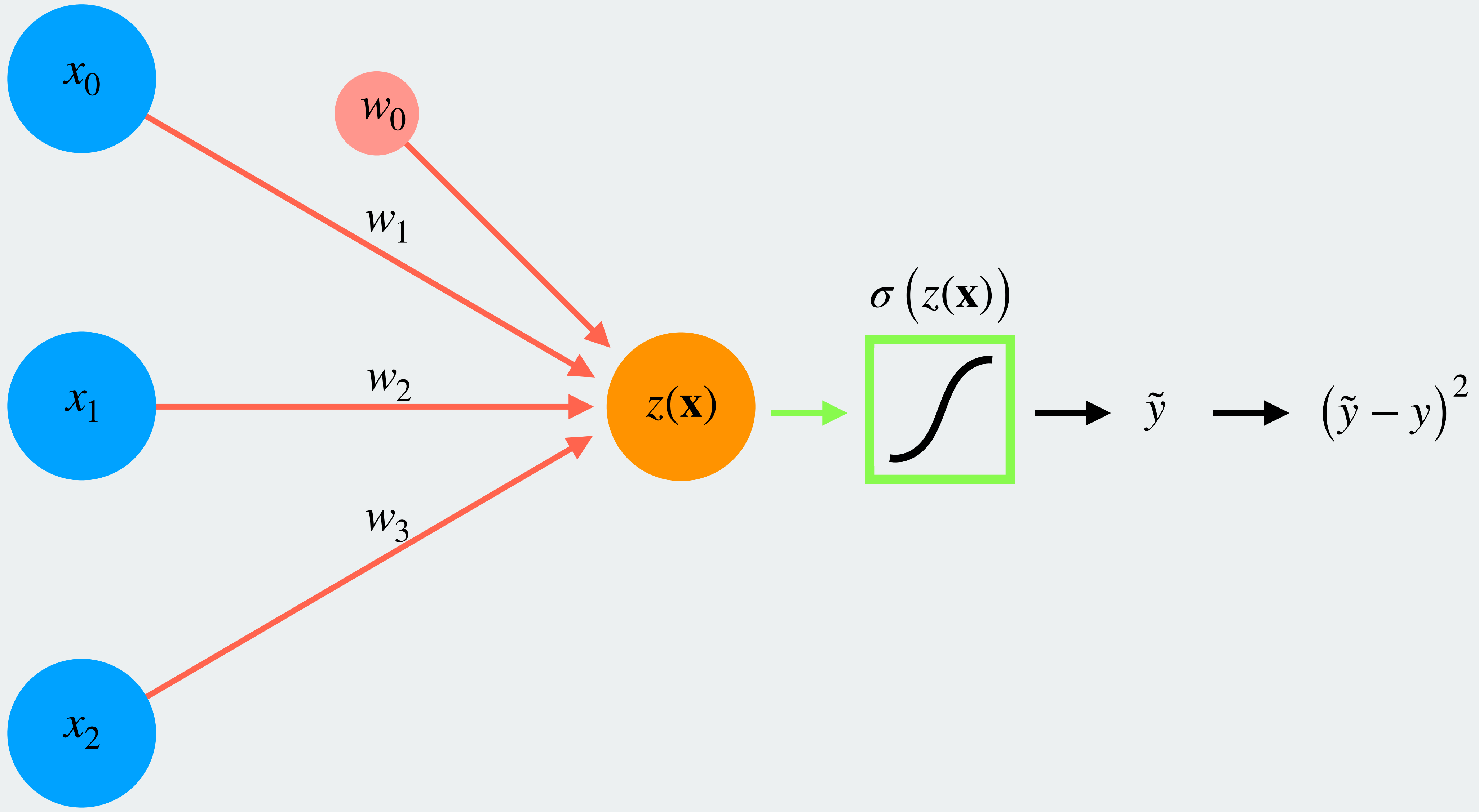

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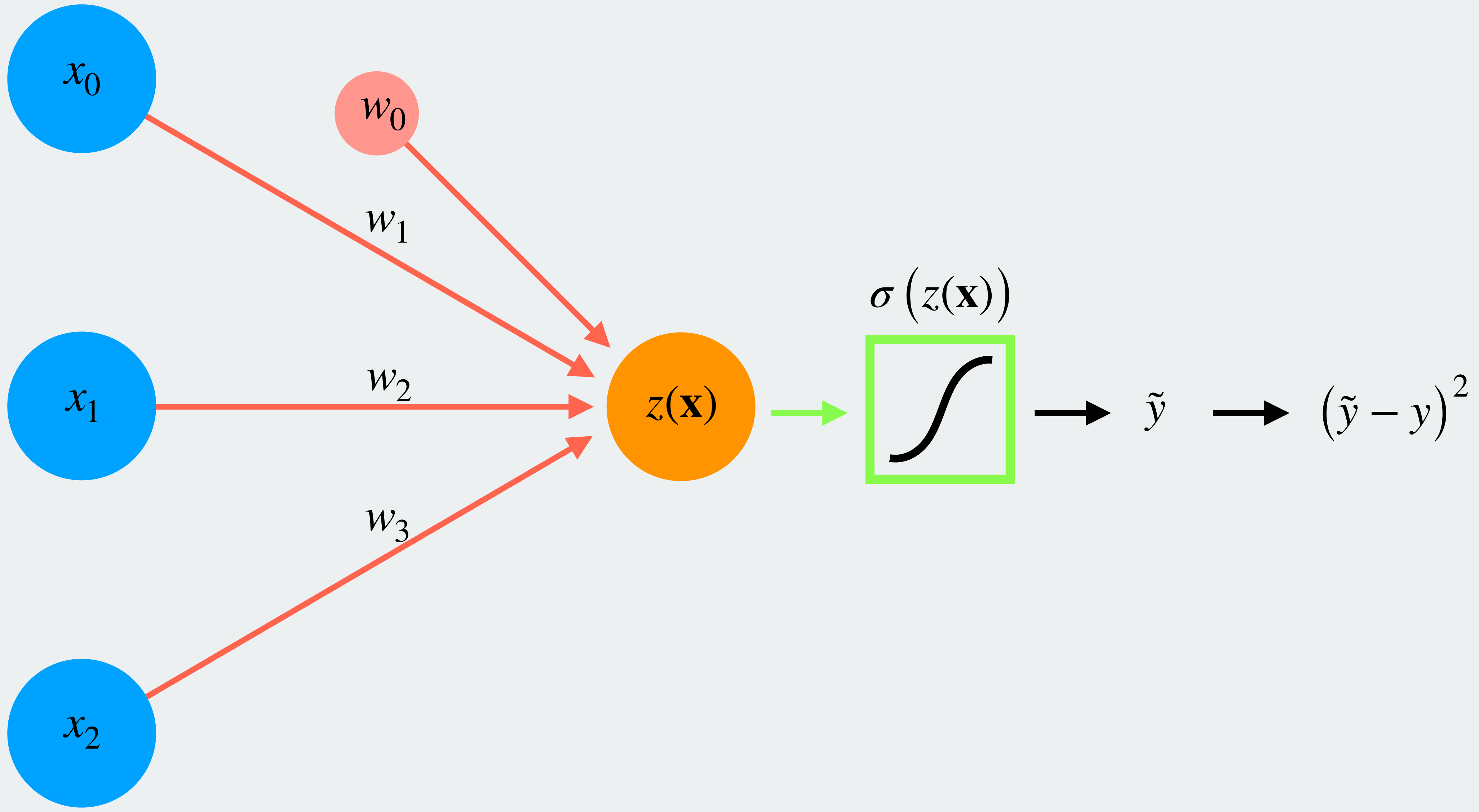

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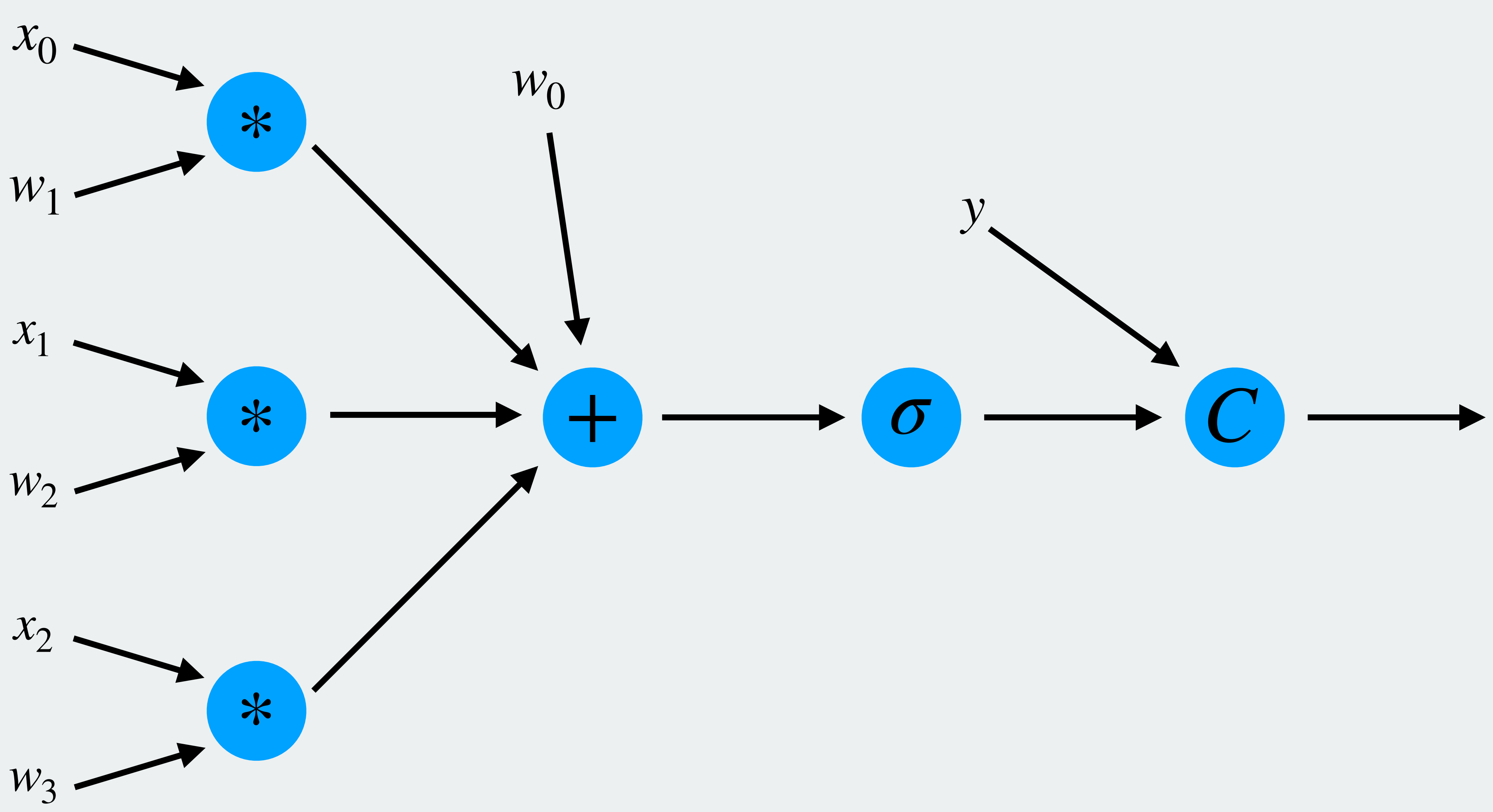

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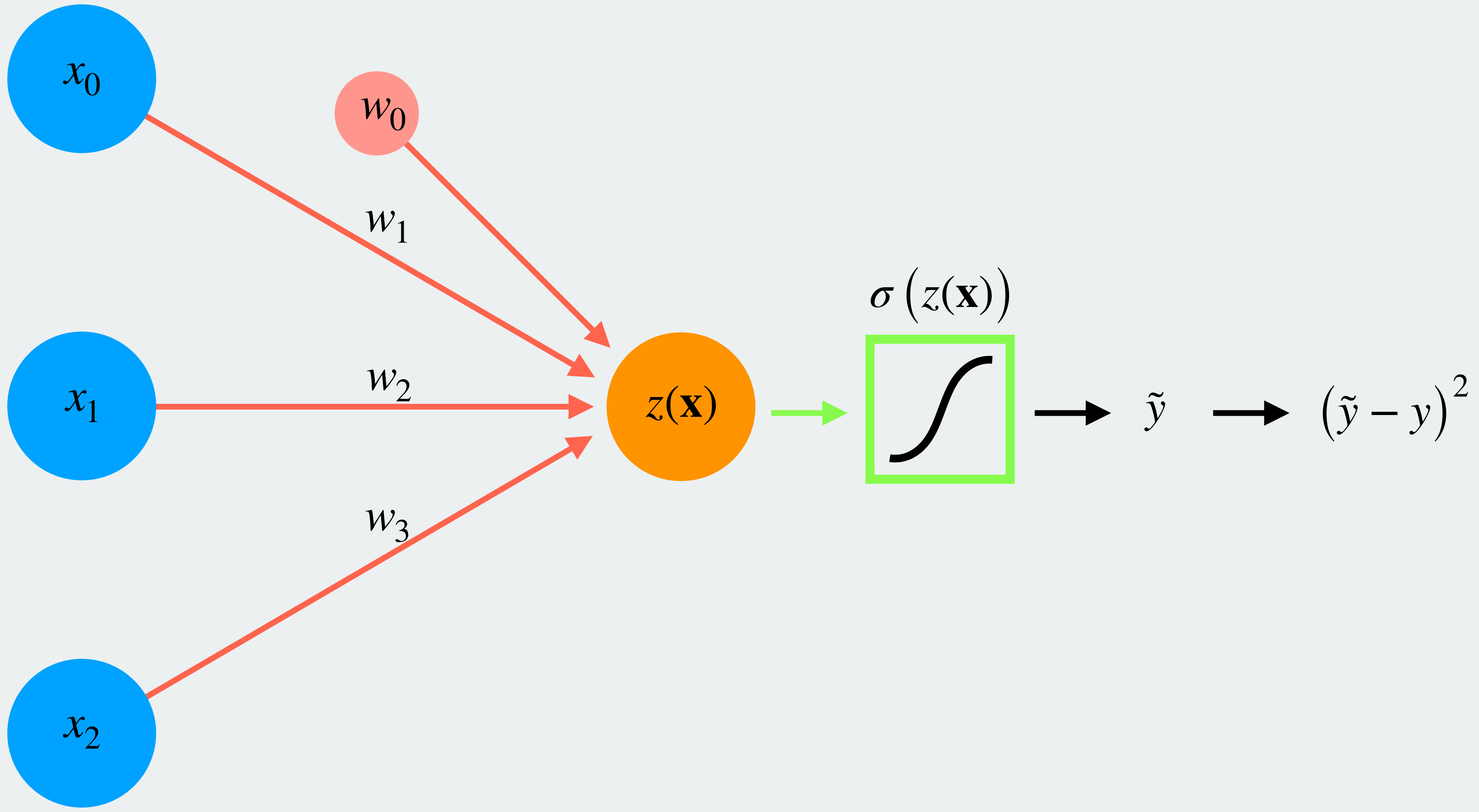

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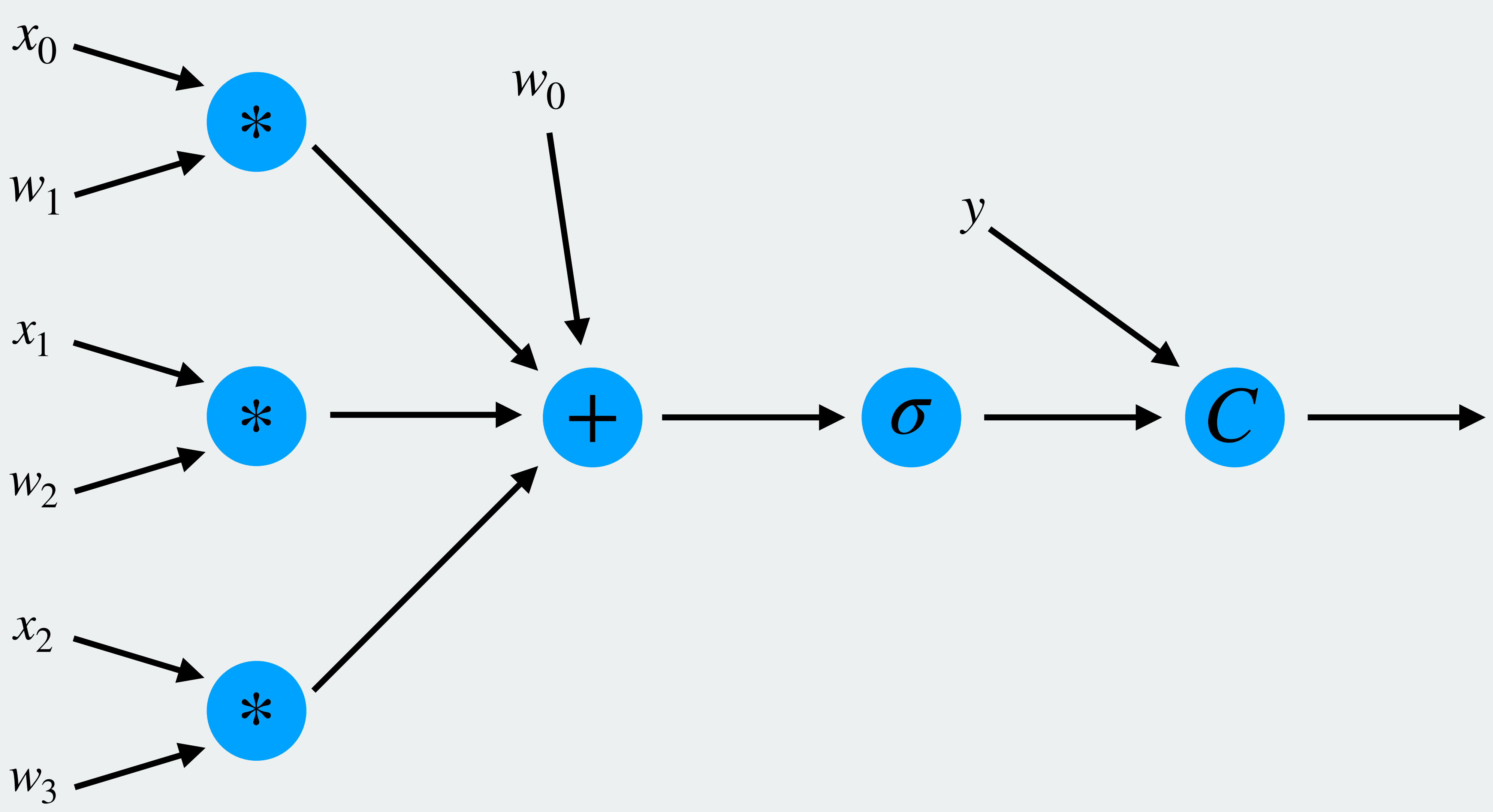

Weights:

$$\mathbf{b} = \begin{bmatrix} -2 \end{bmatrix}$$

$$\mathbf{W} = \begin{bmatrix} -1 & 0.5 & 10 \end{bmatrix}$$

Data:

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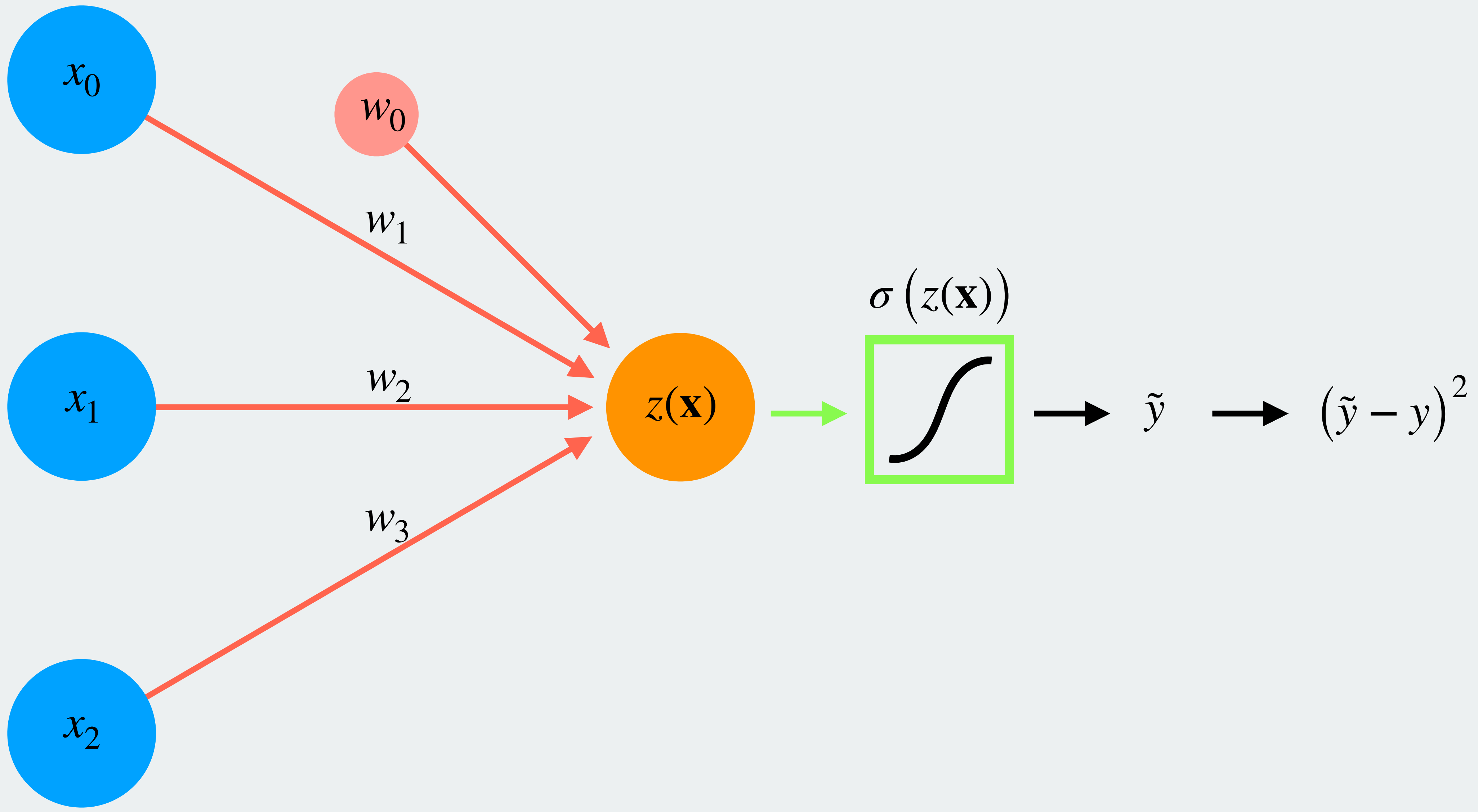

