NEURAL NETWORKS

AND DEEP LEARNING

MICHELLE KUCHERA
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VECC
18 DECEMBER 2024

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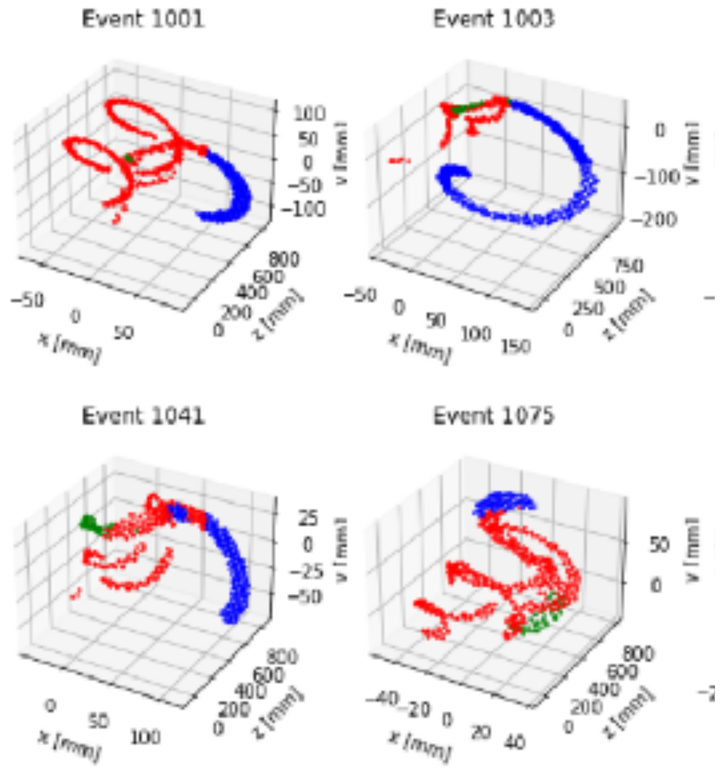
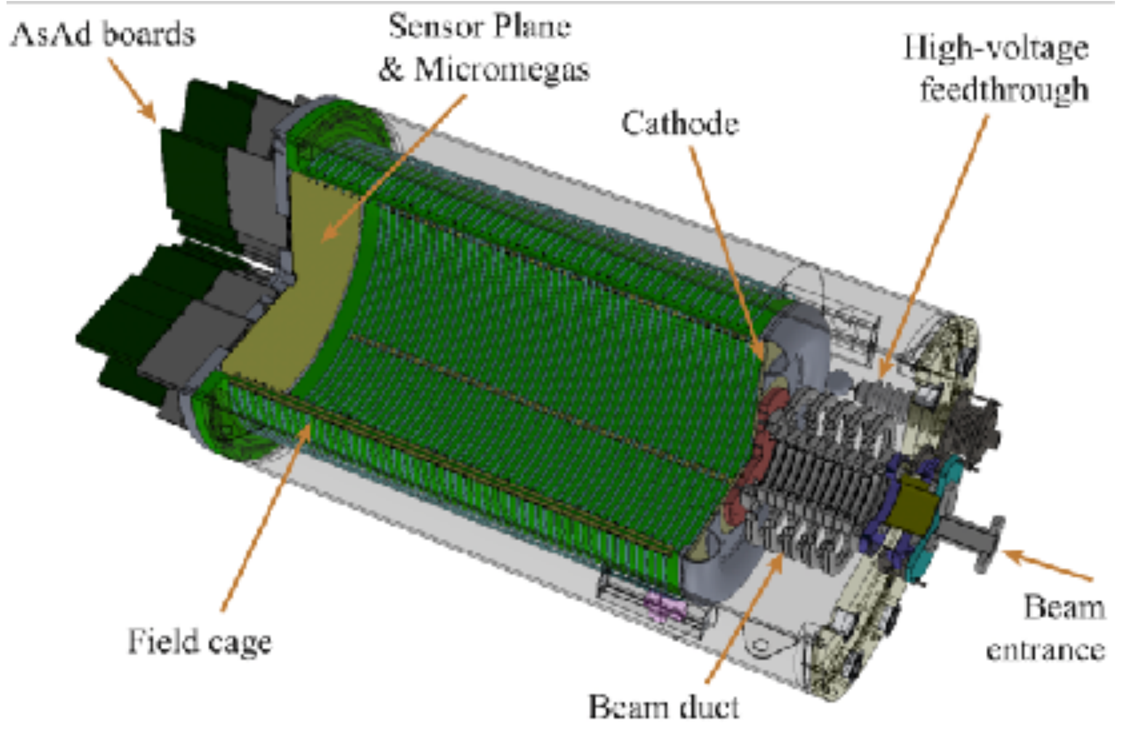
B.S., M.S. PHYSICS
M.S., PH.D. COMPUTATIONAL SCIENCE

ALPhA
DAVIDSON COLLEGE

IAEA
International Atomic Energy Agency





CERN

CMS
Compact Muon Solenoid

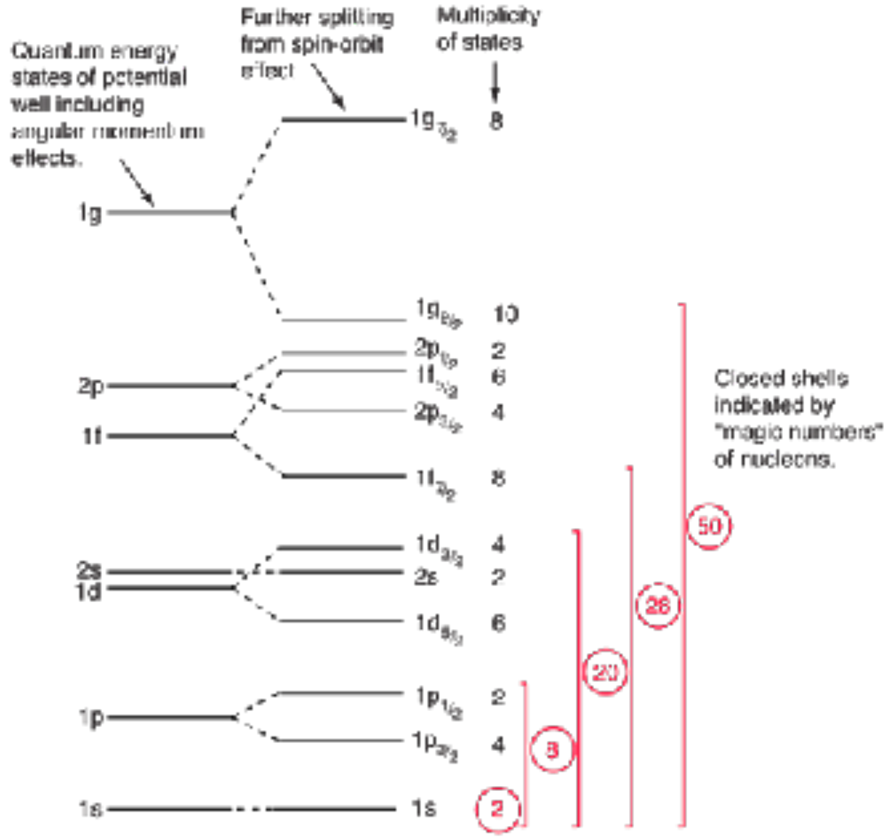
Jefferson Lab

FRIB

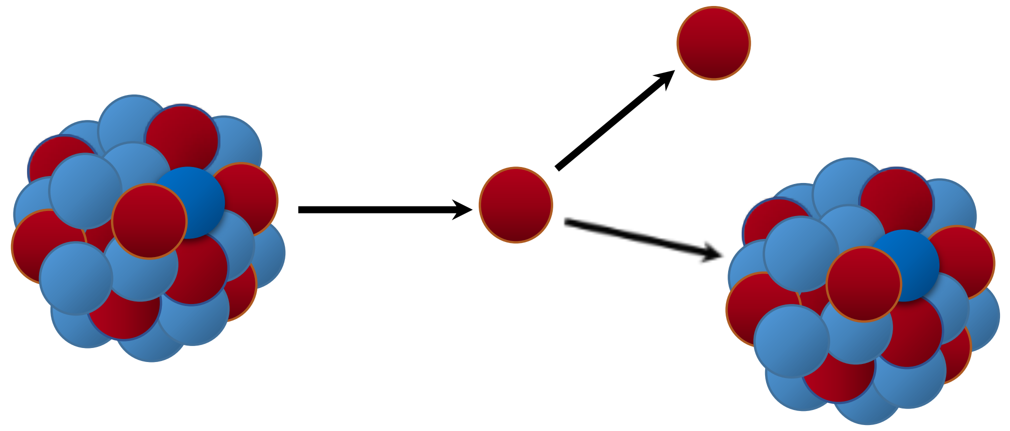
DAVIDSON

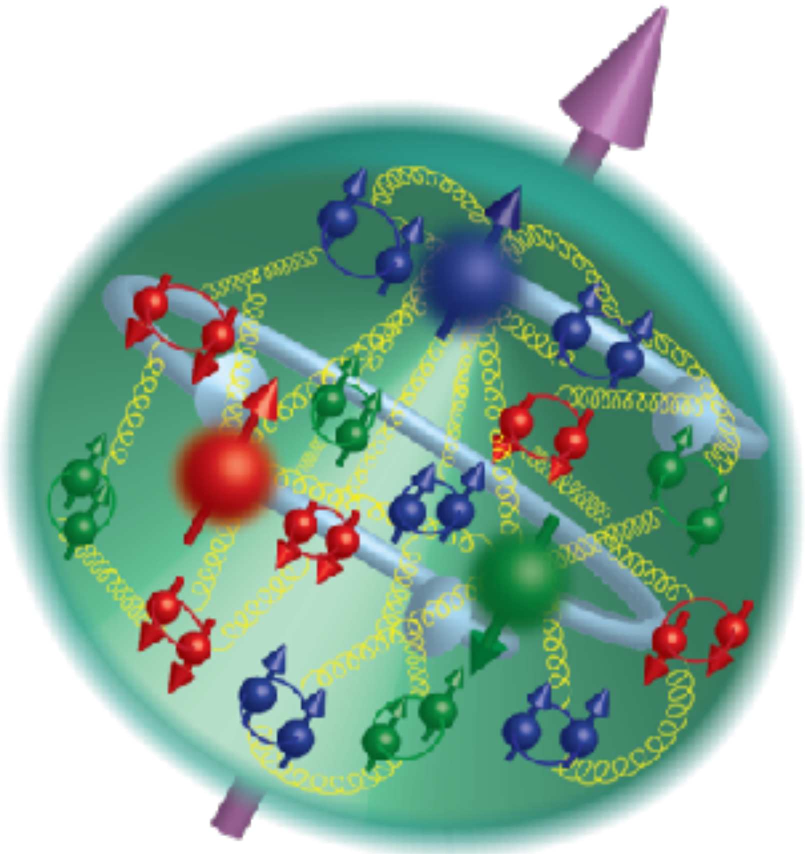
NSCL

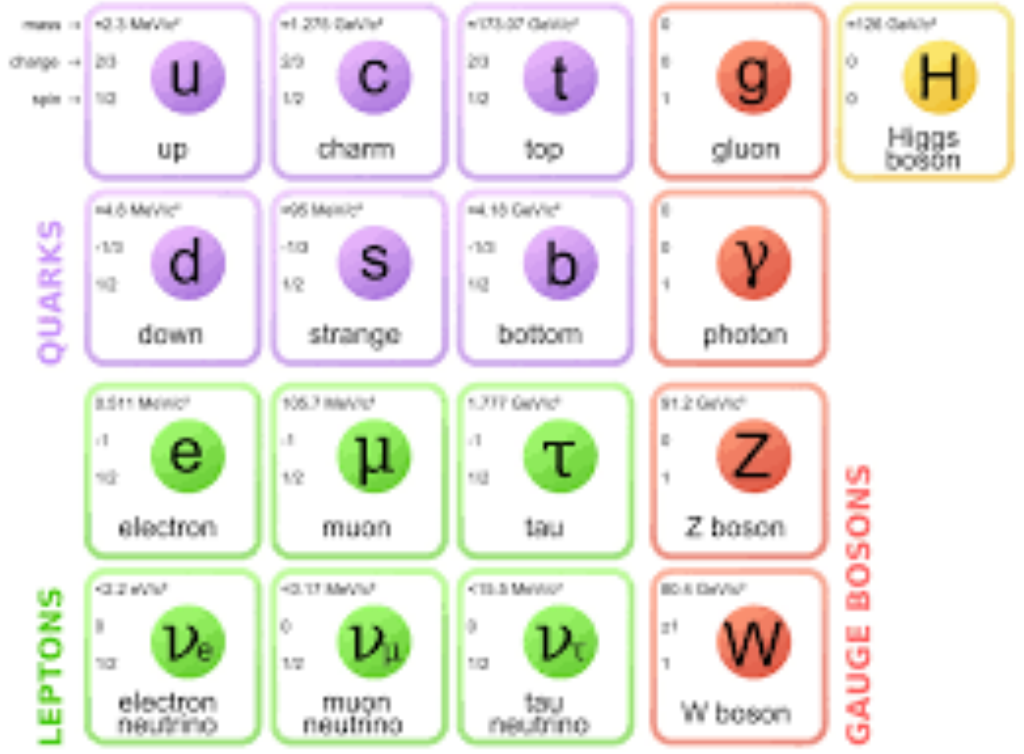
PhD: GPUs for Bayesian Neural Networks (😟)



Quantum energy states of potential well including angular momentum effects.
Further splitting from spin-orbit effect
Multiplicity of states
Closed shells indicated by "magic numbers" of nucleons.
1g
2p
1f
2s
1d
1p
1s
2
8
20
28
50

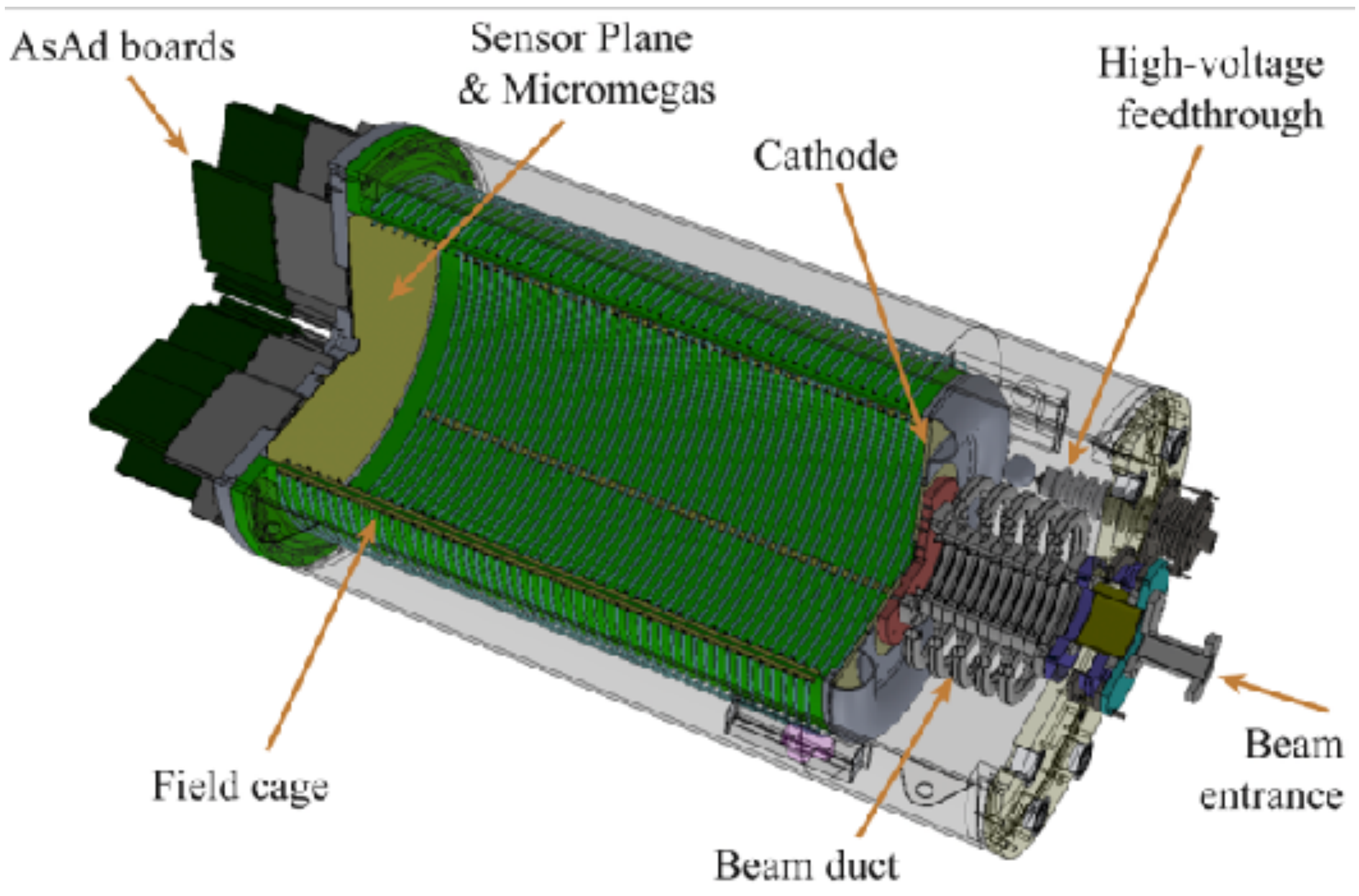




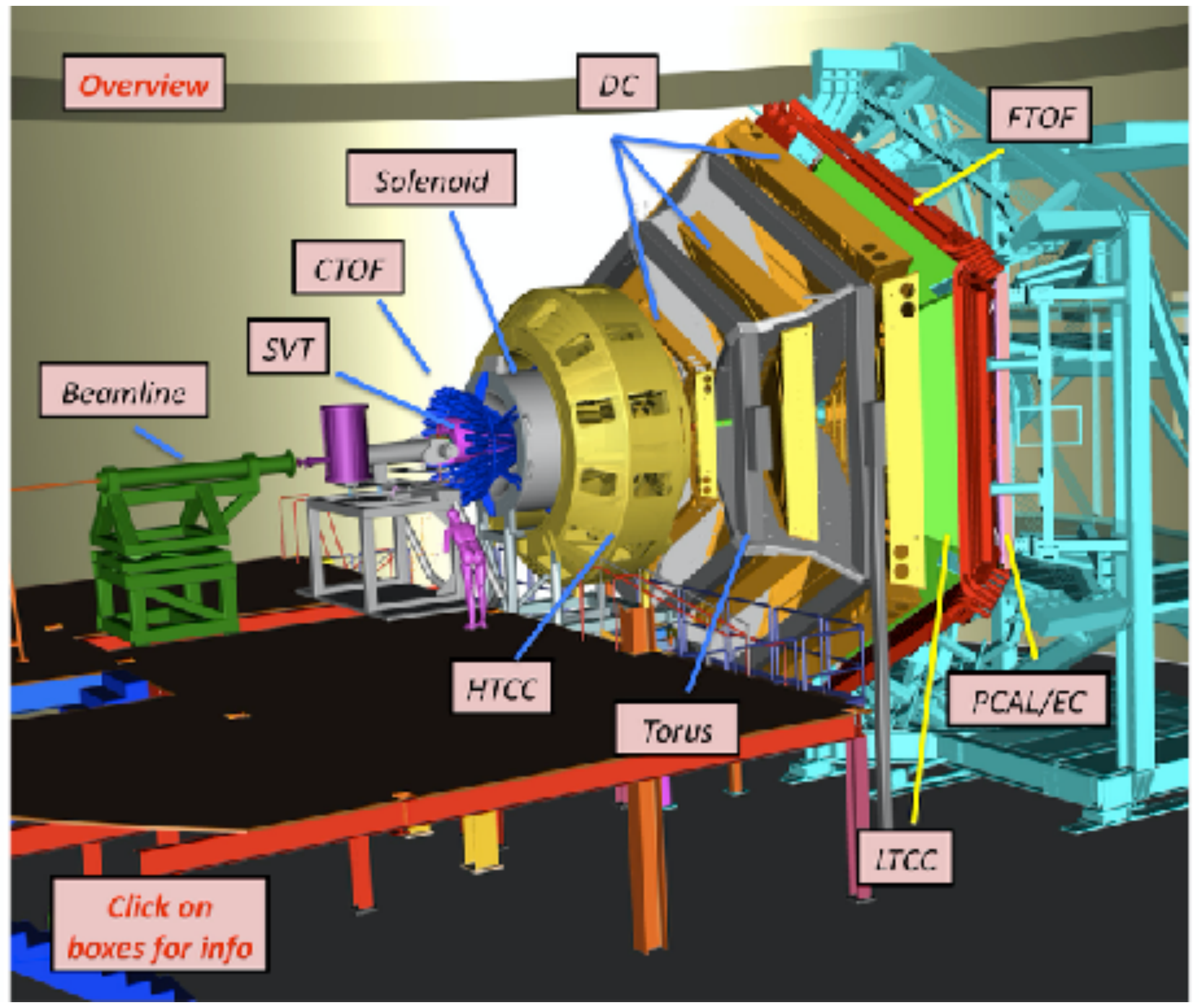


QUARKS
LEPTONS
GAUGE BOSONS
u
up
c
charm
t
top
g
gluon
H
Higgs boson
d
down
s
strange
b
bottom
γ
photon
e
electron
μ
muon
τ
tau
Z
Z boson
ν_e
electron neutrino
ν_μ
muon neutrino
ν_τ
tau neutrino
W
W boson

EXPERIMENTAL DATA



J. BRADT ET. AL., *NUCLEAR INSTRUMENTS AND METHODS*, 2017.



FRIB

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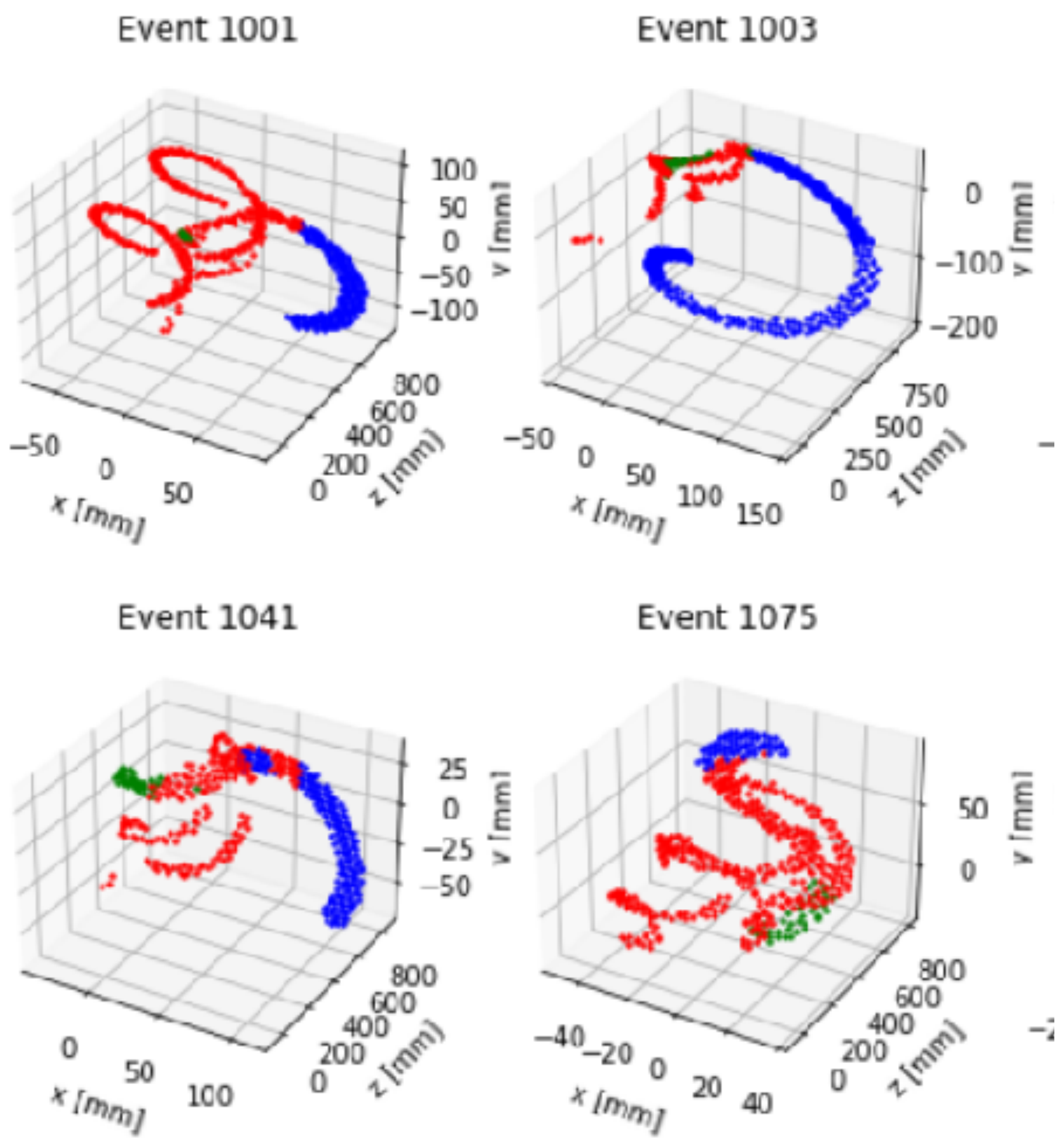
CLAS 12

