

Neural Networks: Basic Structure, Representation Power

Machine Learning Course - CS-433

Nov 8, 2022

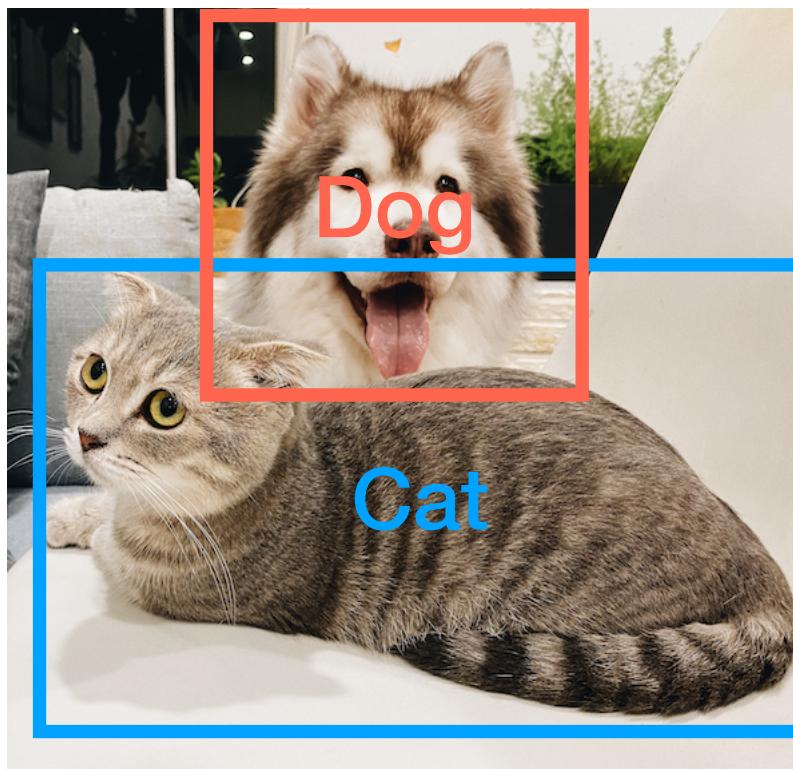
Nicolas Flammarion



Deep Learning: ML Breakthrough

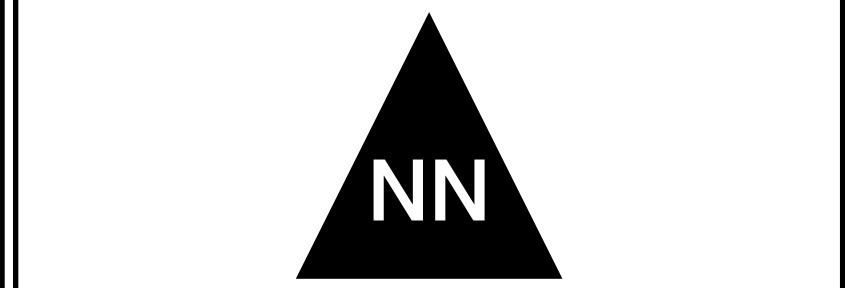
State of the art performance across a broad range of useful tasks

Object Detection



Translation

elle est très intelligente



she is very smart

Speech to Text

hey Siri next song

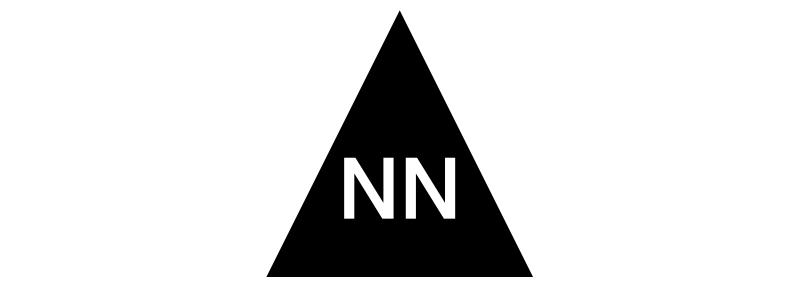
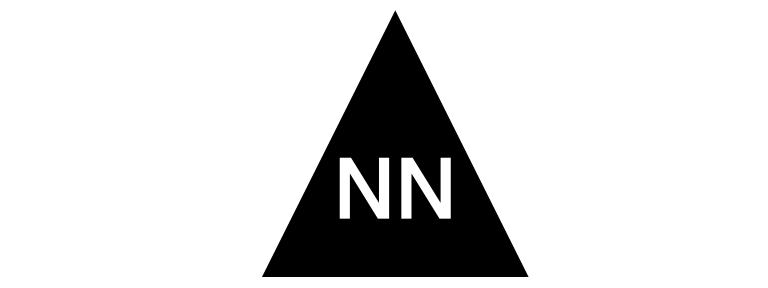
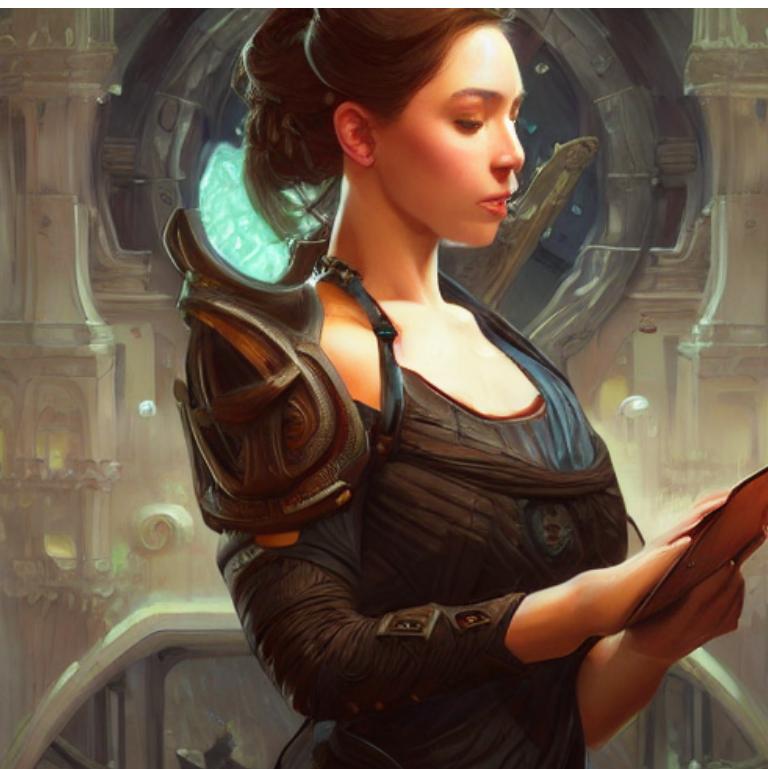
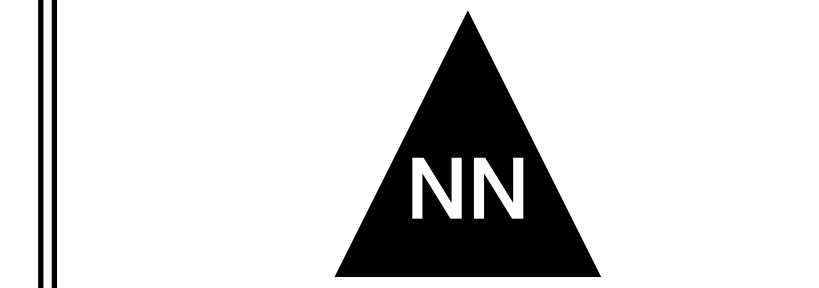


Image Generation

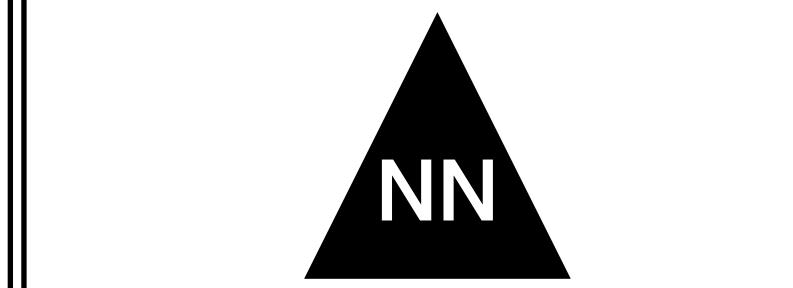


student studying machine learning

Playing Chess



Protein Folding



MAGELVSFAVNKLWDLLSHEYTLFQGVEDQ
VAELKSDLNLLKSFLKDADAKHHTSALVRY
CVEEIKDIVYDAEDVLETFVQKEKLGTTSGIR
KHIKRLTCIVPDRREIALYIGHVSKRITRVIRD
MQSFGVQQMIVDDYMHPLRNRREREIRRTF
PKDNESGFVALEENVKKLVGYFVEEDNYQV
VSITGMGLGLKTTLARQVFNHDMDVTKKFD
KLAWSVSQDFTLKNWQNILGDLKPKEEE
TKEEEKKILEMTEYTLQRELYQLLEMSKSLI
VLDDIWKKEDWEVIKPIFPPTKGWKLLLSR
NESIVAPNTKYFNFKPECLKTDDSWKLQF
RIAFPINDASEFEIDEEMEKLGEKMIEHCGG
LPLAIKVGGMLAEKYTSMDWRRRLSENIGS
HLVGGRTNFNDDNNNSCNYVLSLSFEELPS
YLKHCFLYLAHFPEDYEIKVENLSYYWAAEE
IFQPRHYDGEIIRDVGDVYIEELVRRNM.....