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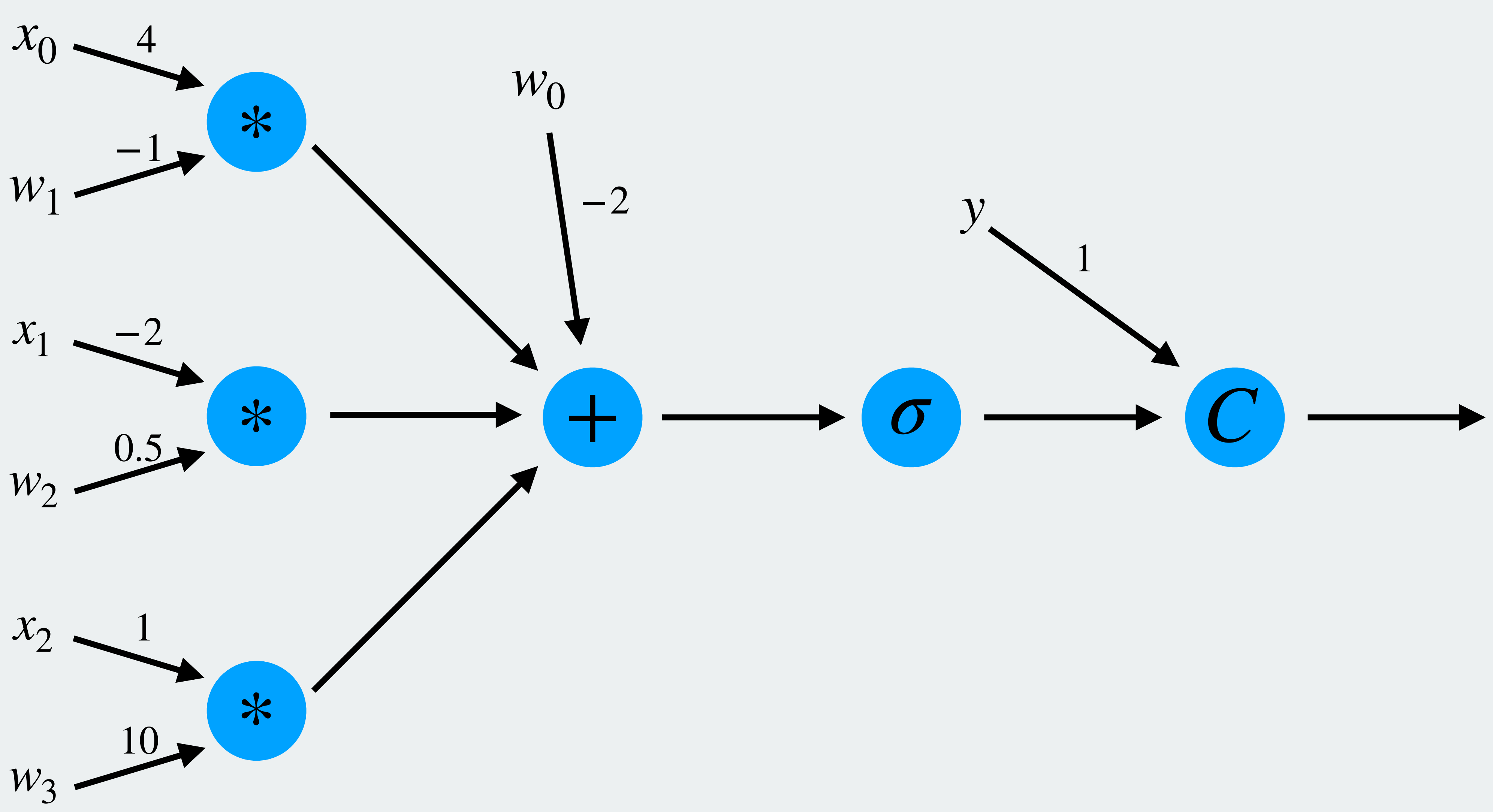
Forward pass



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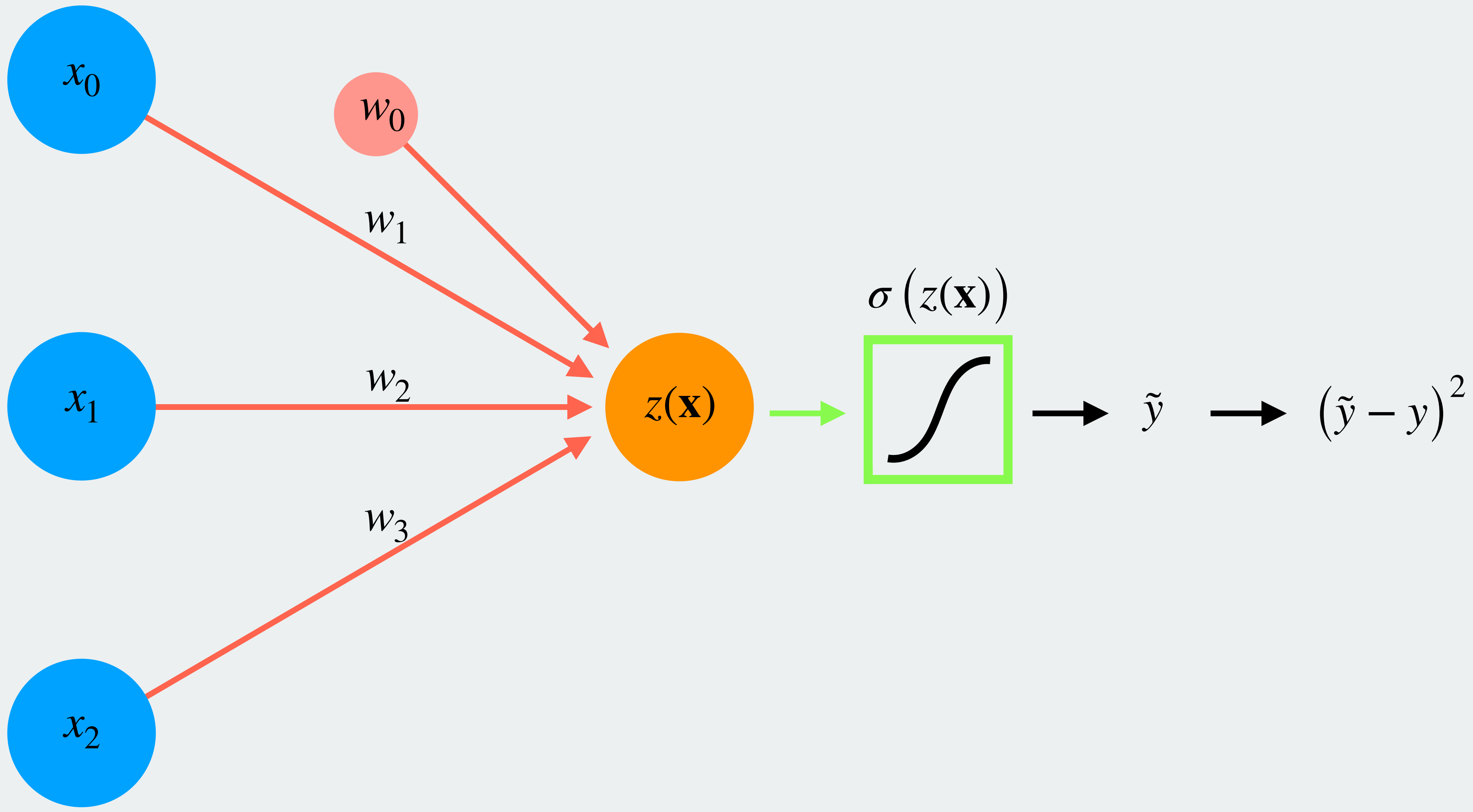

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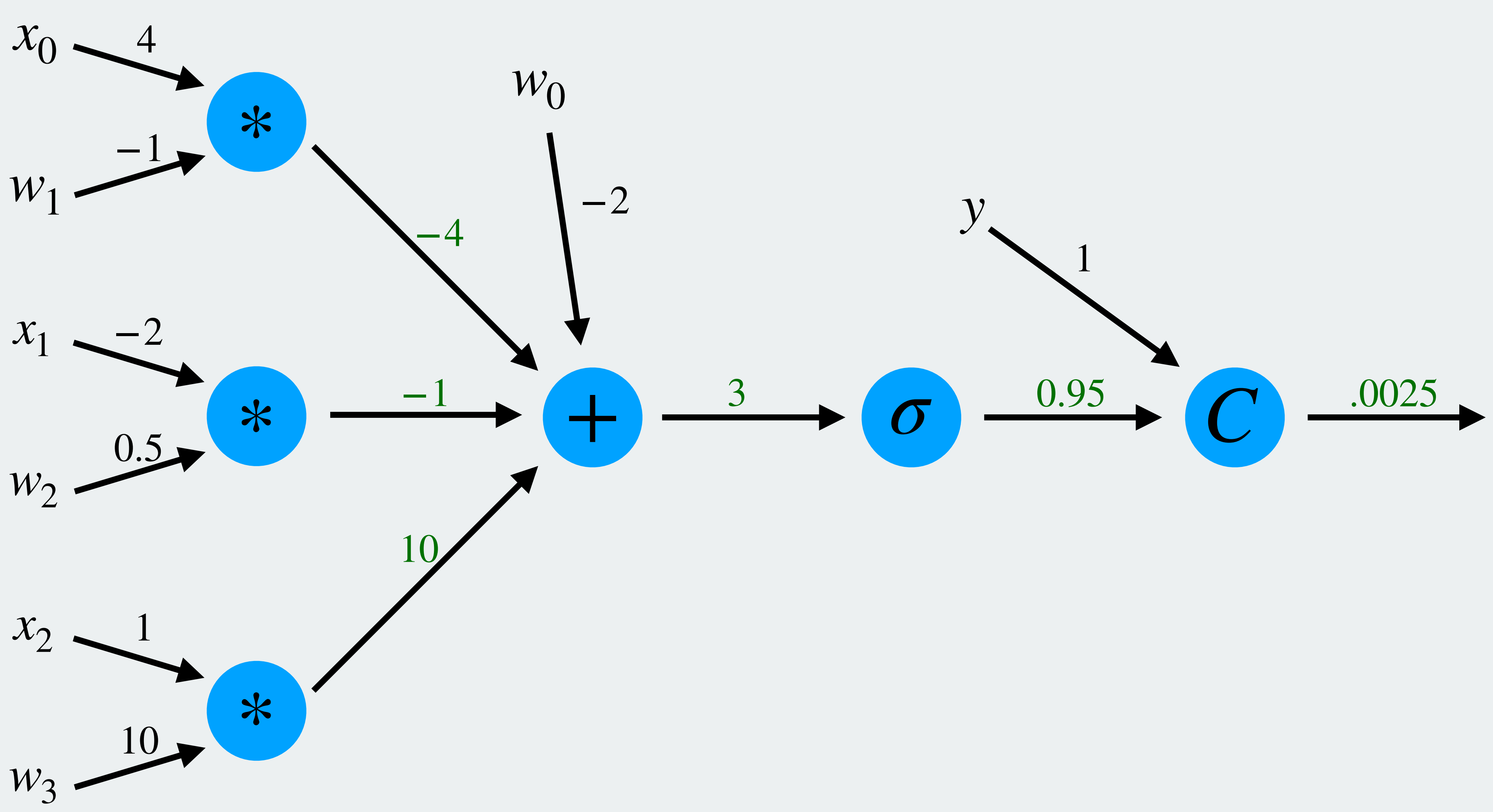

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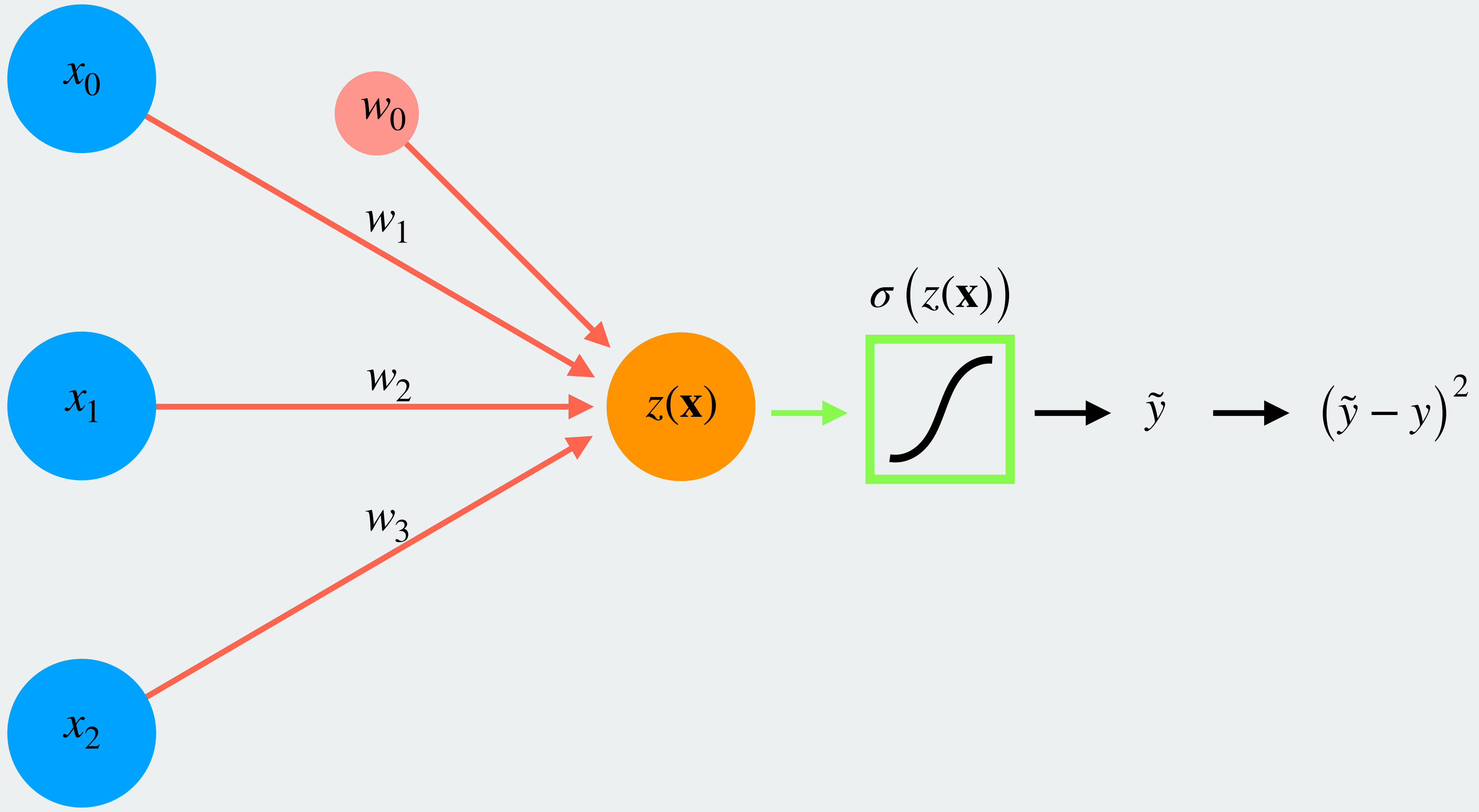

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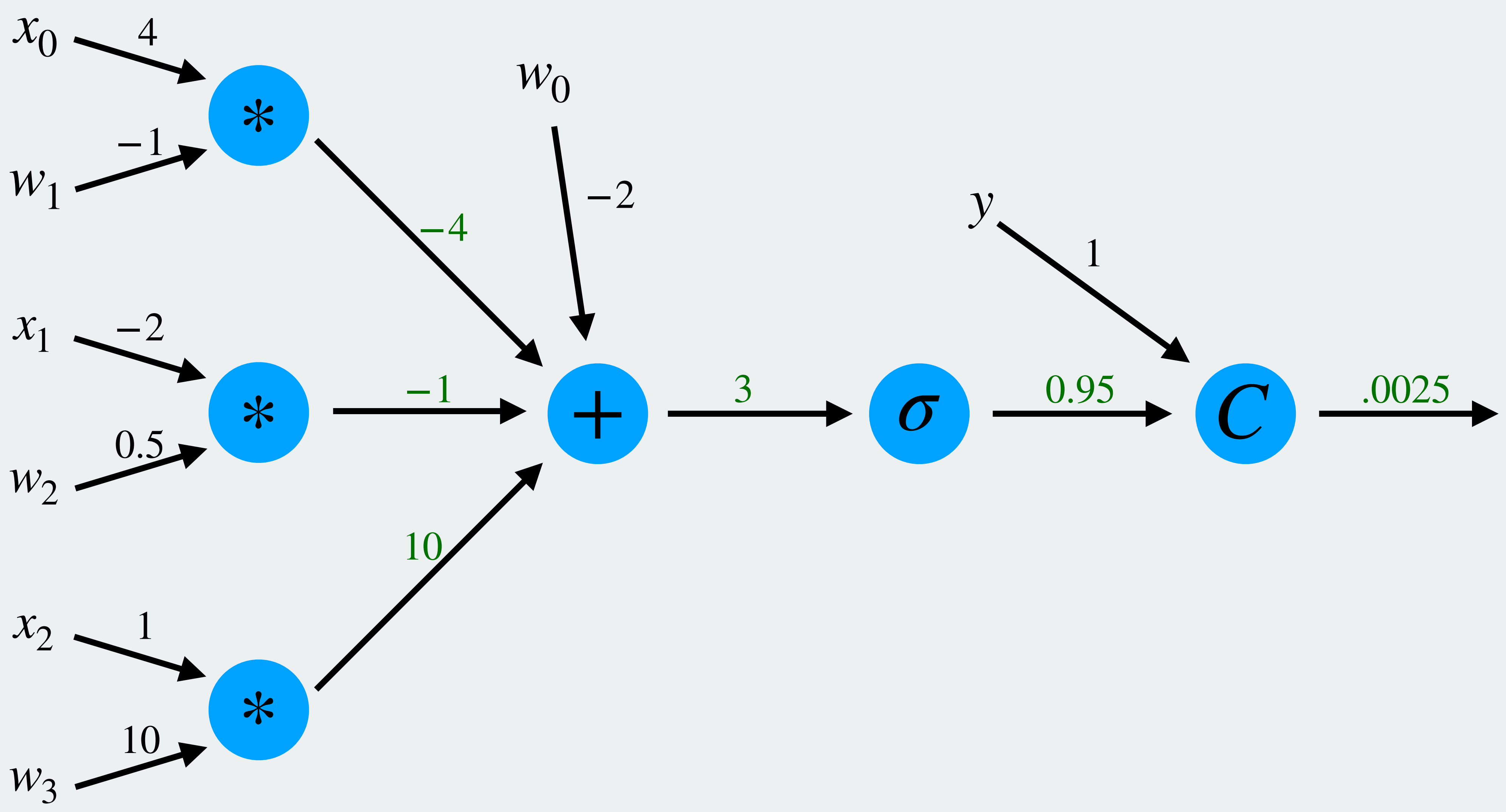
Backward pass



Model:

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$$\sigma(x) = \frac{1}{1 + \exp(-x)}$$

$$C(\tilde{y}, y) = (\tilde{y} - y)^2$$

Model derivatives:

$$C'(\tilde{y}, y) = ?$$

Weights:

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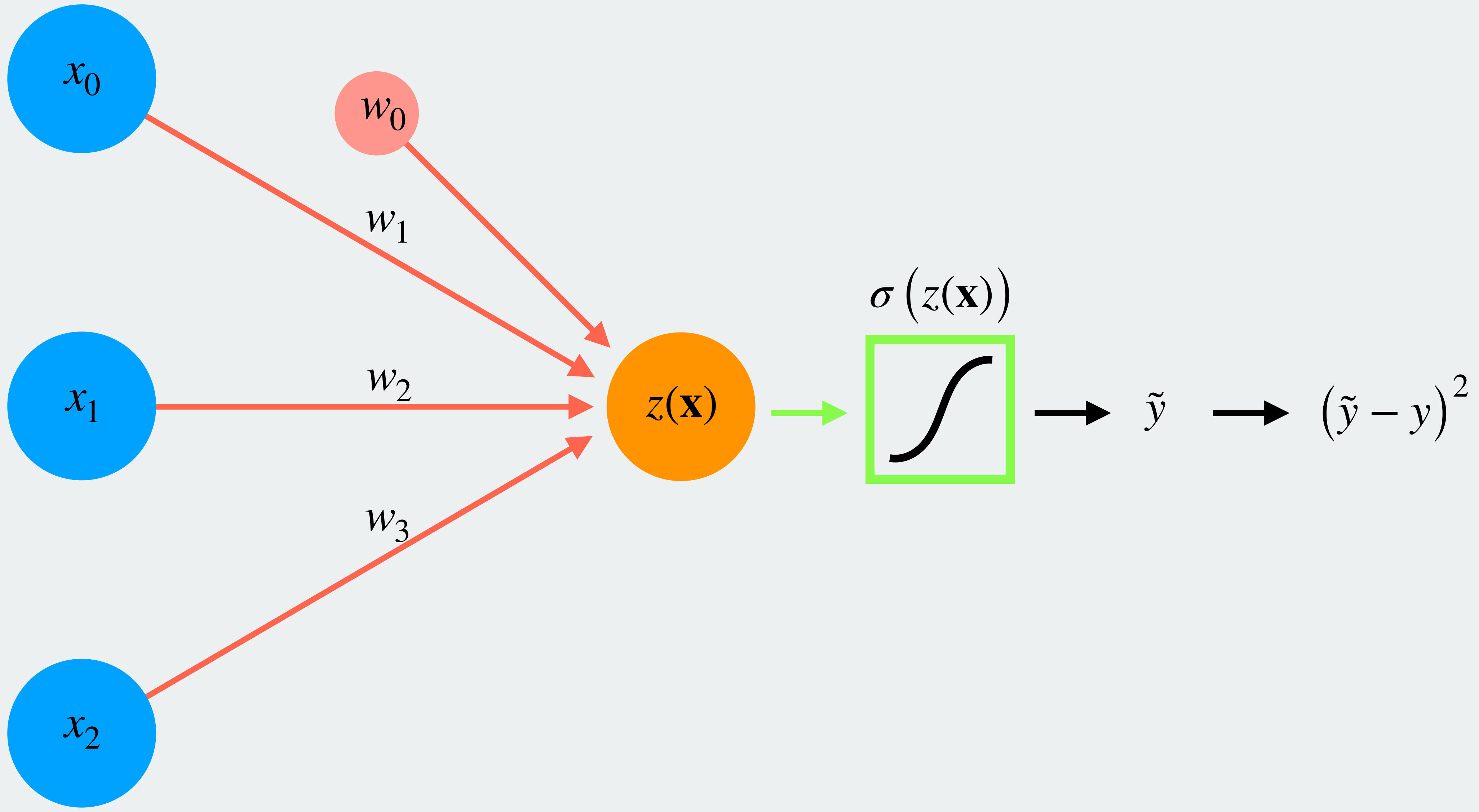

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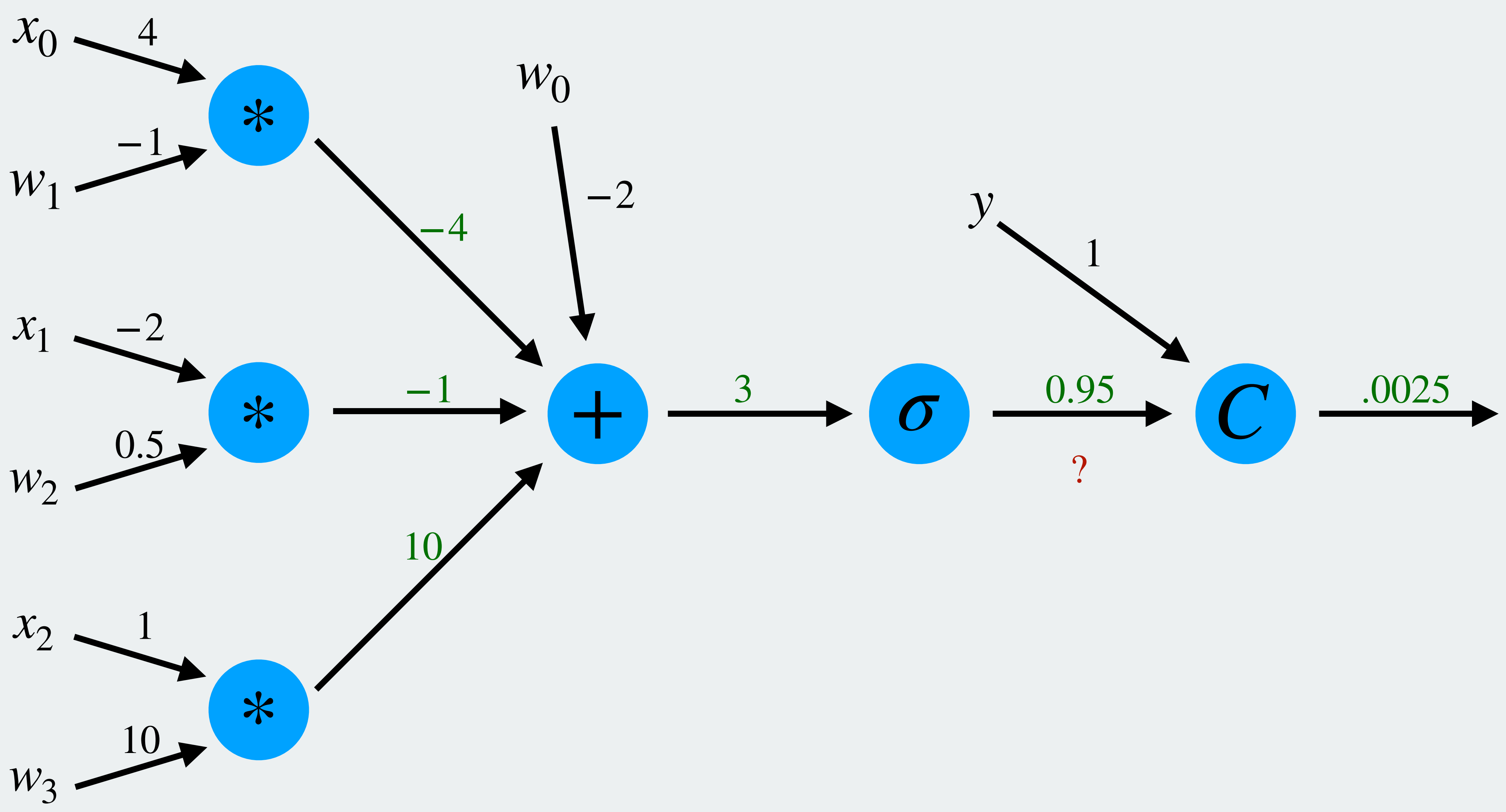

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Model derivatives:

$$C'(\tilde{y}, y) = 2(\tilde{y} - y)$$

Weights:

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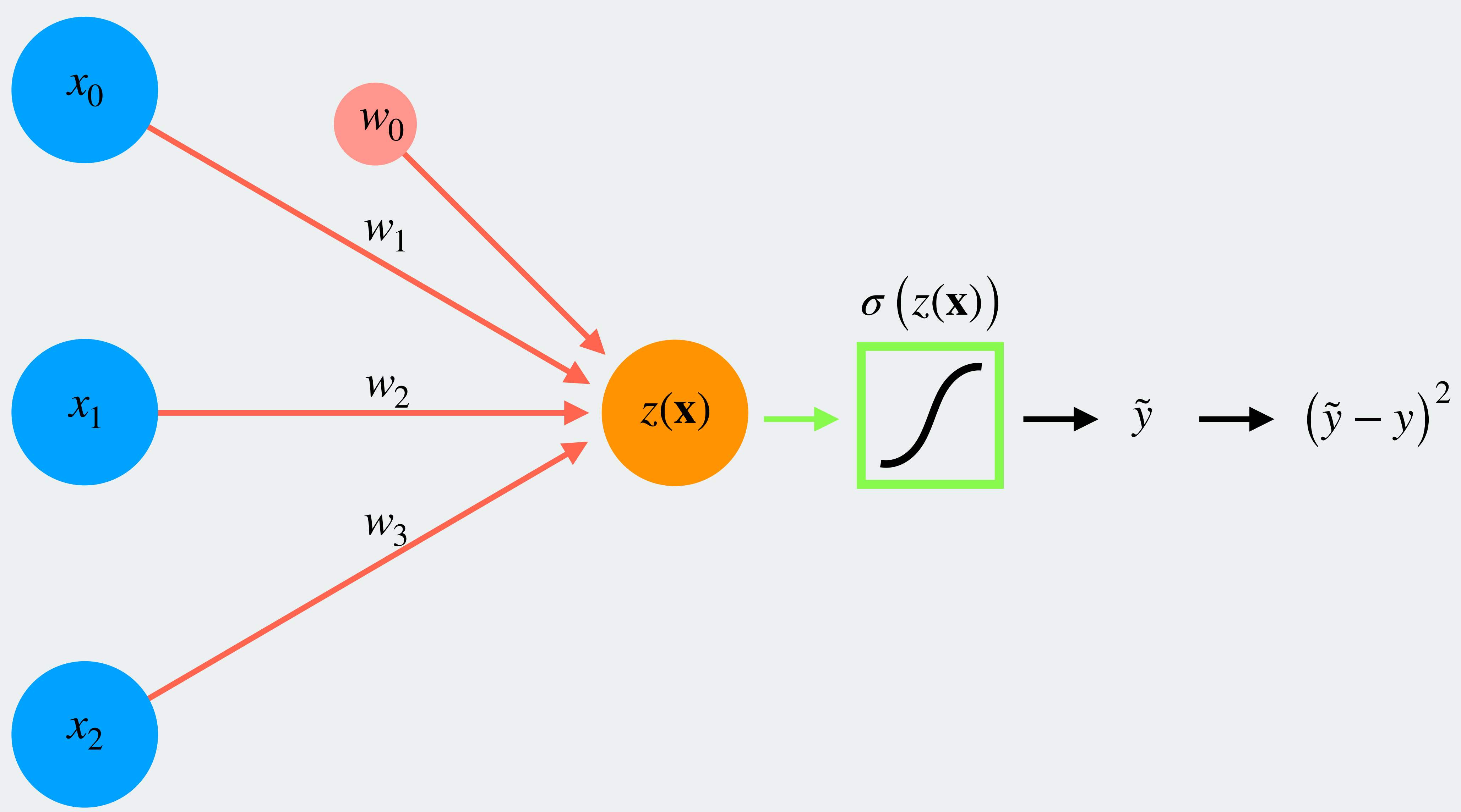

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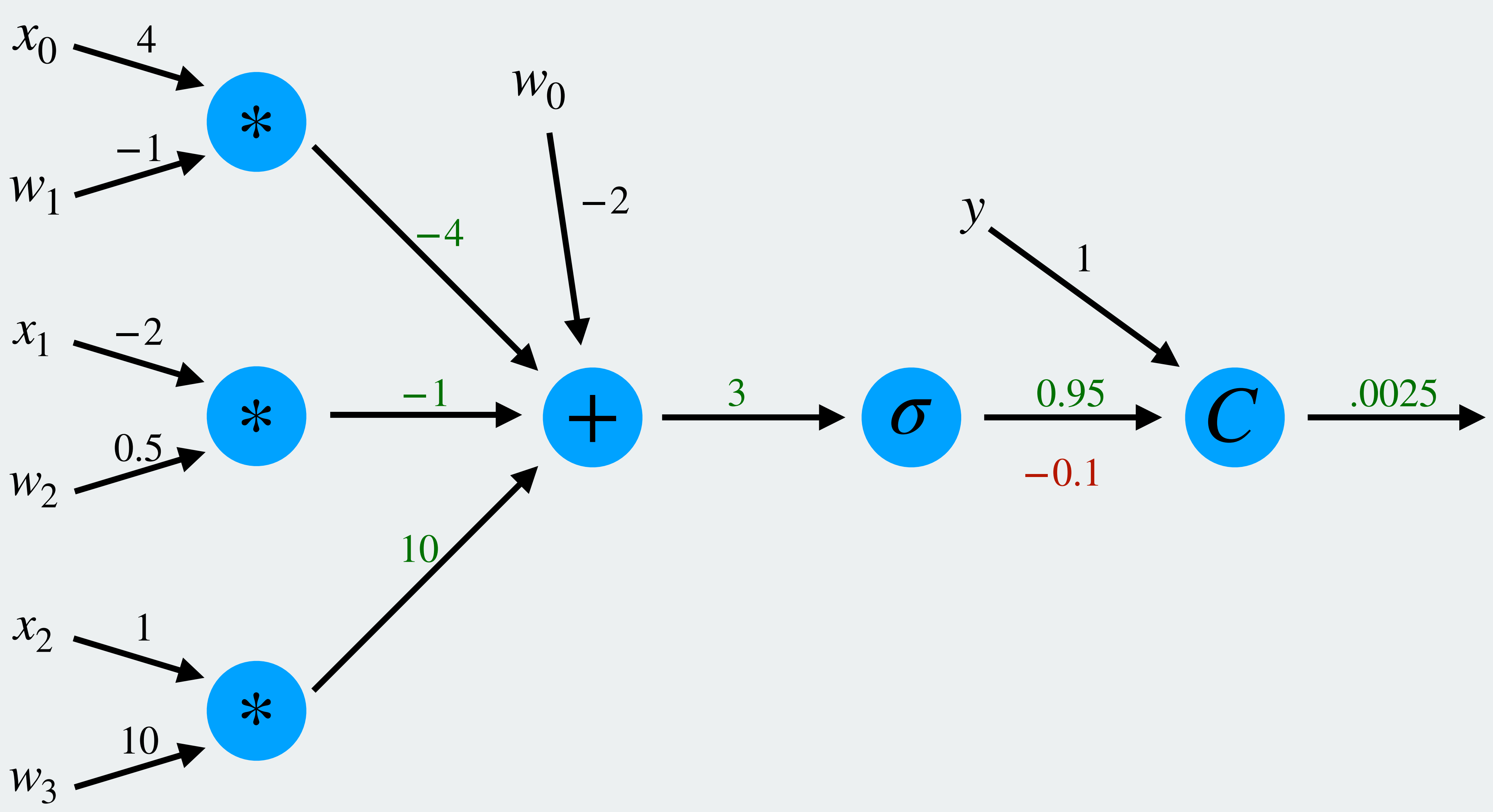

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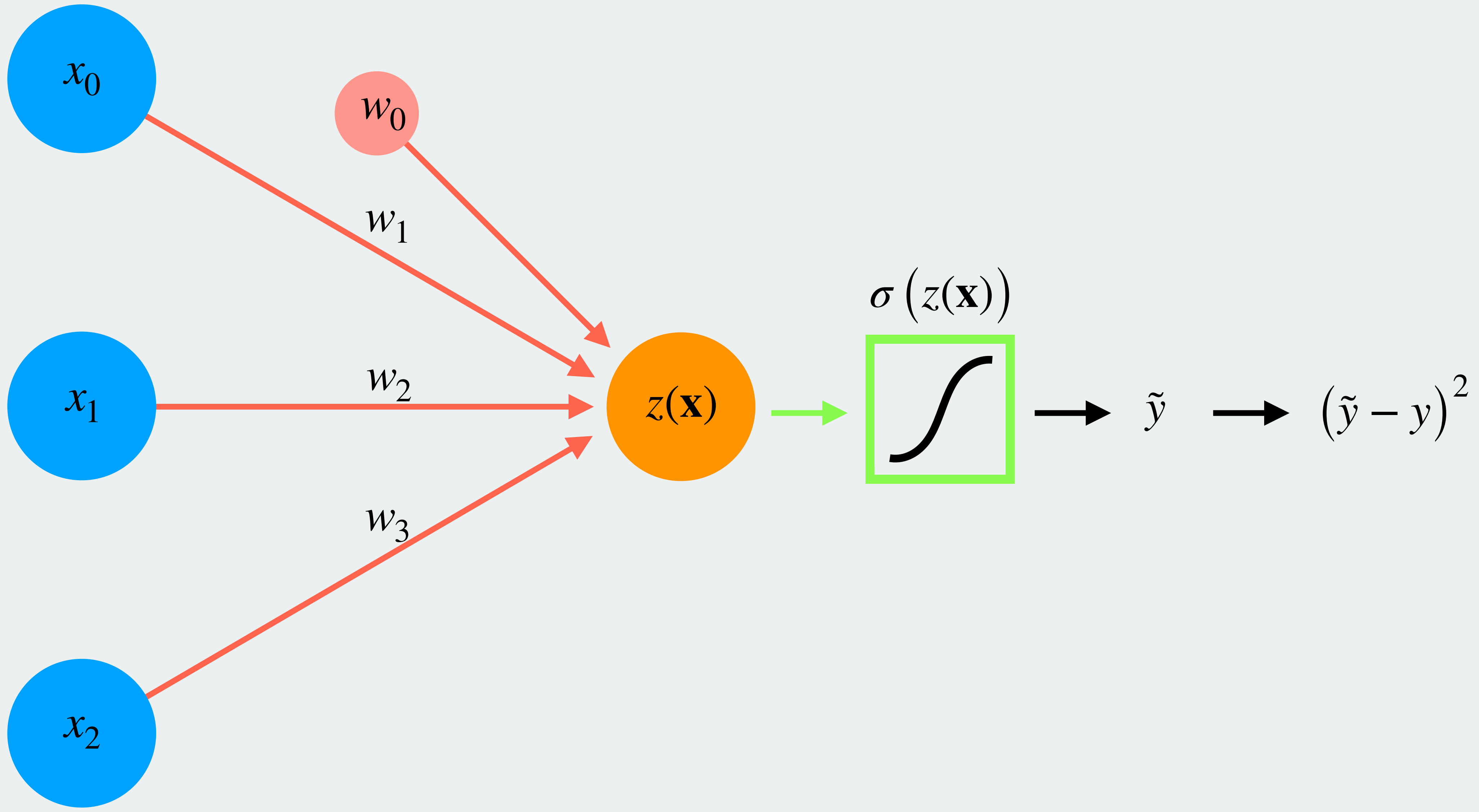

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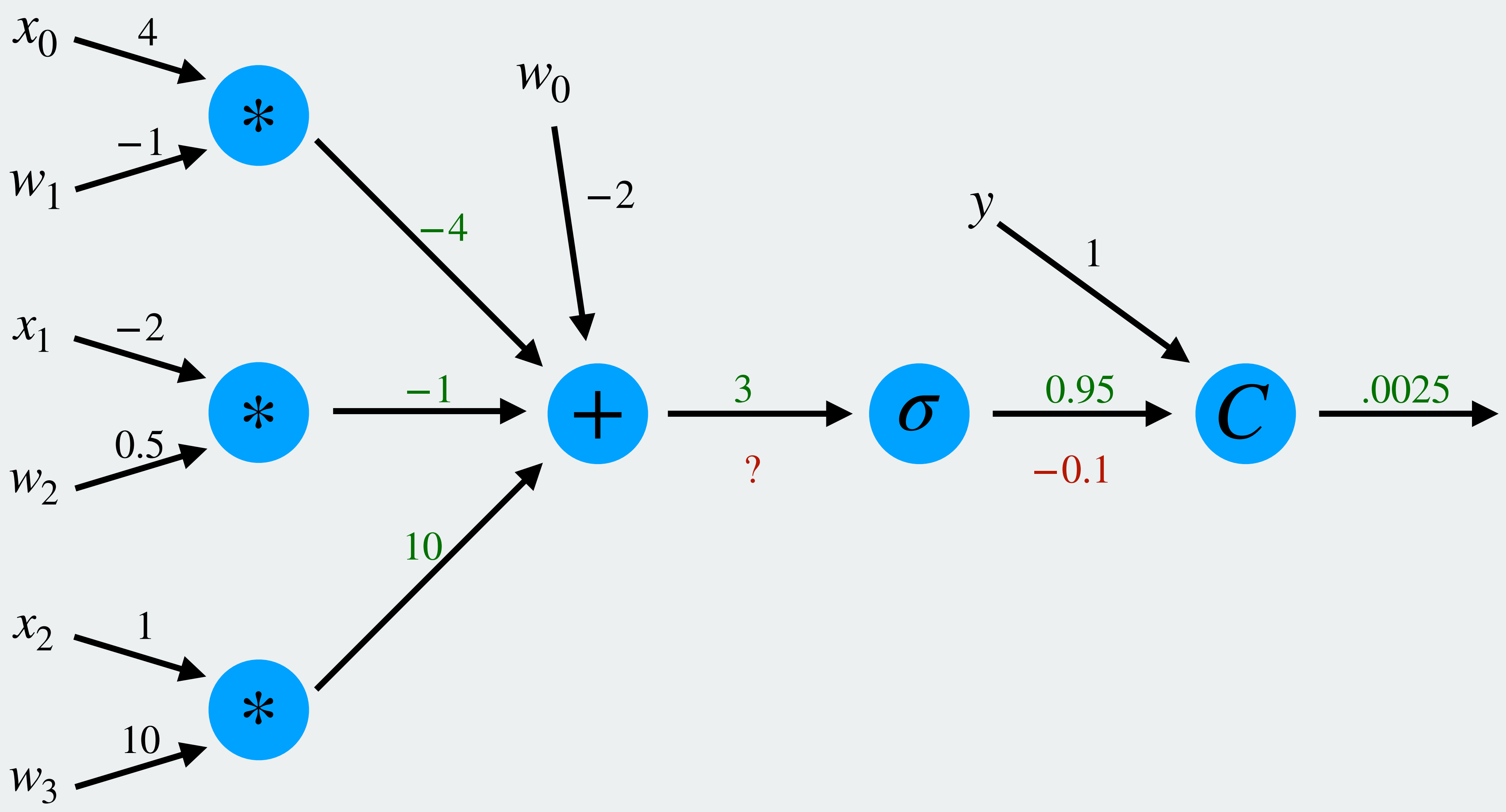