CERN

CMS

EXPERIMENTAL DATA



FRIB

AT-TPC

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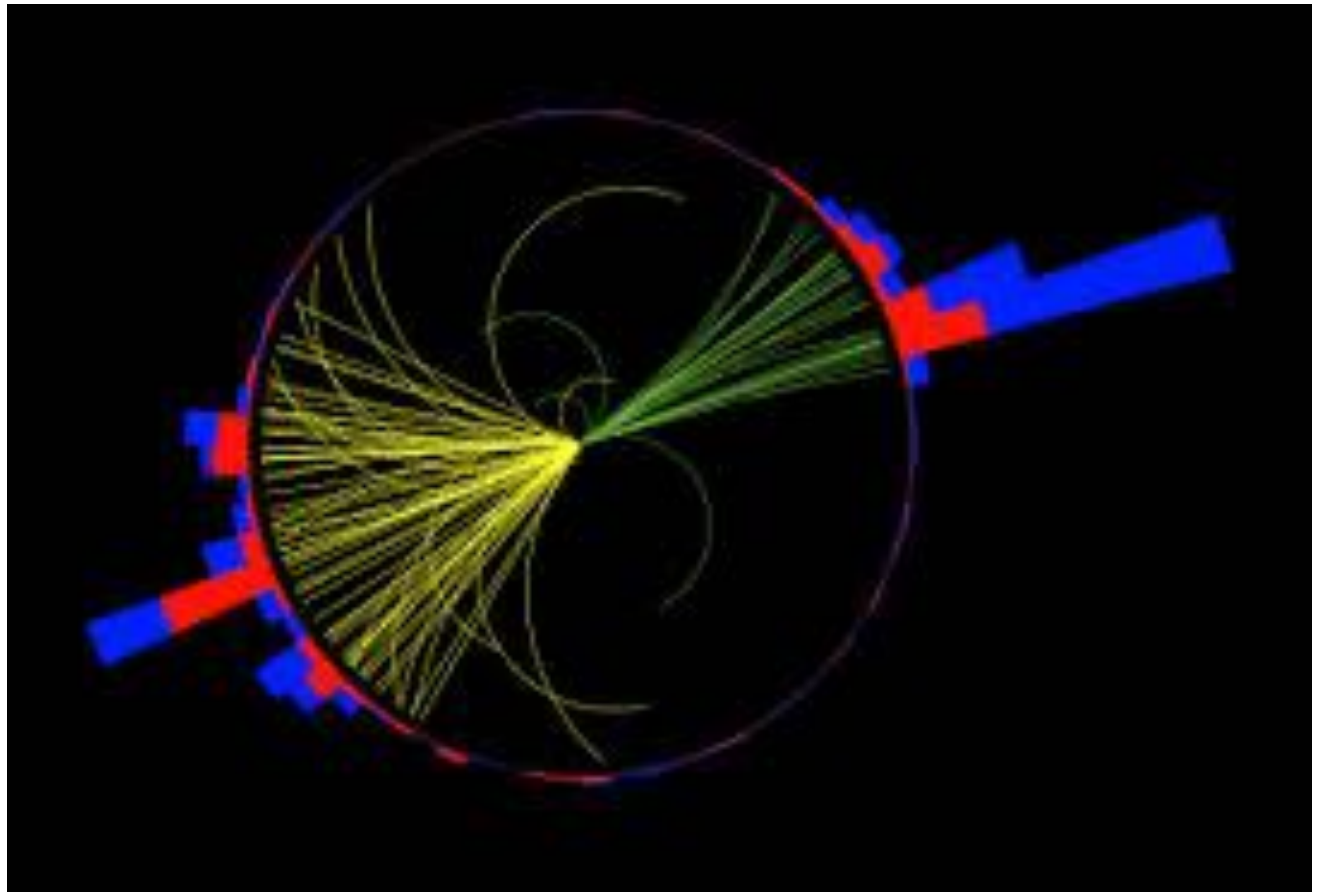
CLAS 12



CERN

CMS

LECTURE 1 TOPICS

- Computational graphs
- Gradient-descent optimization
- Logistic regression
- Regression neural networks

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GOALS

- Each of us learns something today
- Stop me with any questions

MICHELLE KUCHERA
DAVIDSON COLLEGE

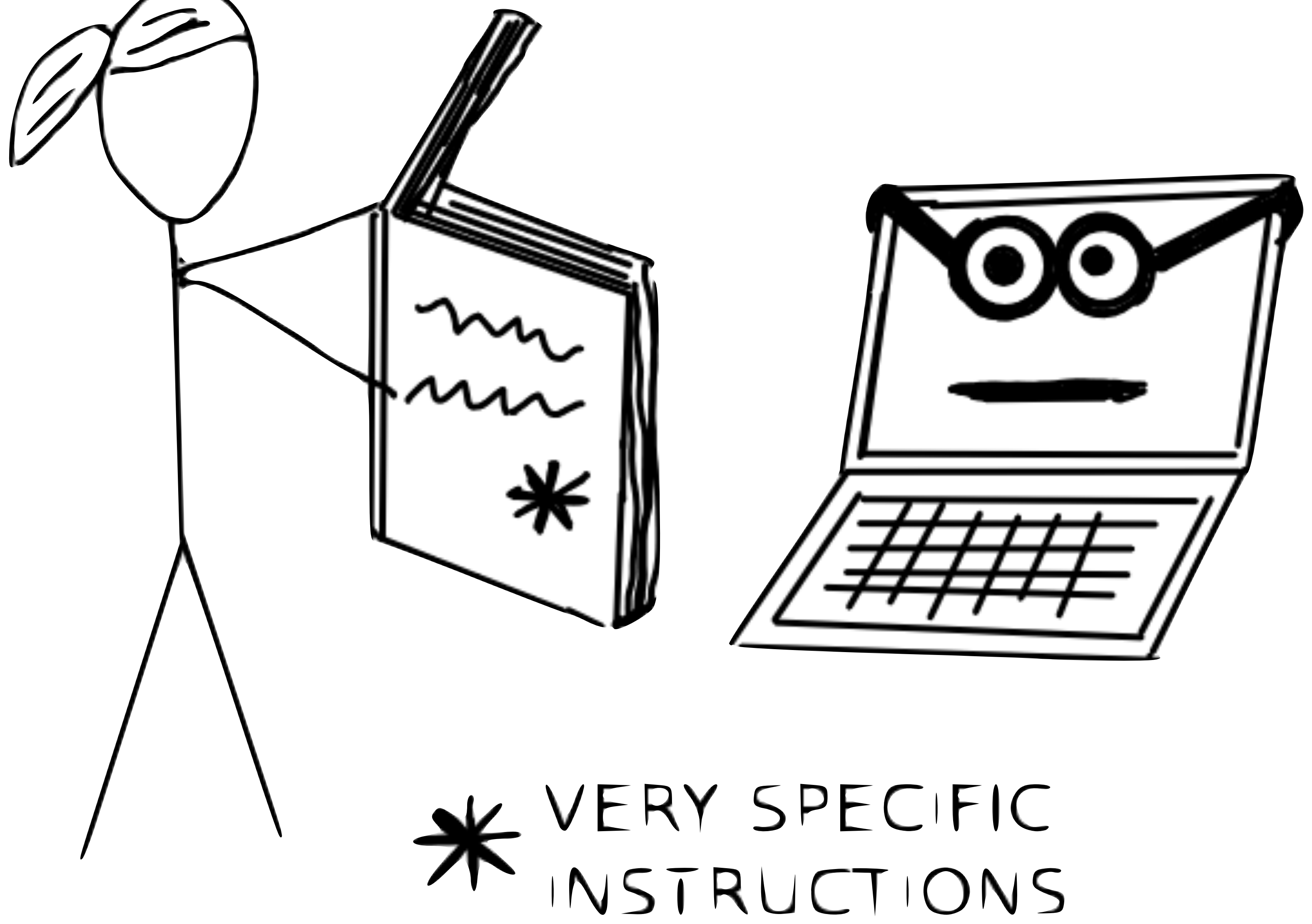
COMMUNITY

- Each of you arrived here with your own backgrounds, specialty, and path in life
- Your experience and expertise are valuable here, no matter what it is
- If the activity is within your background, help others!
- If you are totally (or a little) lost, ask for help!
- It is our shared goal to have **each** of us leave with some new skill/knowledge/understanding

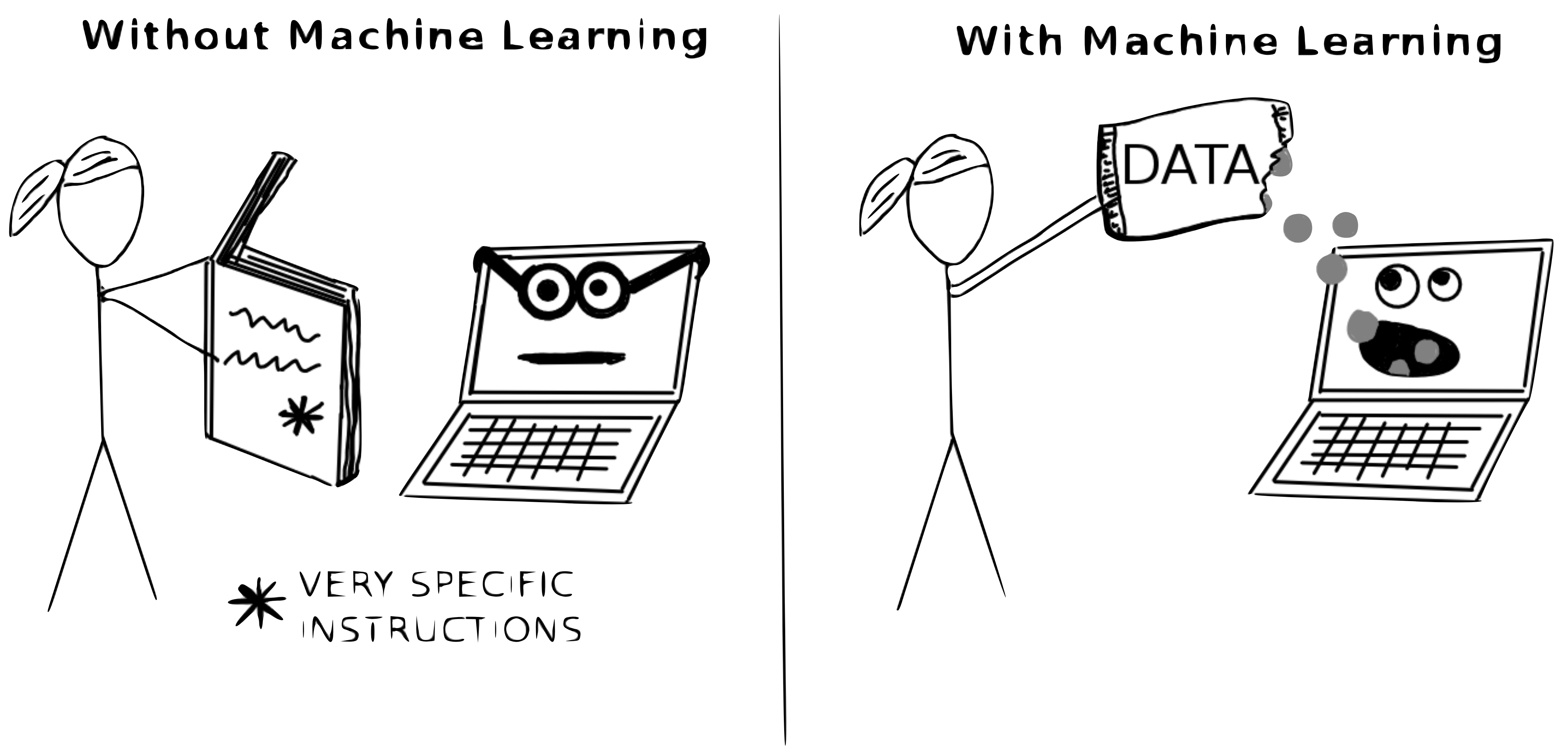
MACHINE LEARNING:

LEARNING FROM DATA

Without Machine Learning



With Machine Learning


Without Machine Learning
* VERY SPECIFIC INSTRUCTIONS
With Machine Learning
DATA

Without Machine Learning

With Machine Learning

Learning from data was a **paradigm shift** in thinking about predictive models

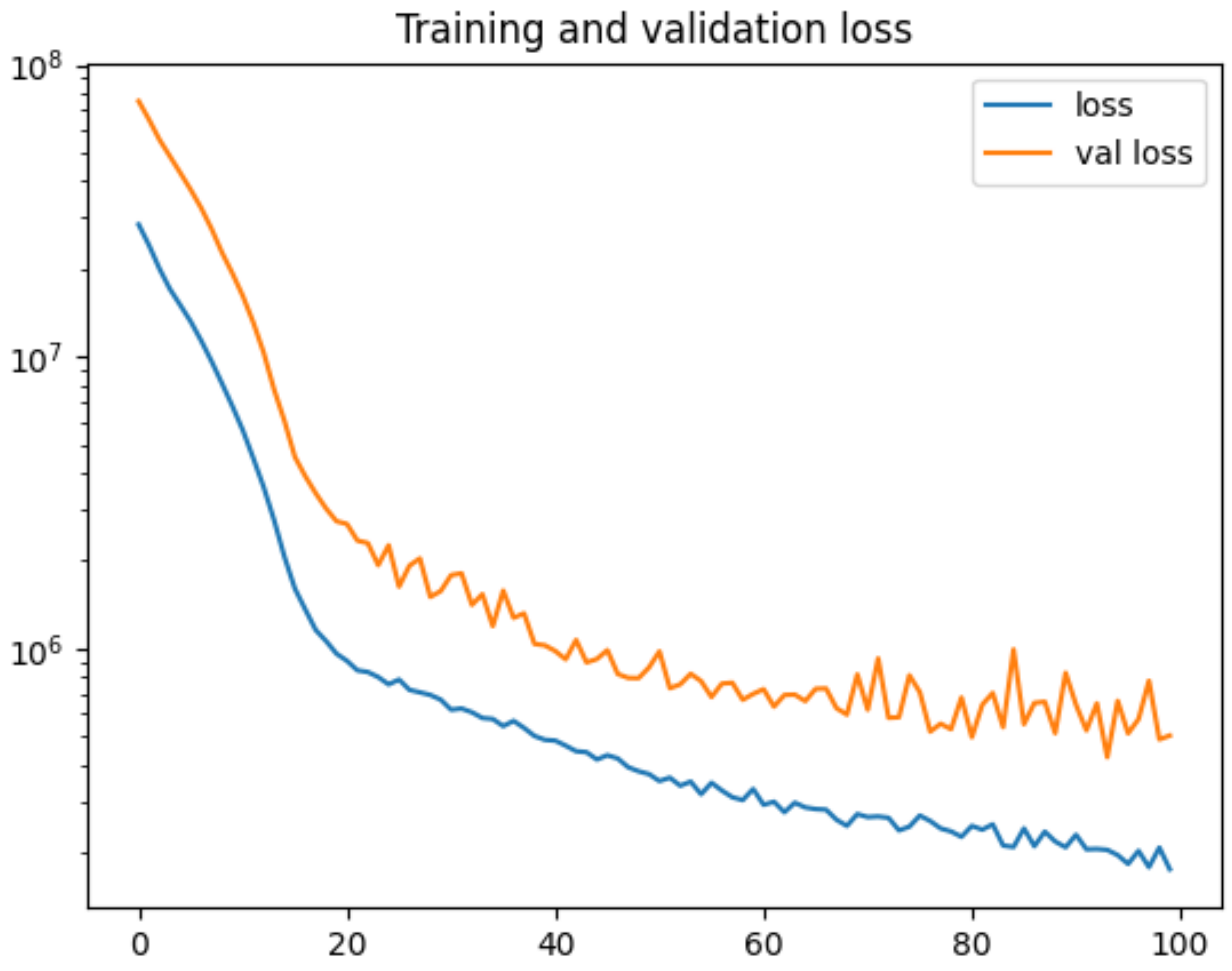
VERY SPECIFIC INSTRUCTIONS

Without Machine Learning

With Machine Learning

Learning from data was a **paradigm shift** in thinking about predictive models

✱ VERY SPECIFIC INSTRUCTIONS

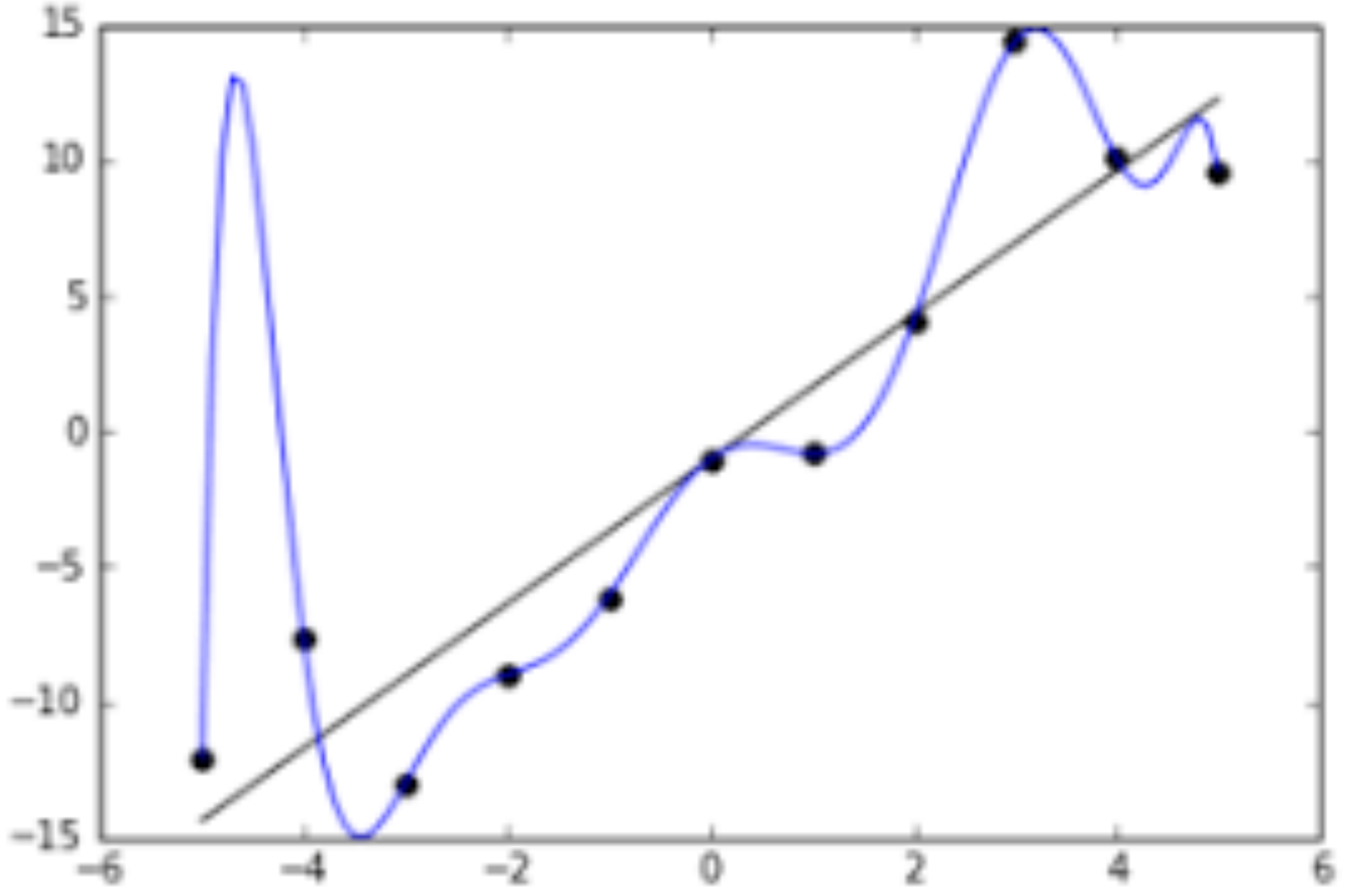


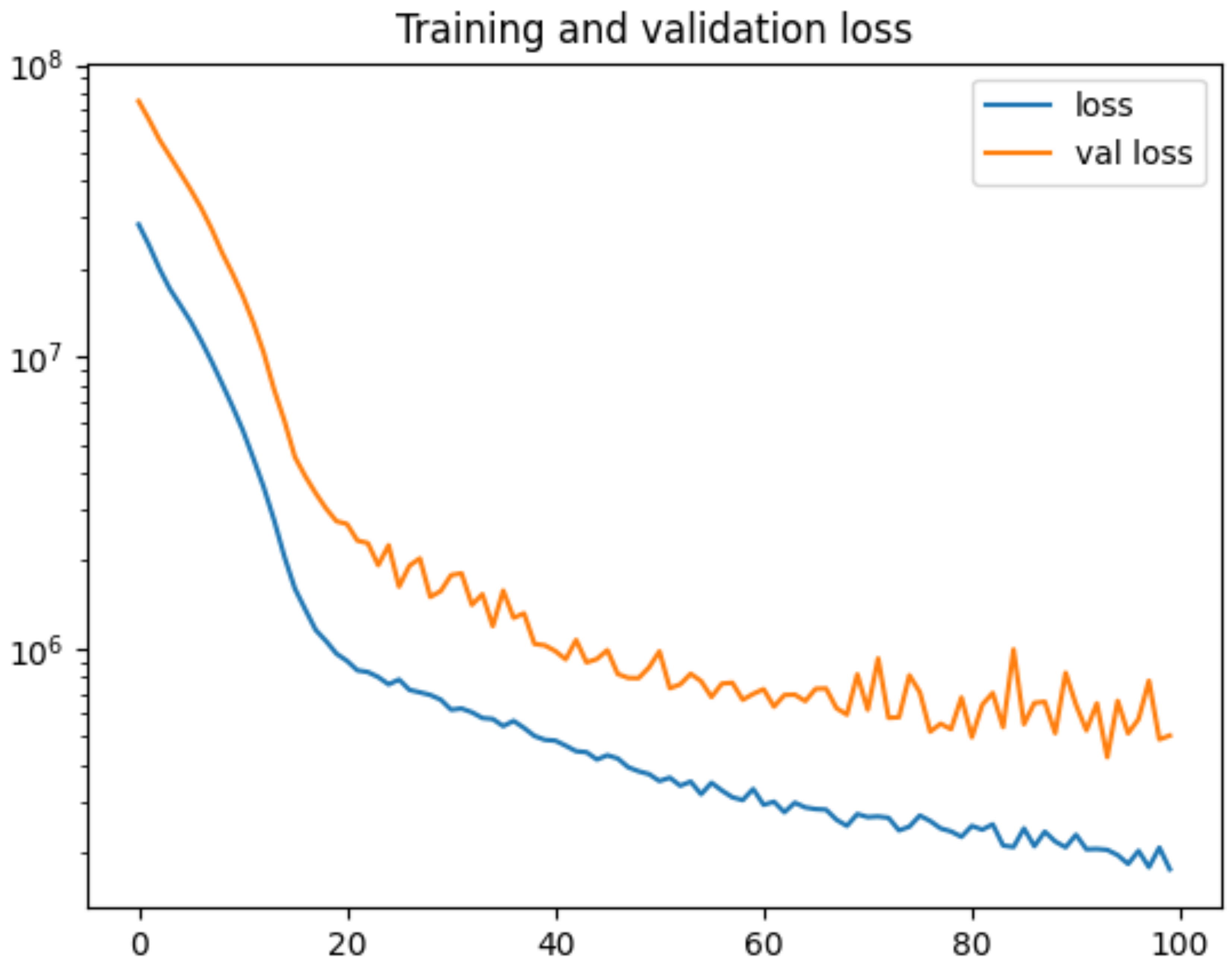
Without Machine Learning

With Machine Learning

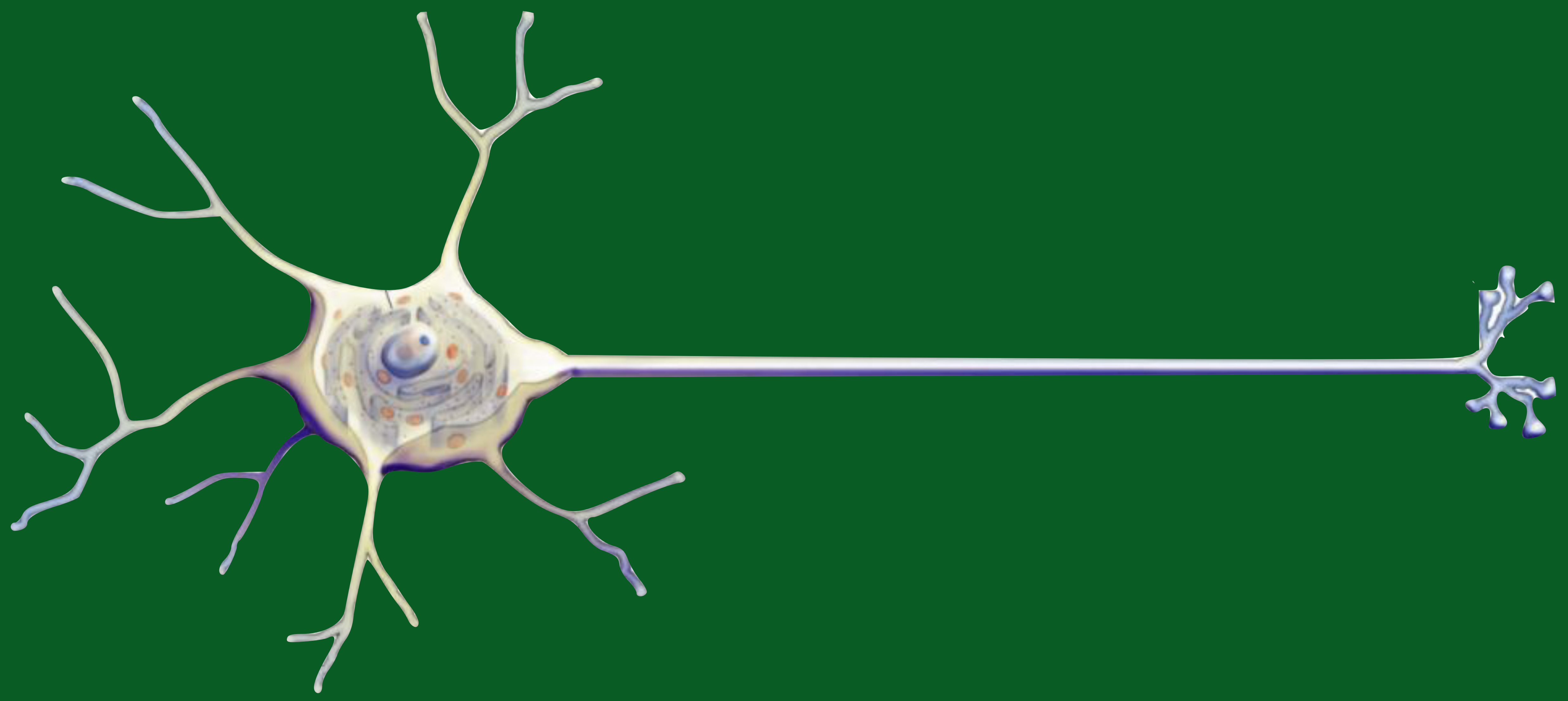
Learning from data was a **paradigm shift** in thinking about predictive models