Why Neural Networks?

Supervised learning:

- Have training data $S_{\text{train}} = \{x_n, y_n\}_{n=1}^N \in \mathcal{X} \times \mathcal{Y}$
- Goal: Find a mapping $\mathcal{X} \rightarrow \mathcal{Y}$ that can predict y for a new x

Classical Machine Learning:

- Relatively simple models on top of **features handcrafted by domain experts**
- Only works well when used with **good features**

Deep Learning:

- Large neural networks that **learn features directly from the data**
- Can be viewed as a complicated feature extractor + linear prediction
- **Requires large amounts of data and compute to train**
- Quality often continues to improve with more data and larger models

The Basic Structure of Neural Networks

Neurons and Logistic Regression

Recap - Logistic Regression:

$$f_{LR}(x) = p(1 | x) = \sigma(x^\top w + b) = \sigma\left(\sum_{i=1}^d x_i w_i + b\right)$$

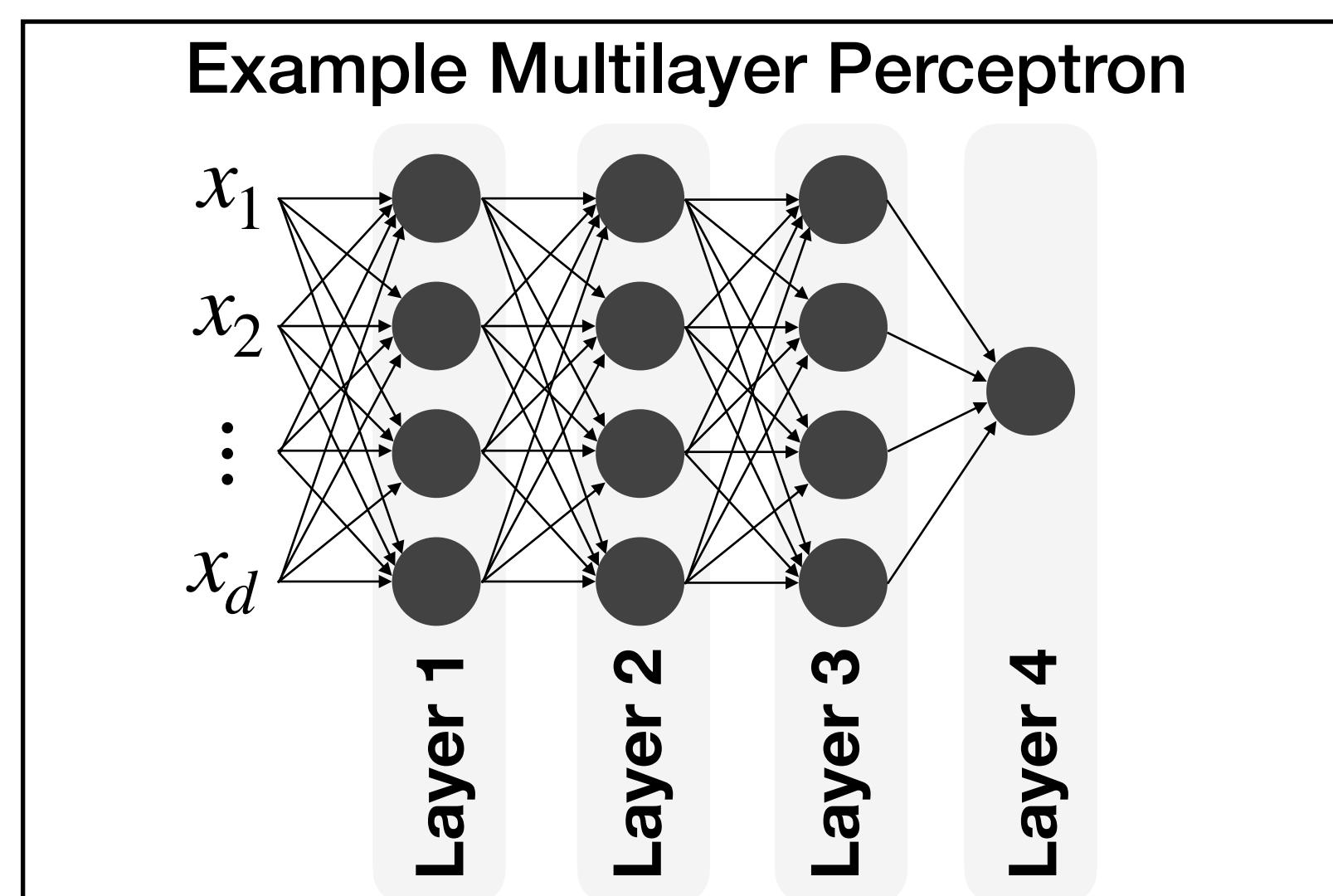
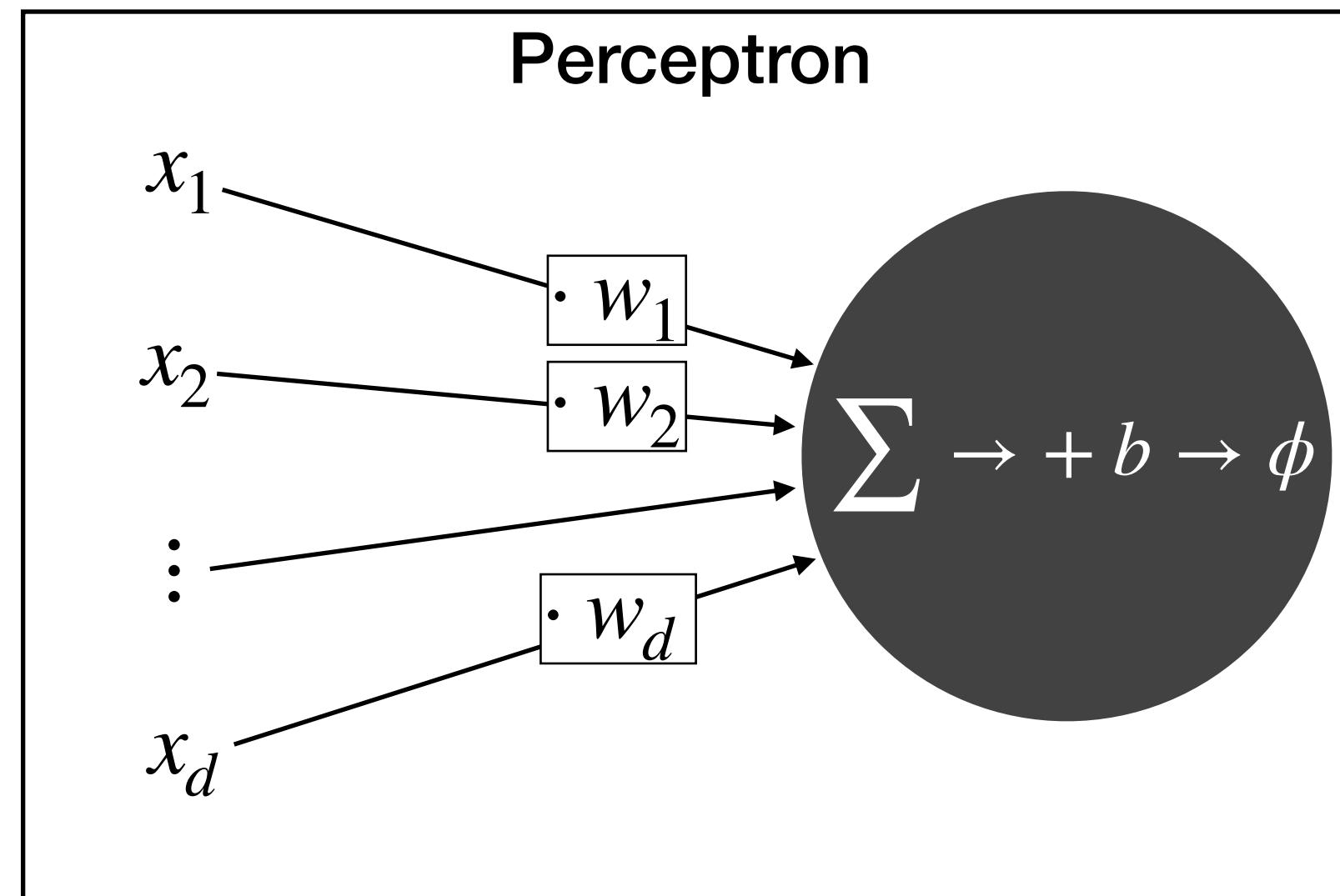
$$\sigma(z) = (1 + \exp(-z))^{-1}$$