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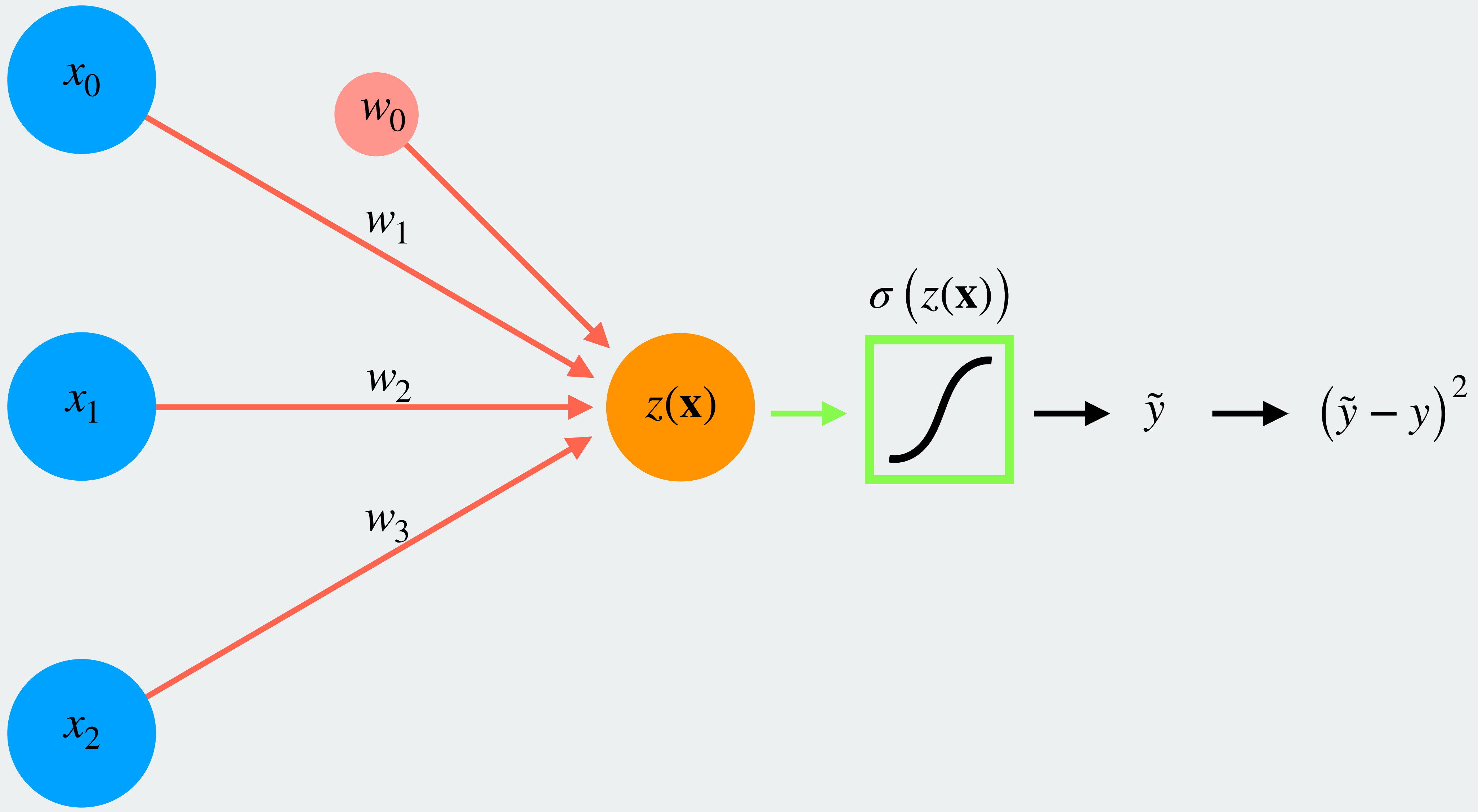

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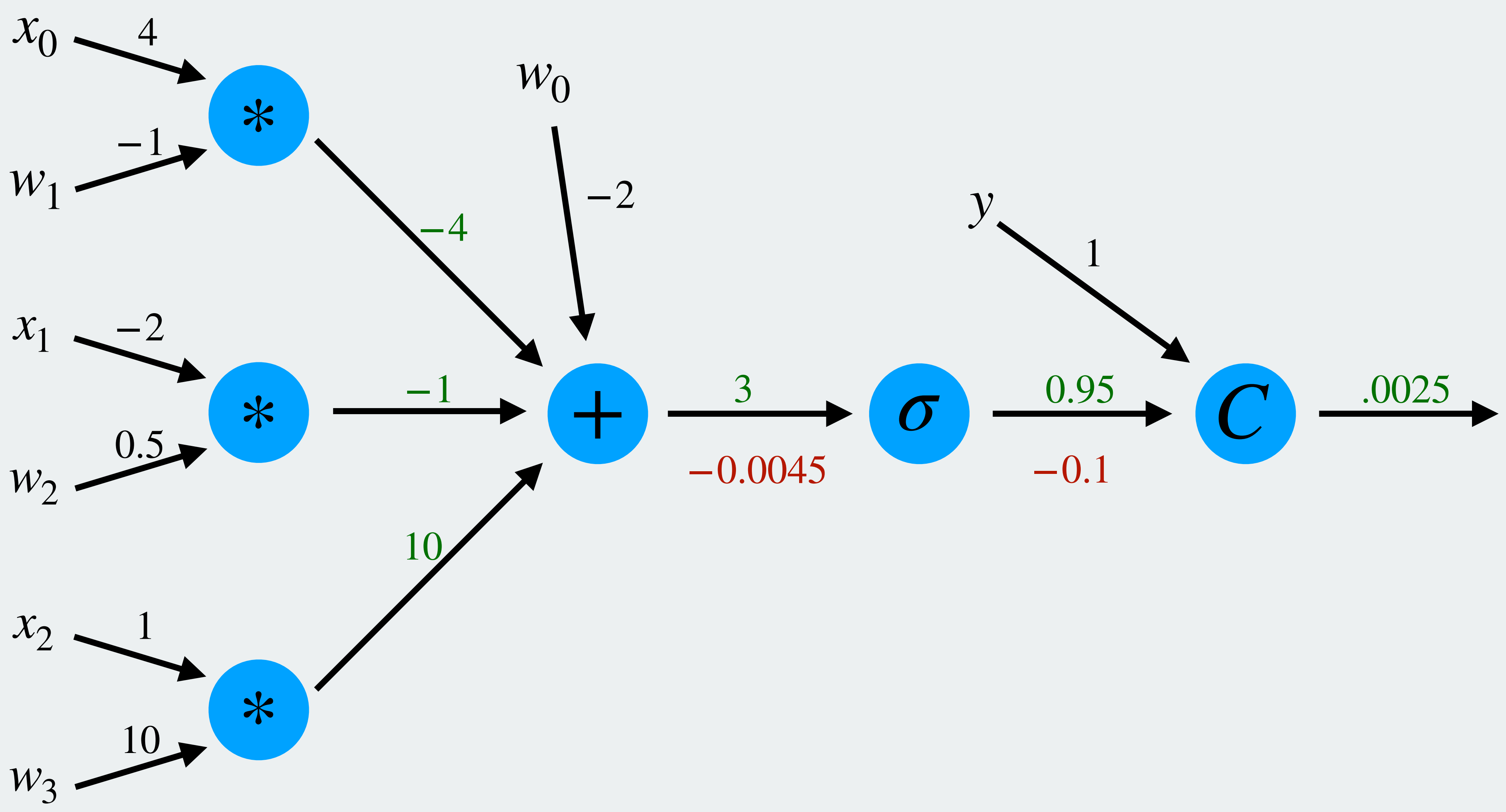

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The + gate is like a function: $y = \sum_{i=0}^{N} z_n$

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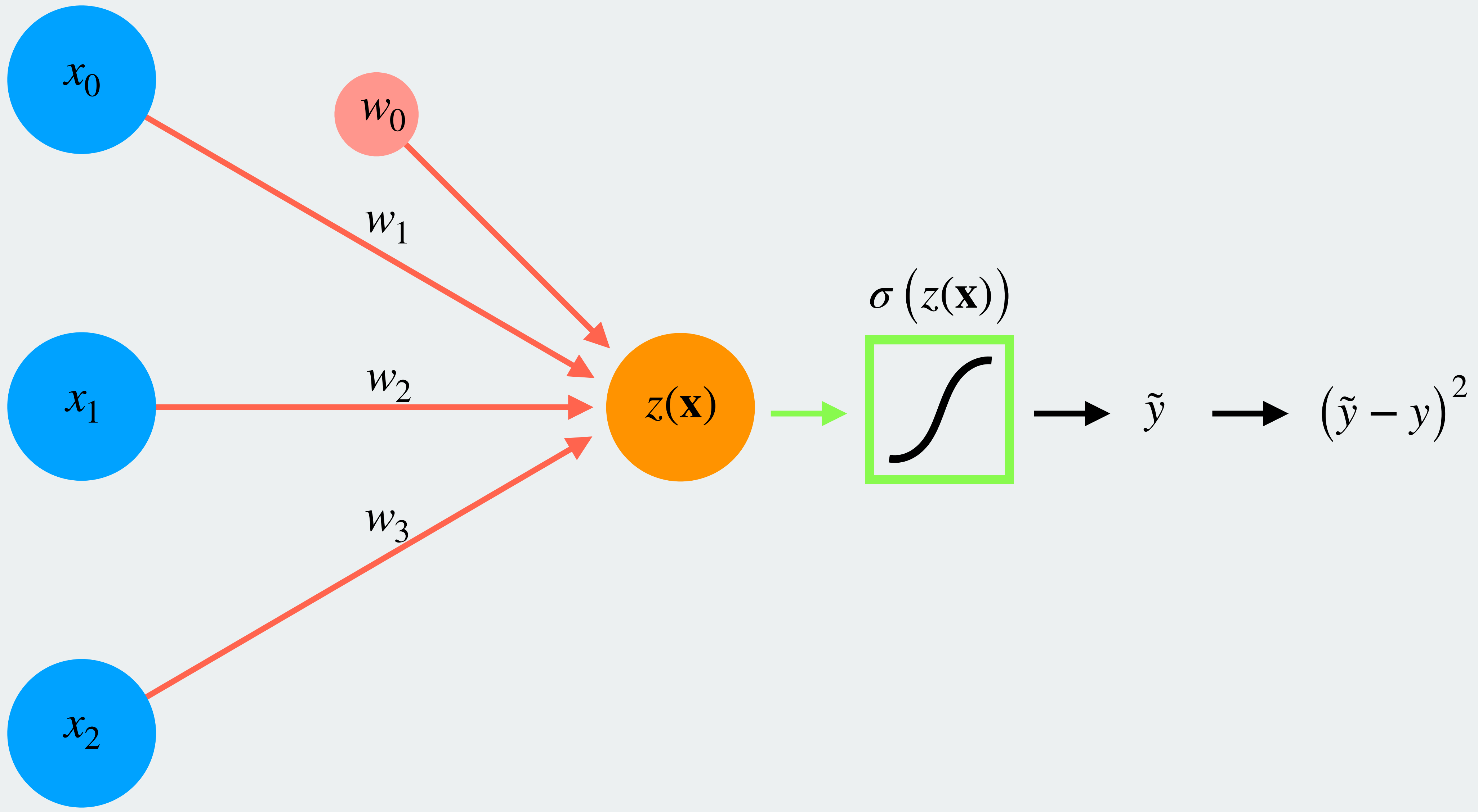

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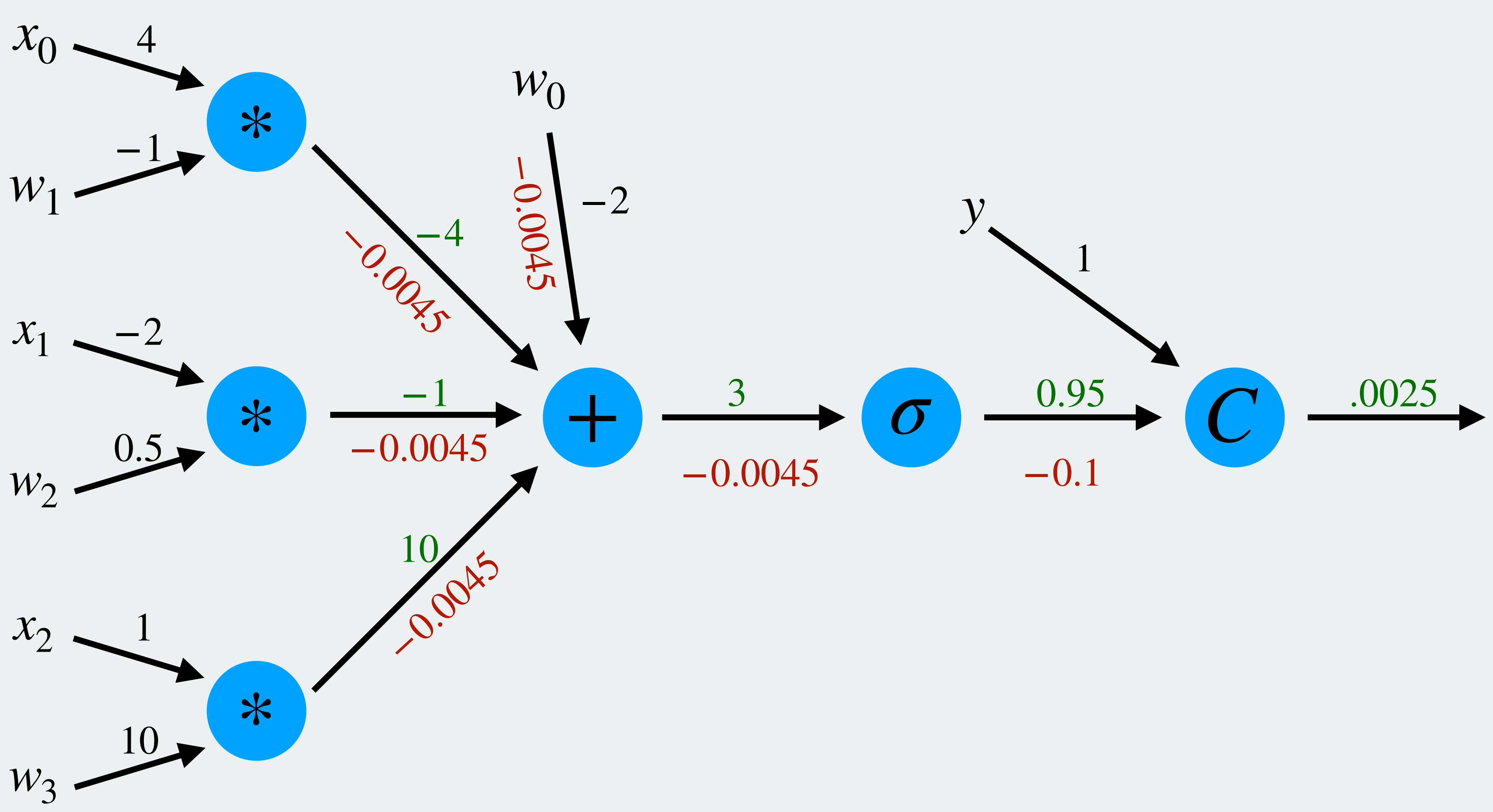

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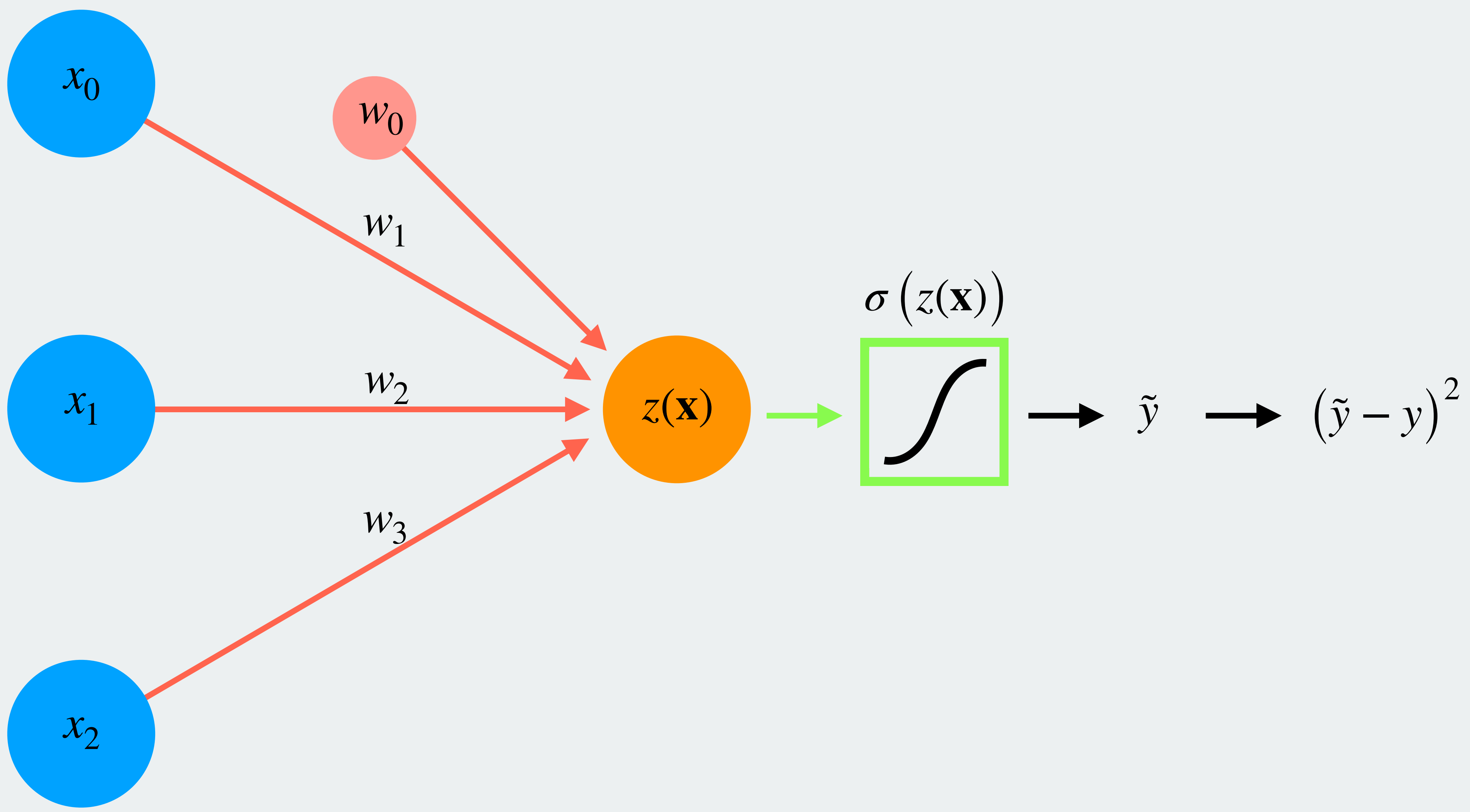