✱ VERY SPECIFIC INSTRUCTIONS





NEURON



MATHEMATICS

ELSEVIER

Neural Networks
Volume 4, Issue 2, 1991, Pages 251-257

Approximation capabilities of multilayer feedforward networks

Kurt Hornik

Show more

Share Cite

https://doi.org/10.1016/0893-6080(91)90009-T

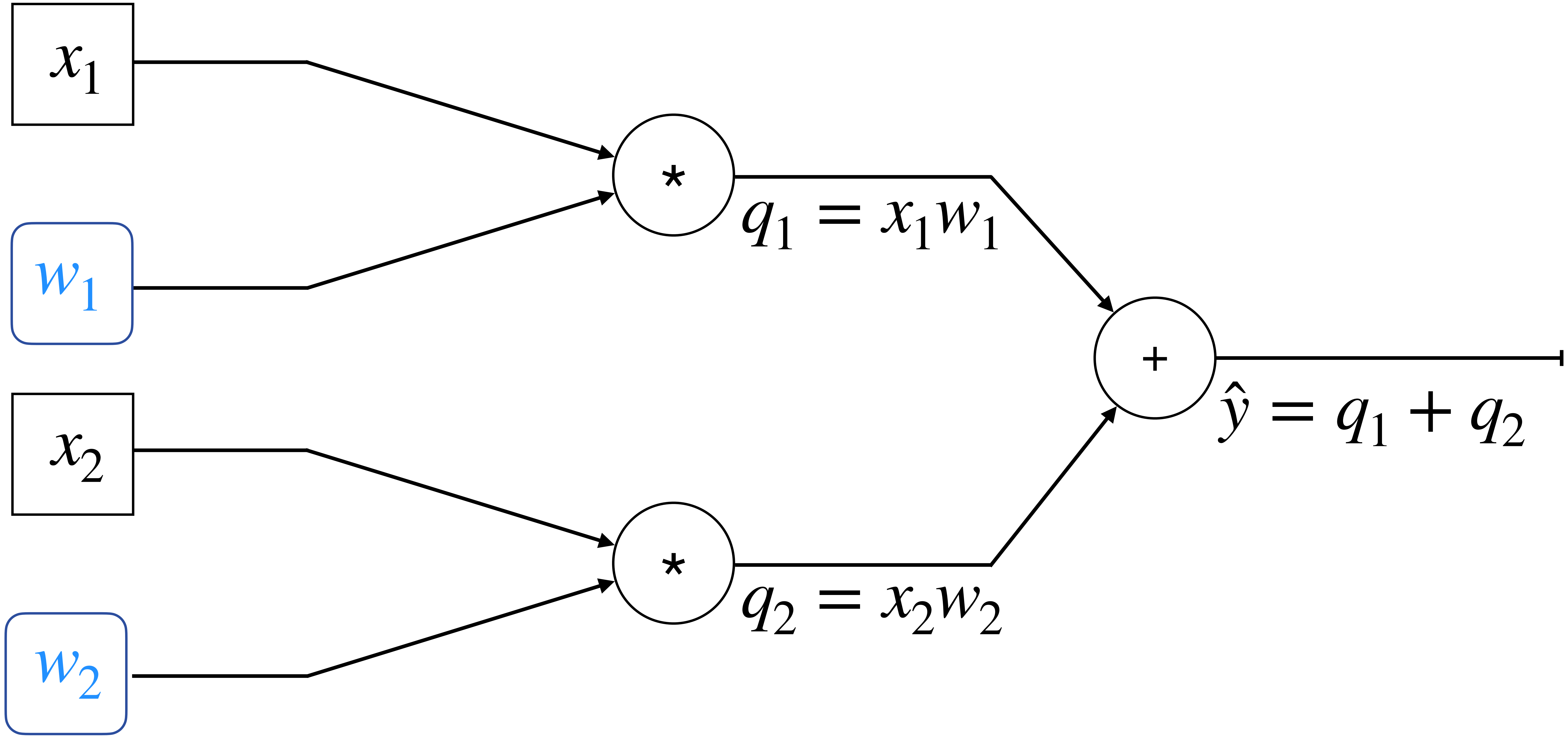
Abstract

We show that standard multilayer feedforward networks with as few as a single hidden layer and arbitrary bounded and nonconstant activation function are universal approximators with respect to $L^p(\mu)$ performance criteria, for arbitrary finite input environment measures μ, provided only that sufficiently many hidden units are available. If the activation function is continuous, bounded and nonconstant, then continuous mappings can be learned uniformly over compact input sets. We also give very general conditions ensuring that networks with sufficiently smooth activation functions are capable of arbitrarily accurate approximation to a function and its derivatives.

MATHEMATICS

COMPUTATIONAL GRAPH

$$\hat{y} = x_1 w_1 + x_2 w_2$$



COMPUTATIONAL GRAPH

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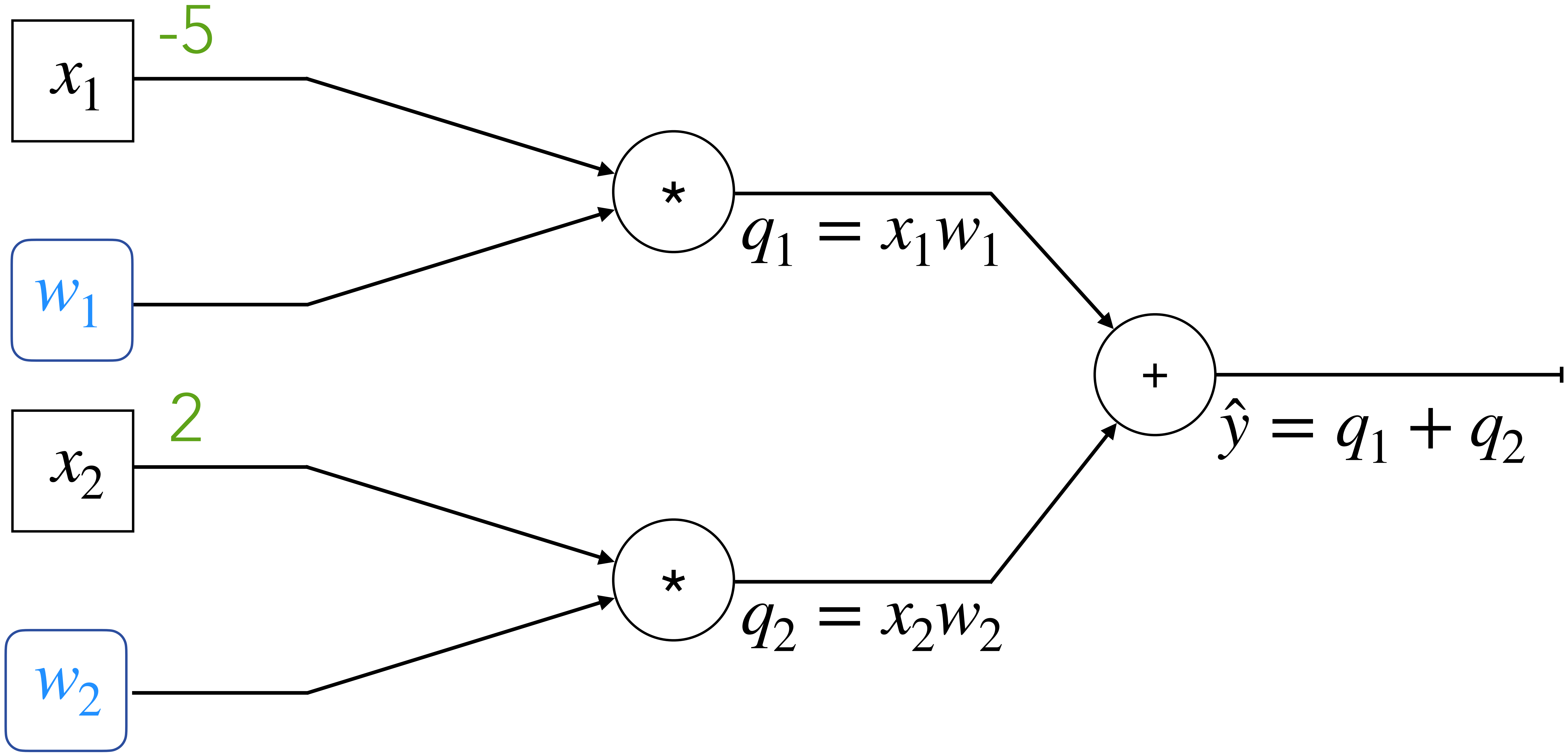

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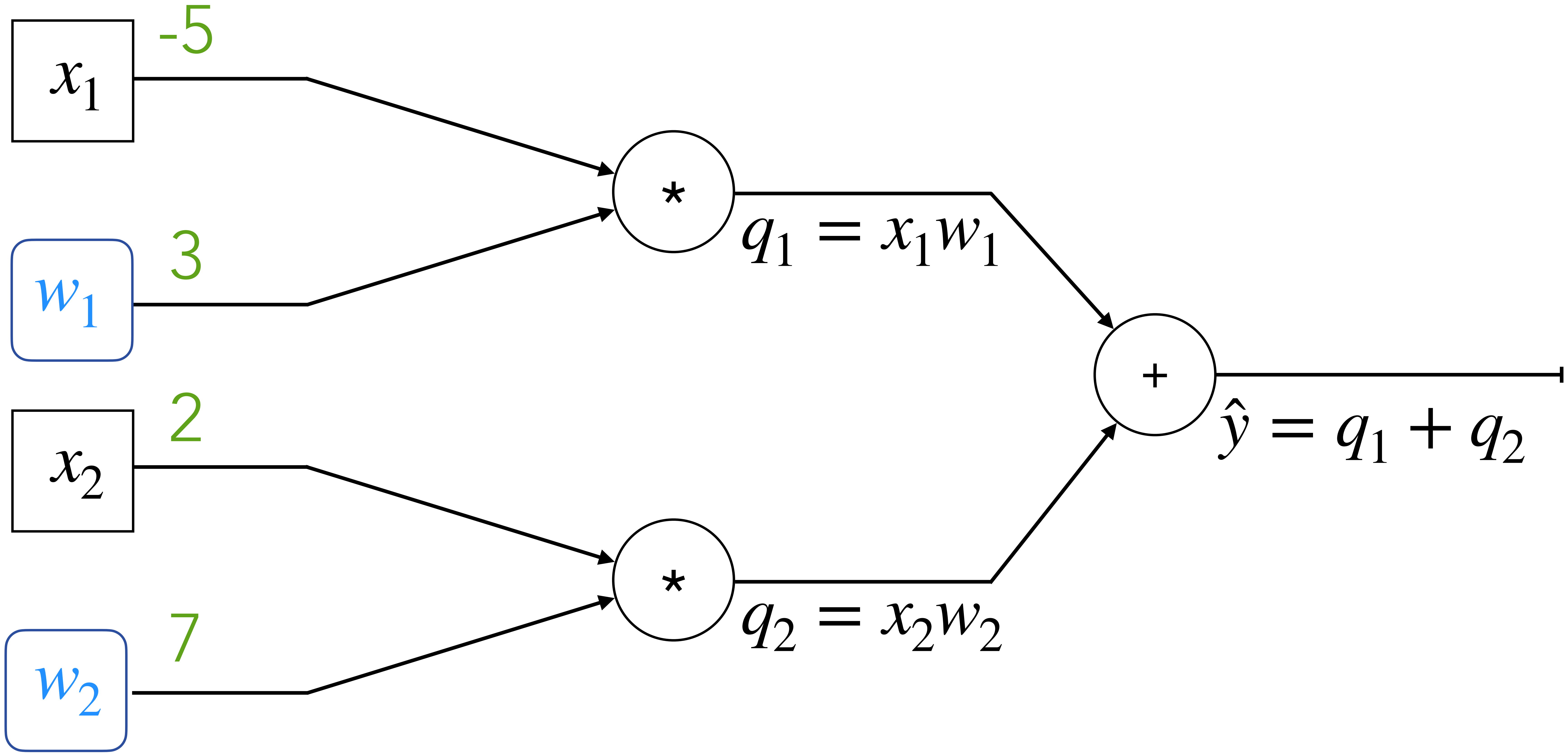

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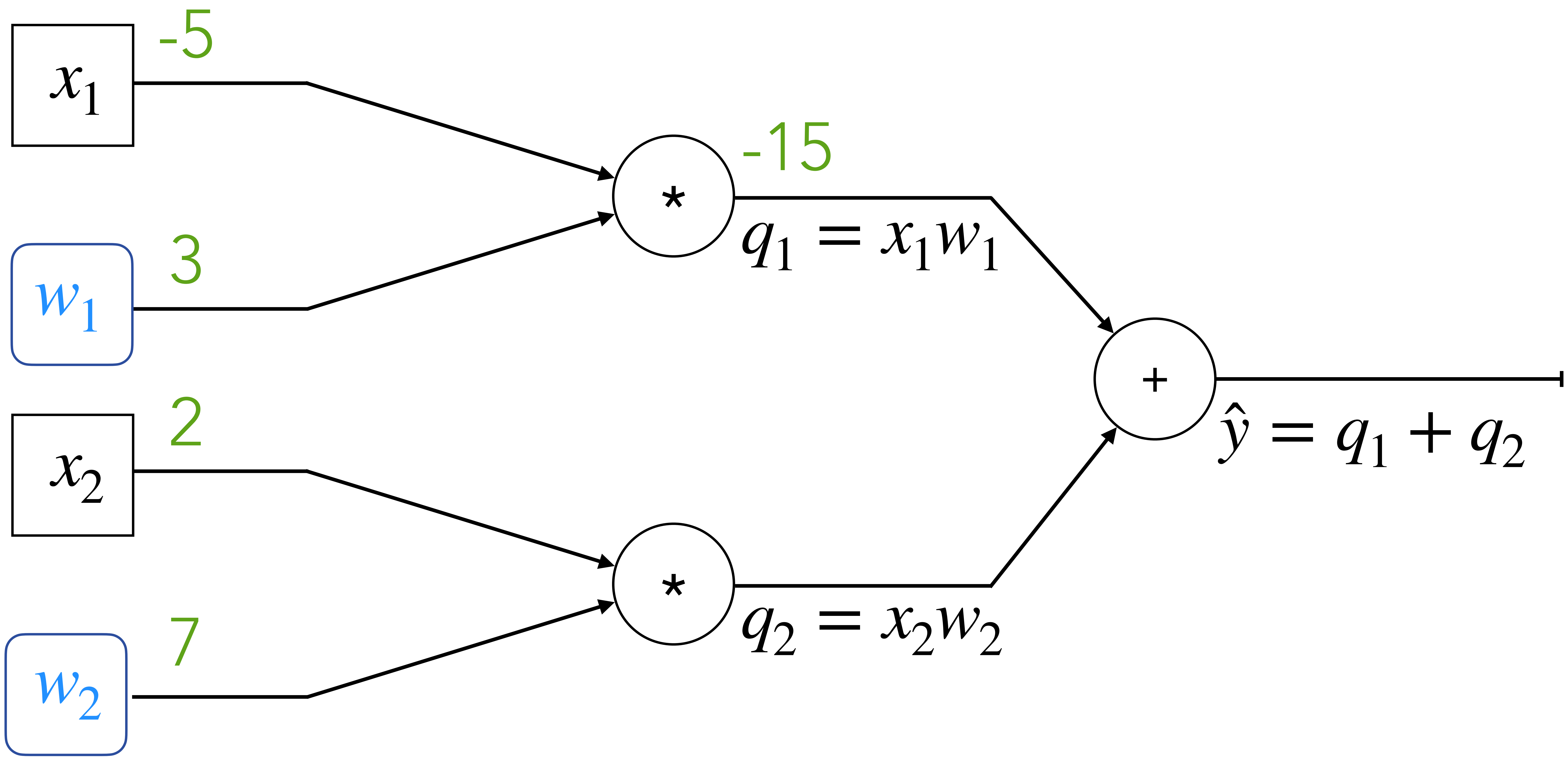

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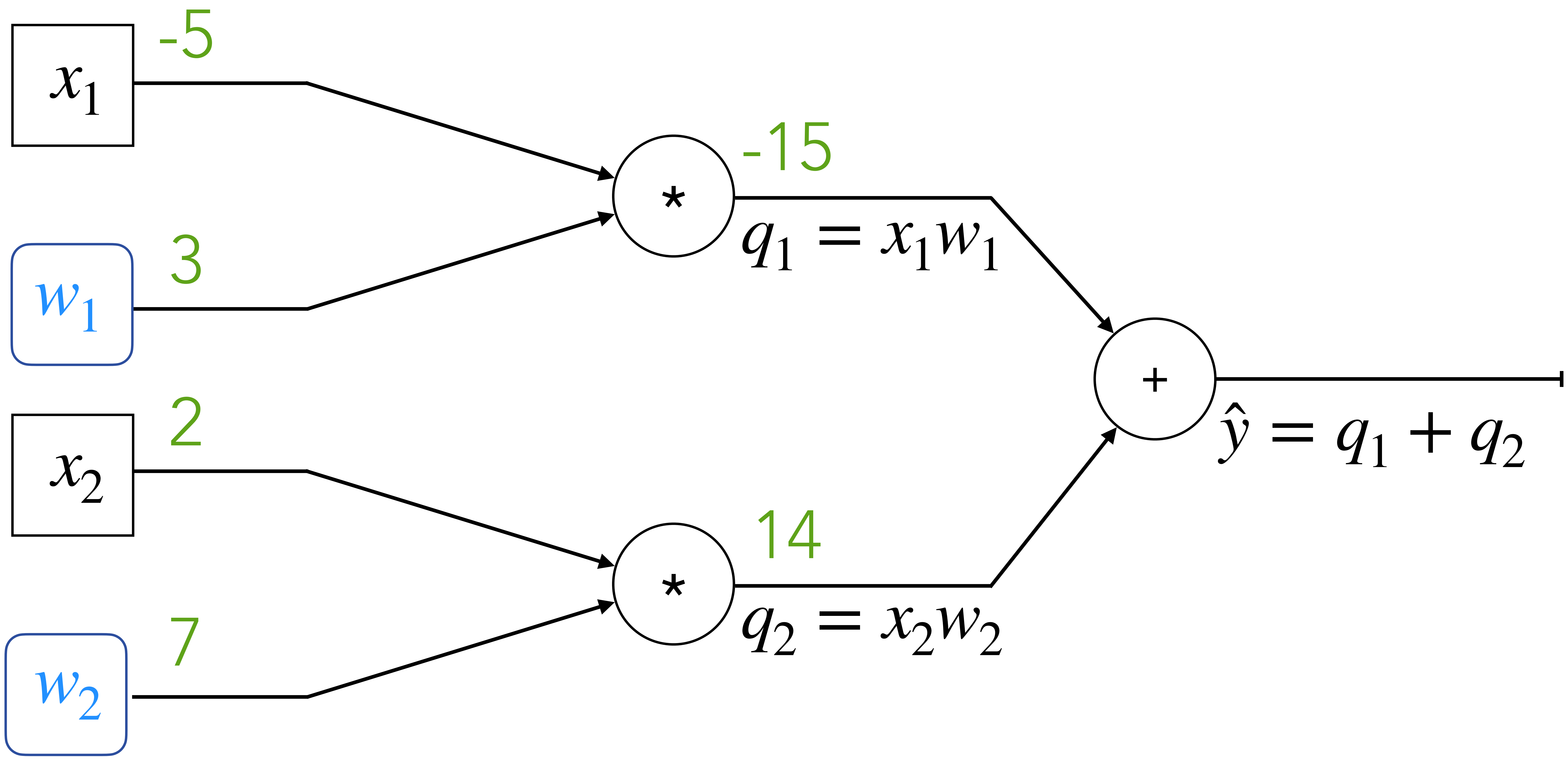
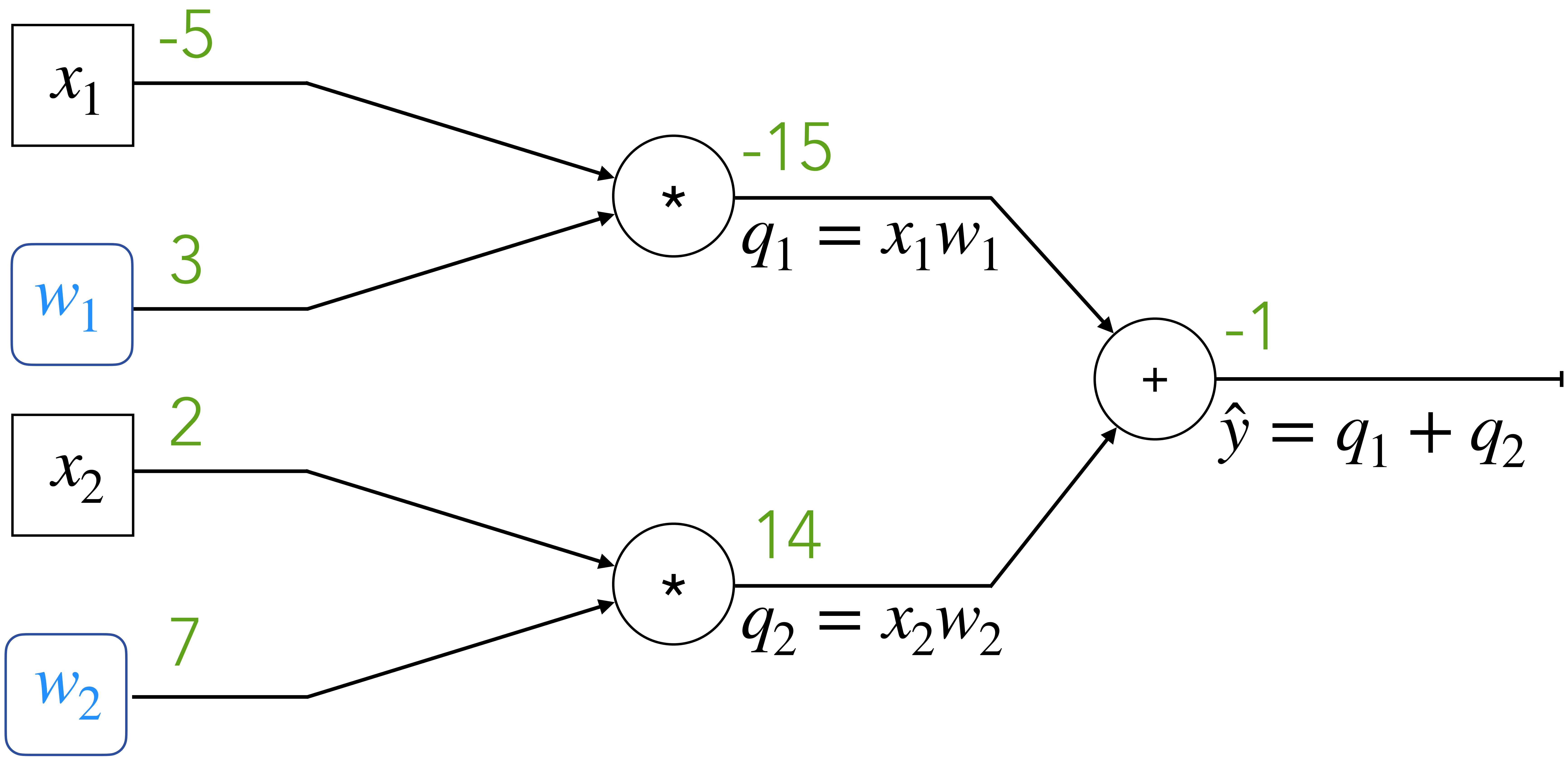