Perceptron:

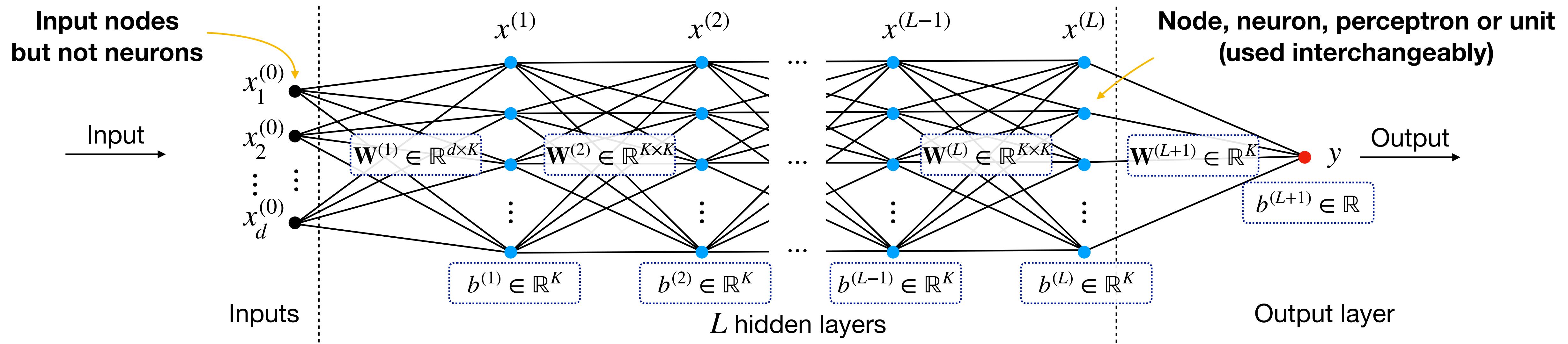
- A simple model of biological neurons
- Activation function ϕ
- Equivalent to f_{LR} when $\phi = \sigma$

Multilayer Perceptron (MLP):

- Arrange perceptrons into layers
- Neurons in later layers receive inputs from prior layer
- Also known as a **fully connected neural network**



Fully Connected Neural Networks



Assume L hidden layers with K neurons each + output layer with single node

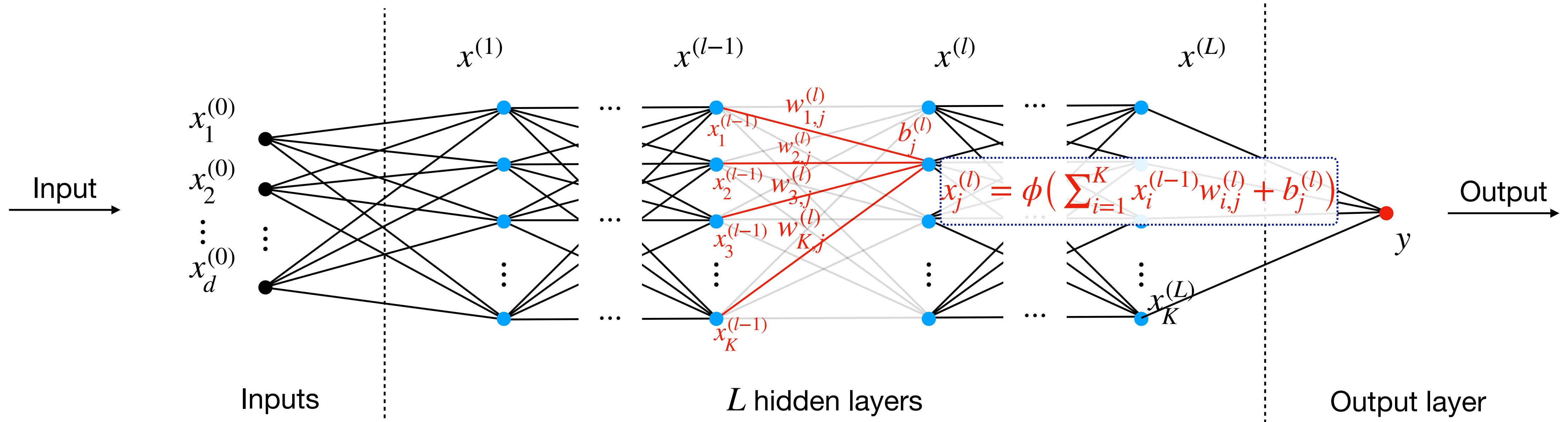
Outputs of hidden layer l given by vector: $x^{(l)} = f^{(l)}(x^{(l-1)}) := \phi((\mathbf{W}^{(l)})^\top x^{(l-1)} + b^{(l)})$

Elementwise

Learnable Parameters: Weight matrices $\mathbf{W}^{(l)}$ and bias vectors $b^{(l)}$ for $1 \leq l \leq L + 1$

- Each column of $\mathbf{W}^{(l)}$ corresponds to the weights of one perceptron

Single Neuron View



$$x_j^{(l)} = \phi\left(\sum_{i=1}^K x_i^{(l-1)} w_{i,j}^{(l)} + b_j^{(l)}\right)$$

Important: ϕ is non-linear
otherwise we can only
represent linear functions

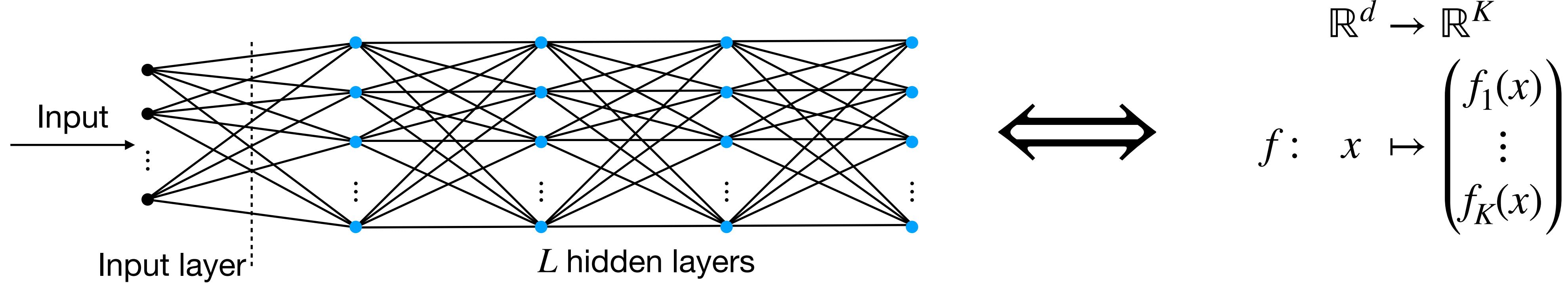
weight of the edge going from node i
in layer $l - 1$ to node j in layer l

bias term associated with
node j in layer l

NNs extract suitable features from the input

A NN can be decomposed into a feature extractor and the output layer.

Feature extractor from \mathbb{R}^d to \mathbb{R}^K :

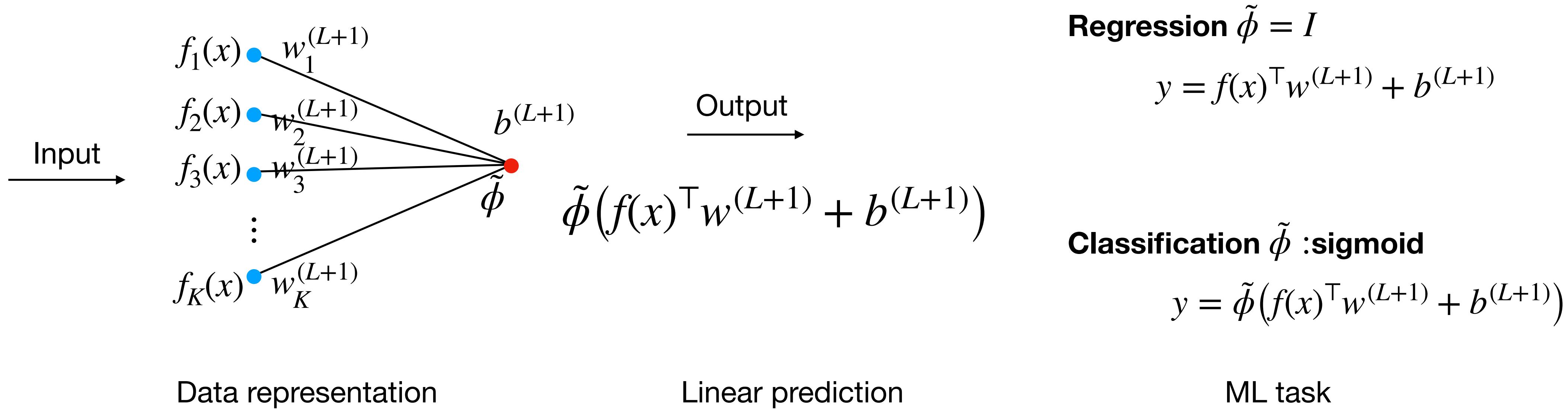


This function is defined by

- The biases $\{b^{(l)}\}_{l \in [L]}$ and weights $\{\mathbf{W}^{(l)}\}_{l \in [L]}$ so we learn
 → $O(dK + K^2L) \approx O(K^2L)$ parameters
- The activation function ϕ we pick

In practice: both L and K are large - overparametrized NNs

The last layer performs the desired ML task



A suitable representation of the data in hands, the last layer only performs a linear regression or classification step

Representational Power of NNs

Three theoretical questions in Deep Learning

- **Expressive power** of NNs: Why are the functions we are interested in so **well approximated** by NNs?
- **Success of naive optimization**: Why does **gradient descent** lead to a good local minimum?
- **Generalization miracle**: Why is there **no overfitting** with so many parameters?