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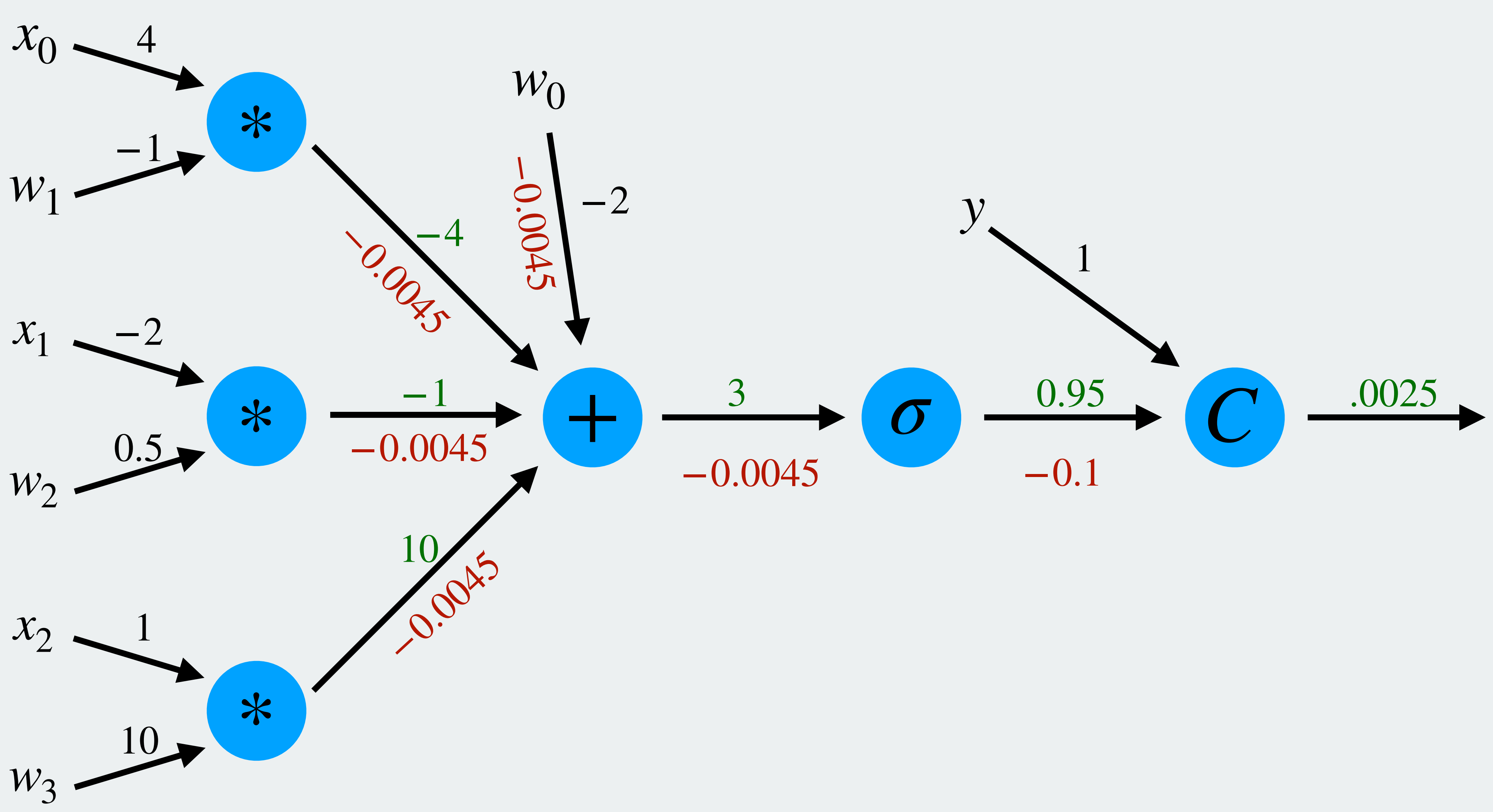

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Model derivatives:

Each branch is a function: $y = wx$

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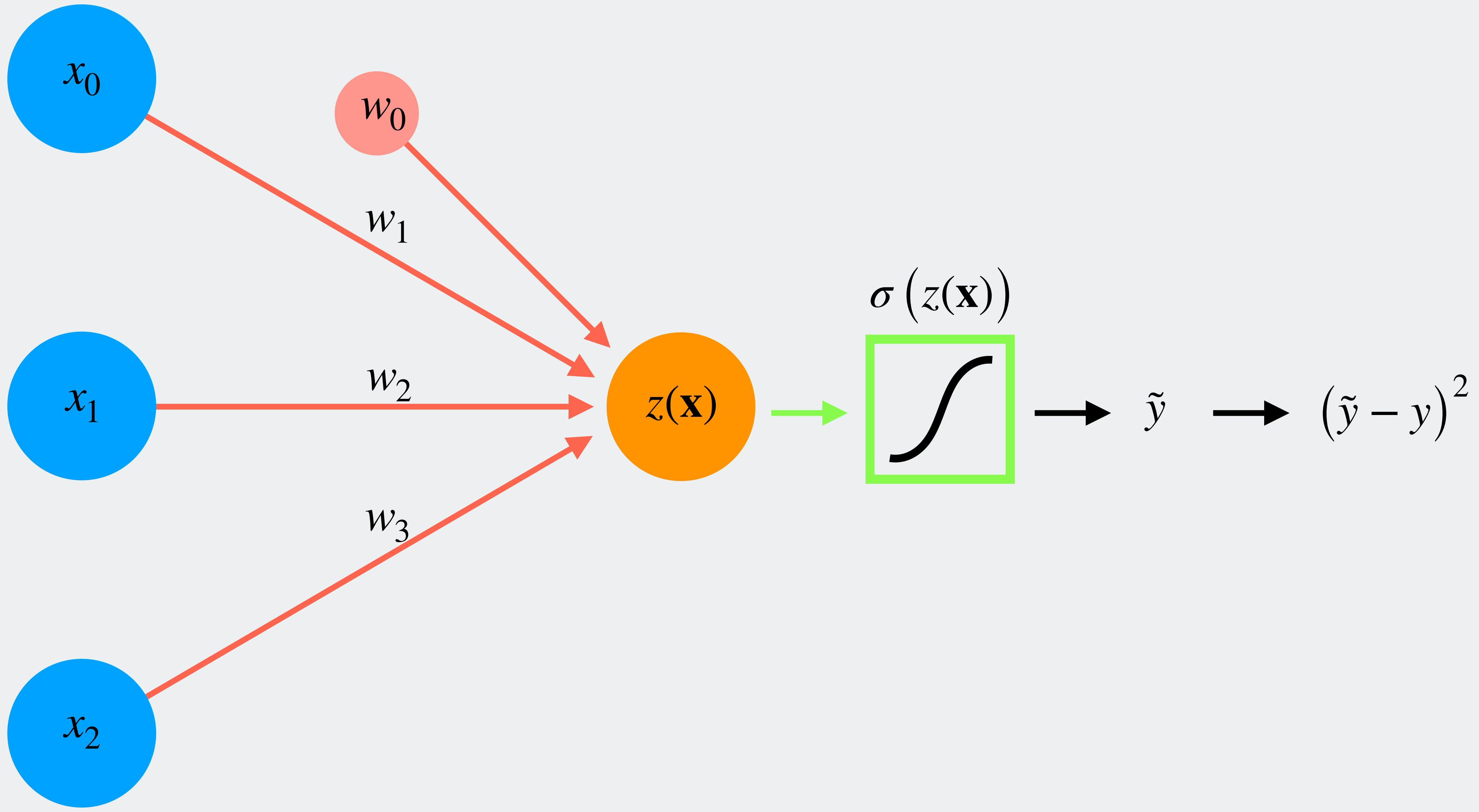

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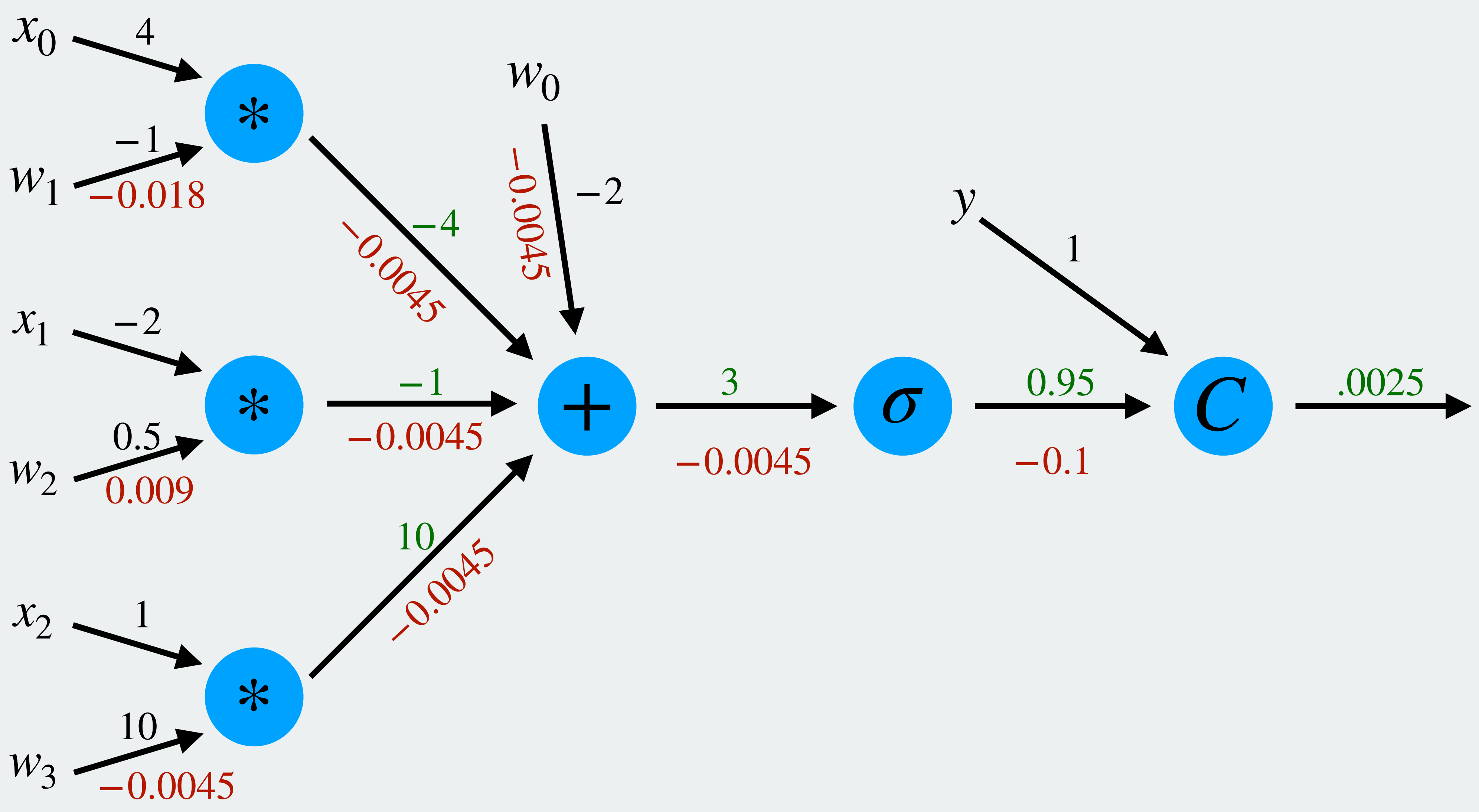

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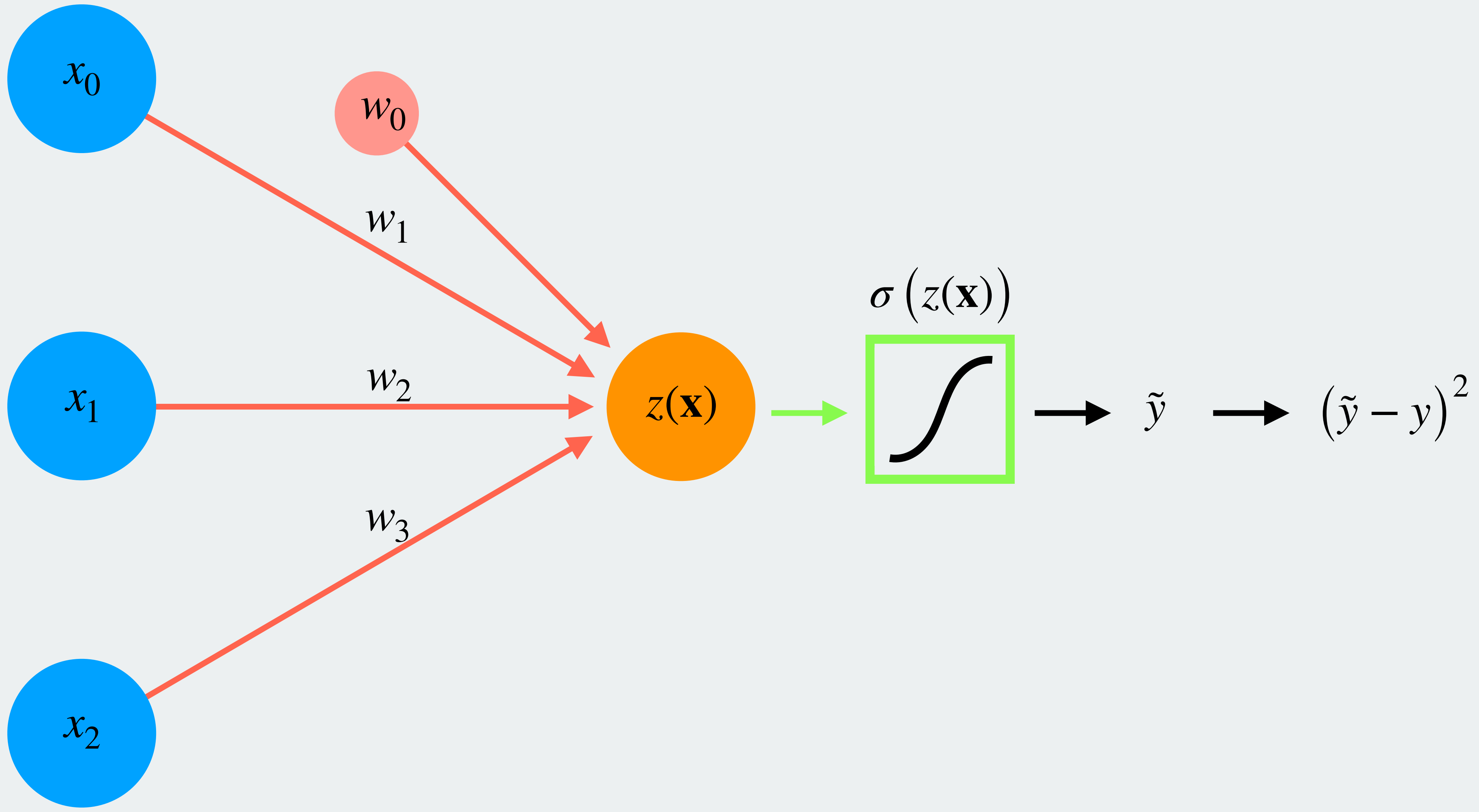

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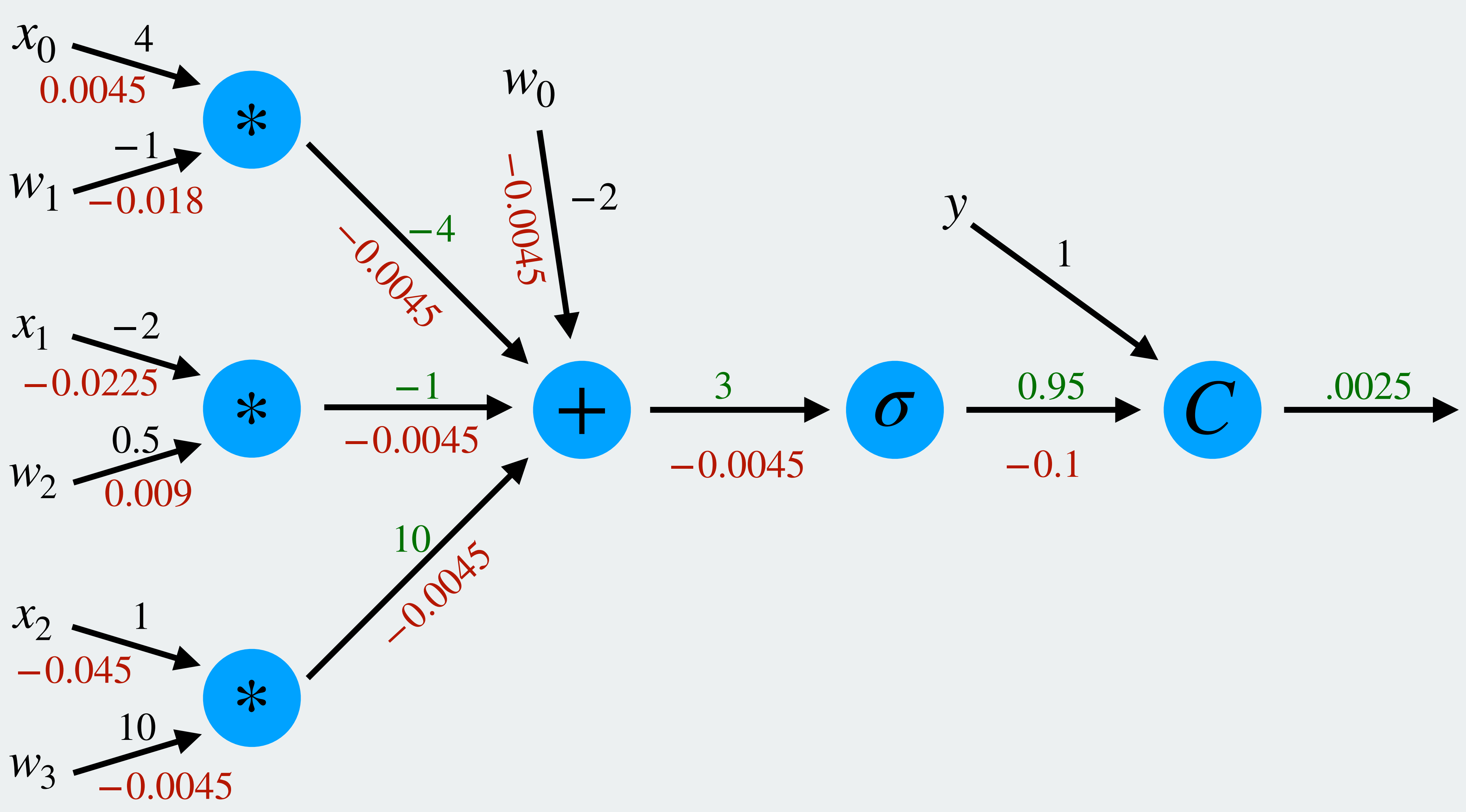

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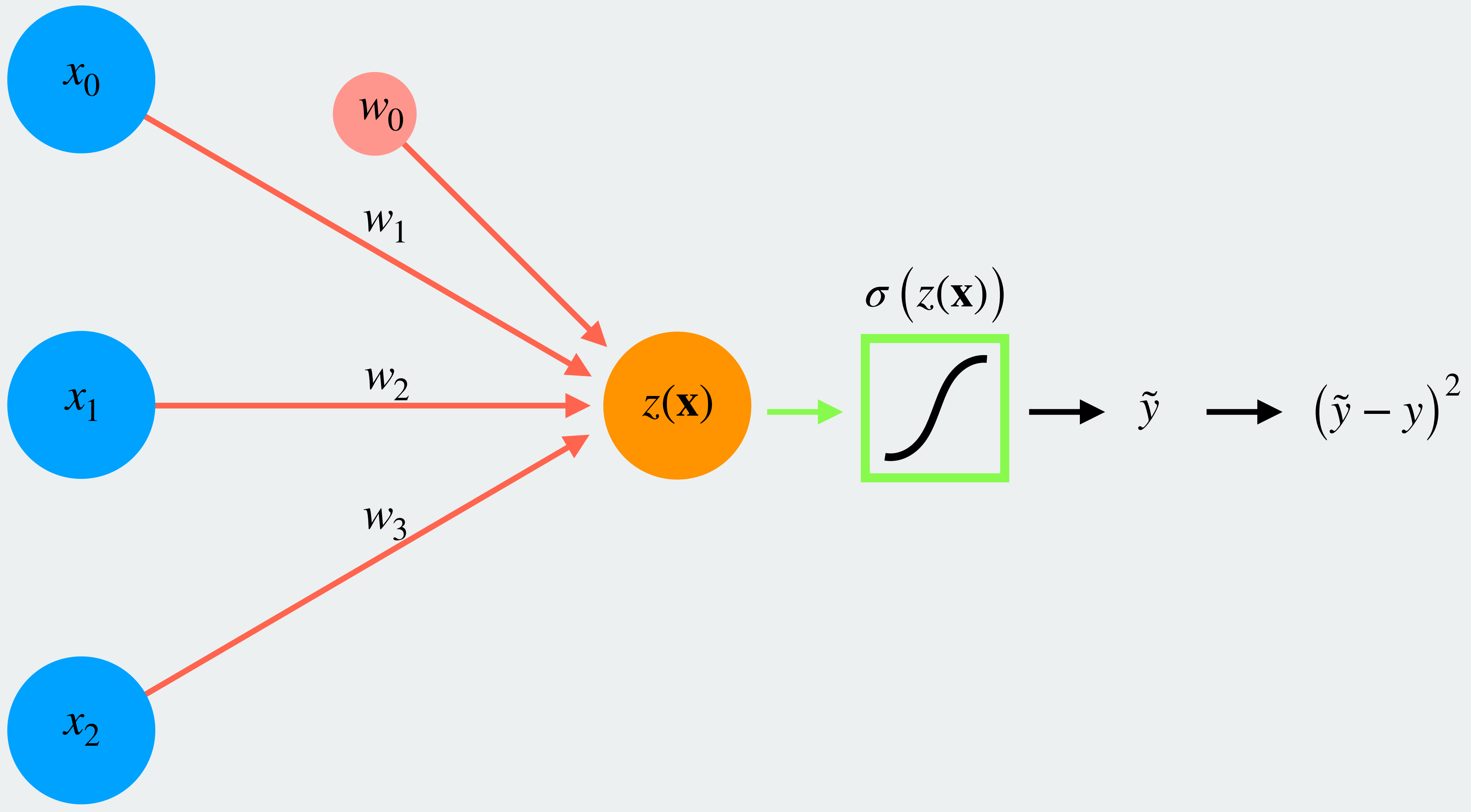