COMPUTATIONAL GRAPH

$$\hat{y} = x_1 w_1 + x_2 w_2$$



COMPUTATIONAL GRAPH

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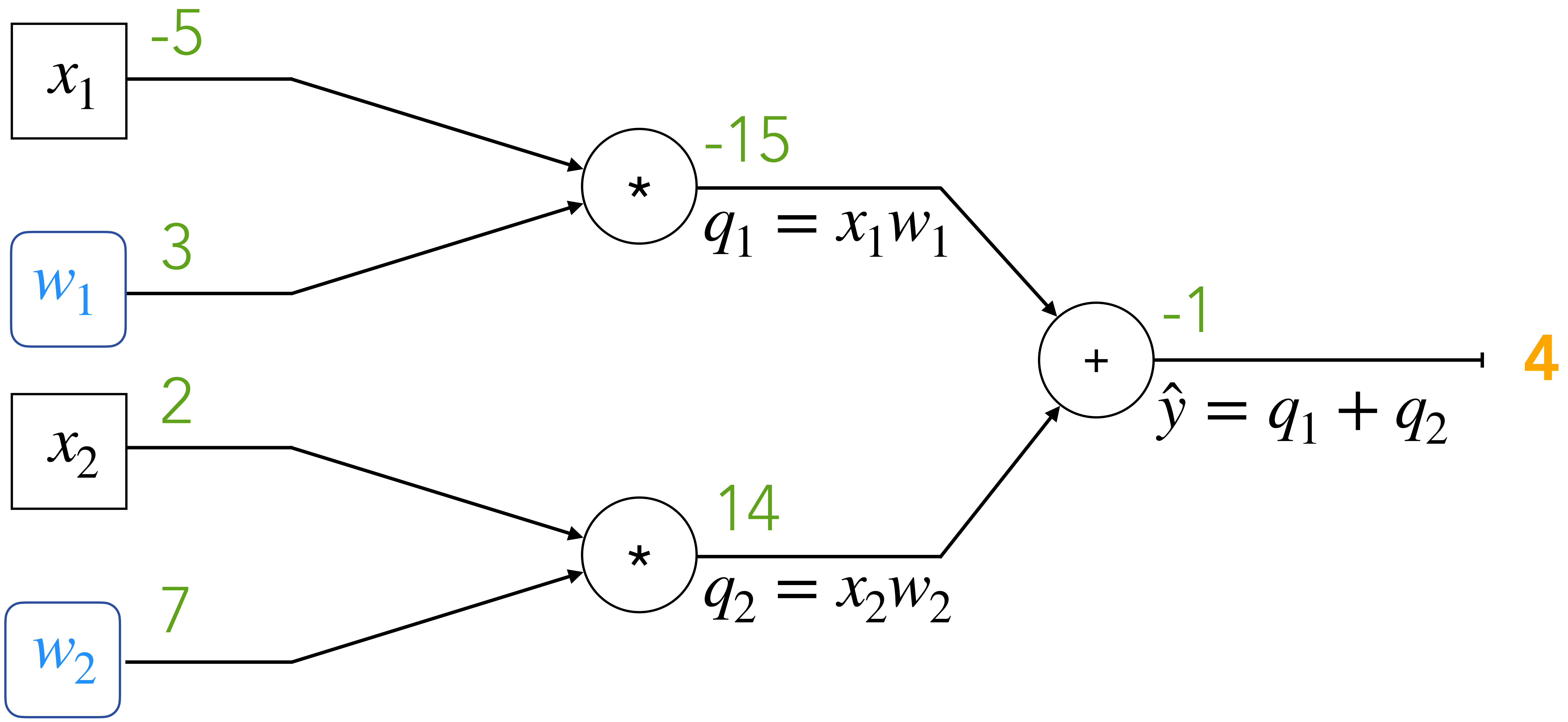
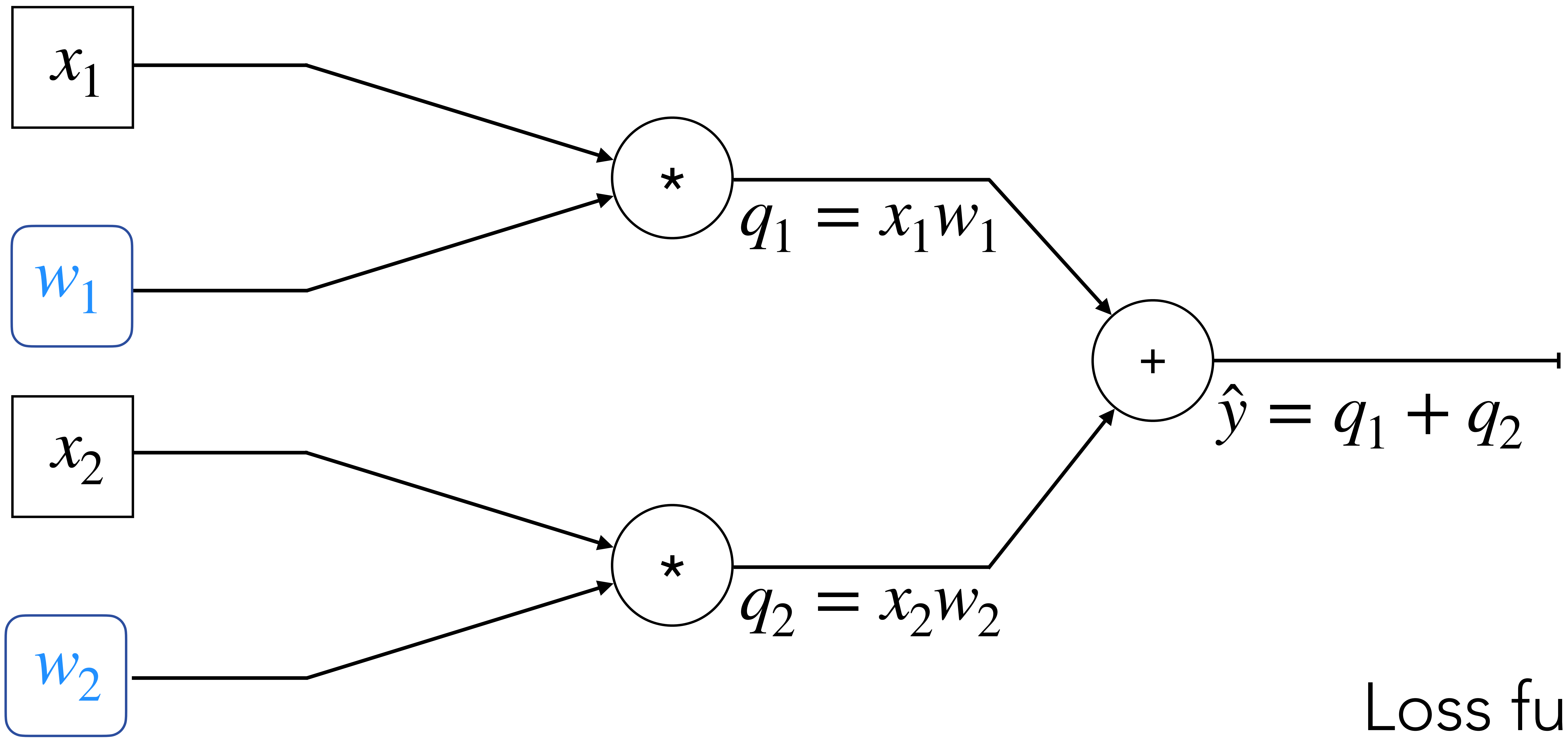


MACHINE LEARNING

SUPERVISED LEARNING

REGRESSION

$$\hat{y} = x_1 w_1 + x_2 w_2$$

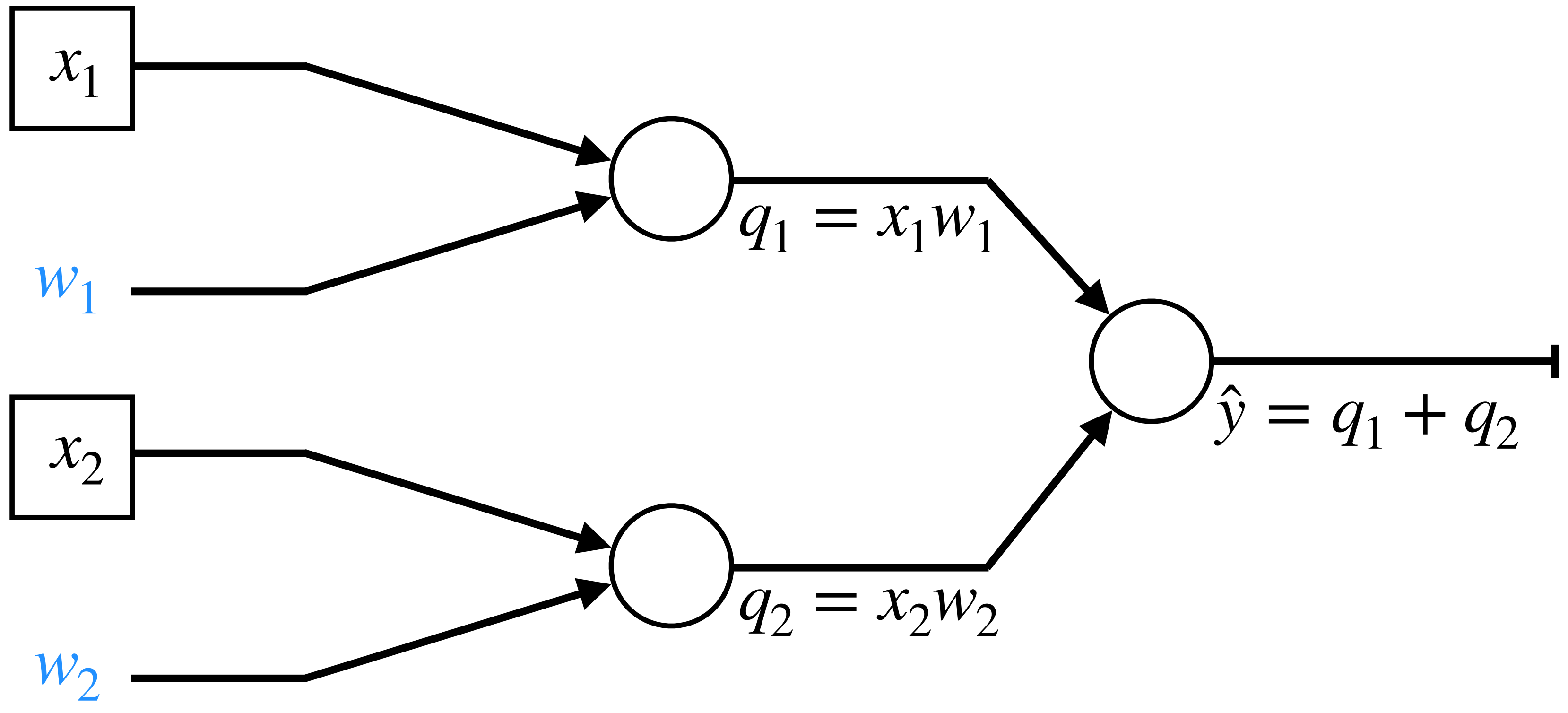


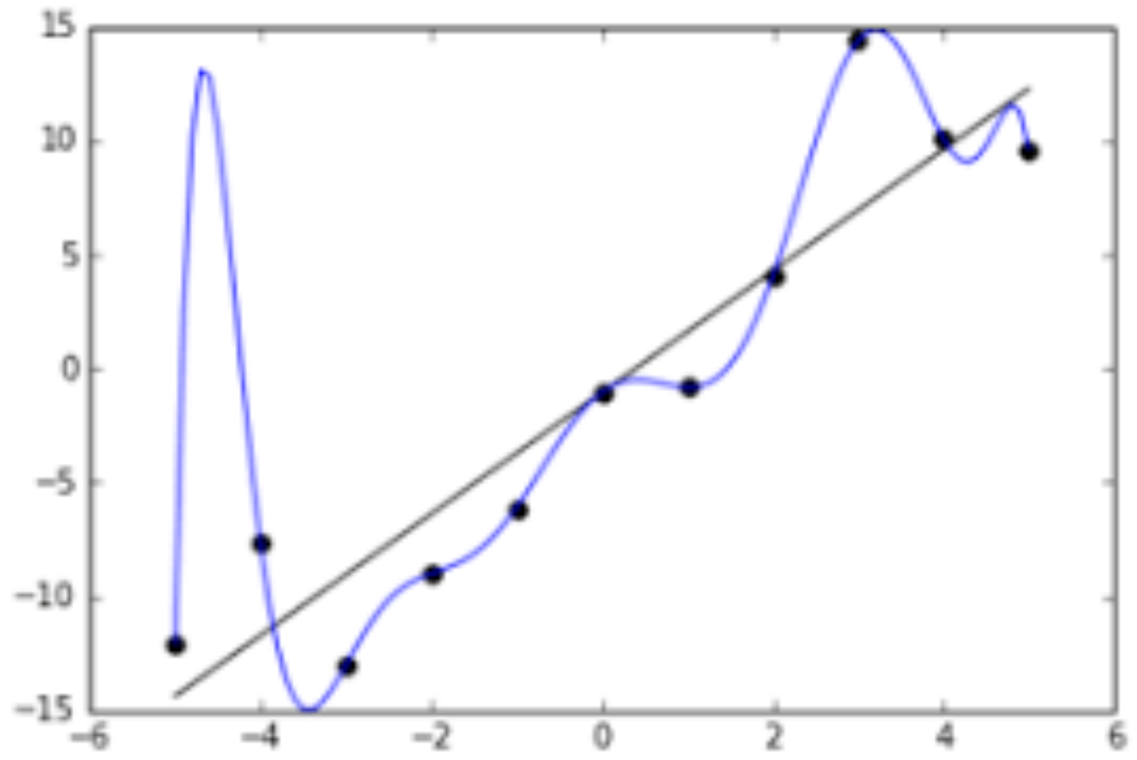
Loss function

$$J(w) = \hat{y} - y$$

SUPERVISED LEARNING

$$\hat{y} = x_1 w_1 + x_2 w_2$$





	Feature 1	Feature 2	Feature 3	Target
Example 1				
Example 2				
Example 3				
Example 4				

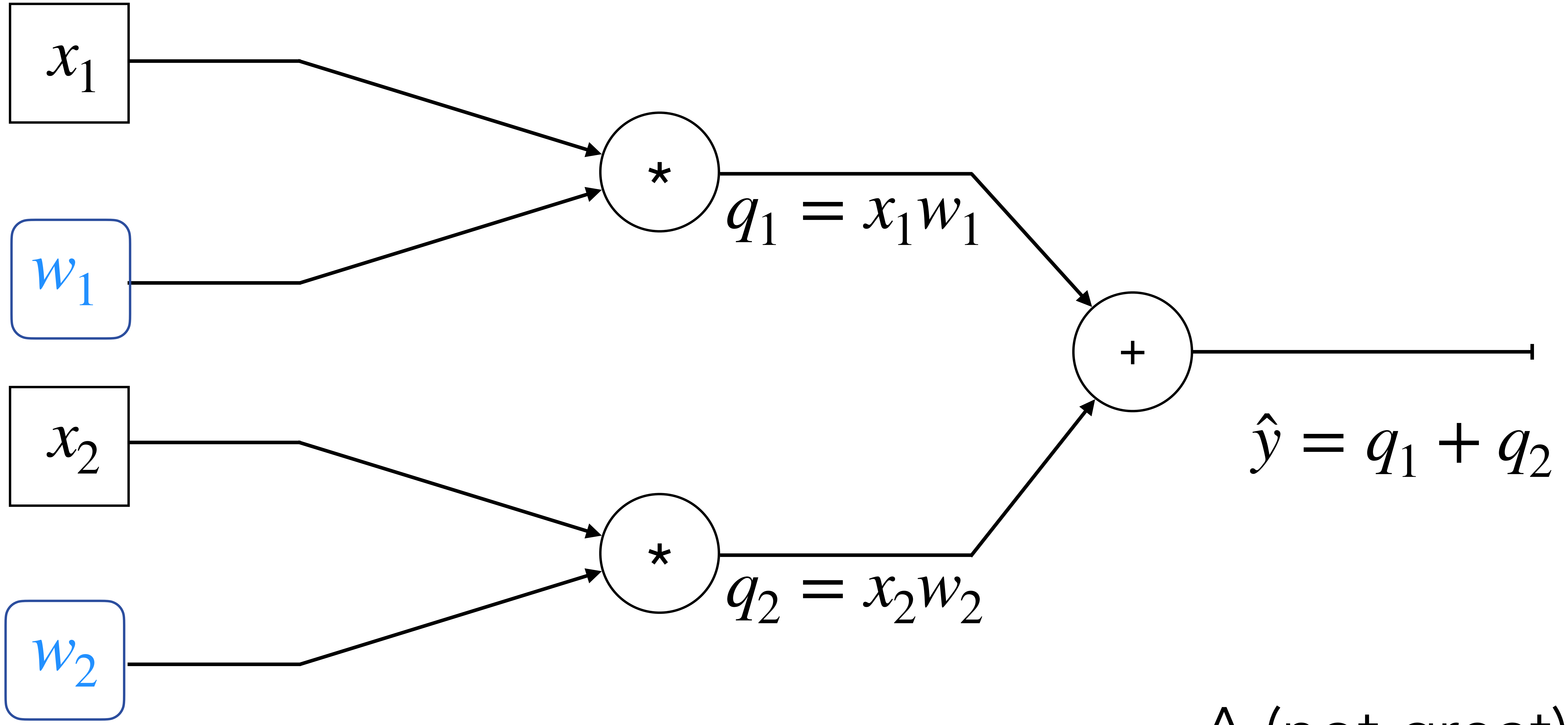
Loss function

MSE across N examples

$$J(w) = \frac{1}{N} \sum_{i=0}^{N} (\hat{y}_i - y_i)^2$$

BACKPROPAGATION

$$w_1 = w_1 - \eta * \frac{\partial J}{\partial w_1}$$



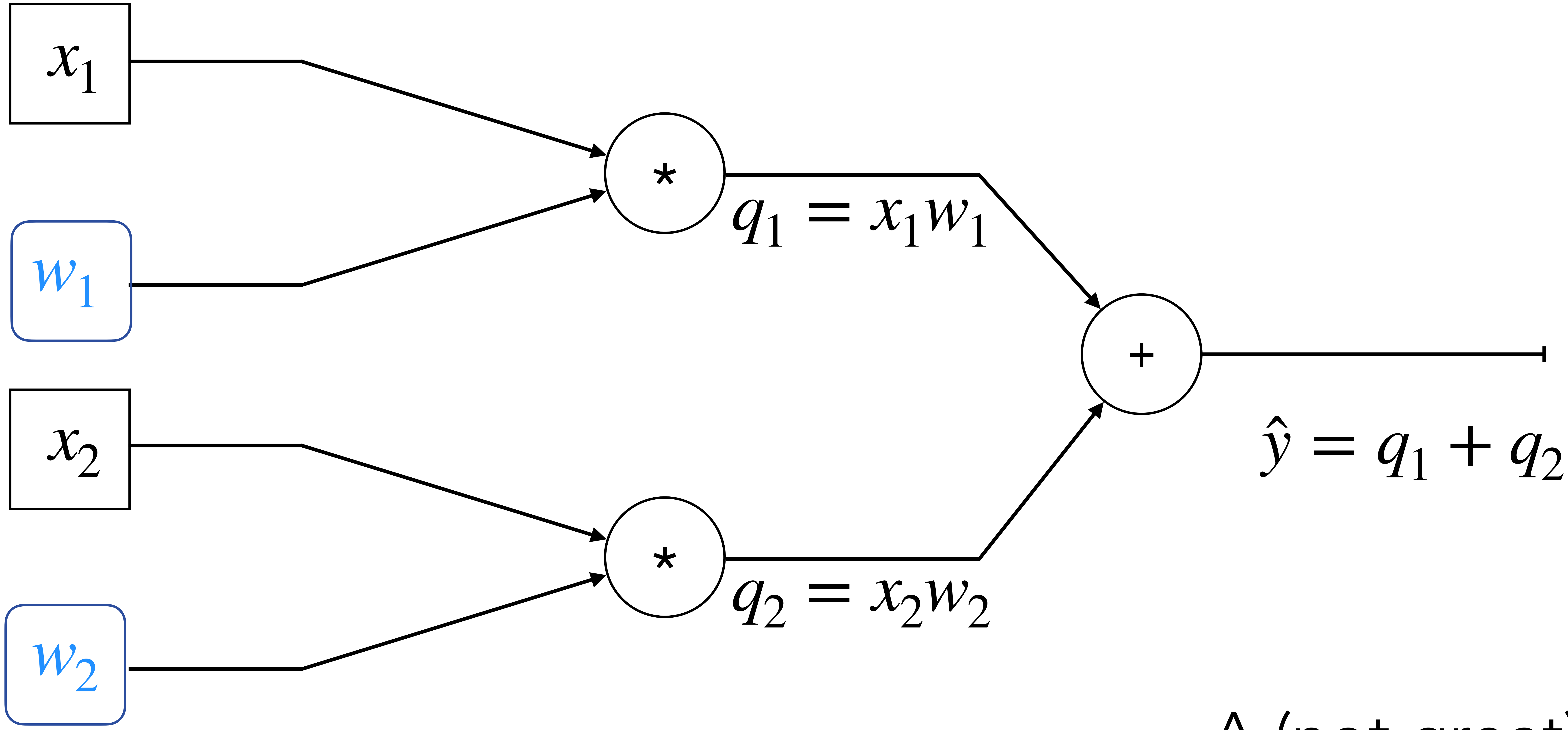
$$w_2 = w_2 - \eta * \frac{\partial J}{\partial \hat{w}_2}$$

A (not great) loss function:

$$J(w) = \hat{y} - y$$

BACKPROPAGATION

$$w_1 = w_1 - \eta * \frac{\partial J}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial q_1} \frac{\partial q_1}{\partial w_1}$$



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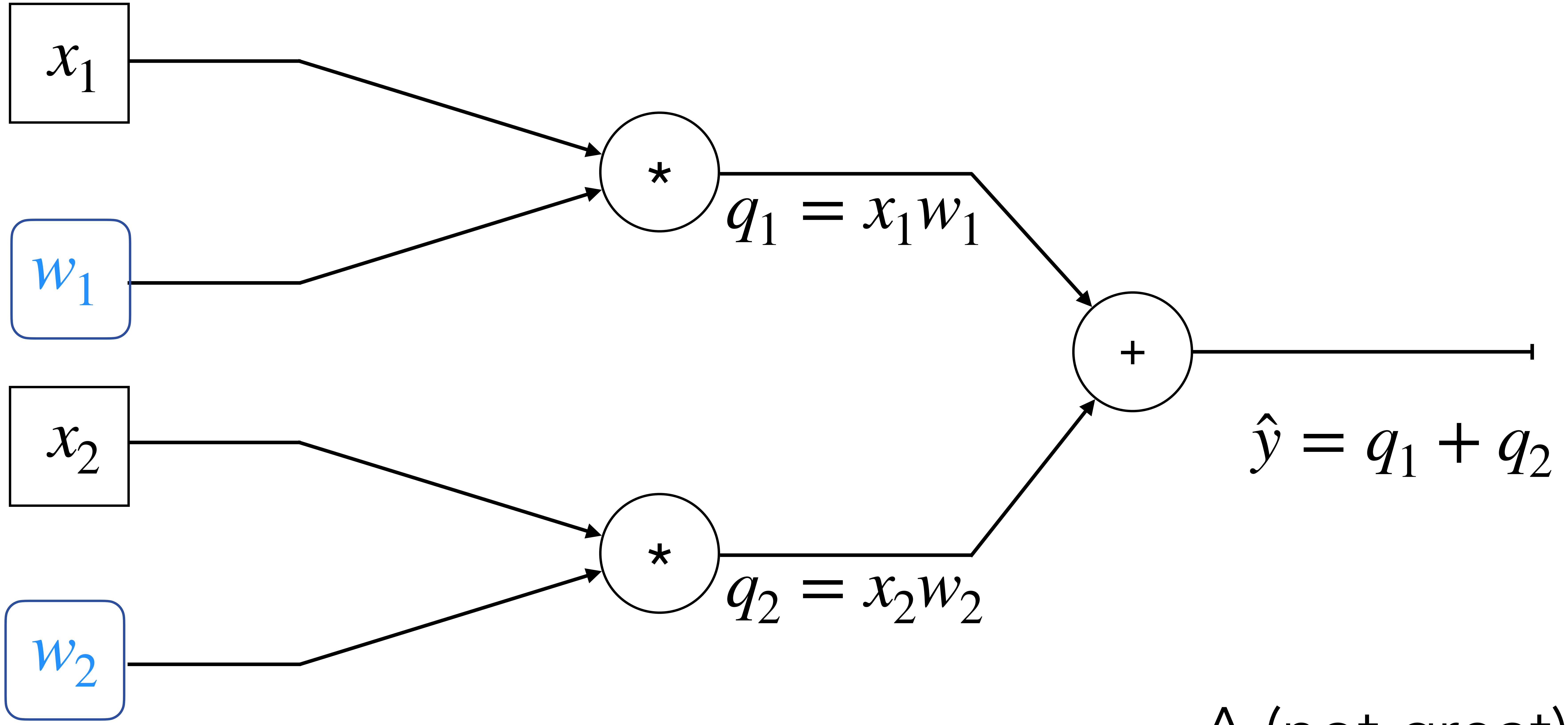

$$w_2 = w_2 - \eta * \frac{\partial J}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial q_2} \frac{\partial q_1}{\partial w_2}$$