L_2 Approximation: Barron's result

Let $f: \mathbb{R}^d \rightarrow \mathbb{R}$ and define $\hat{f}(\omega) = \int_{\mathbb{R}^d} f(x) e^{-i\omega^\top x} dx$ its Fourier transform

Assumption: $\int_{\mathbb{R}^d} |\omega| |\hat{f}(\omega)| d\omega \leq C$ (smoothness assumption)

Claim: For all $n \geq 1$, it exists a function f_n of the form

$$f_n(x) = \sum_{j=1}^n c_j \phi(x^\top w_j + b_j) + c_0$$

so that

$$\int_{|x| \leq r} (f(x) - f_n(x))^2 dx \leq \frac{(2Cr)^2}{n}$$

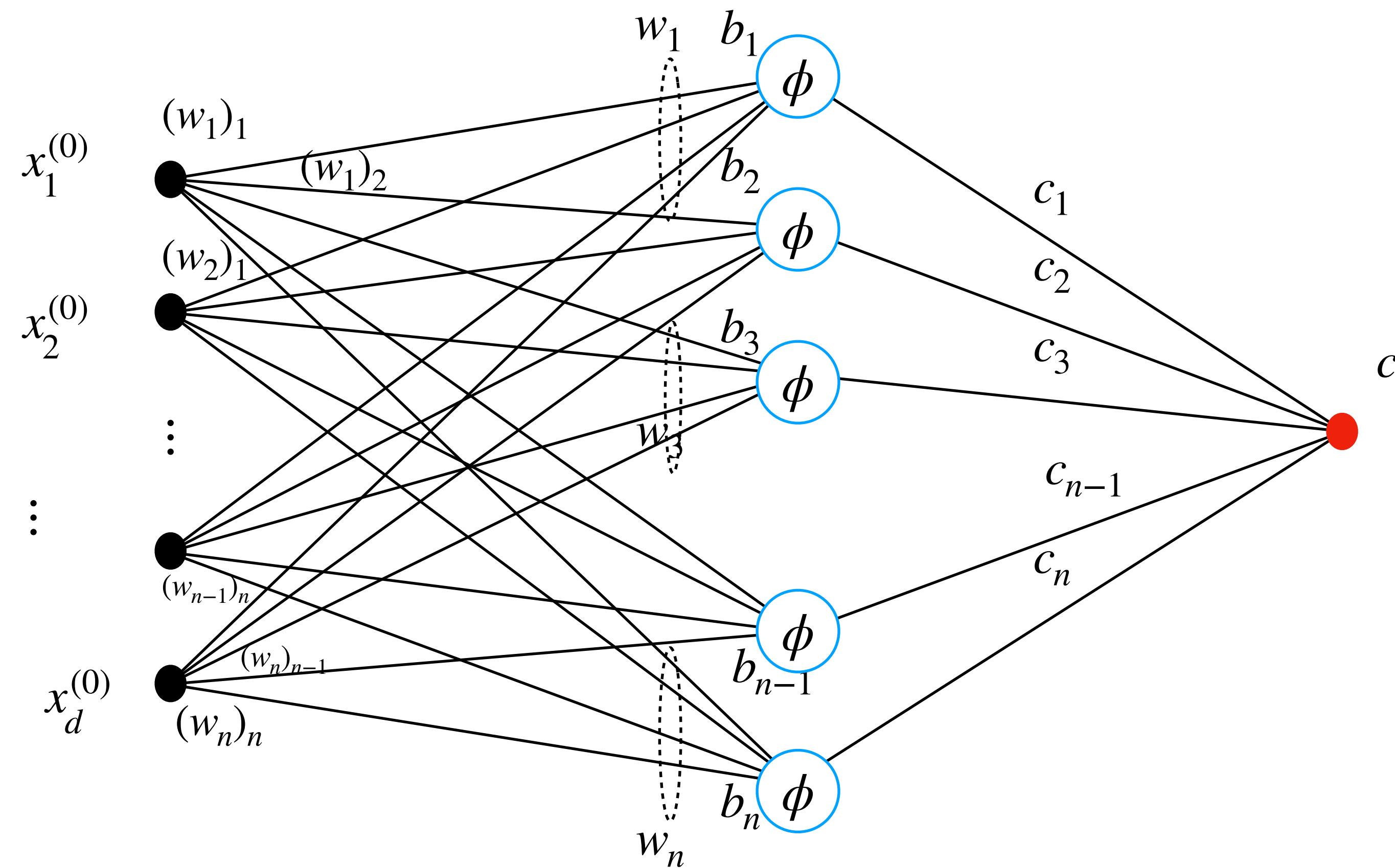
All sufficiently smooth function can be approximated by a one-hidden-layer NN

$$\int_{|x| \leq r} (f(x) - f_n(x))^2 dx \leq \frac{(2Cr)^2}{n}$$

- The more neurons we allow, the smaller the error
- The smoother the function is (the smaller C), the smaller the error
- The larger the domain (the larger r), the worse the error
- Approximation in average (in ℓ_2 -norm)
- For any “sigmoid-like” activation function

The function f_n is a one-hidden-layer NN with n nodes

$$f_n(x) = \sum_{j=1}^n c_j \phi(x^\top w_j + b_j) + c_0 = c^\top \phi(W^\top x + b) + c_0$$