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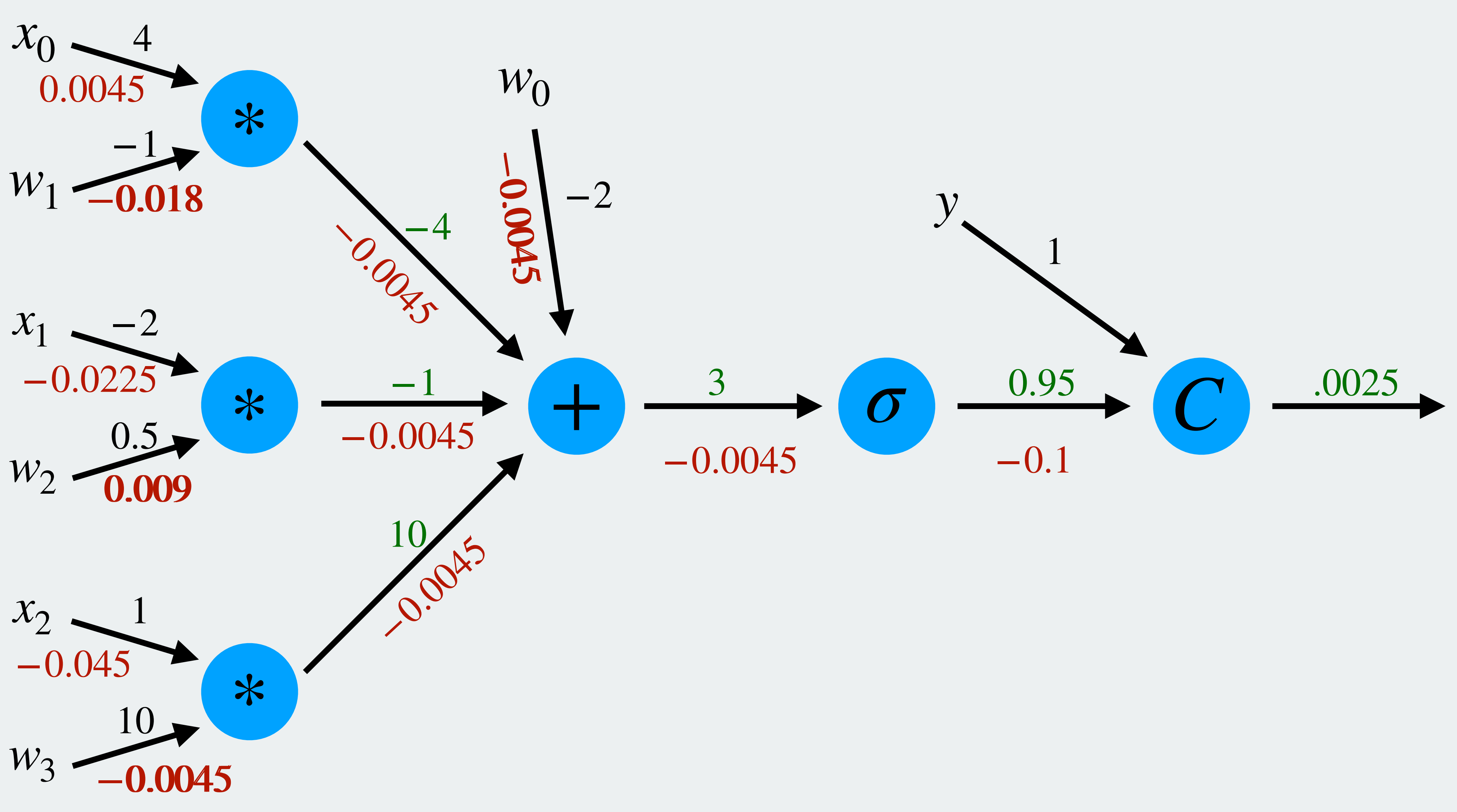

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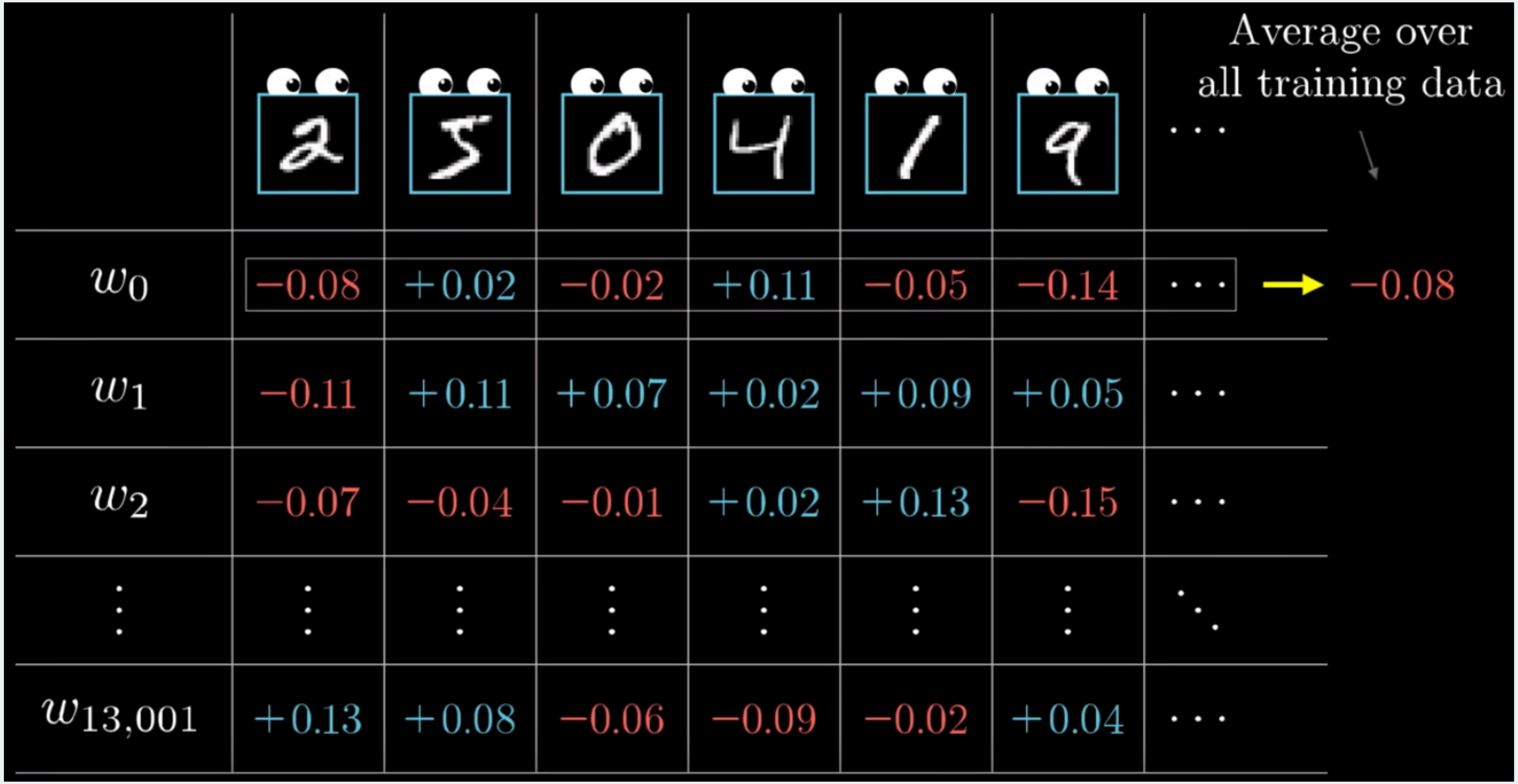
Backpropagation – on a neural network

> When **multiple** gradients come into a neuron you **add** them

Backpropagation – in the computer



	2	5	0	4	1	9	$\cdots$	Average over all training data
w_0	-0.08	$+0.02$	-0.02	$+0.11$	-0.05	-0.14	$\cdots$	$\rightarrow -0.08$
w_1	-0.11	$+0.11$	$+0.07$	$+0.02$	$+0.09$	$+0.05$	$\cdots$	
w_2	-0.07	-0.04	-0.01	$+0.02$	$+0.13$	-0.15	$\cdots$	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	
$w_{13,001}$	$+0.13$	$+0.08$	-0.06	-0.09	-0.02	$+0.04$	$\cdots$	

https://www.youtube.com/watch?v=Ilg3gGewQ5U

Regularization

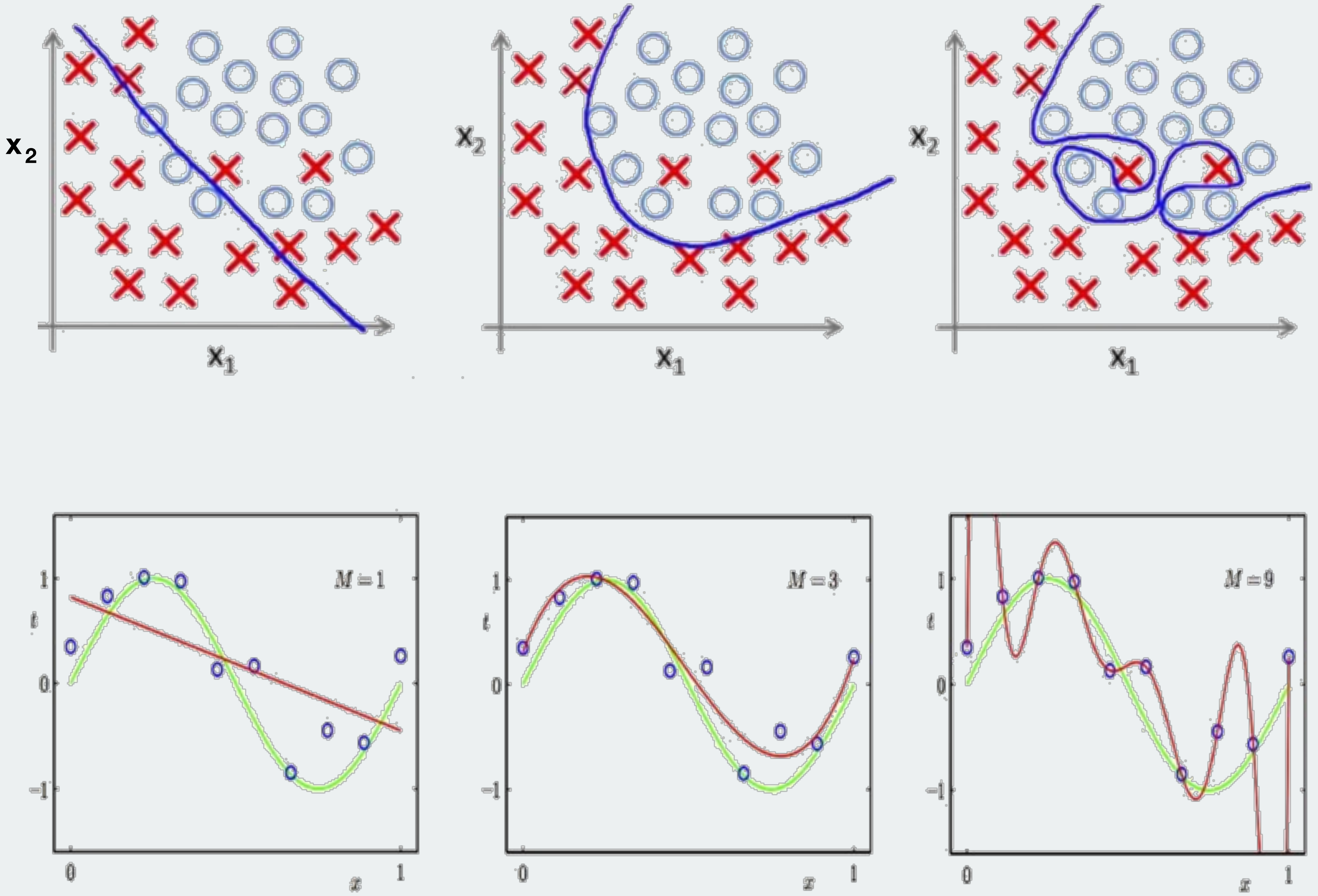
Tricks to avoid overfitting

Regularization – underfitting and overfitting

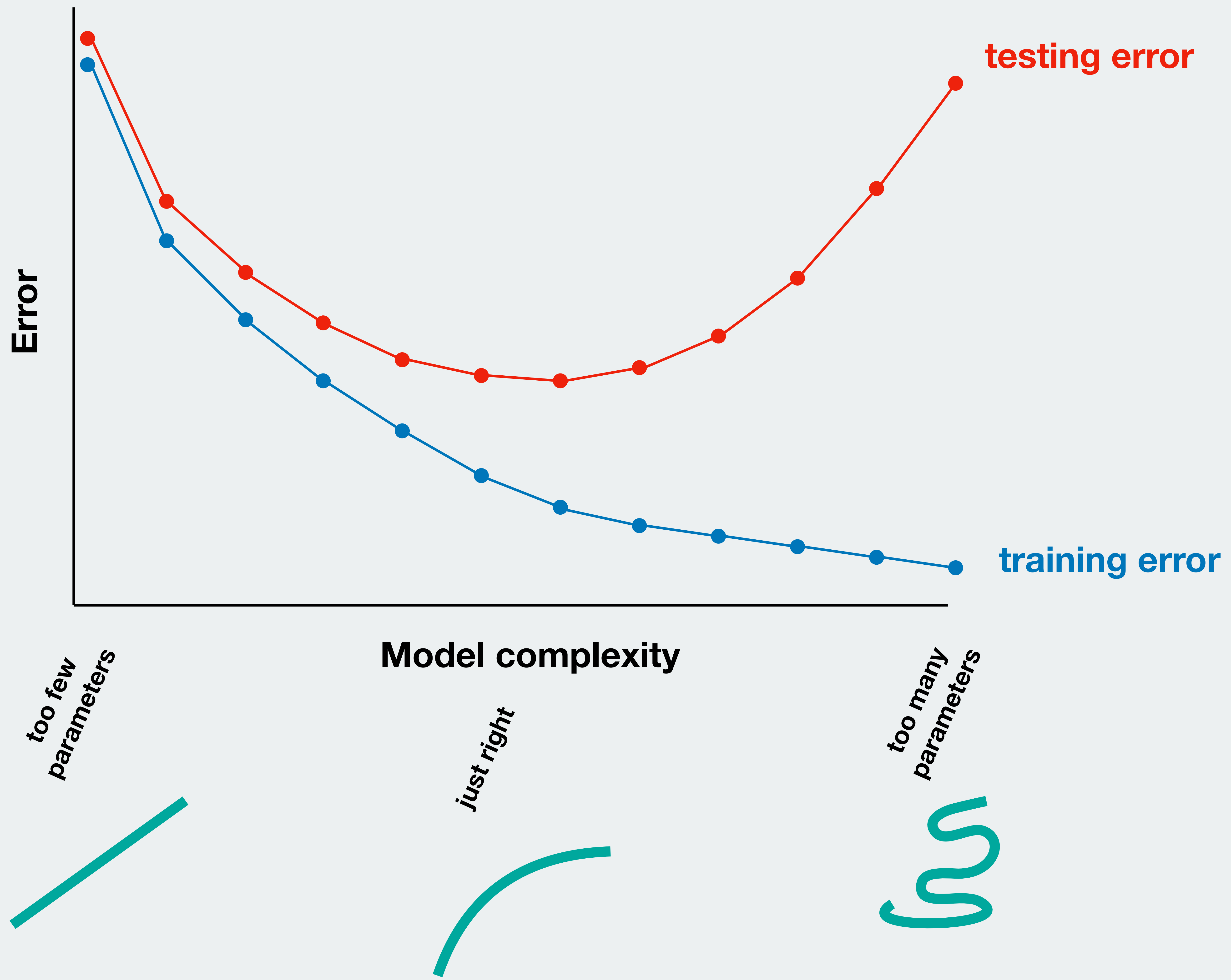
Underfitting **Overfitting**

Classification

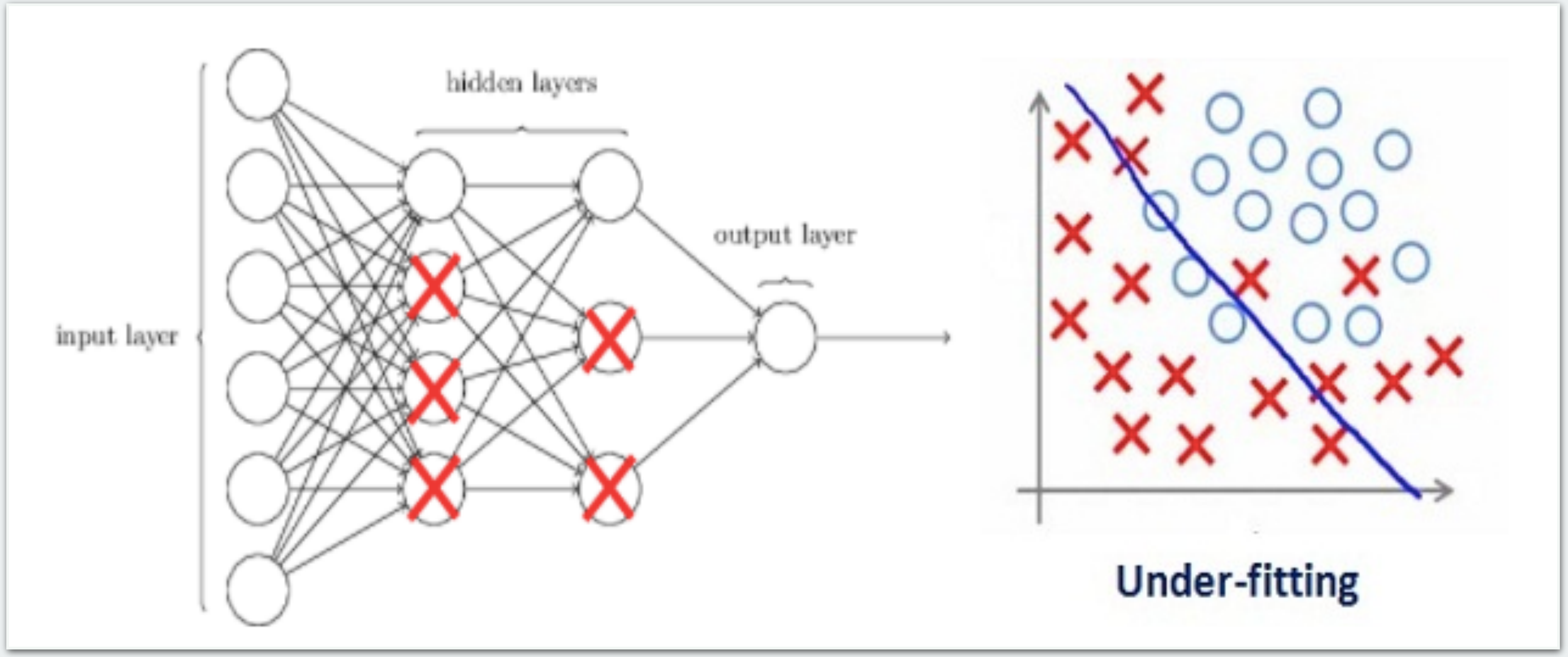
Regression



Regularization – underfitting and overfitting



Regularization – *how* does regularization reduce overfitting?



https://www.analyticsvidhya.com/blog/2018/04/fundamentals-deep-learning-regularization-techniques/