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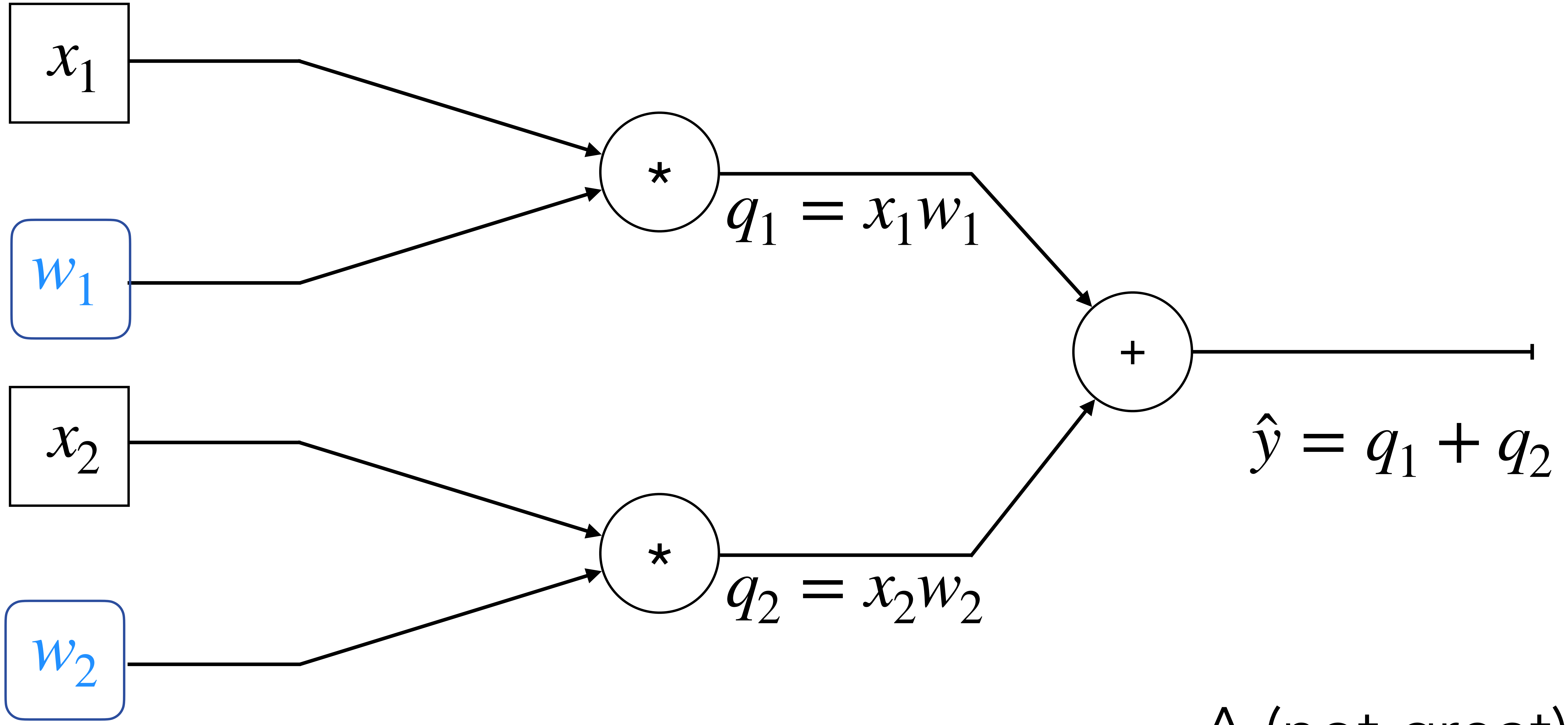
BACKPROPAGATION

$$w_1 = w_1 - \eta * \frac{\partial J}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial q_1} \frac{\partial q_1}{\partial w_1}$$



$$\frac{\partial J}{\partial \hat{y}} = 1$$

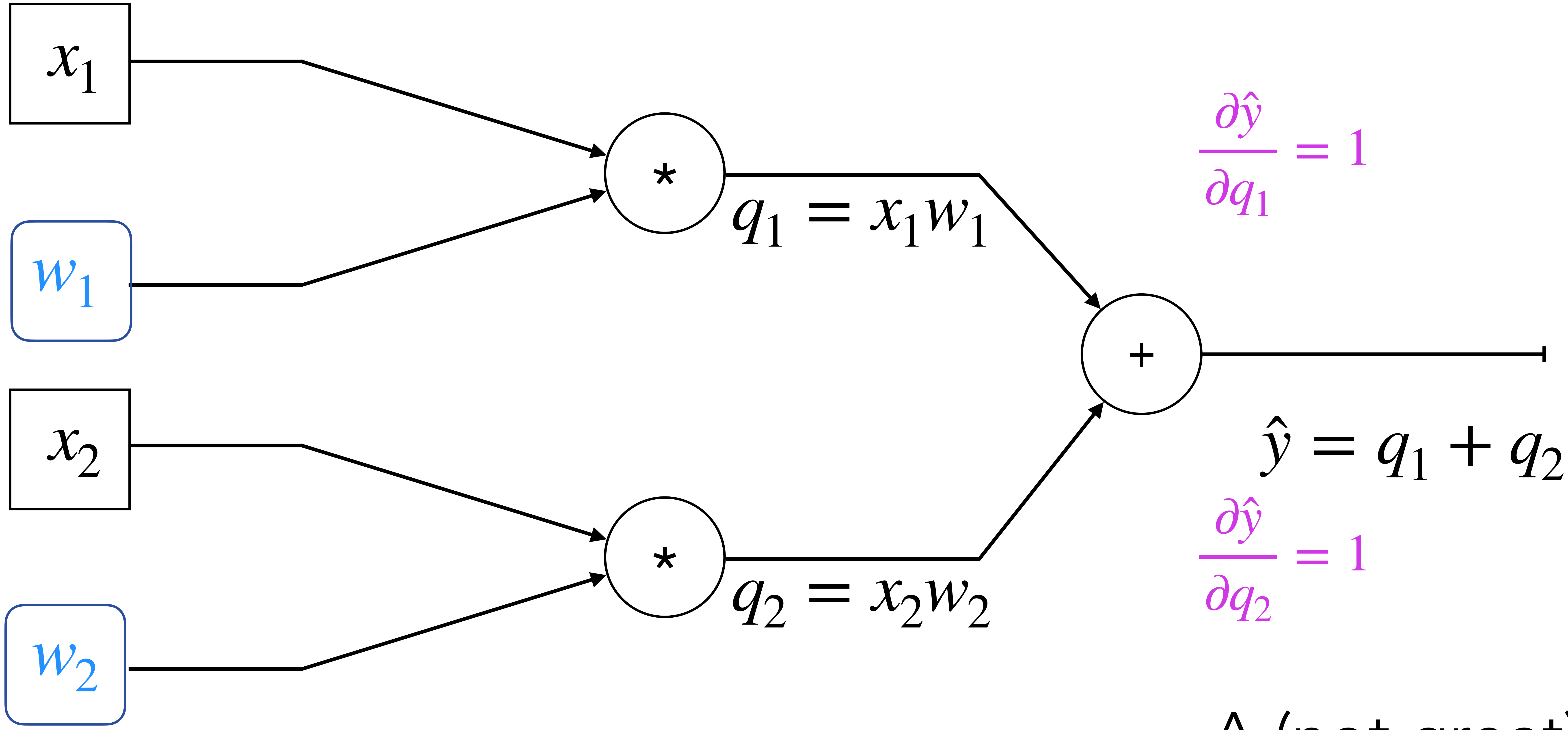
$$w_2 = w_2 - \eta * \frac{\partial J}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial q_2} \frac{\partial q_1}{\partial w_2}$$

A (not great) loss function:

$$J(w) = \hat{y} - y$$

BACKPROPAGATION

$$w_1 = w_1 - \eta * \frac{\partial J}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial q_1} \frac{\partial q_1}{\partial w_1}$$



$$\frac{\partial \hat{y}}{\partial q_1} = 1$$

$$\frac{\partial J}{\partial \hat{y}} = 1$$

$$\frac{\partial \hat{y}}{\partial q_2} = 1$$

A (not great) loss function:

$$J(w) = \hat{y} - y$$

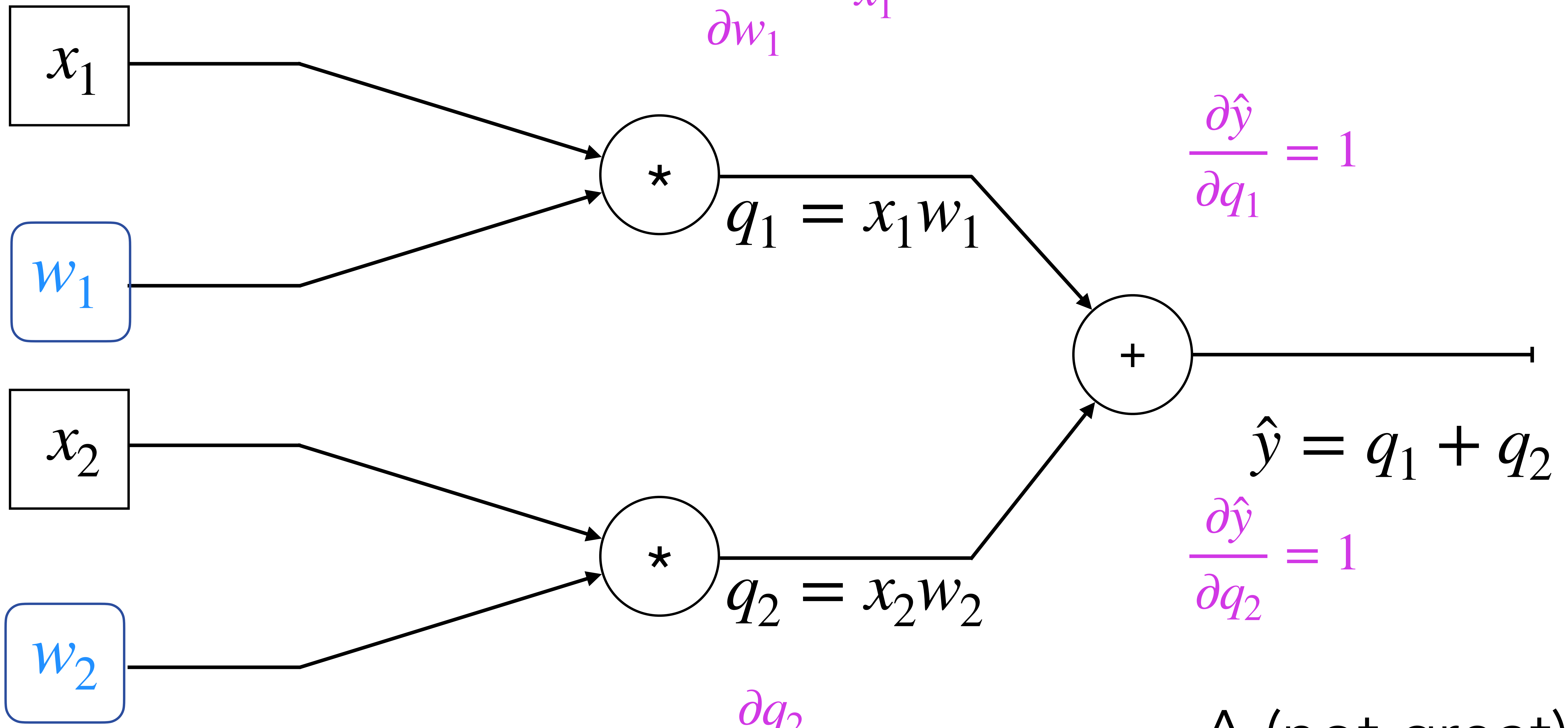
$$w_2 = w_2 - \eta * \frac{\partial J}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial q_2} \frac{\partial q_1}{\partial w_2}$$

BACKPROPAGATION

$$w_1 = w_1 - \eta * \frac{\partial J}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial q_1} \frac{\partial q_1}{\partial w_1}$$

$$\frac{\partial q_1}{\partial w_1} = x_1$$

$$\frac{\partial \hat{y}}{\partial q_1} = 1$$



$$\frac{\partial J}{\partial \hat{y}} = 1$$

$$\frac{\partial \hat{y}}{\partial q_2} = 1$$

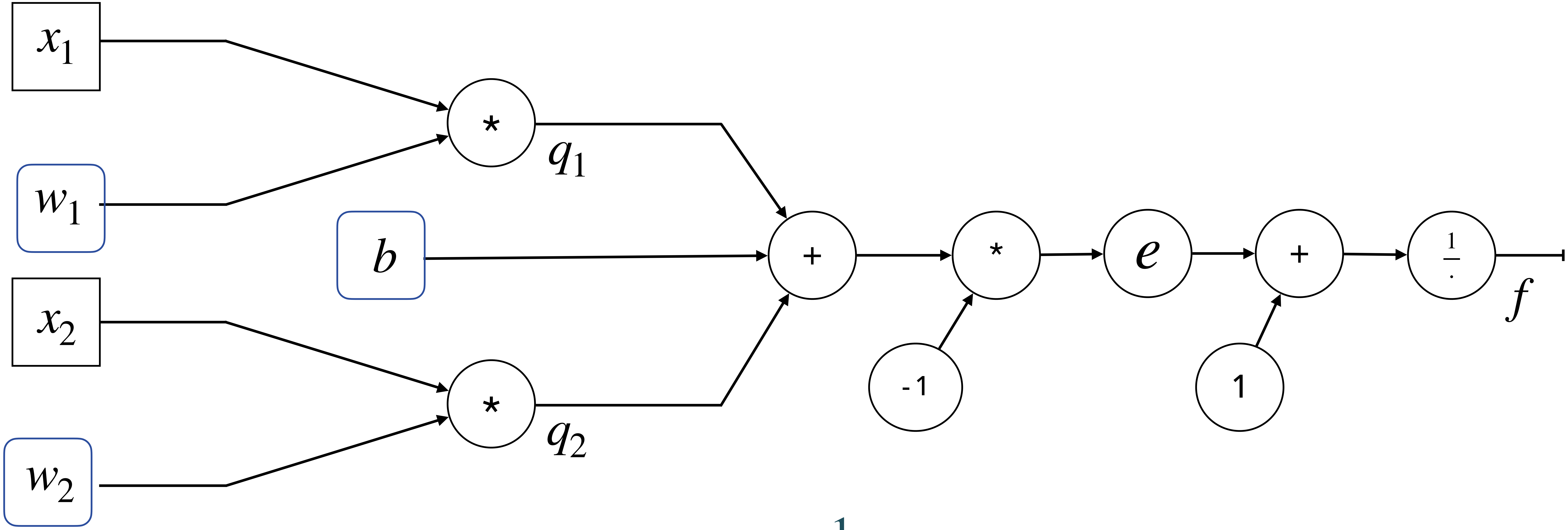
$$\frac{\partial q_2}{\partial w_2} = x_2$$

$$w_2 = w_2 - \eta * \frac{\partial J}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial q_2} \frac{\partial q_1}{\partial w_2}$$

A (not great) loss function:

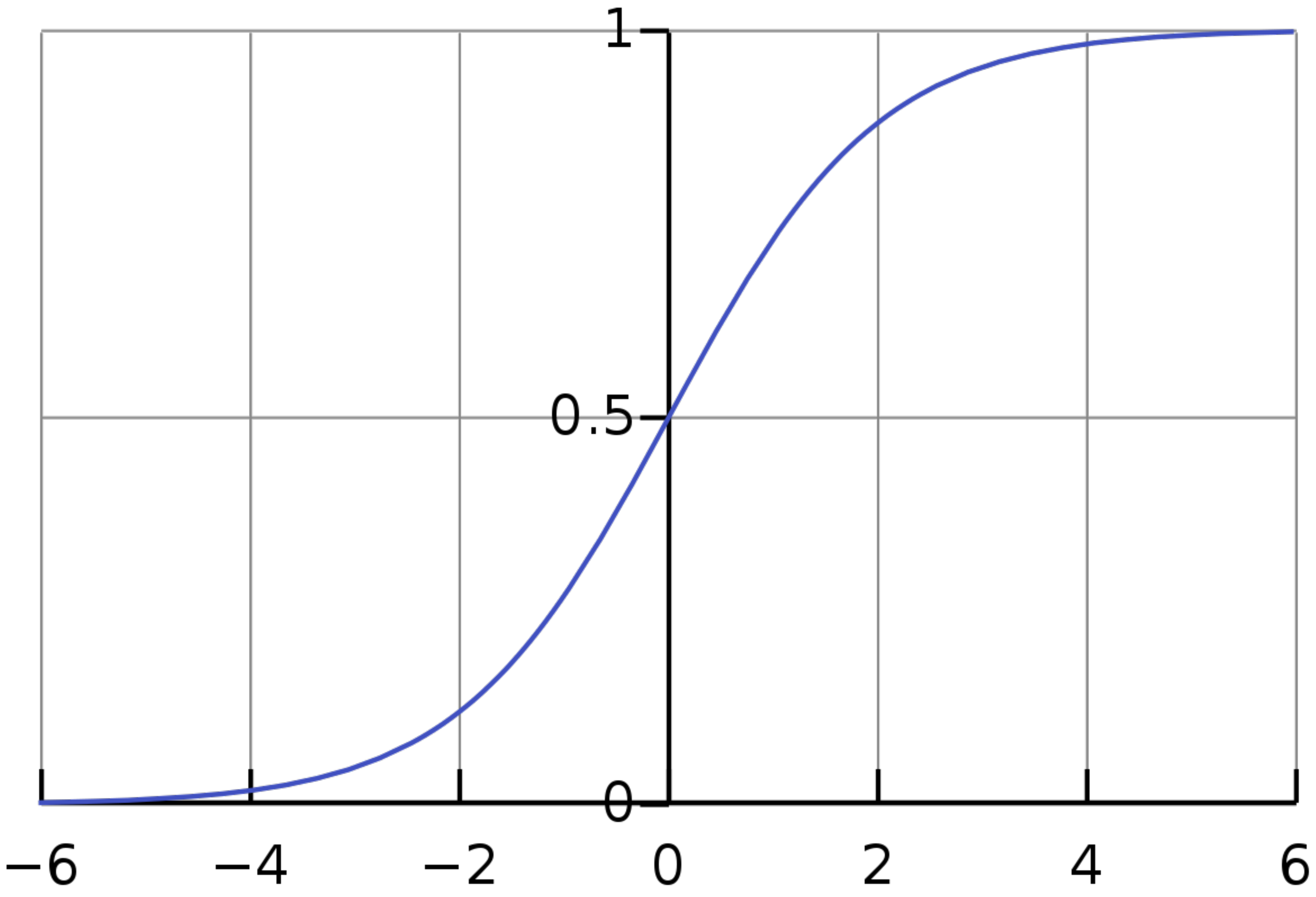
$$J(w) = \hat{y} - y$$

LOGISTIC REGRESSION

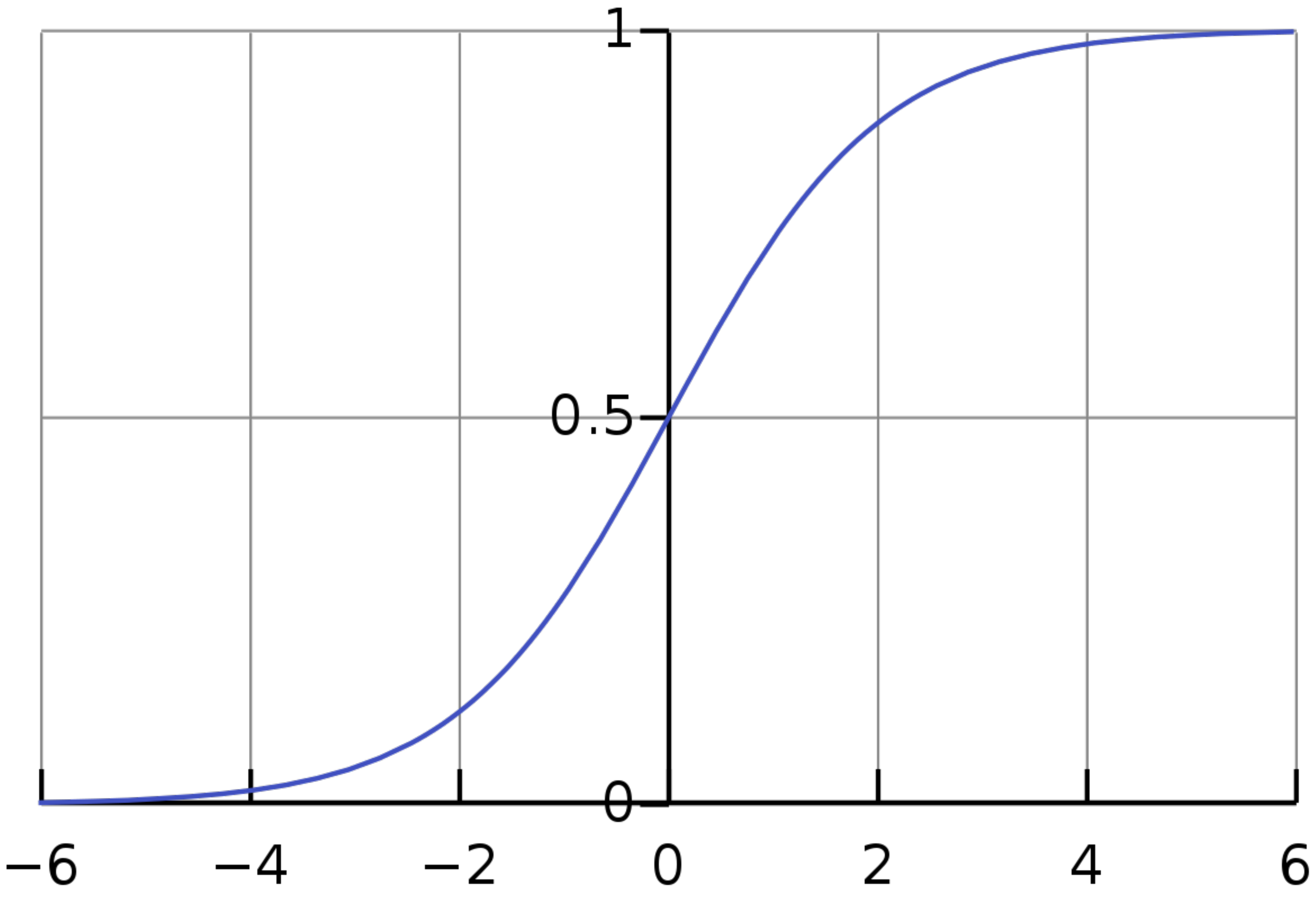


$$f = \frac{1}{1 + e^{-(x_1 w_1 + x_2 w_2 + b)}}$$

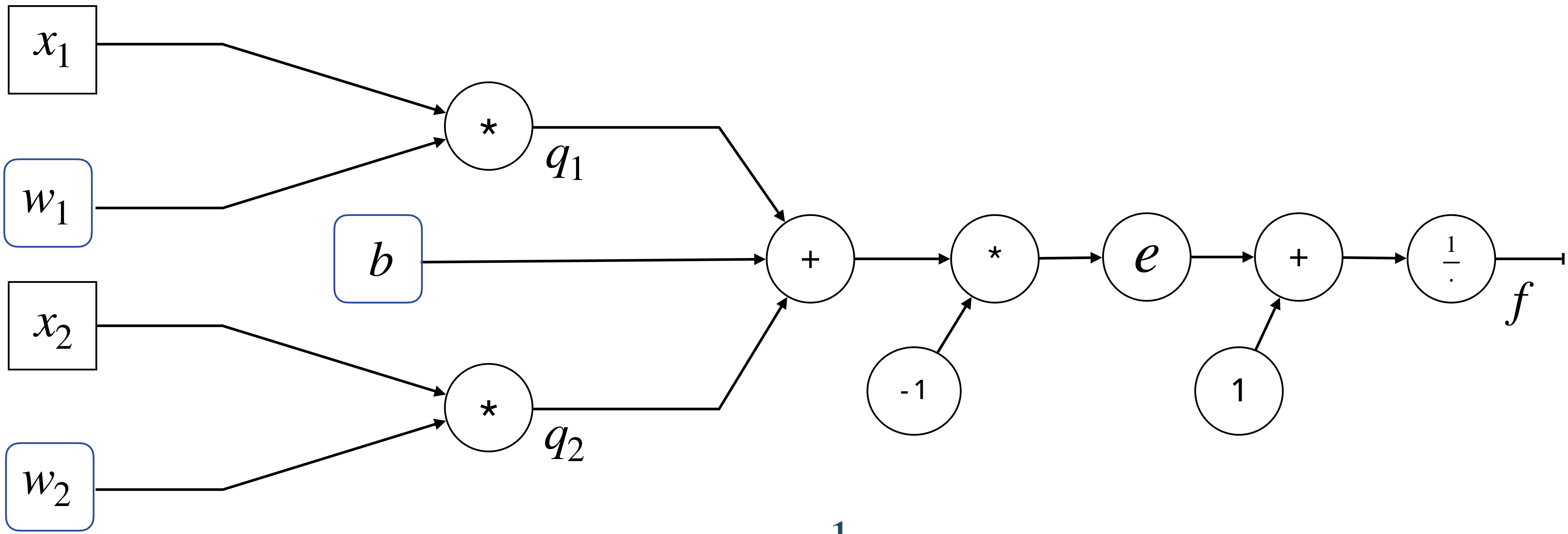
LOGISTIC REGRESSION



CLASSIFICATION

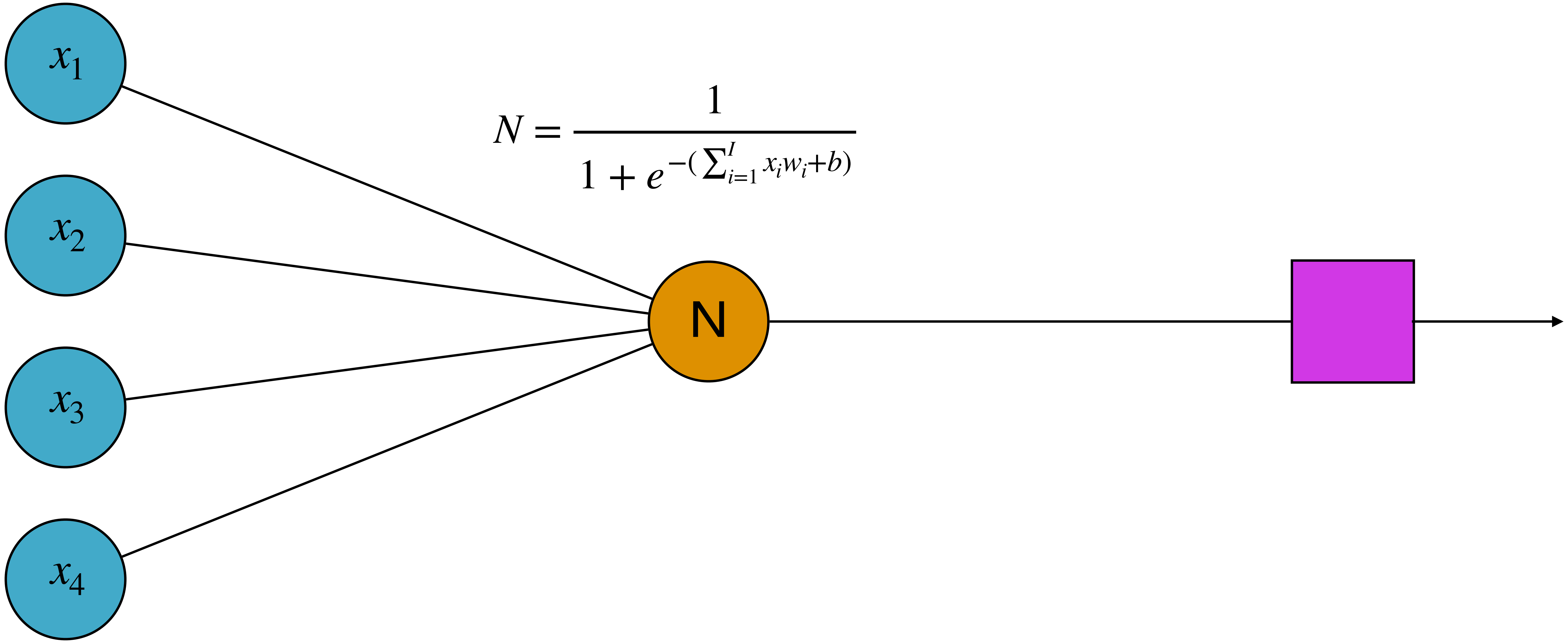


LOGISTIC REGRESSION

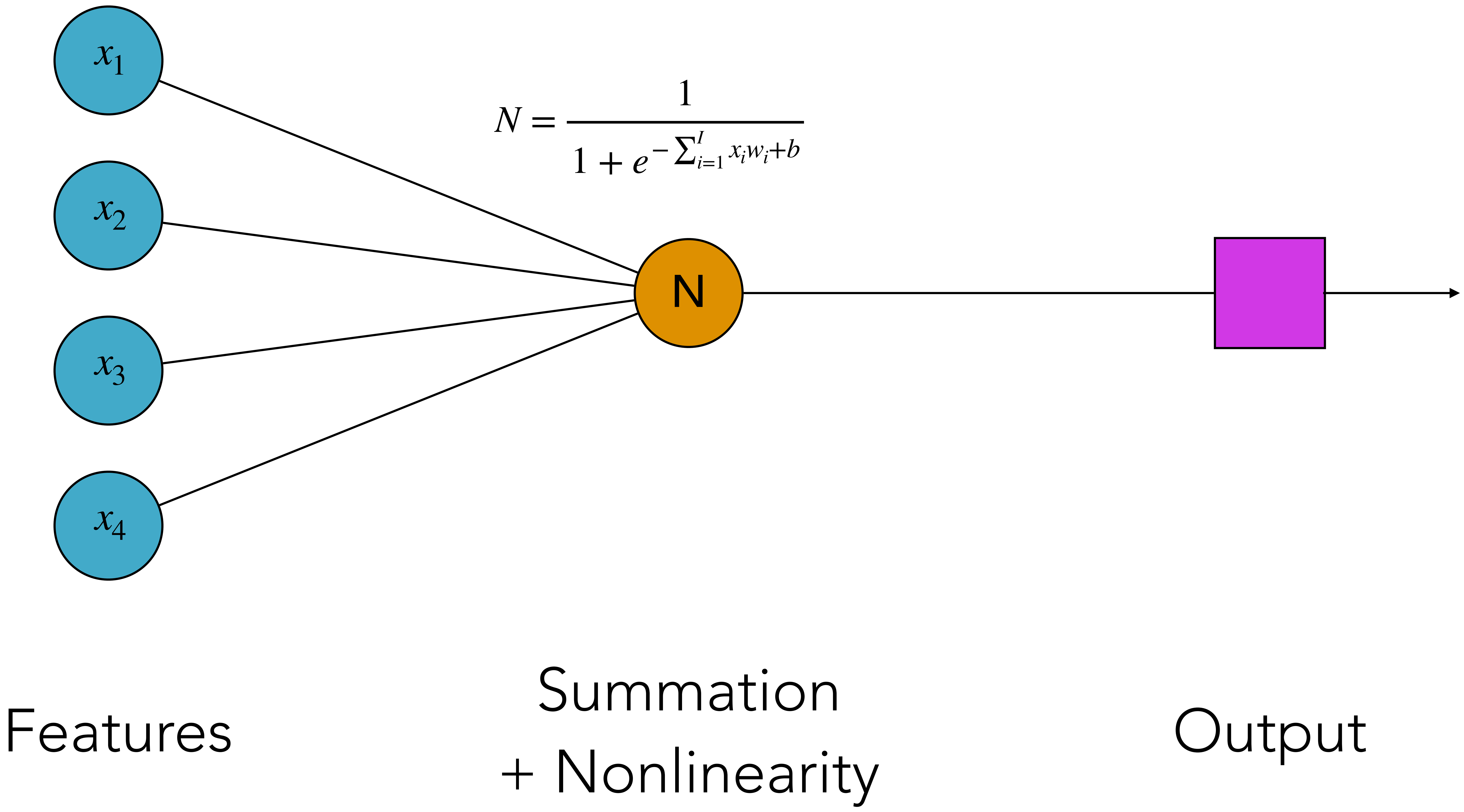


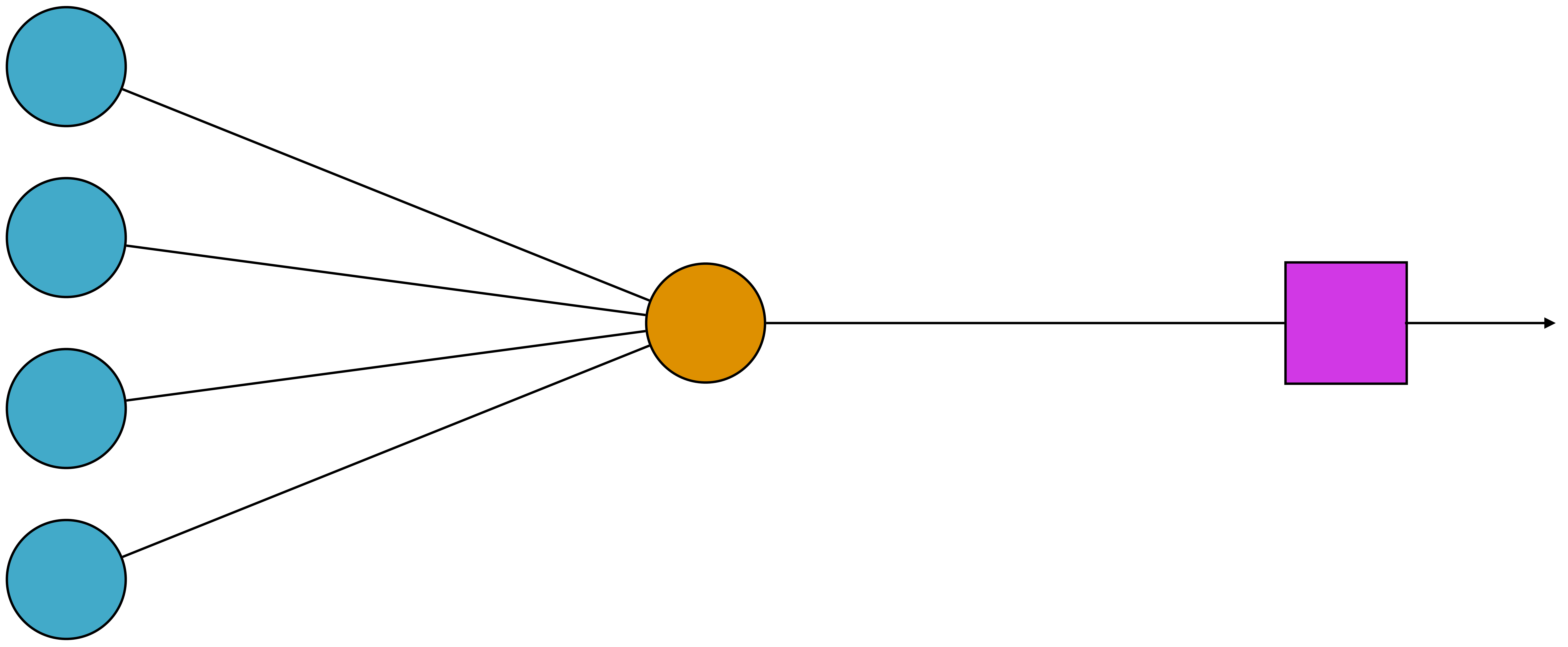
$$f = \frac{1}{1 + e^{-(x_1 w_1 + x_2 w_2 + b)}}$$

$$N = \frac{1}{1 + e^{-\left(\sum_{i=1}^{I} x_i w_i + b\right)}}$$

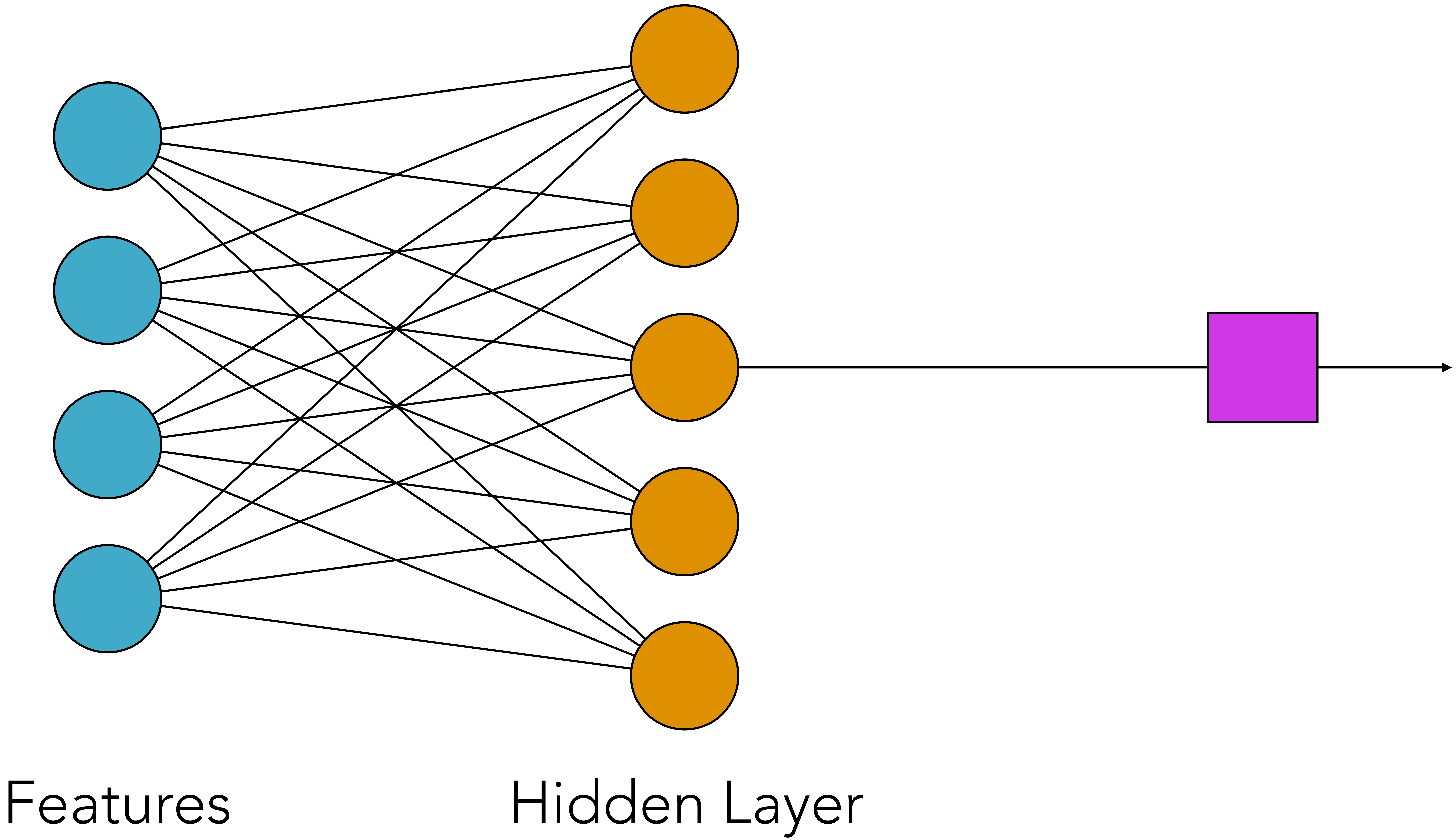


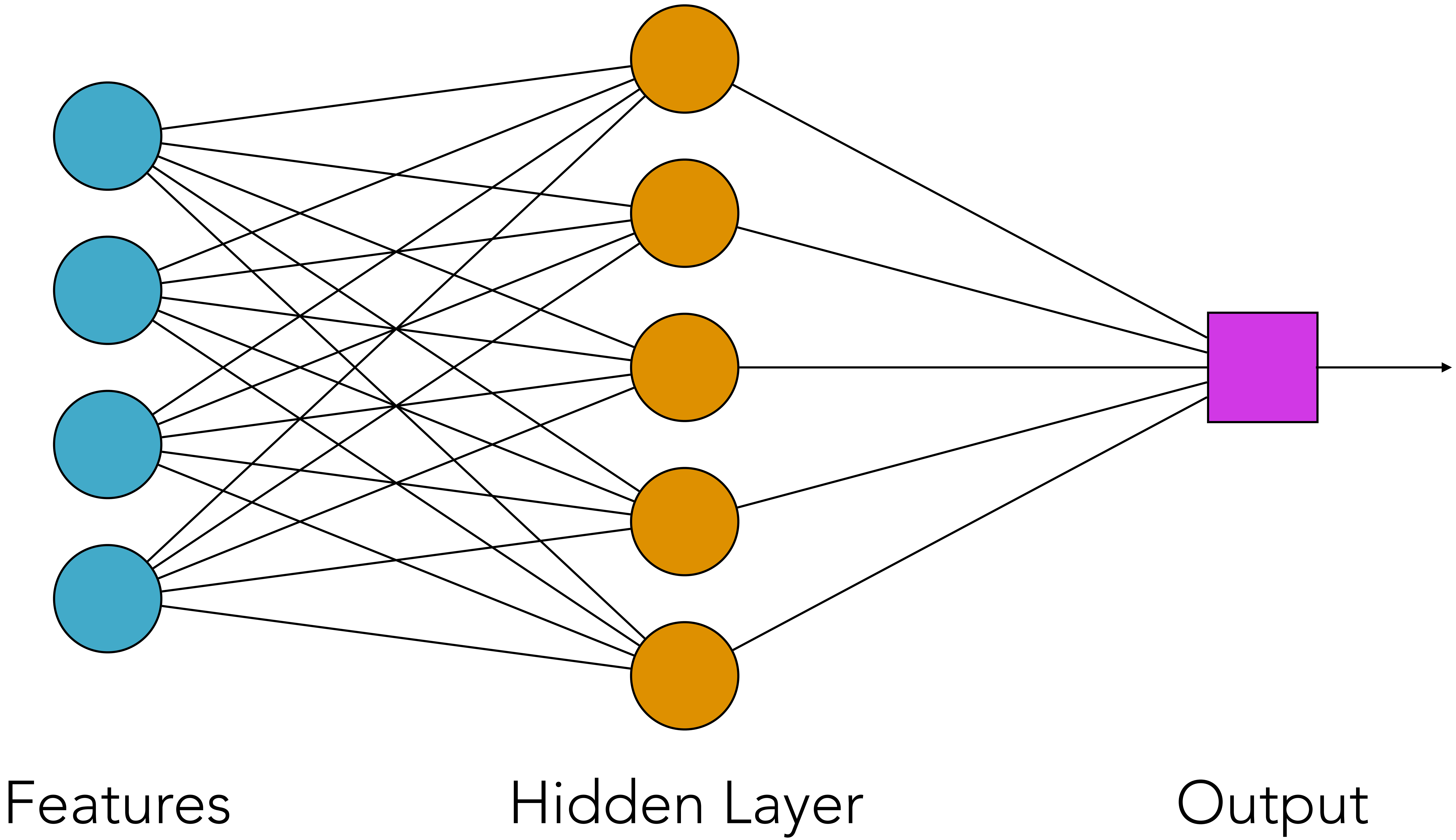
CHECK: HOW MANY TRAINABLE PARAMETERS?

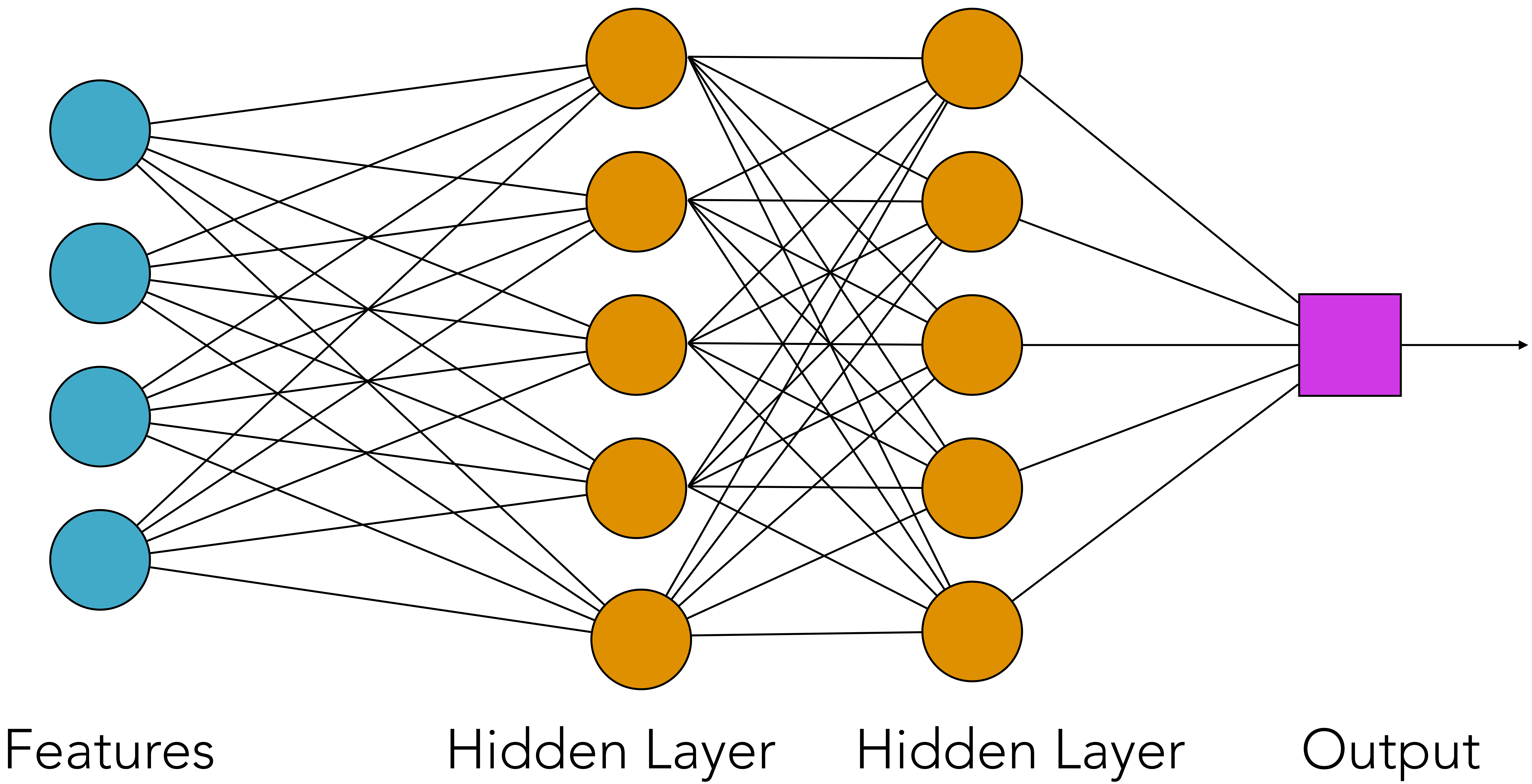




Features

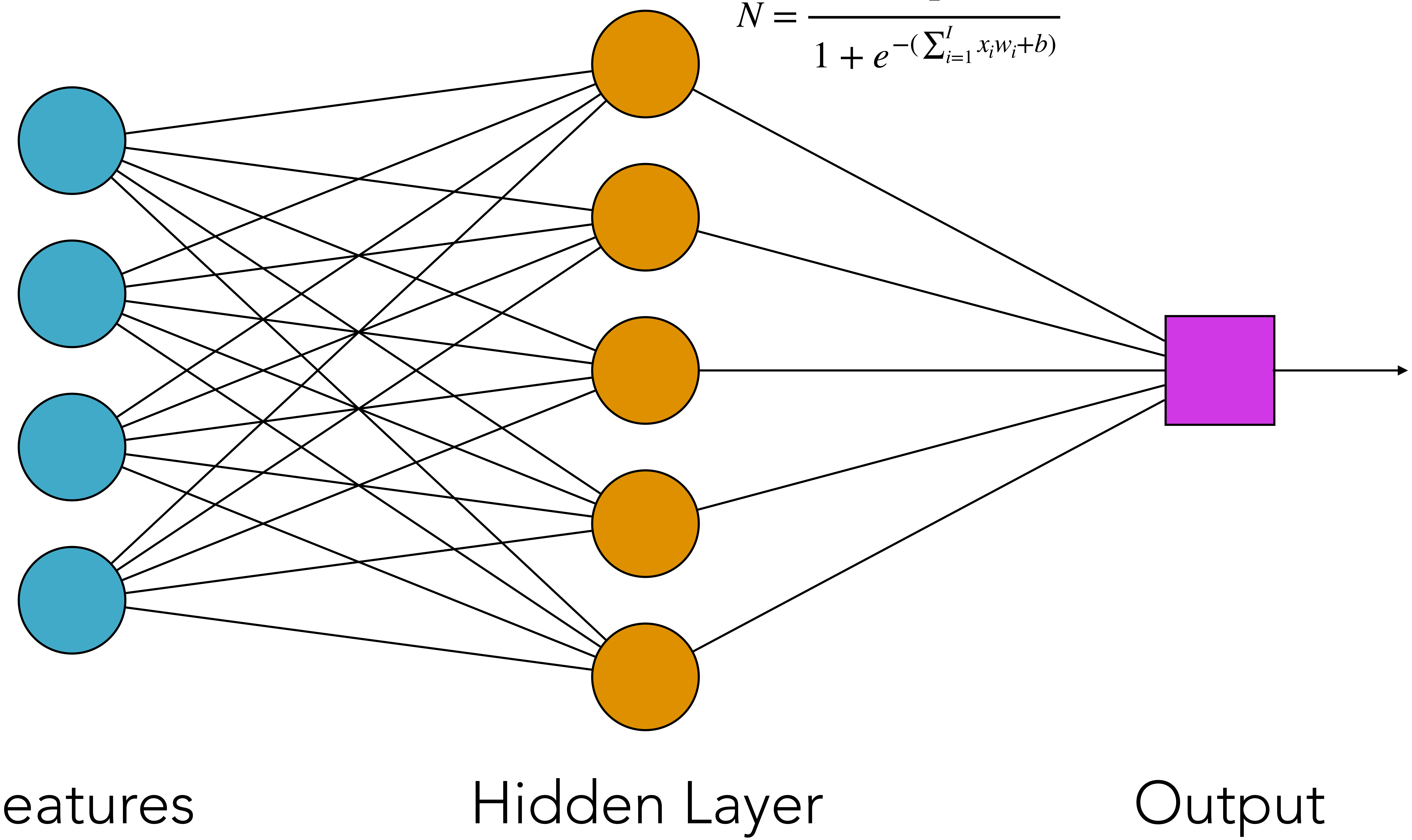

Features
Hidden Layer


Features
Hidden Layer
Output


Features
Hidden Layer
Hidden Layer
Output

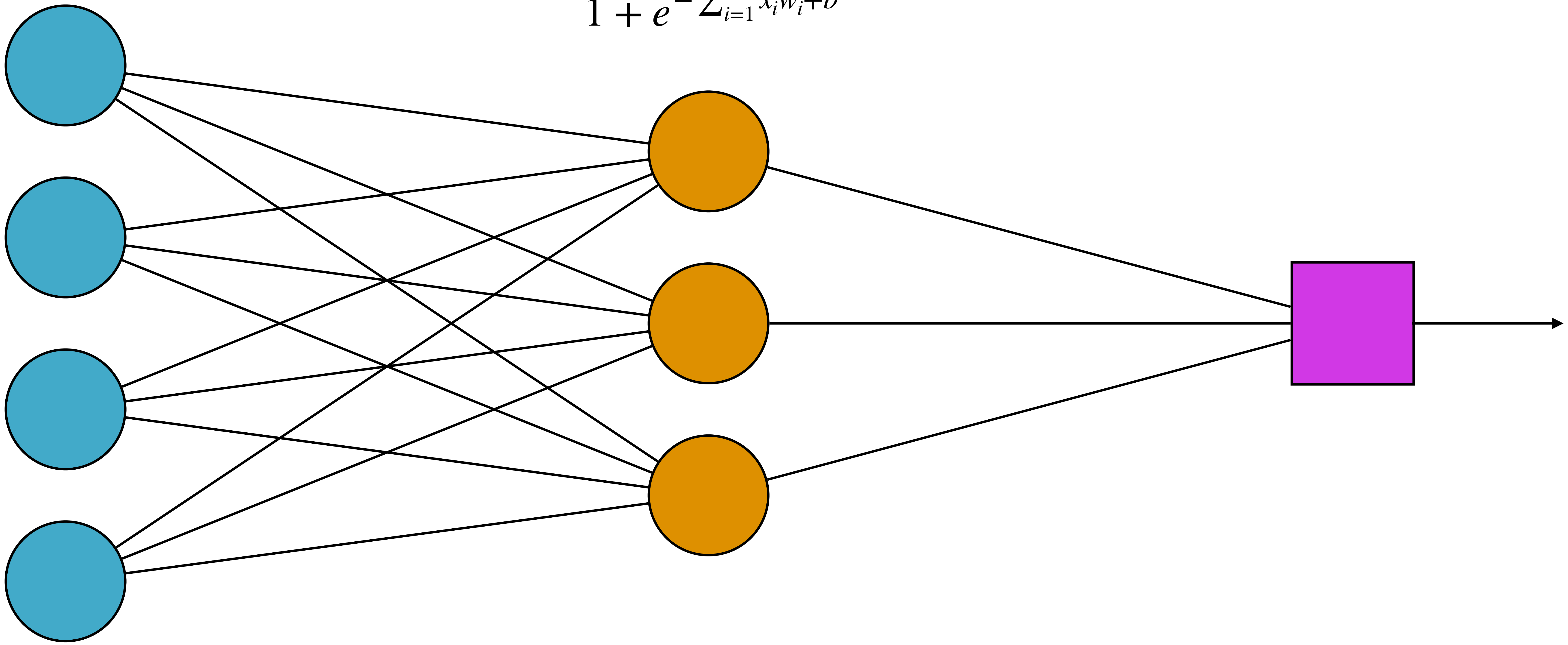
CHECK: HOW MANY TRAINABLE PARAMETERS?