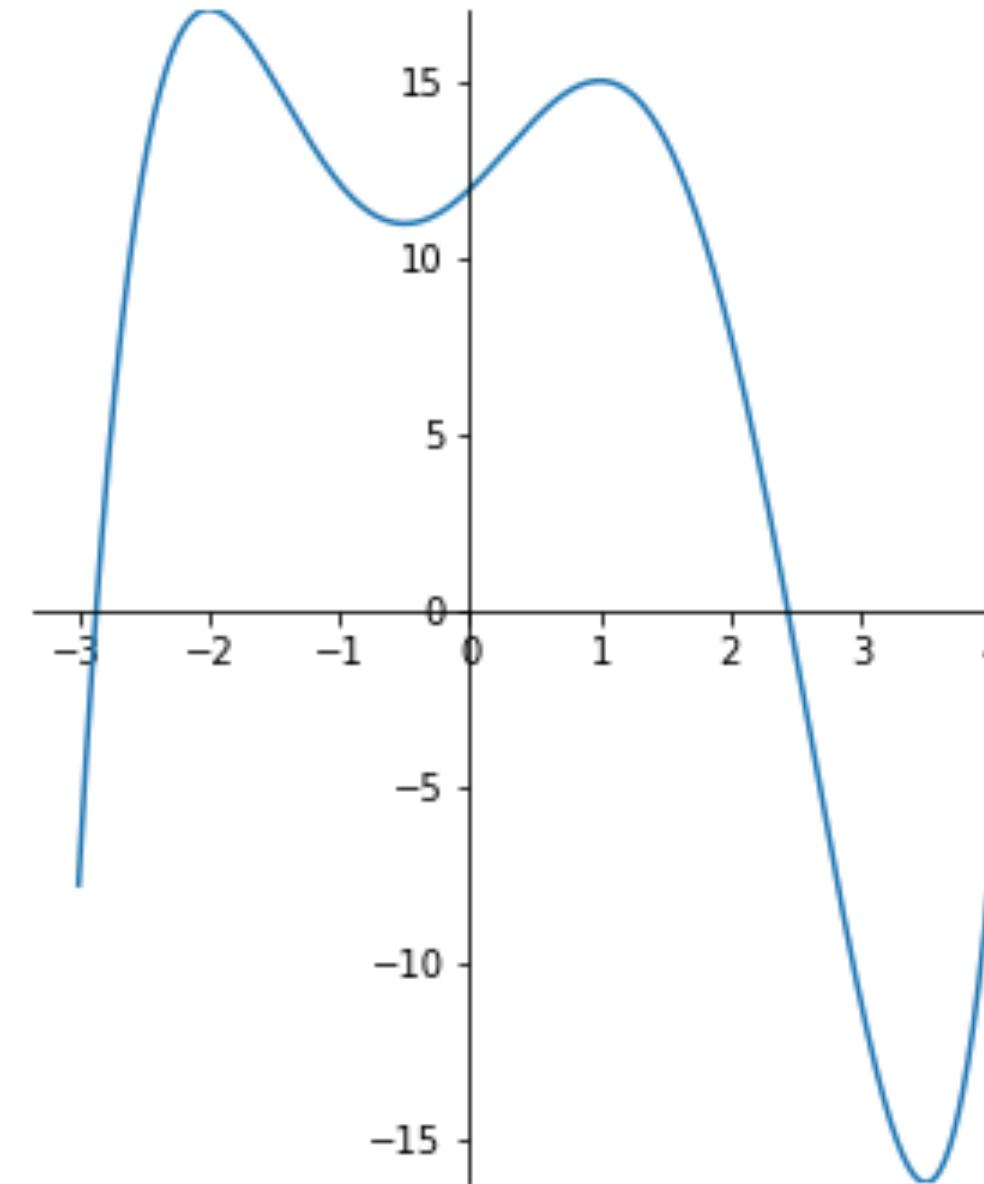


L_1 Approximation: Proof by picture

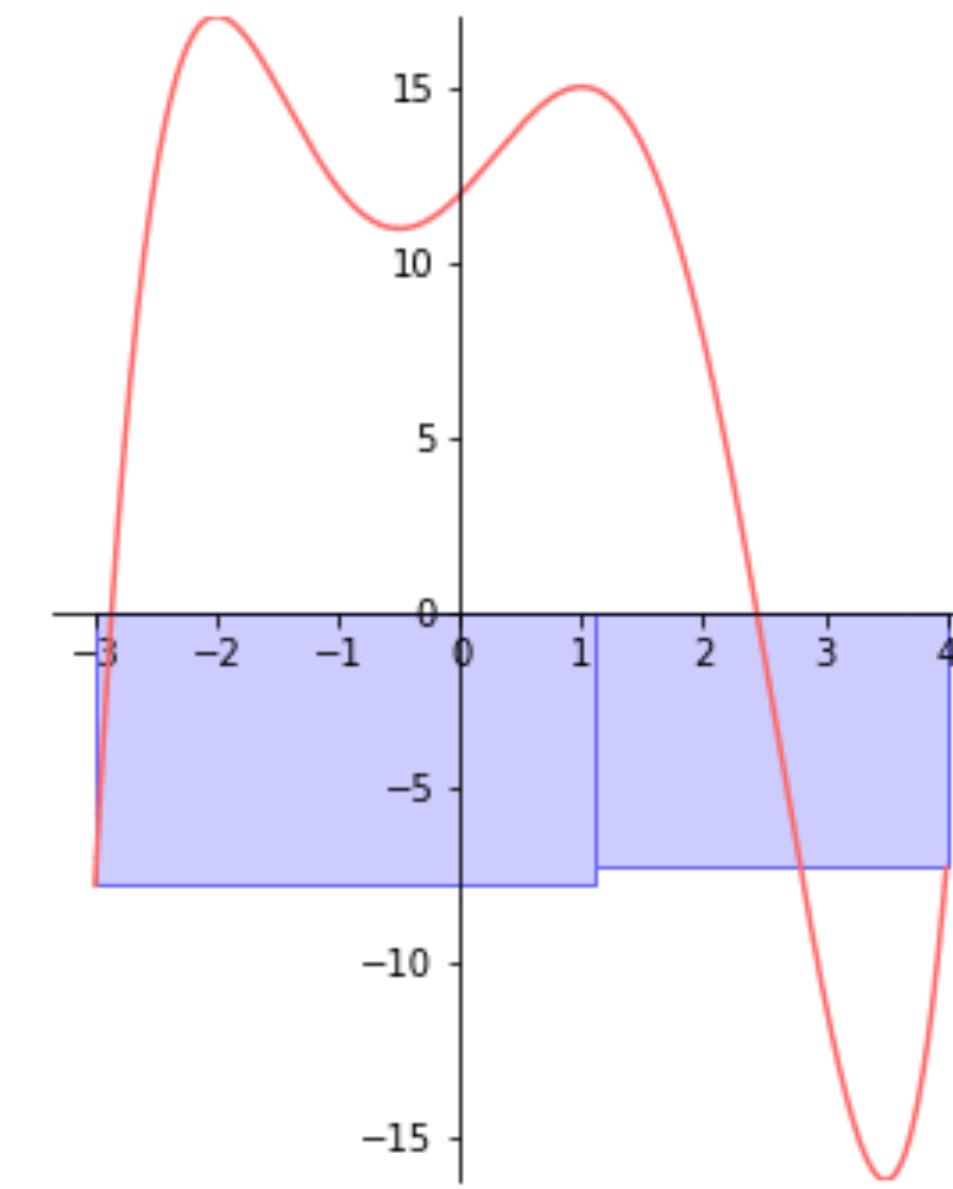
Simple and intuitive explanation of a slightly different result:

“A NN with sigmoid activation and at most two hidden layers can approximate well a smooth function in average, i.e, in ℓ_1 -norm”

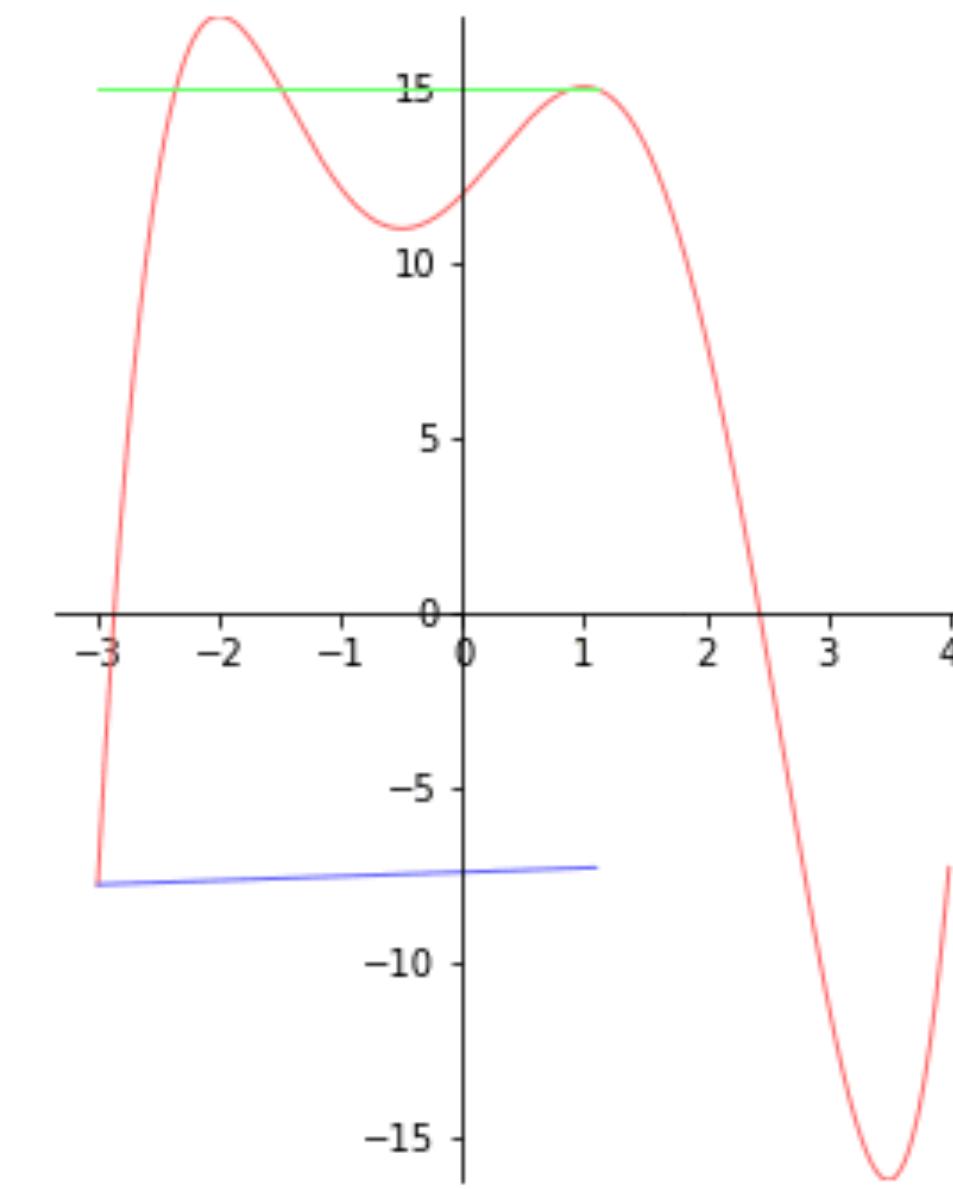
Consider a function $f: \mathbb{R} \rightarrow \mathbb{R}$ on a bounded domain