Regularization – Different techniques

L-norm regularization: “Introduce a cost for large weights”

$$C = Loss + Regularization\ term$$

Regularization – Different techniques

<u>L-norm regularization:</u> "Introduce a cost for large weights"

$$C = Loss + Regularization\ term$$

L1: $$C = Loss + \lambda \sum_{l=1}^{L} \|\mathbf{W_l}\|$$

L2: $$C = Loss + \lambda \sum_{l=1}^{L} \|\mathbf{W_l^2}\|$$

Regularization – Different techniques

L-norm regularization: "Introduce a cost for large weights"

$$C = Loss + Regularization\ term$$

L1: $$C = Loss + \lambda \sum_{l=1}^{L} \|\mathbf{W_l}\|$$

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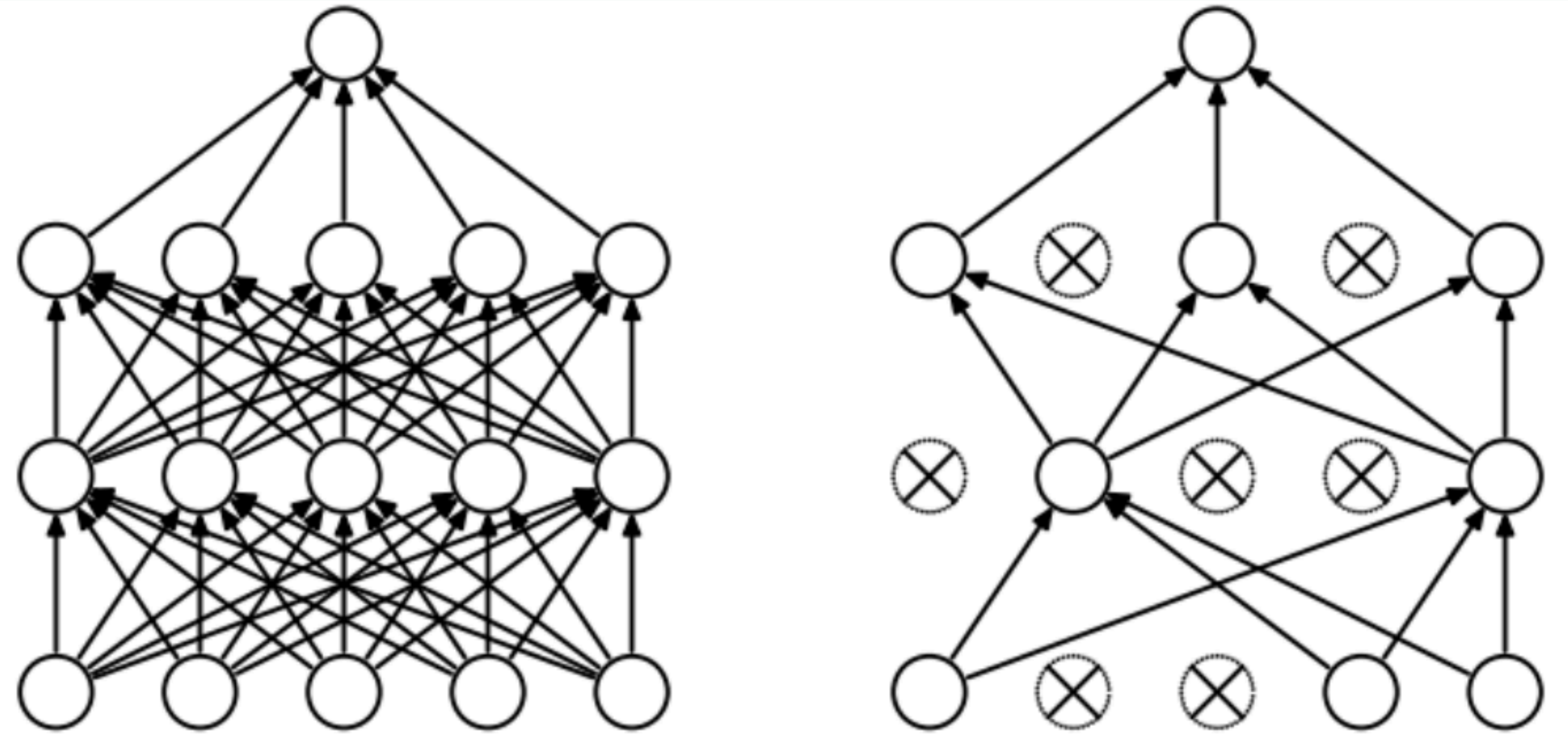
Dropout:

"In each SGD step, randomly ignore a fraction p of neurons"



(a) Standard Neural Net (b) After applying dropout.

Srivastava, Nitish, et al. "Dropout: a simple way to prevent neural networks from overfitting", JMLR 2014

- Can select p in wide range. Typical is 0.2 – 0.8, dependent on size of ANN
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Regularization – Different techniques

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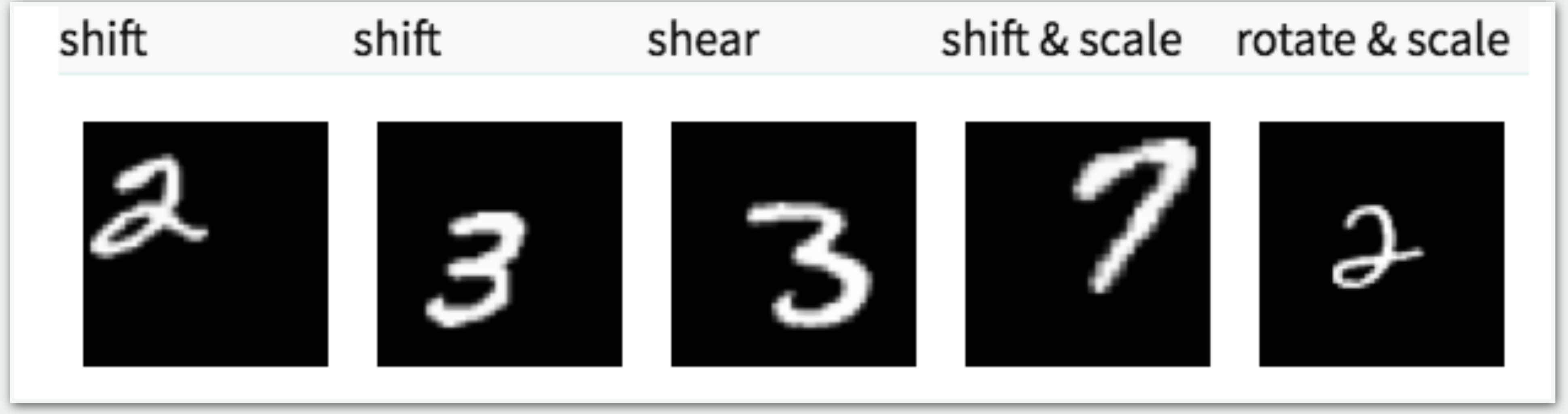
"Shear, shift, scale and/or rotate input data"



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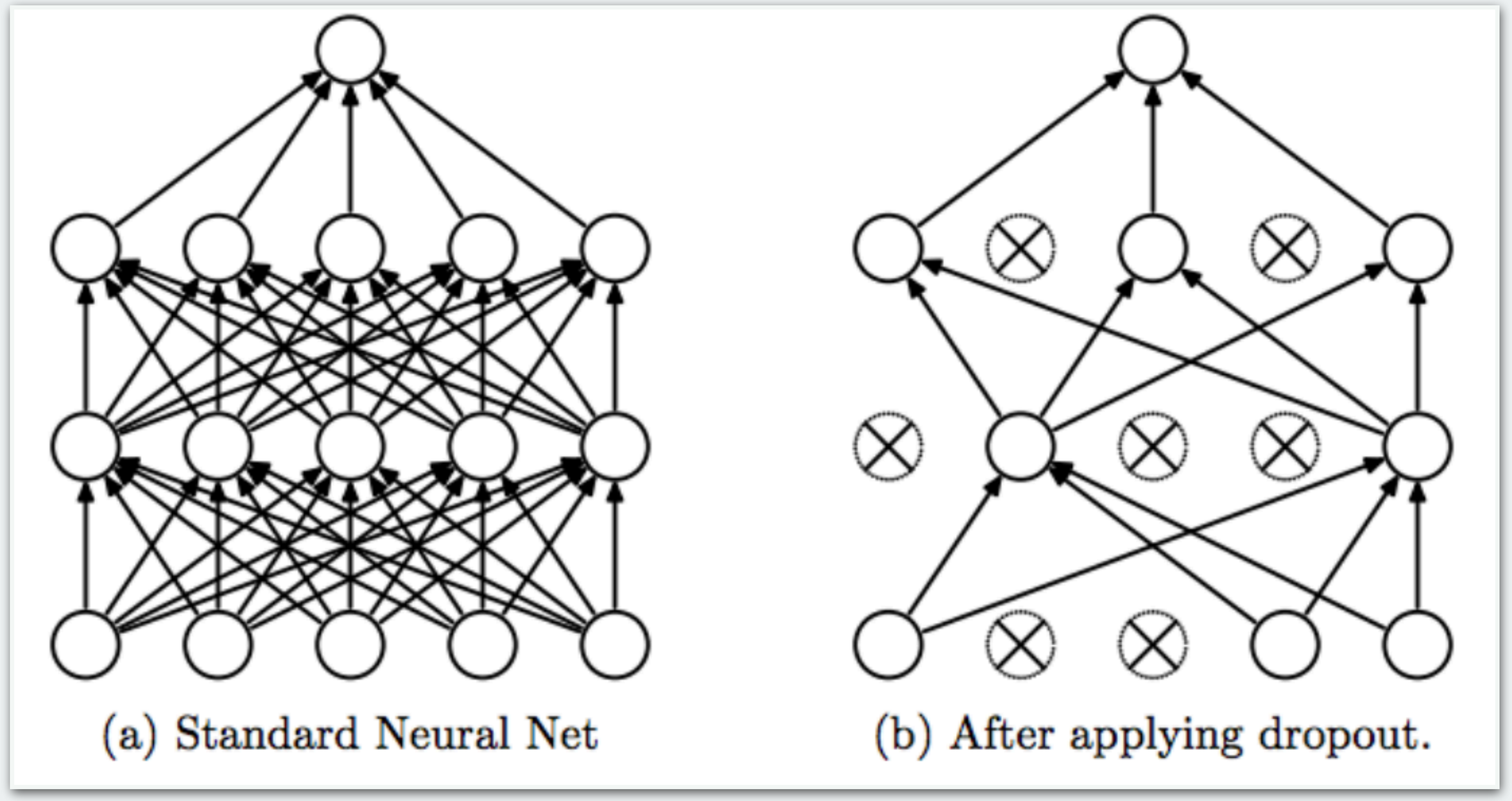

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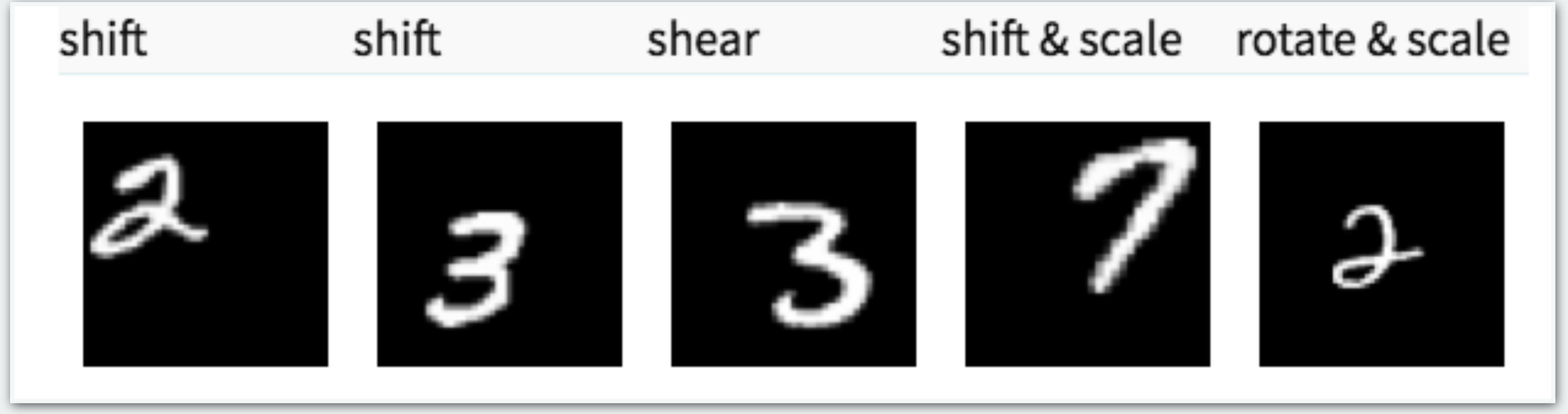
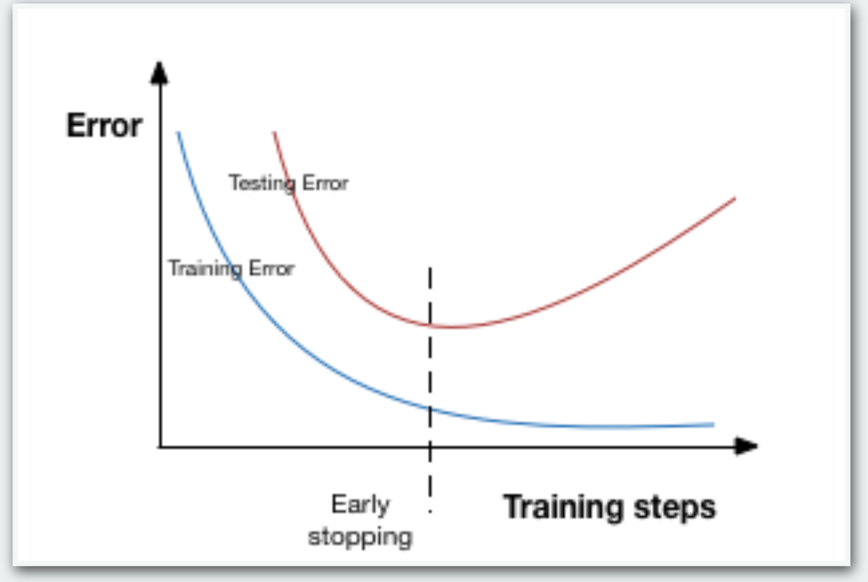


Early stopping

"Stop training when performance on validation dataset starts worsening"



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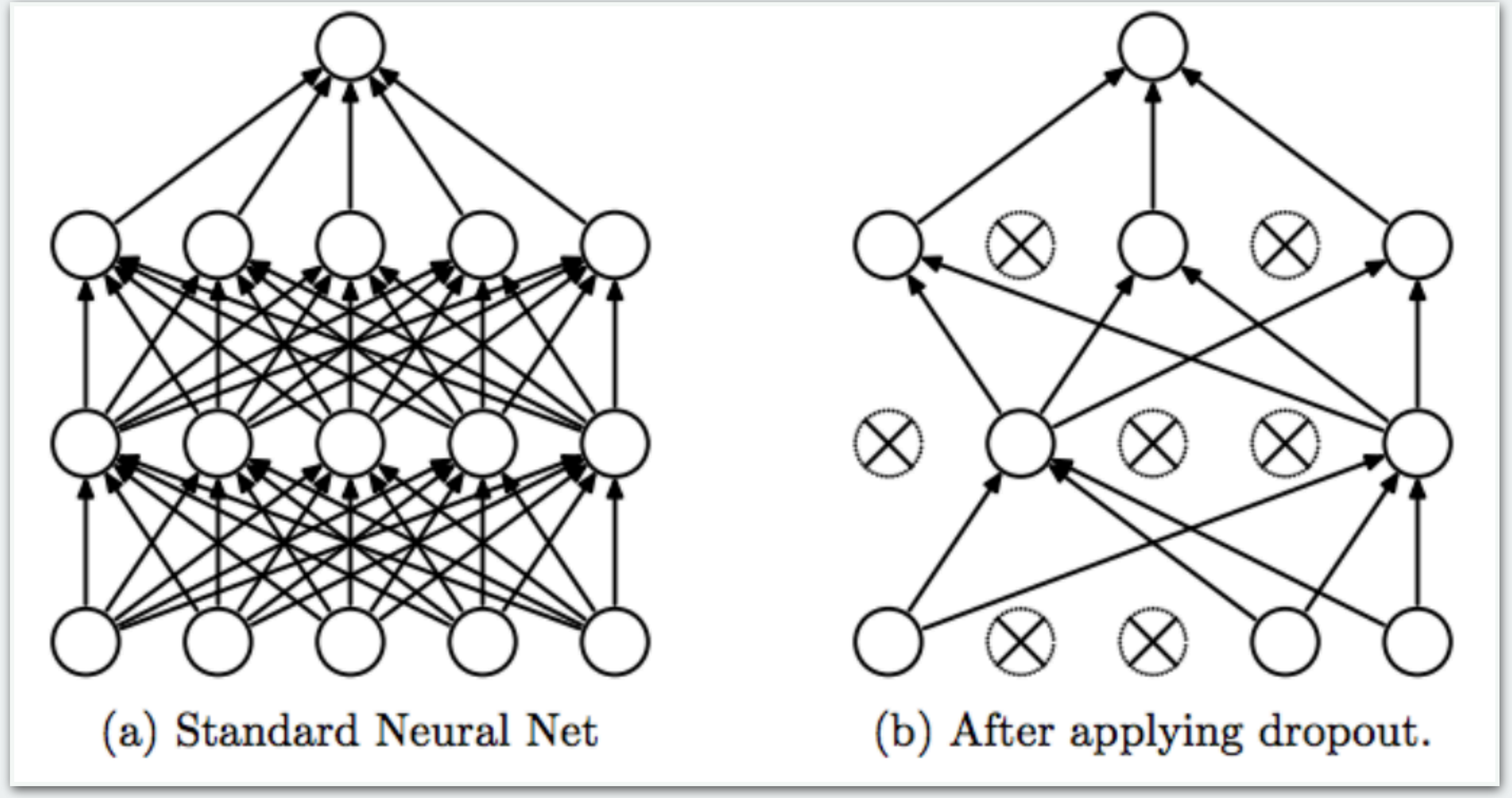

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A quick word on:

The Vanishing Gradient Problem

Vanishing gradients – A problem in *deep* neural nets

Problem:

- Gradients closer and closer to the input tend to get smaller and smaller
- Leads to smaller weight updates near input and larger weight updates near output
- Bad because layers near input take part in recognizing “simple” patterns, which are important to learning

$$\frac{\partial C}{\partial b_1} = \sigma'(z_1) \times w_2 \times \sigma'(z_2) \times w_3 \times \sigma'(z_3) \times w_4 \times \sigma'(z_4) \times \frac{\partial C}{\partial a_4}$$

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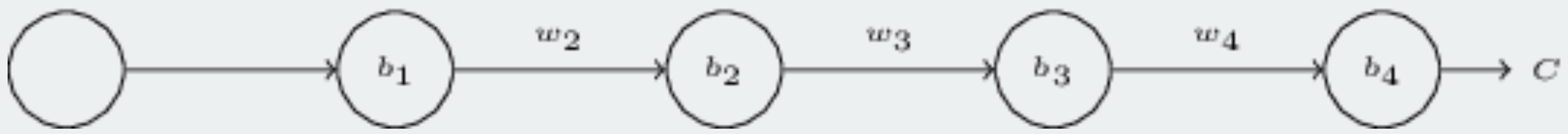

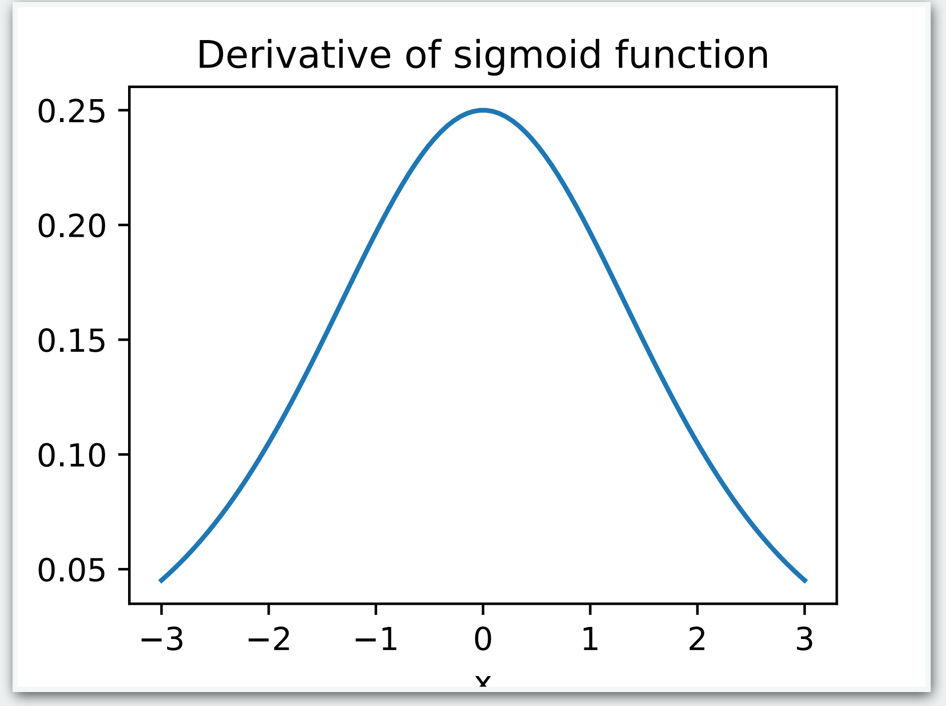

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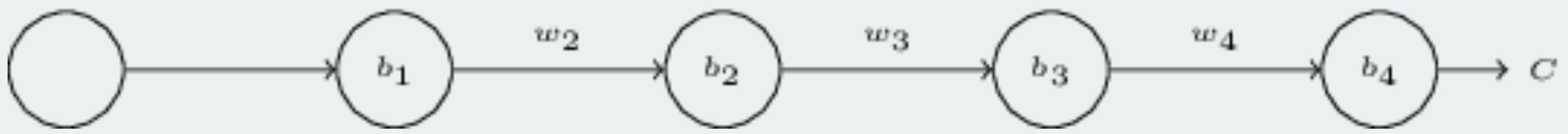