$$N = \frac{1}{1 + e^{-(\sum_{i=1}^{I} x_i w_i + b)}}$$



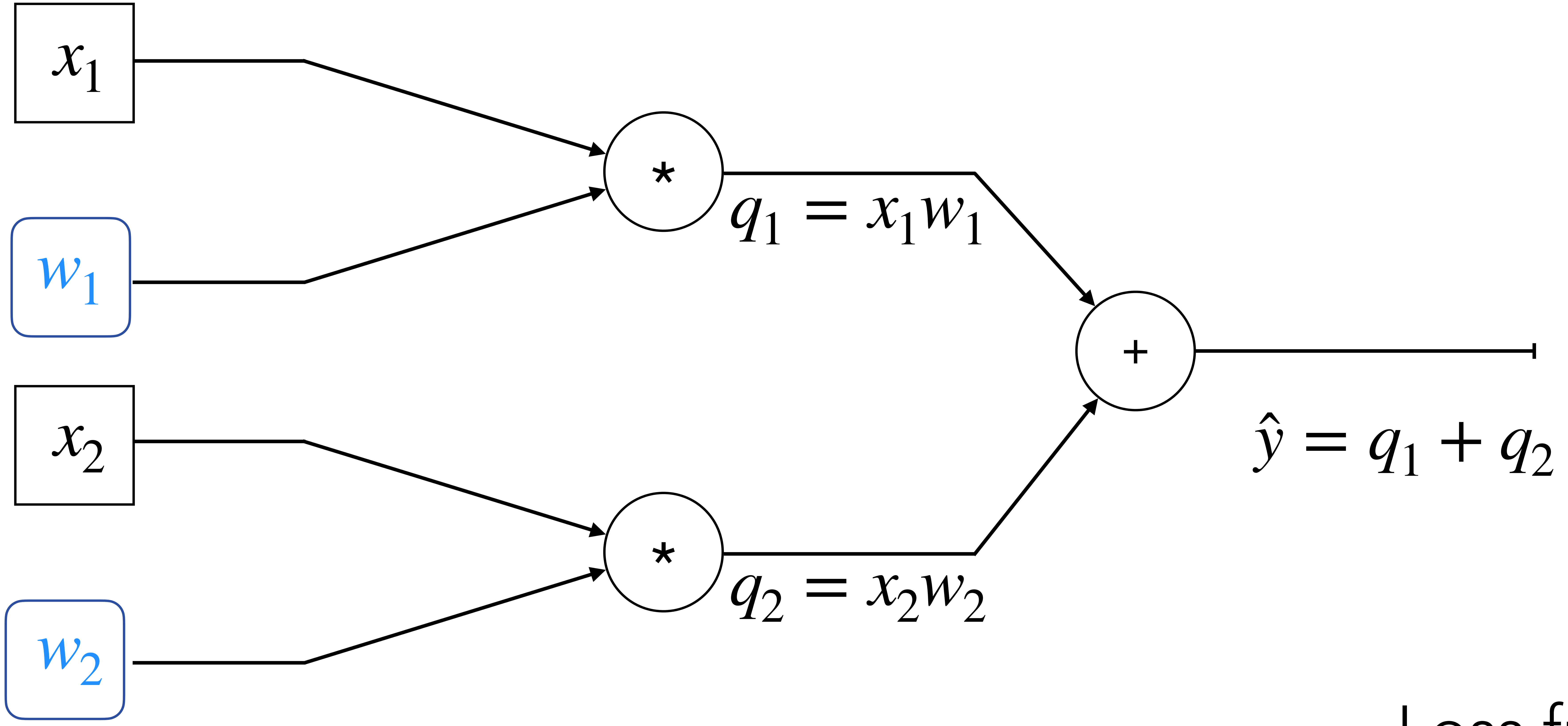
CHECK: HOW MANY TRAINABLE PARAMETERS?

$$N = \frac{1}{1 + e^{-\sum_{i=1}^{I} x_i w_i + b}}$$



Features Hidden Layer Output

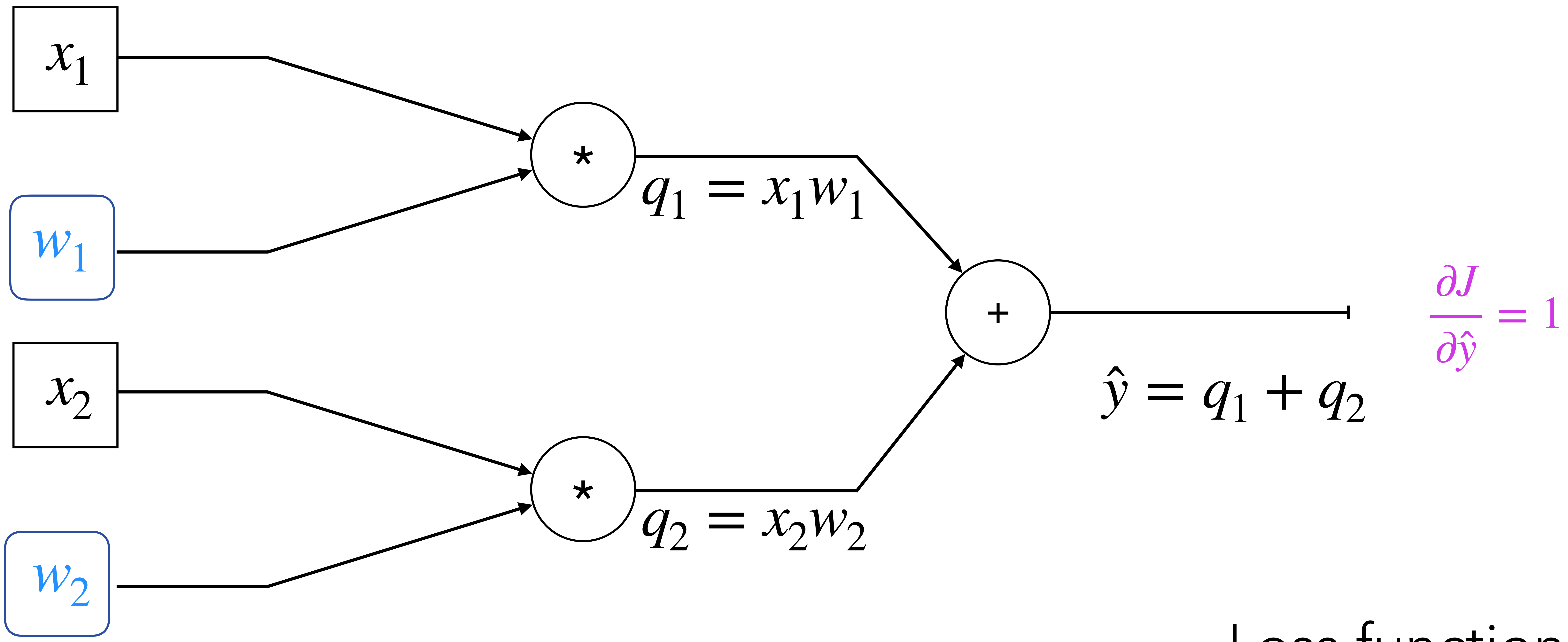
BACKPROPAGATION



Loss function

$$J(w) = \hat{y} - y$$

BACKPROPAGATION



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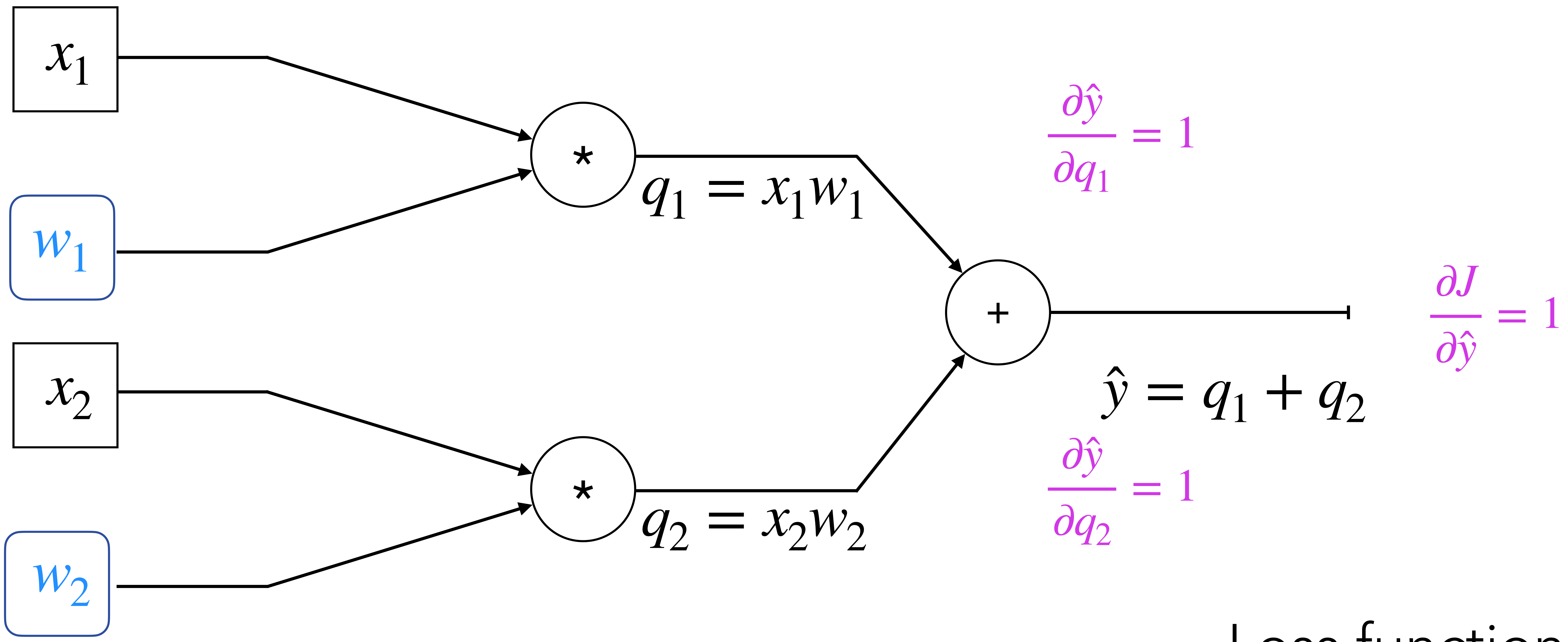

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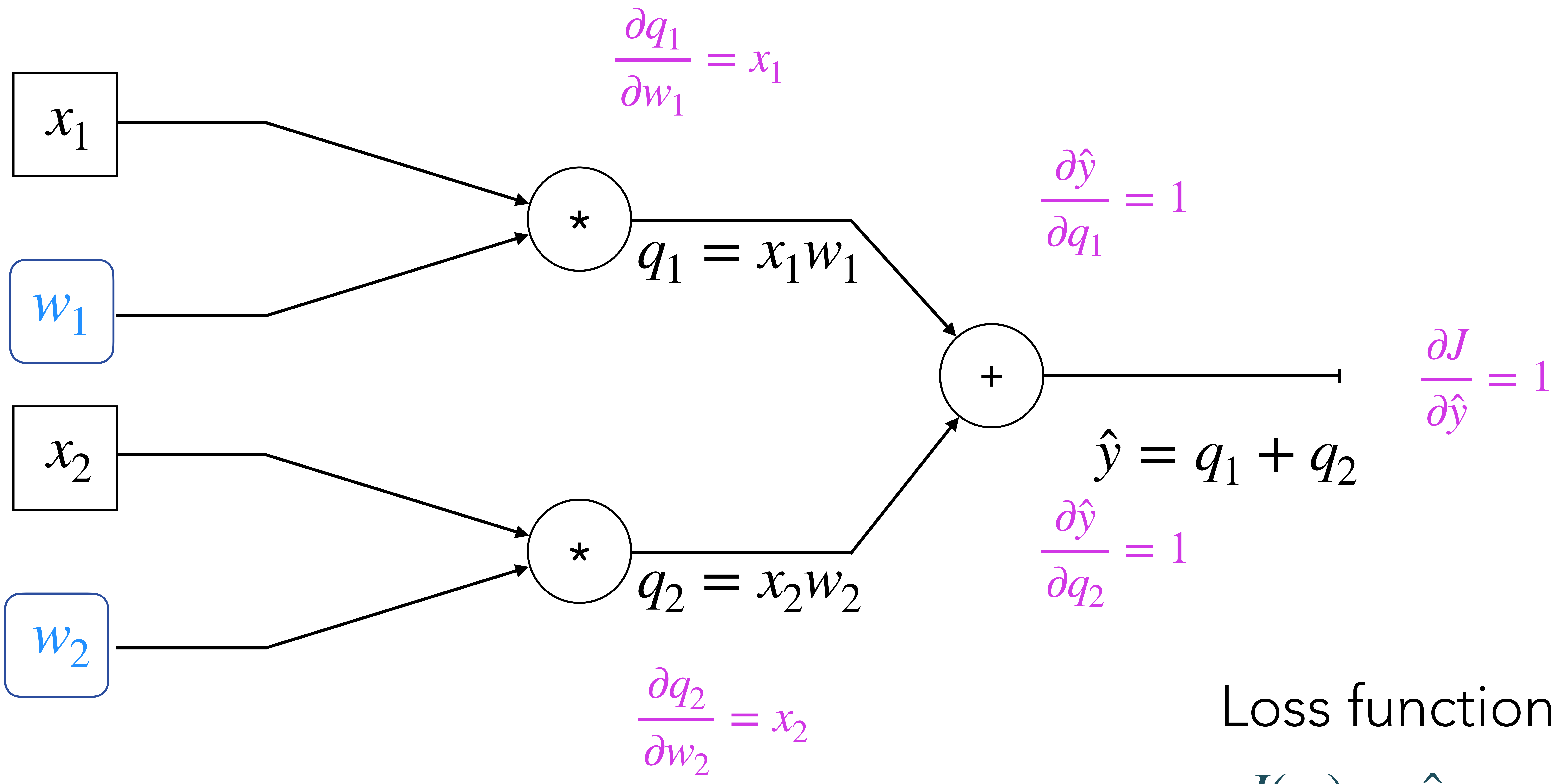

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BACKPROPAGATION

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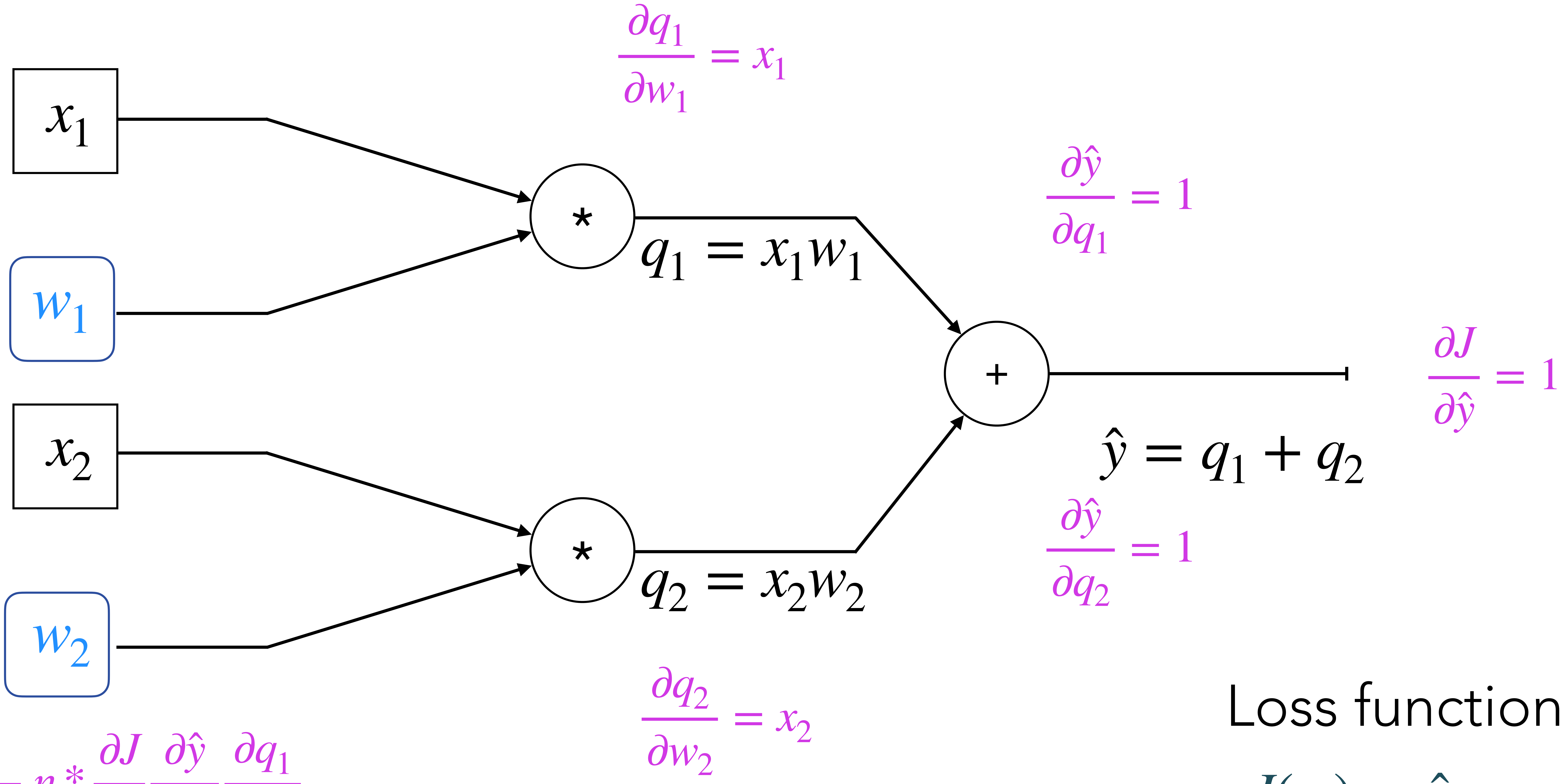
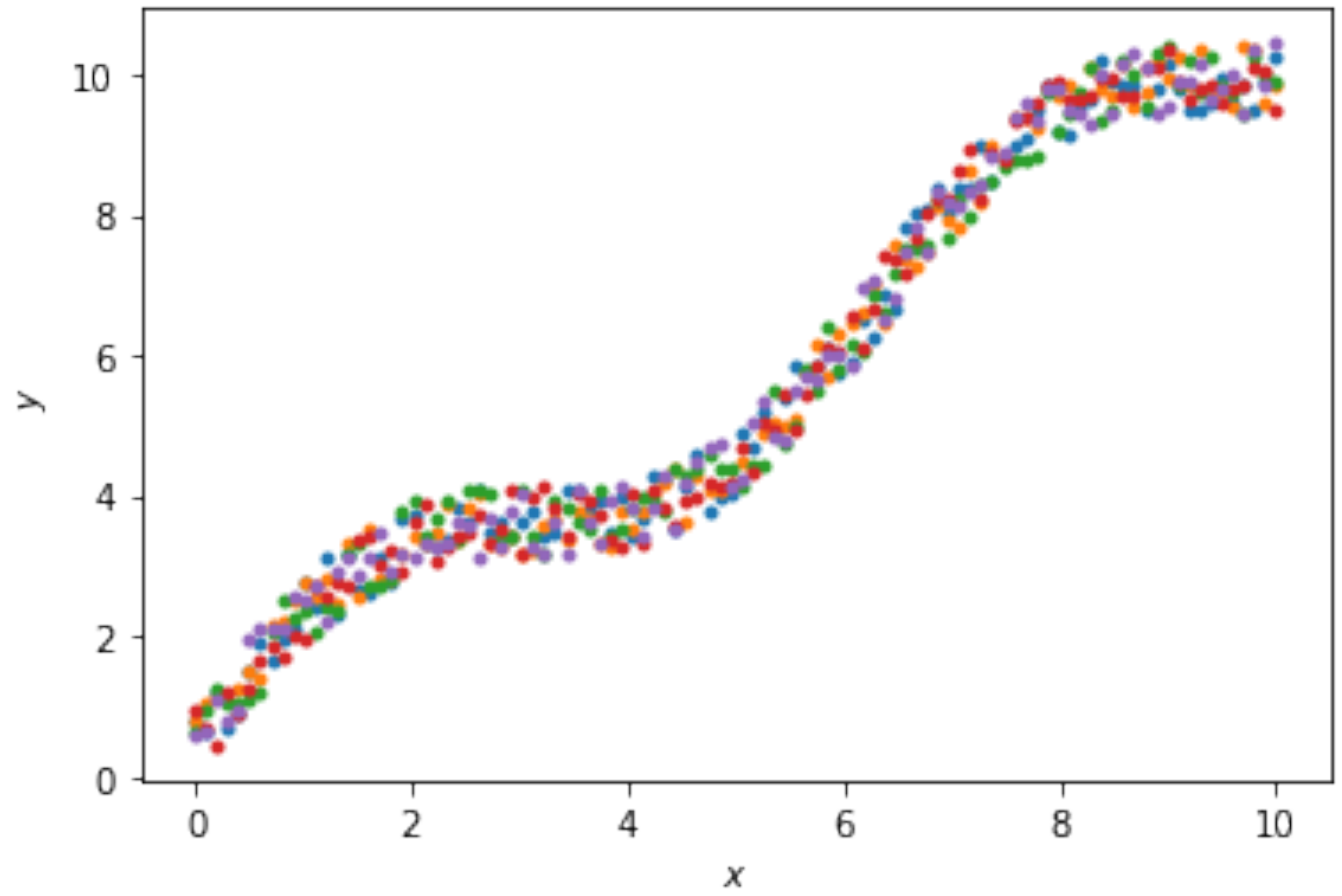


$$w_2 = w_2 - \eta * \frac{\partial J}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial q_2} \frac{\partial q_1}{\partial w_2}$$