Approximation of the function by a sum of rectangles



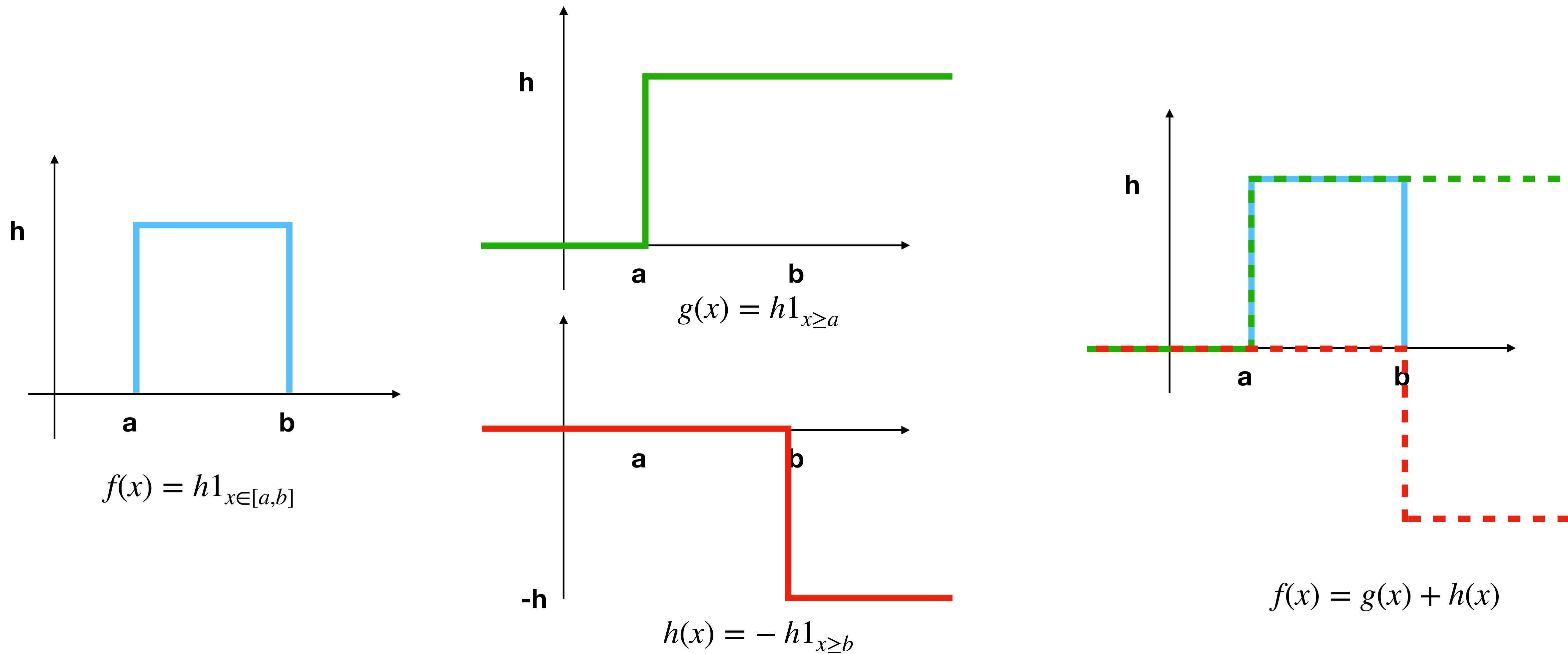
From below



From above

The function is Riemann integrable - can be approximated arbitrarily closely by “lower” and “upper” sums of rectangle

A rectangle is equal to the sum of two step functions



Approximate a step function with a sigmoid

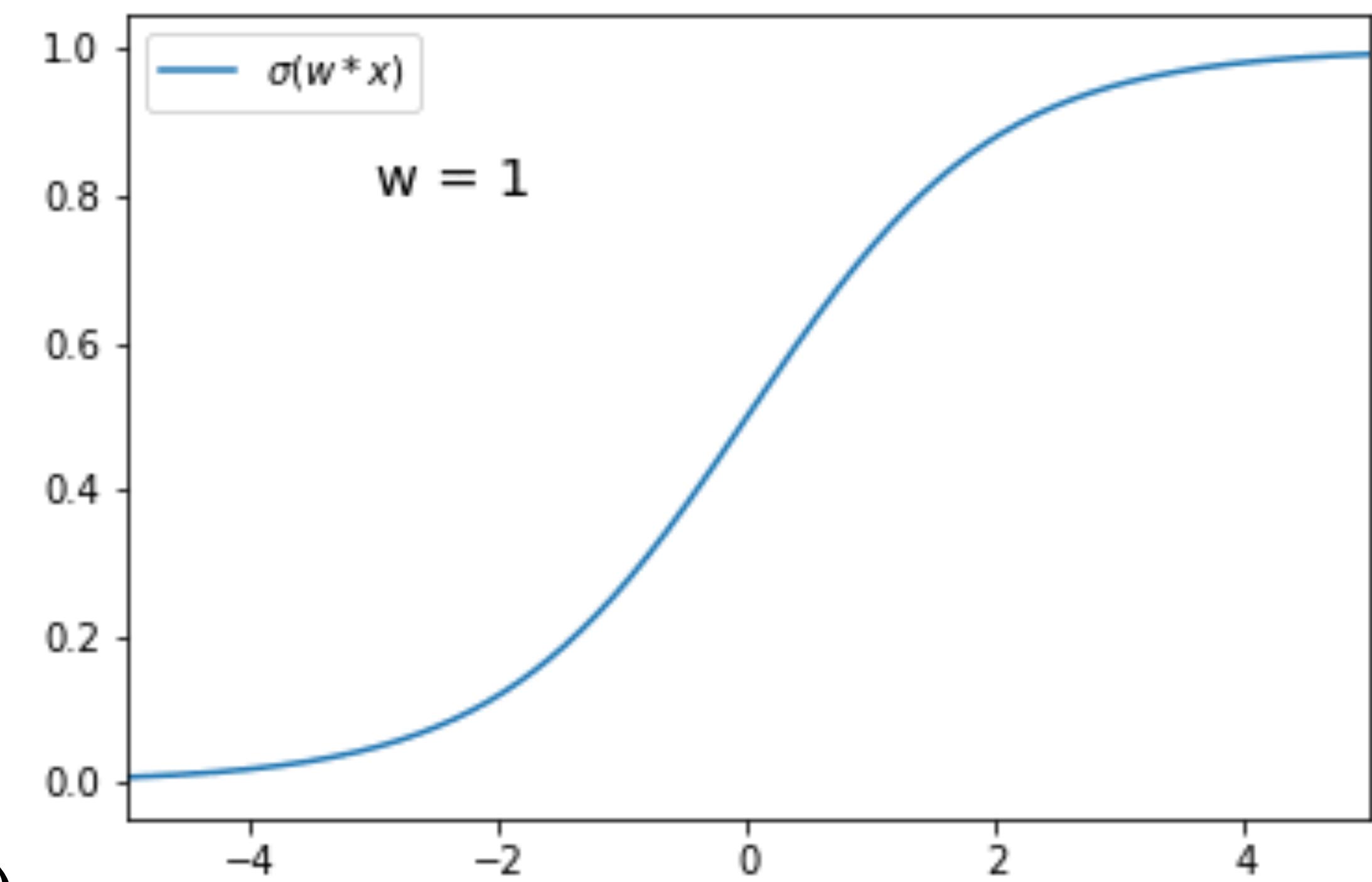
$$\tilde{\phi}(x) = \phi(w(x - b))$$

By setting:

- b : where the transition happens
- w : makes the transition steeper

Derivative: $\tilde{\phi}'(b) = w/4$

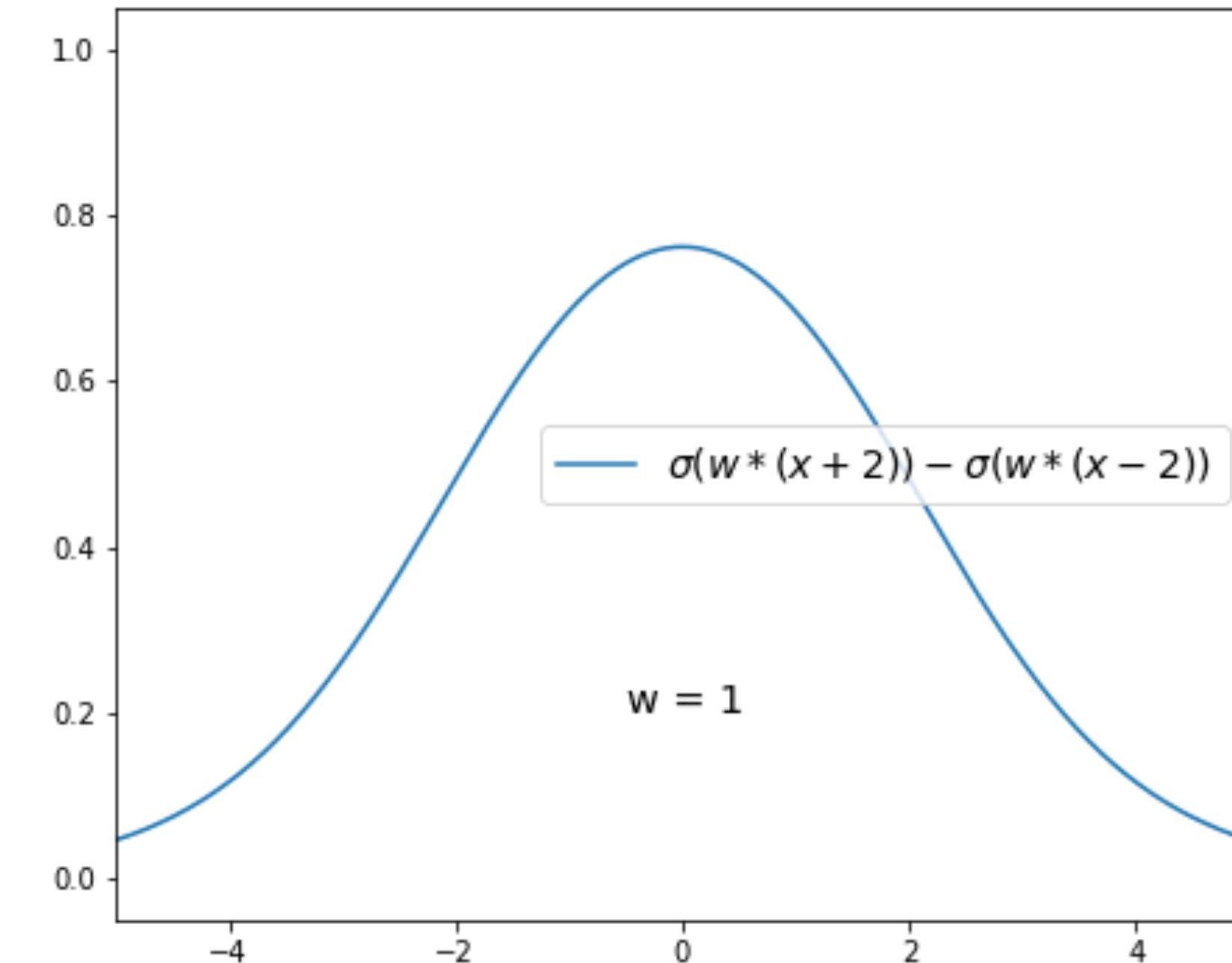
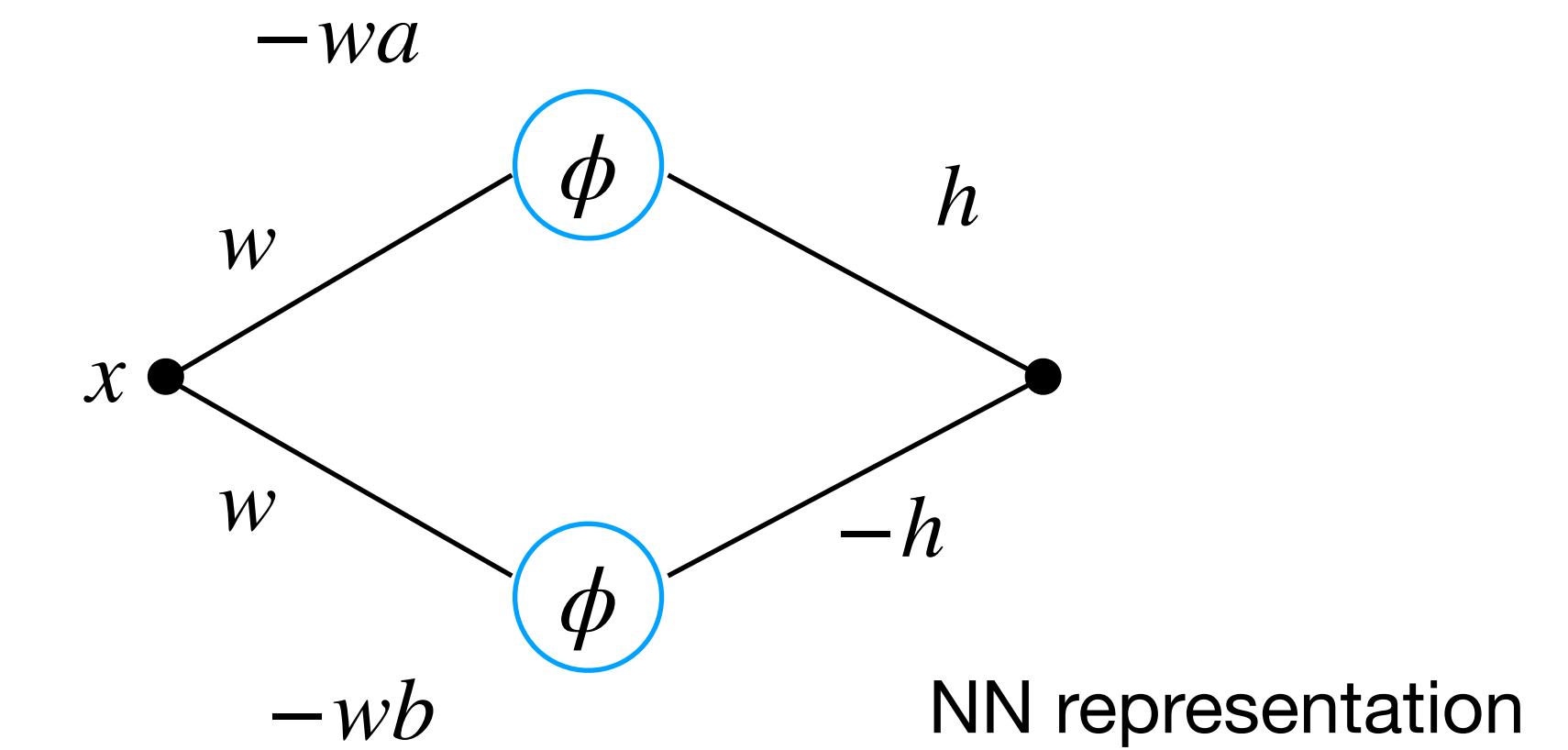
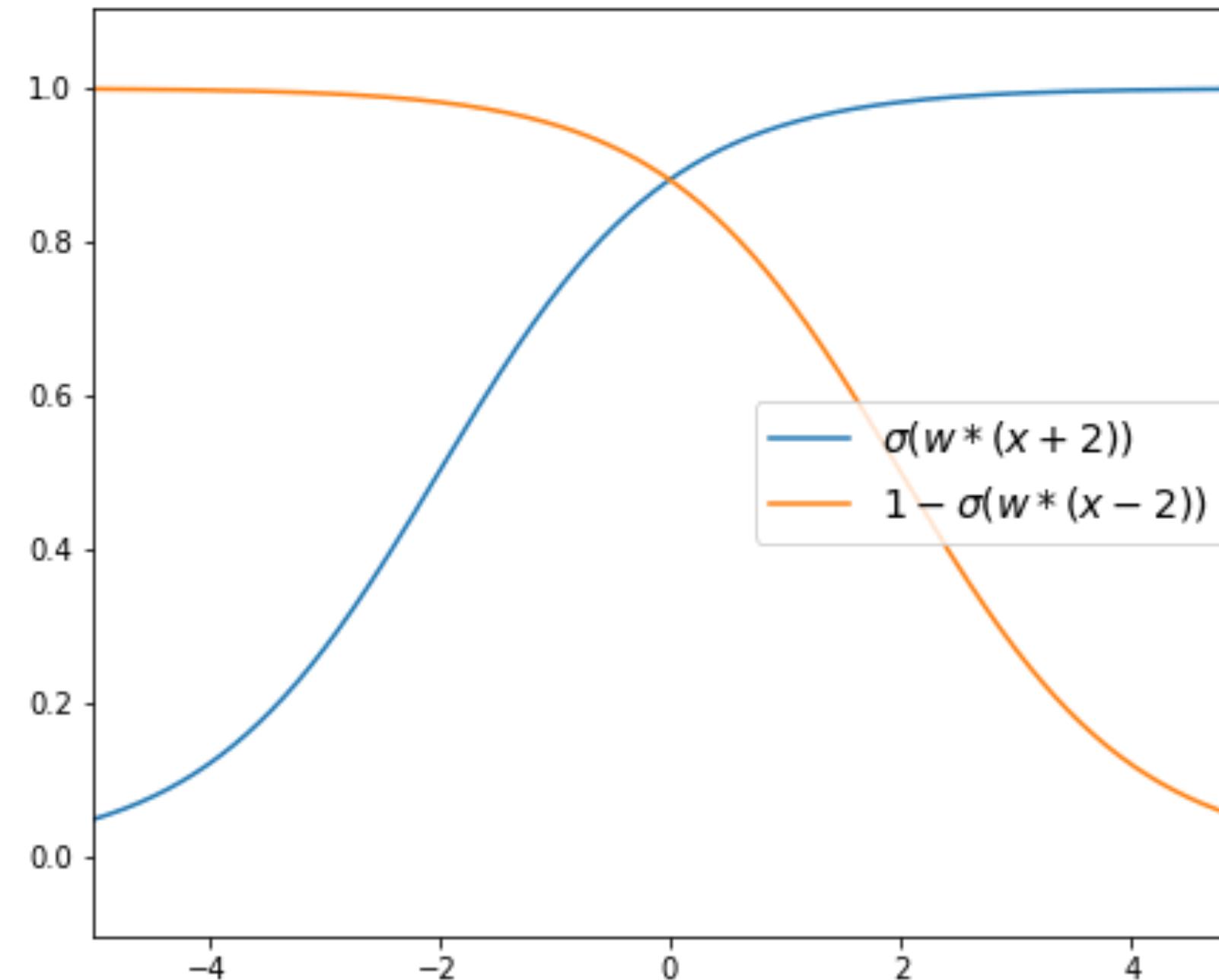
→ The width of the transition is $O(4/w)$