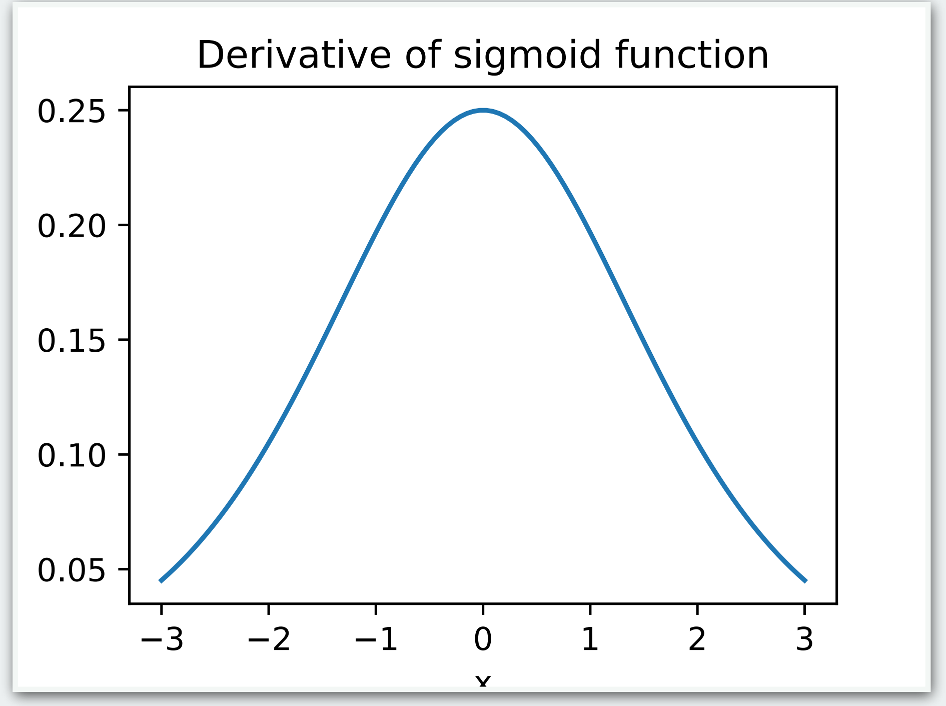

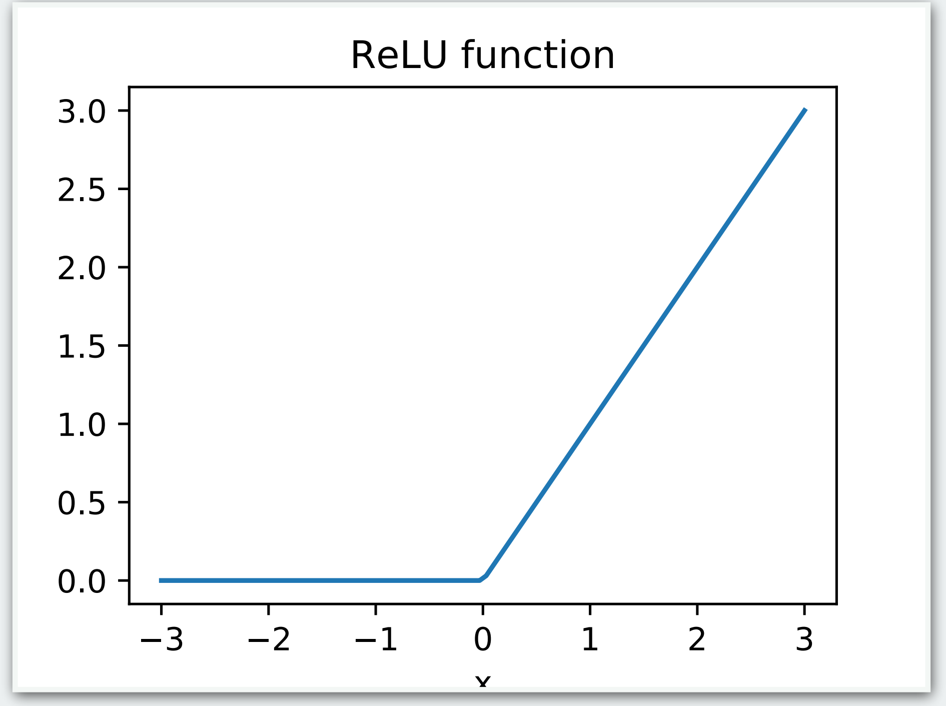

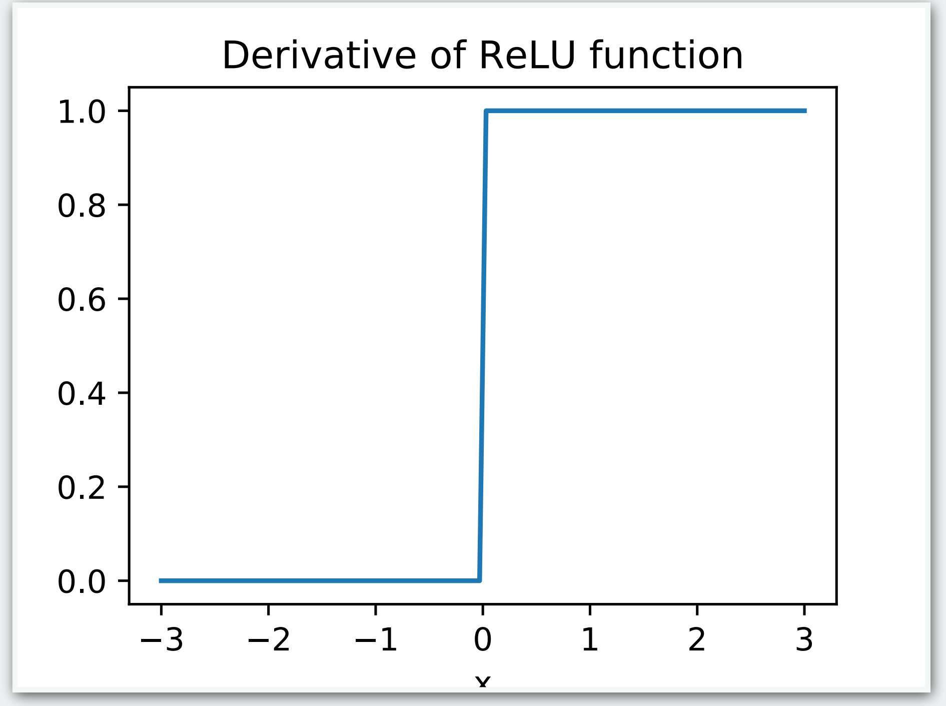

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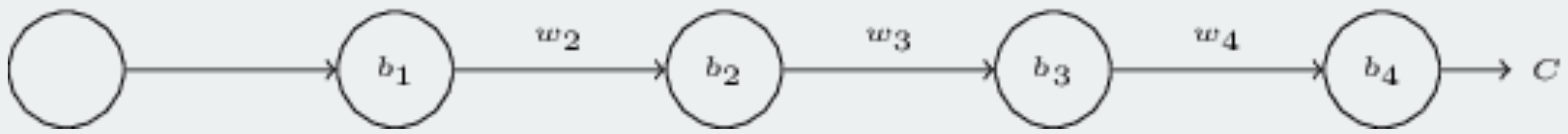

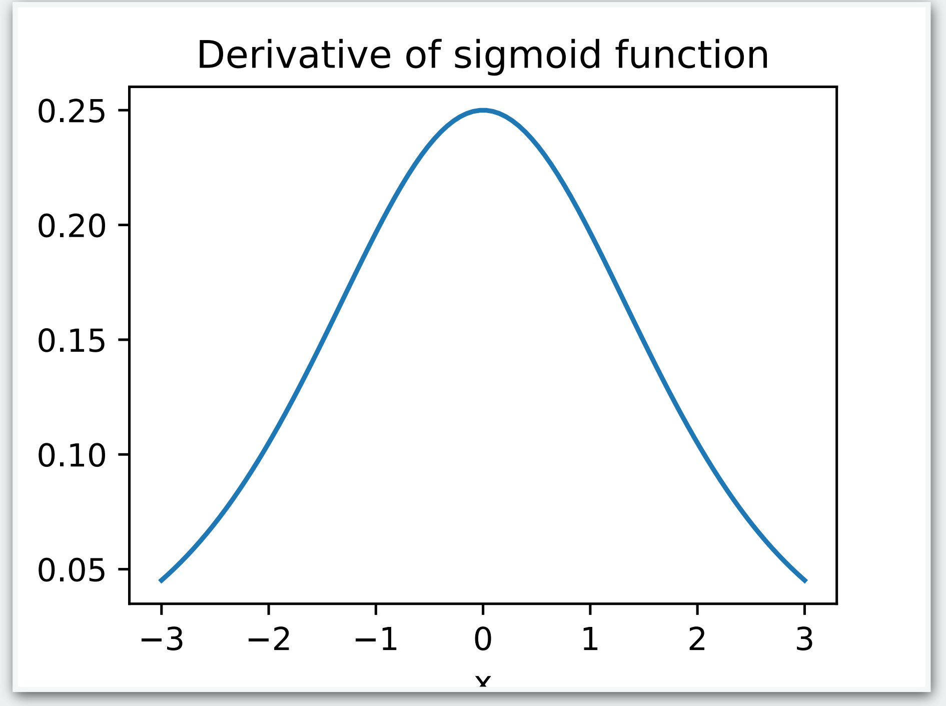

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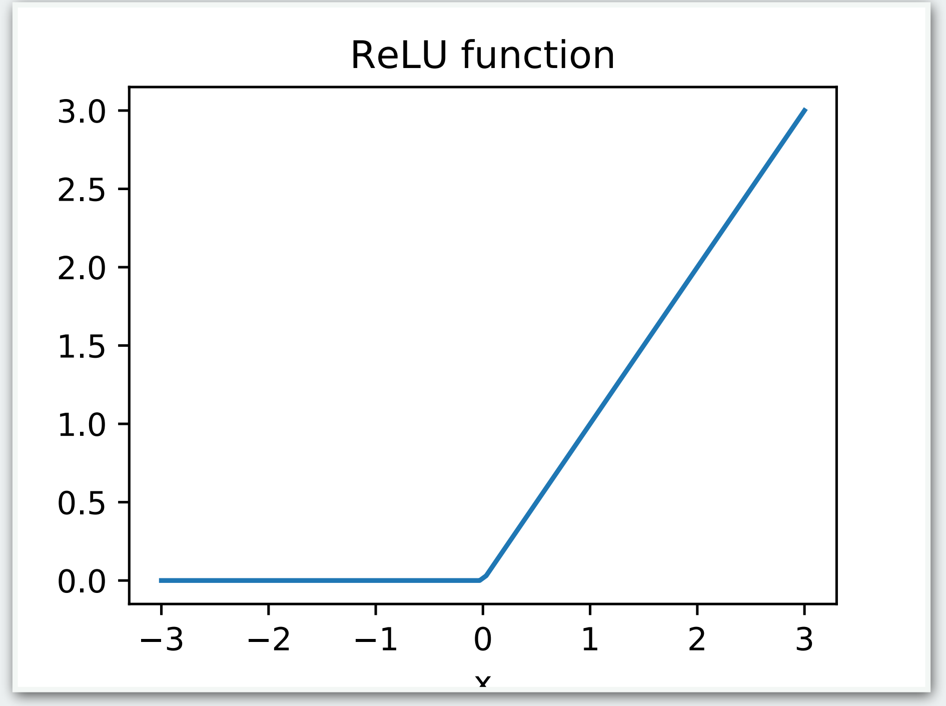

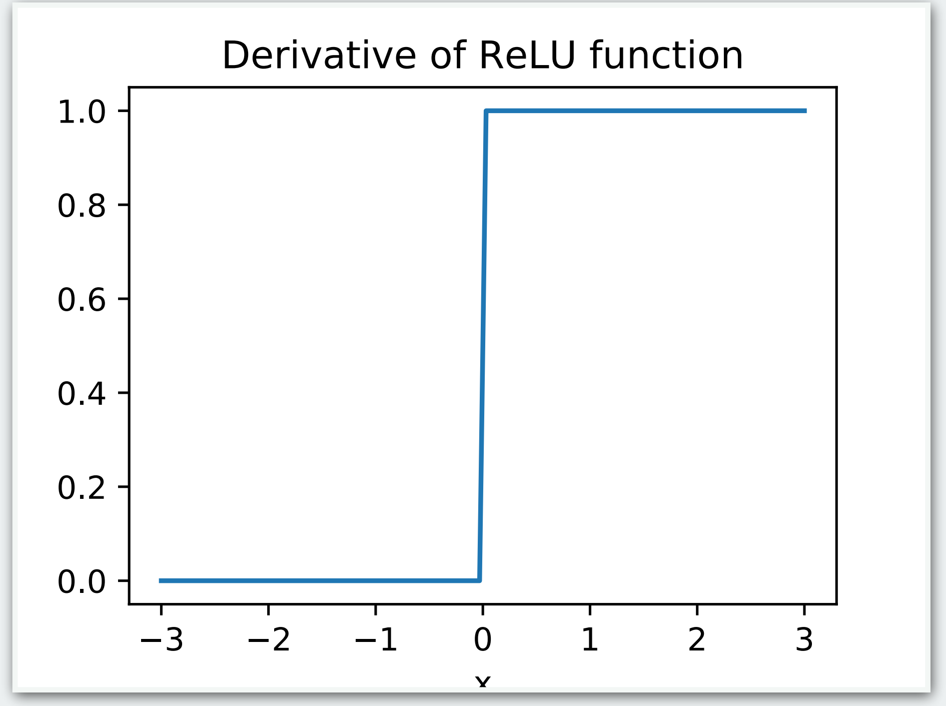

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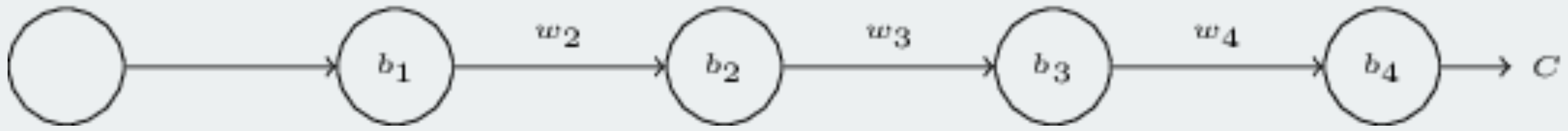

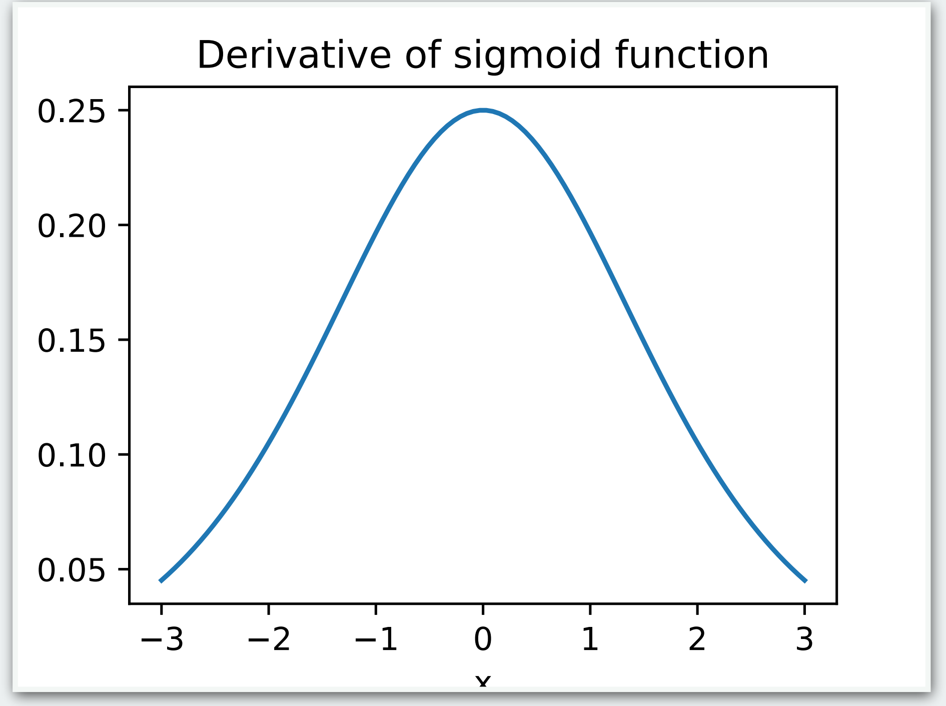

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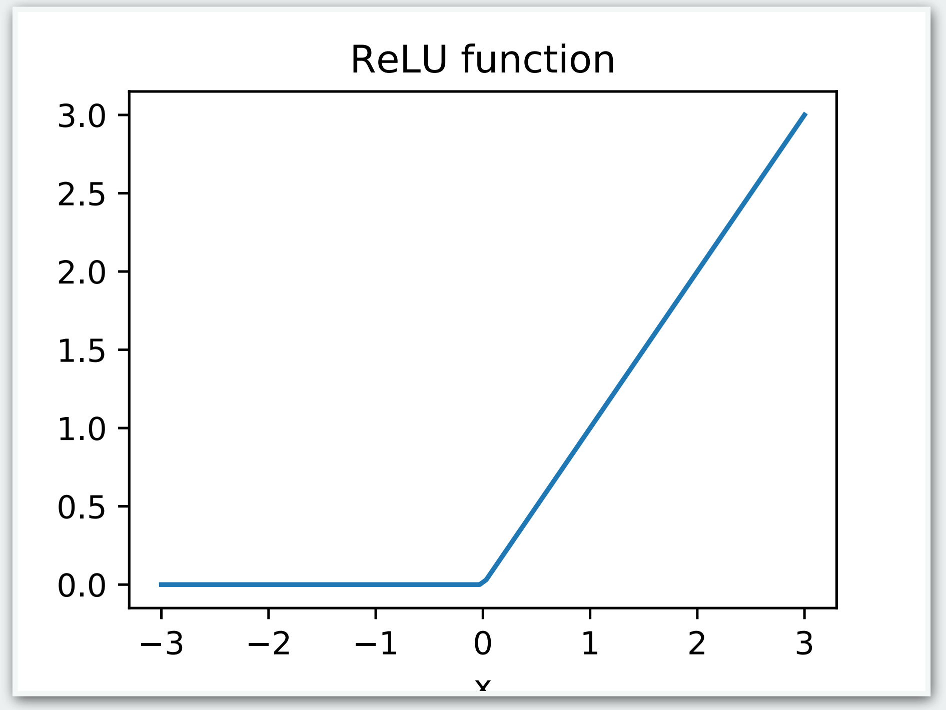

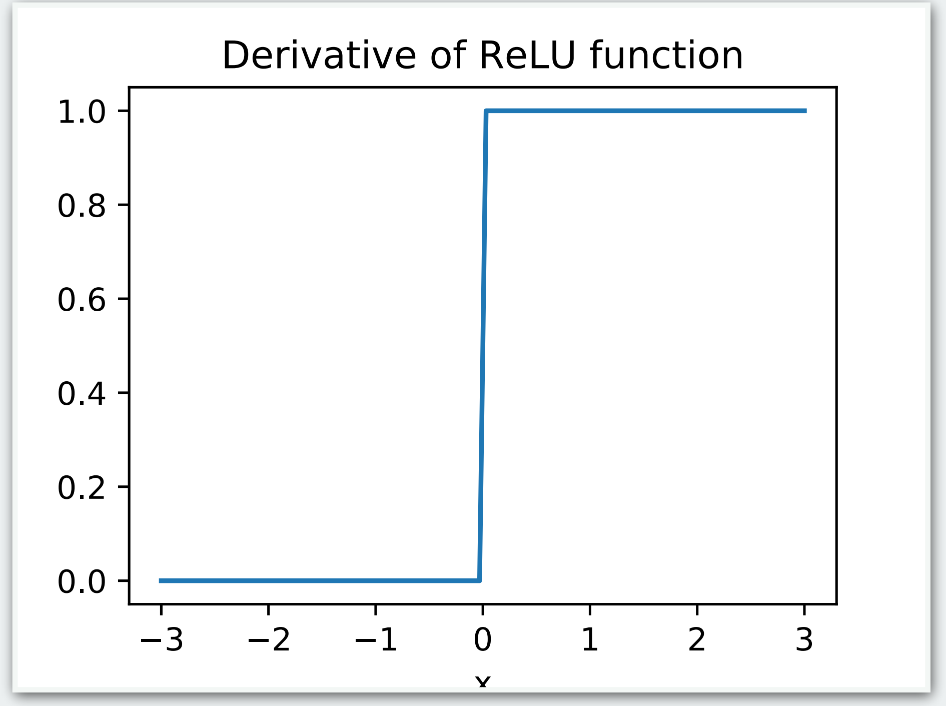

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