Loss function

$$J(w) = \hat{y} - y$$

LOSS FUNCTIONS



Loss function

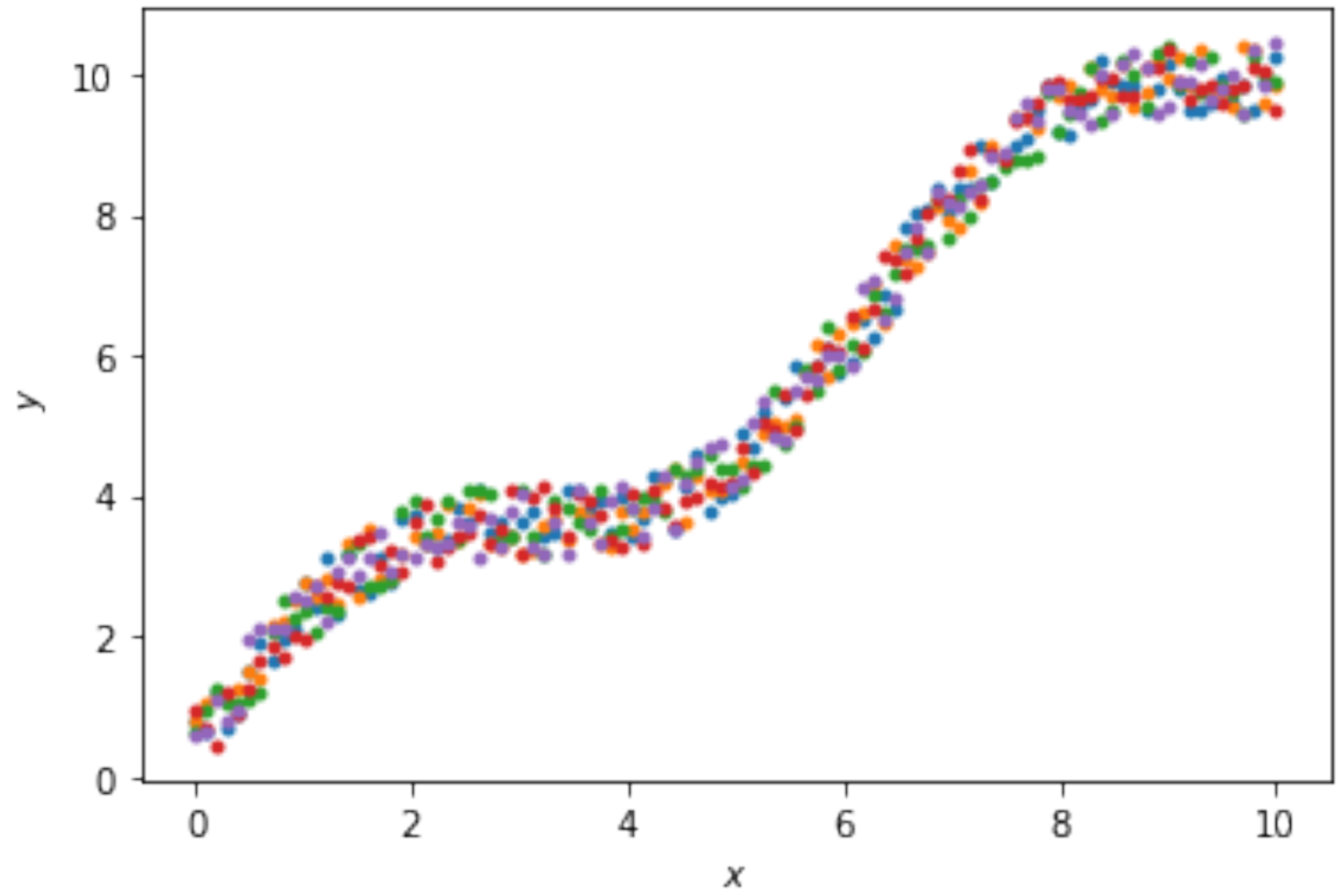
Mean squared error (MSE)

$$J(w) = \frac{1}{N}\sum_{i=0}^{N}(\hat{y}_i - y_i)^2$$

Mean absolute error (MAE)

$$J(w) = \frac{1}{N}\sum_{i=0}^{N}|\hat{y}_i - y_i|$$

LOSS FUNCTIONS



Loss function

Mean squared error

mean

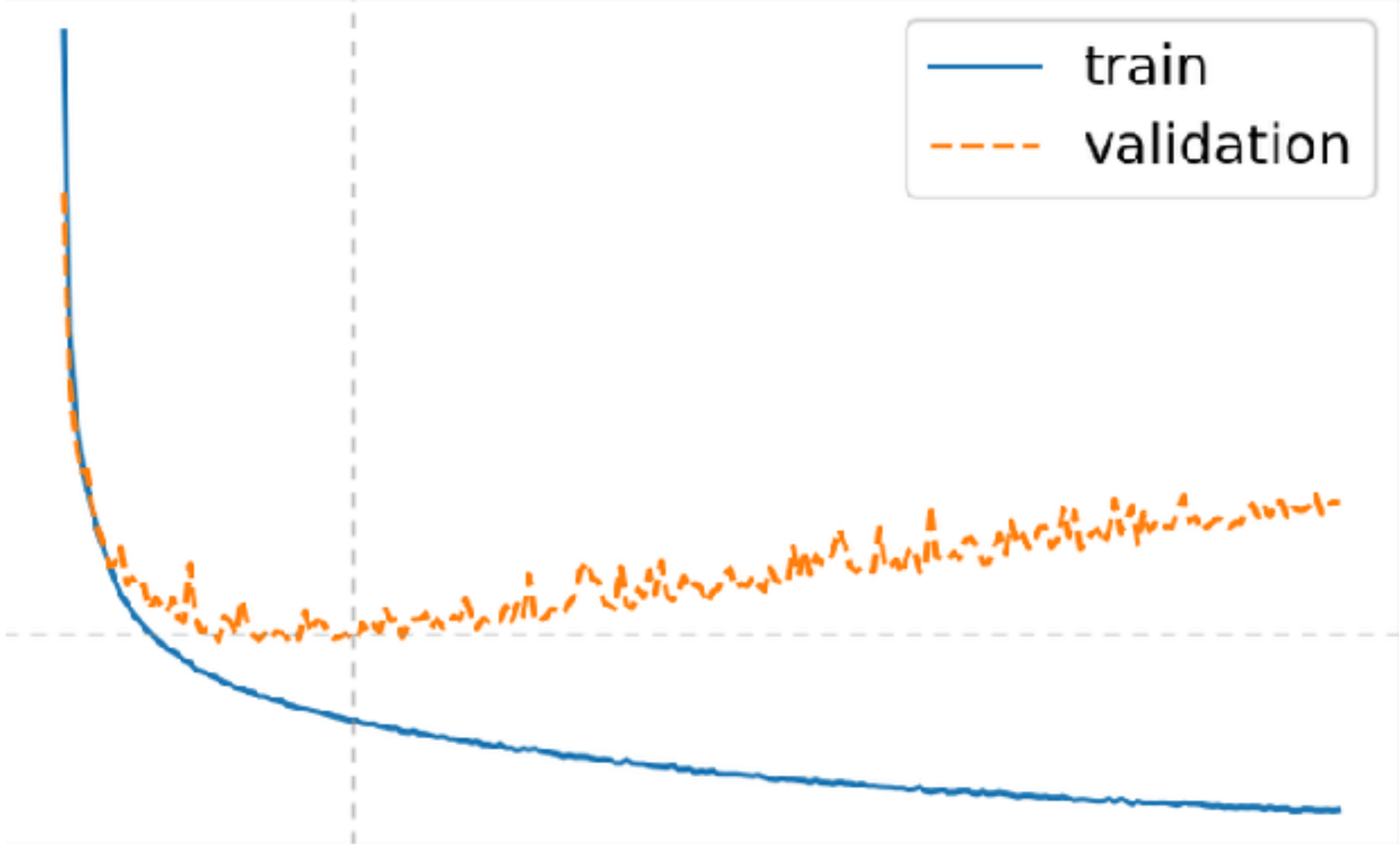
$$J(w) = \frac{1}{N} \sum_{i=0}^{N} (\hat{y}_i - y_i)^2$$

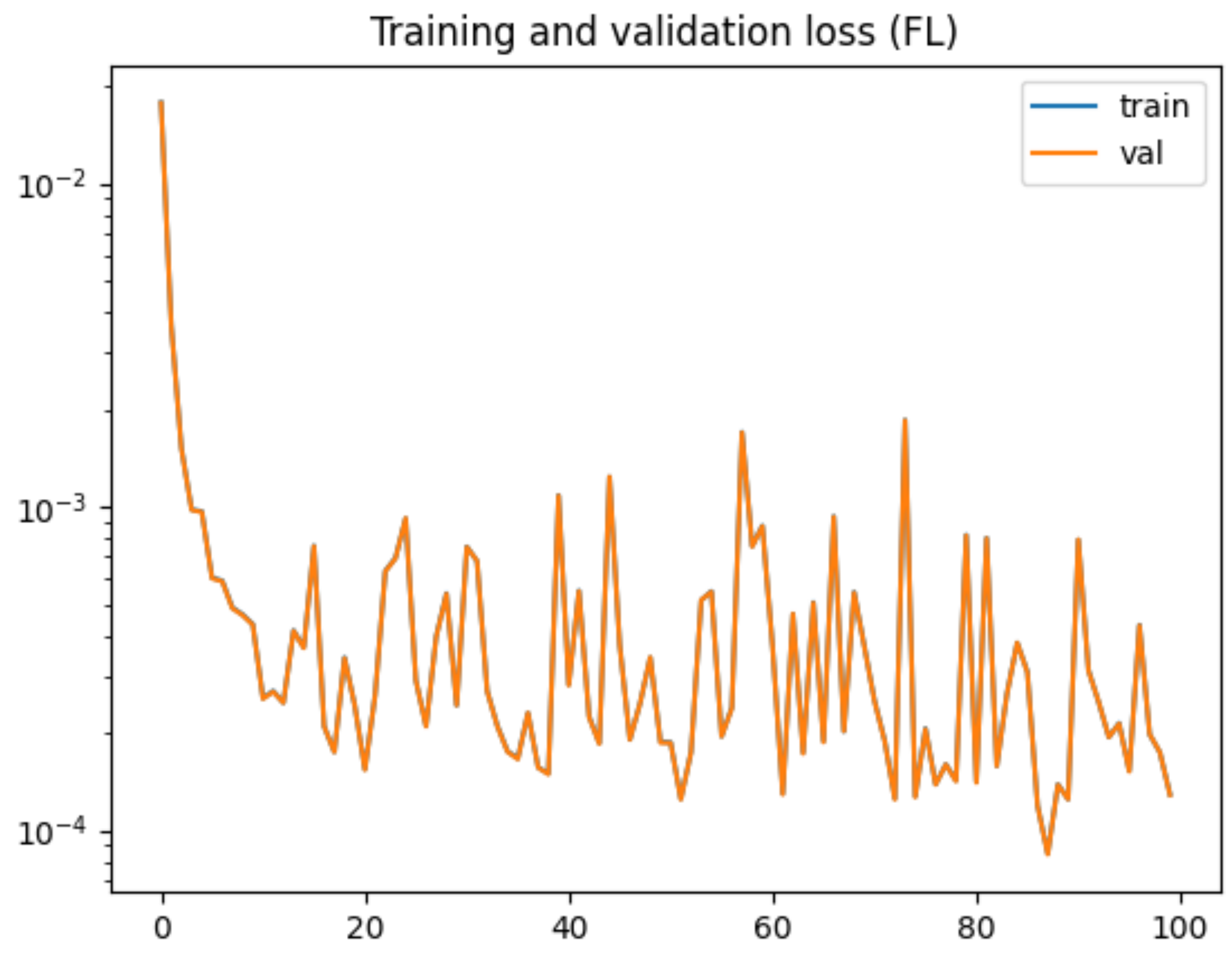
Mean absolute error

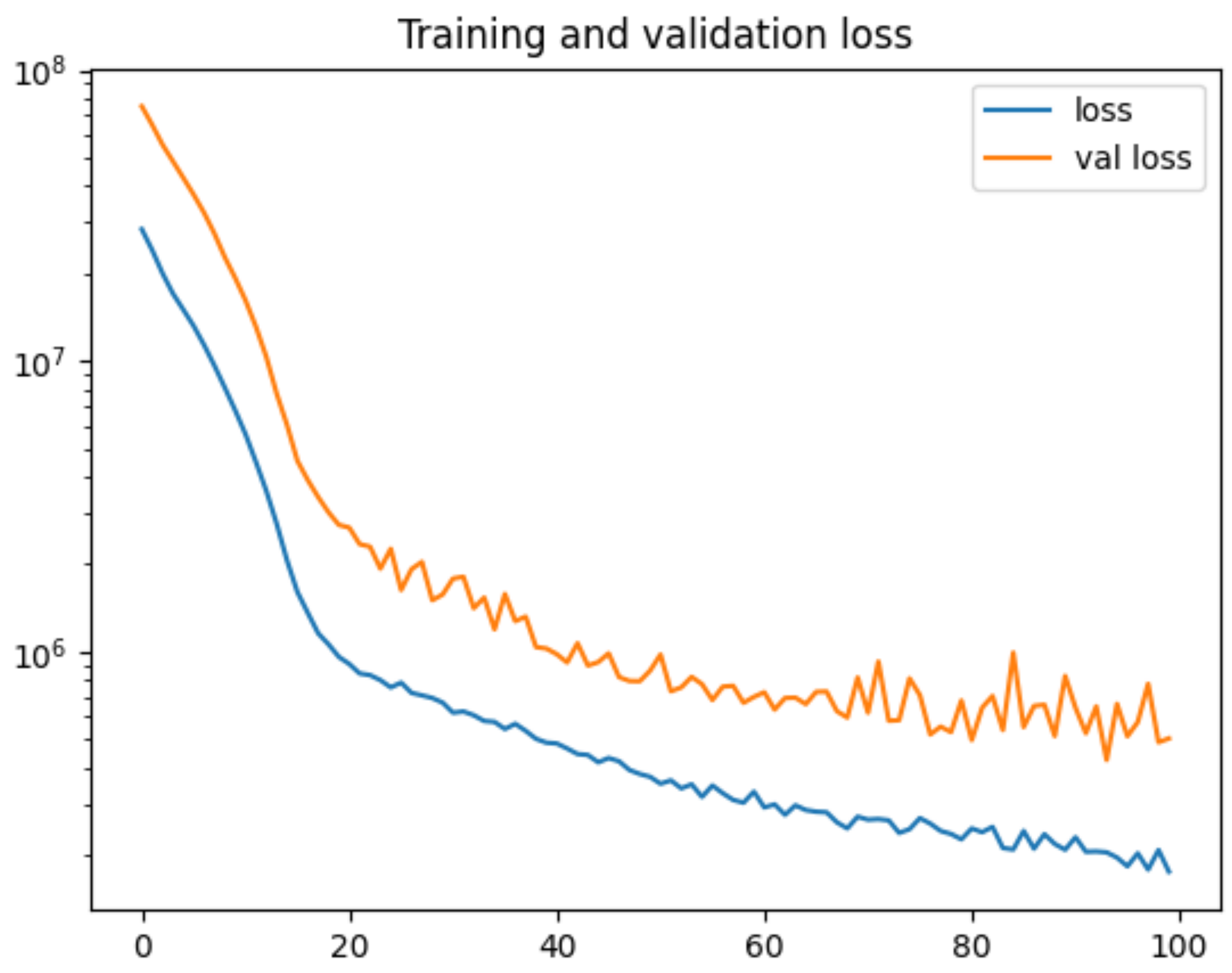
median

$$J(w) = \frac{1}{N} \sum_{i=0}^{N} |\hat{y}_i - y_i|$$

LEARNING (LOSS) CURVES



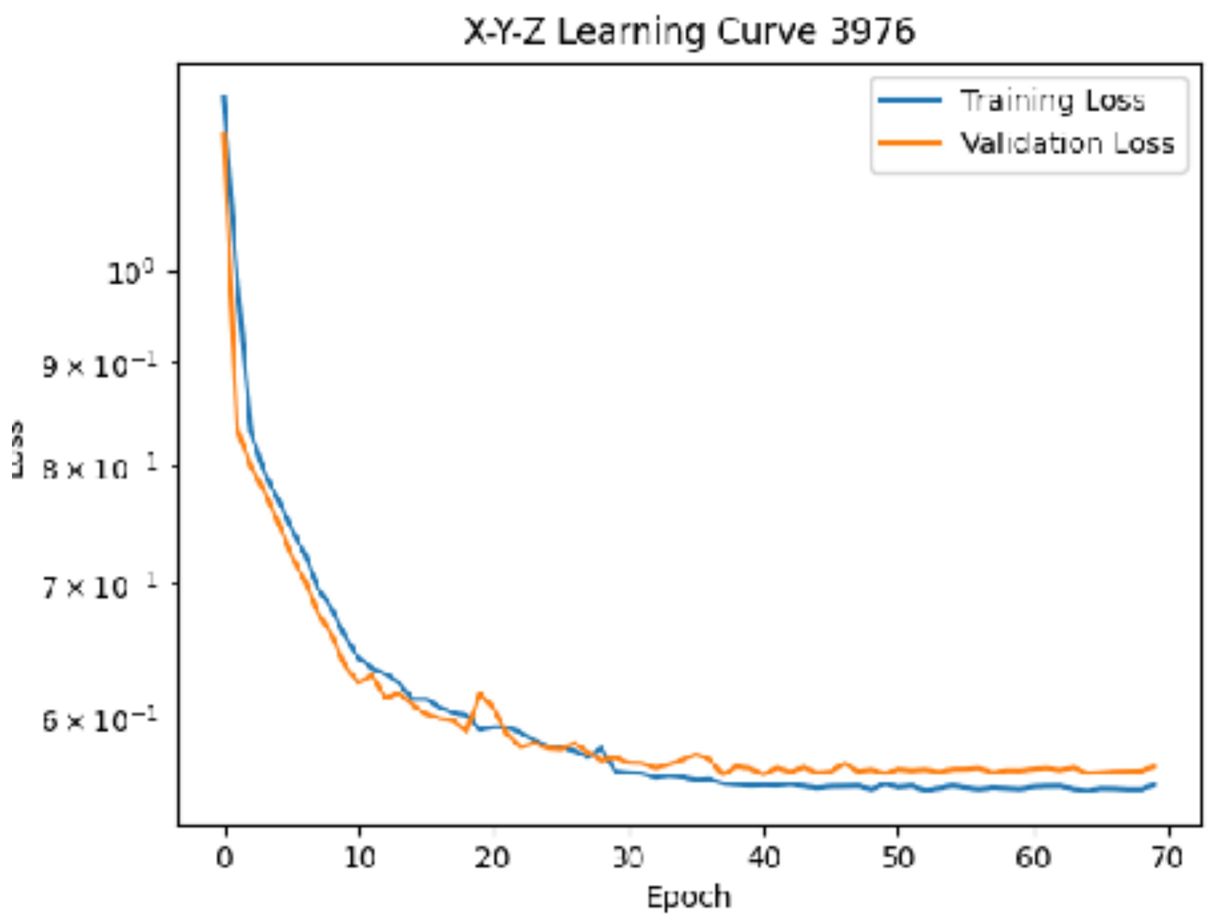


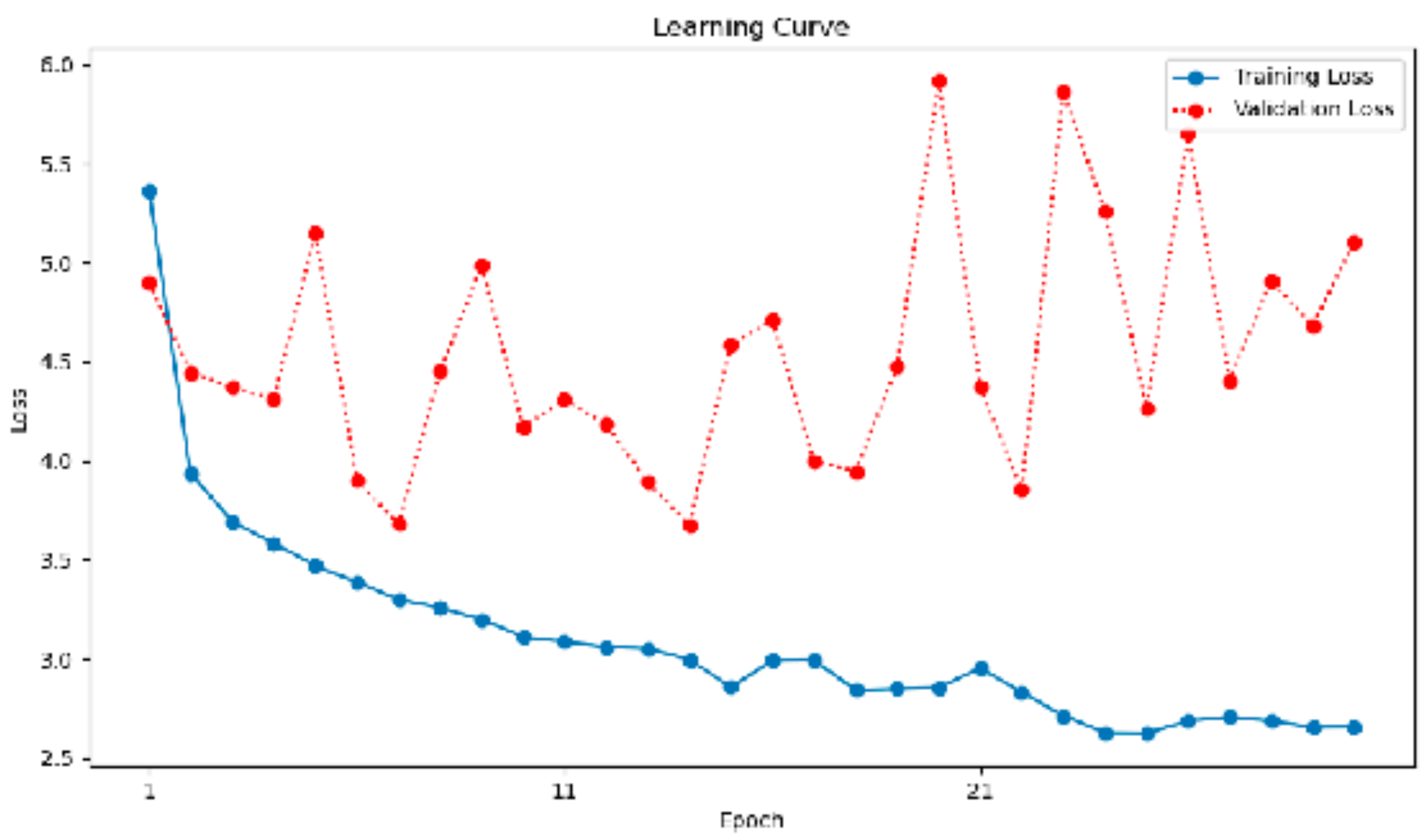


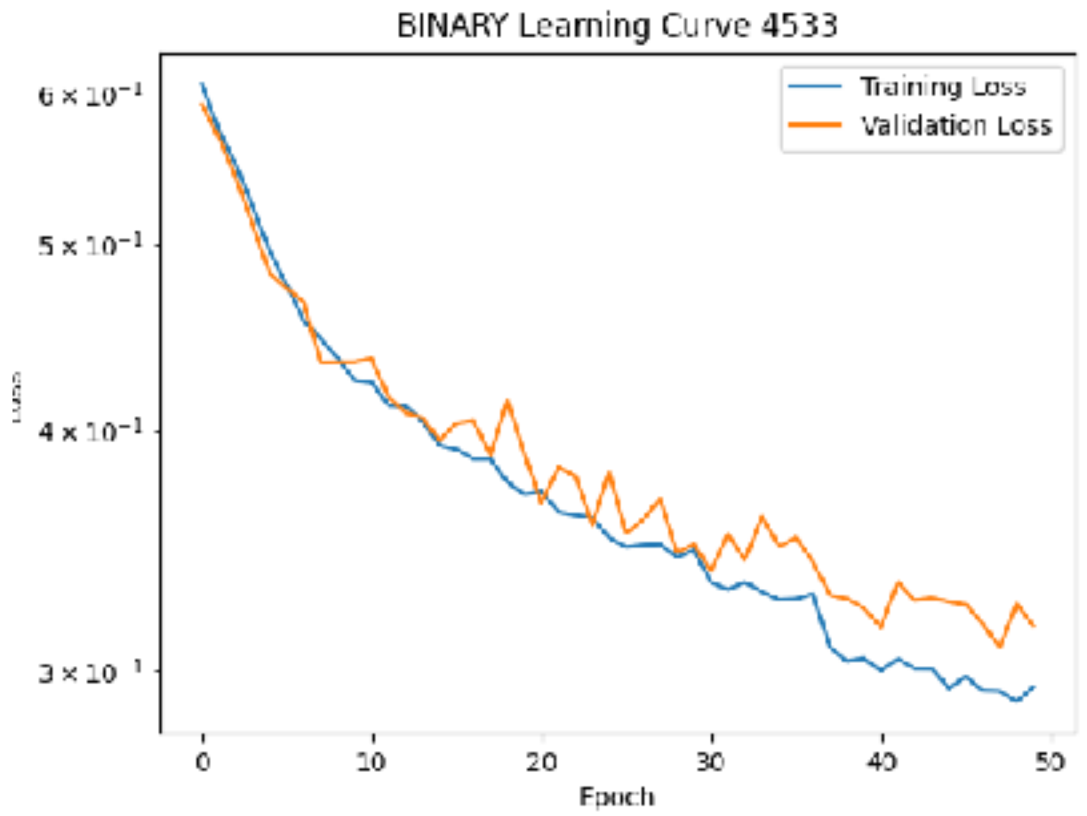
TRAINING

Remember that our goal is NOT to minimize loss on training data!

Learning curves







AUTOMATIC DIFFERENTIATION

TensorFlow PyTorch

Keras

MODERN NEURAL NETWORK ARCHITECTURES

CHRISTIAN SZEGEDY ET. AL. GOING DEEPER WITH CONVOLUTIONS.

“GoogLeNet network with all the bells and whistles”

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PRACTICAL TIPS FOR TRAINING MODELS

DATA

	Feature 1	Feature 2	Feature 3	Target
Example 1				
Example 2				
Example 3				
Example 4				

NORMALIZATION

- Puts each feature on same scale
- Allows default hyperparamters to be a good starting point
  - learning rate, initialization of weights, etc.
- Options depend on data distribution
  - Standardization: mean: 0 stdev: 1
  - Min-max: [0,1]

DATA

	Feature 1	Feature 2	Feature 3	Target
Example 1				
Example 2				
Example 3				
Example 4				

ENCODING

- Non-numeric data
- Class-based features:
  - One-hot encoding: 3 → [0 0 1] [0 1 0] [1 0 0]

WHY??

DATA

	Feature 1	Feature 2	Feature 3	Target
Example 1				
Example 2				
Example 3				
Example 4				

ENCODING

- Non-numeric data
- Class-based features:
  - One-hot encoding: 3 → [0 0 1] [0 1 0] [1 0 0]
  - When classes do not have sequential meaning: ✅ cars vs dogs vs plants ❌ months

BUILDING AND TRAINING MODELS

TRAINING

- The most challenging part of machine learning is gaining the experience for tuning models well.
- We will work on this skill!

COMMUNITY

- Each of you arrived here with your own backgrounds, specialty, and path in life
- Your experience and expertise are valuable here, no matter what it is
- If the activity is within your background, help others!
- If you are totally (or a little) lost, ask for help!
- It is our shared goal to have **each** of us leave with some new skill/knowledge/understanding