Approximation of the rectangle

$$h(\phi(w(x - a)) - \phi(w(x - b)))$$

$$\begin{aligned}a &= -2 \\b &= 2 \\h &= 1\end{aligned}$$

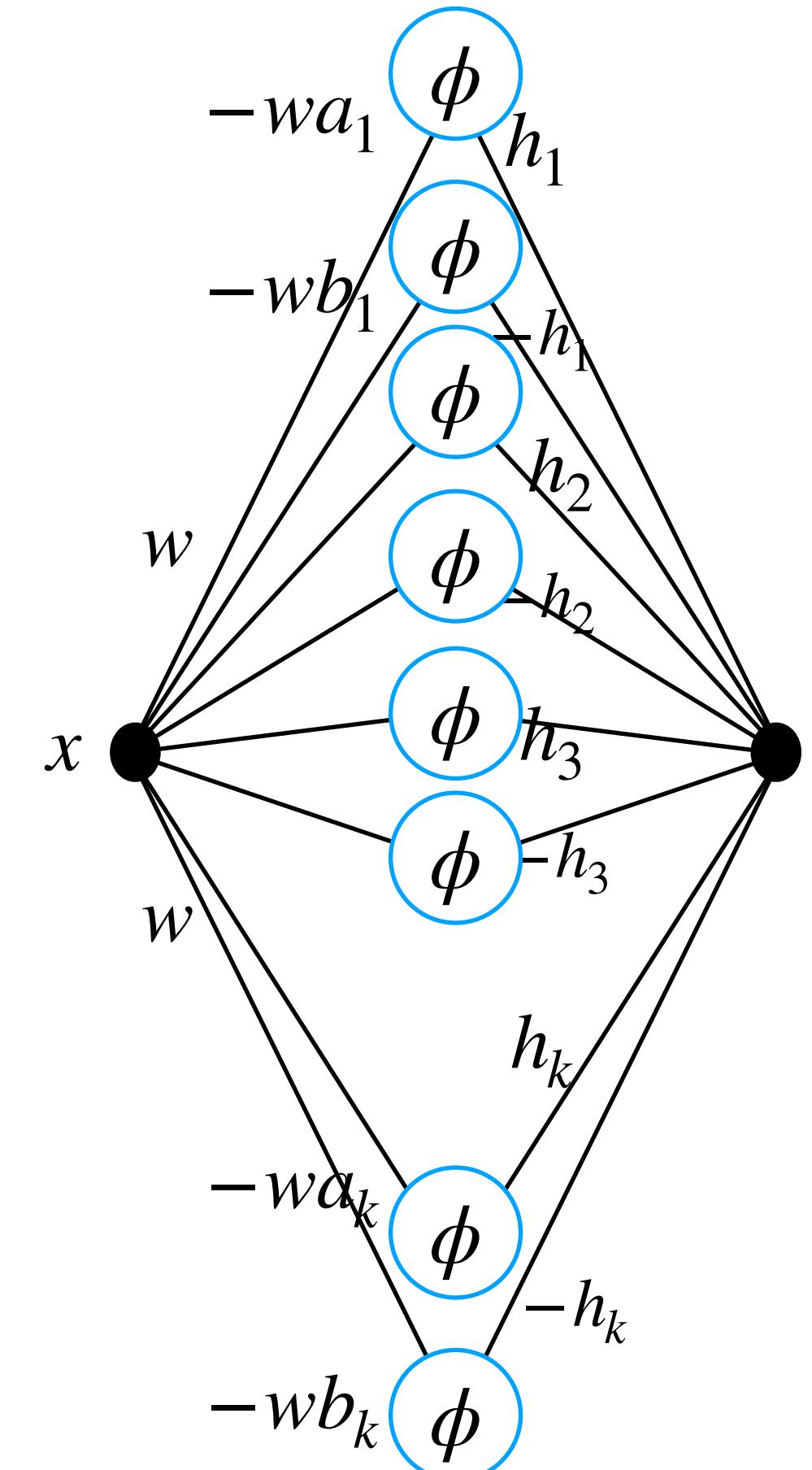


Conclusion in the 1D case

1. Approximate the function in the Riemann sense by a sum of k rectangles
2. Approximate each rectangle, by means of two nodes in the hidden layer of a NN
3. Compute the sum (with appropriate sign) of all the hidden layers at the output node
→ NN with one hidden layer containing $2k$ nodes for a Riemann sum with k rectangles

Remarks:

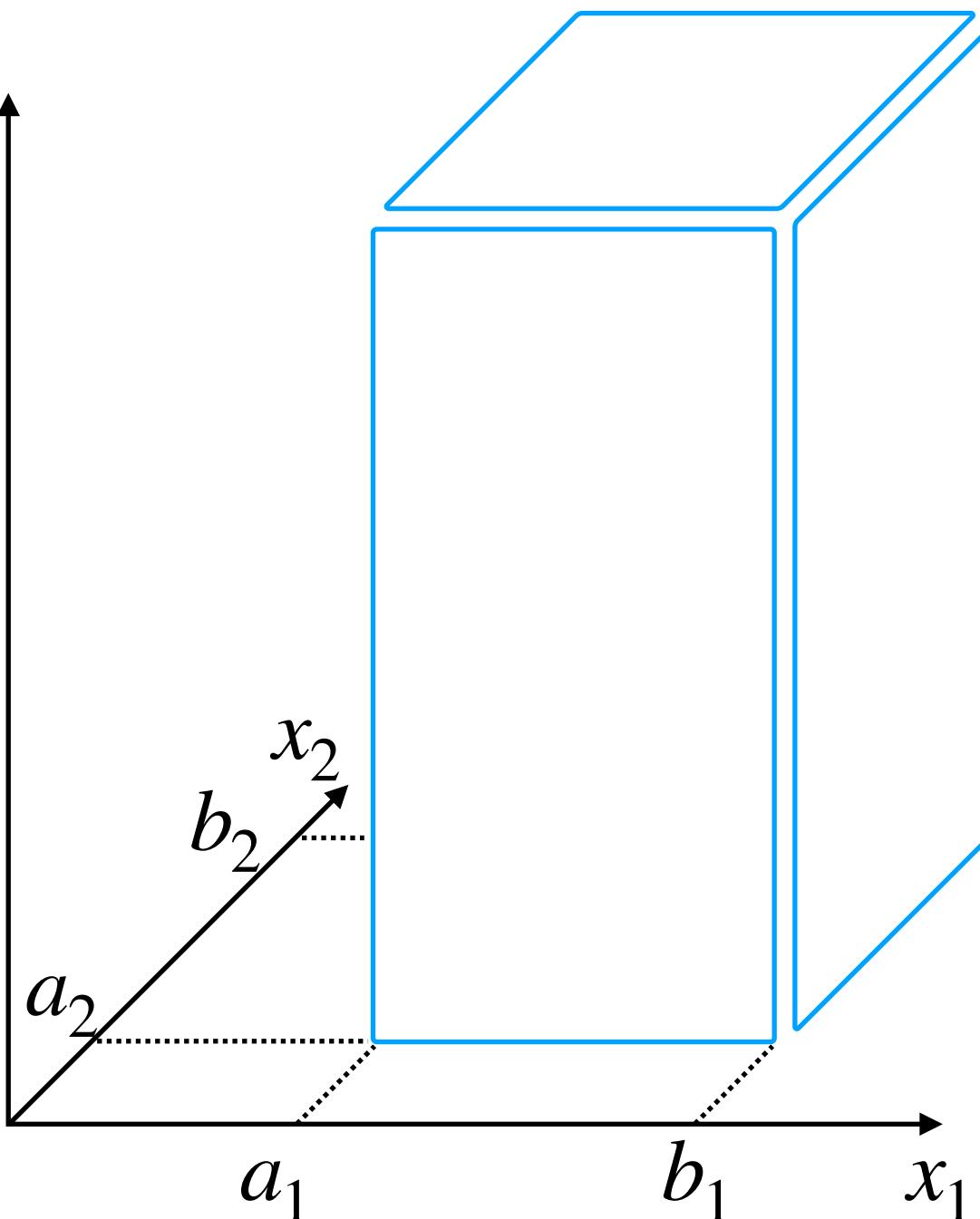
- Same intuition hold for any sigmoid like function
- Only intuition, not quantitative
- Need the weights w to be large



Larger dimension: $d = 2$

Same idea:

- Approximate the function by 2D rectangles
- Approximate a 2D rectangle by sigmoids

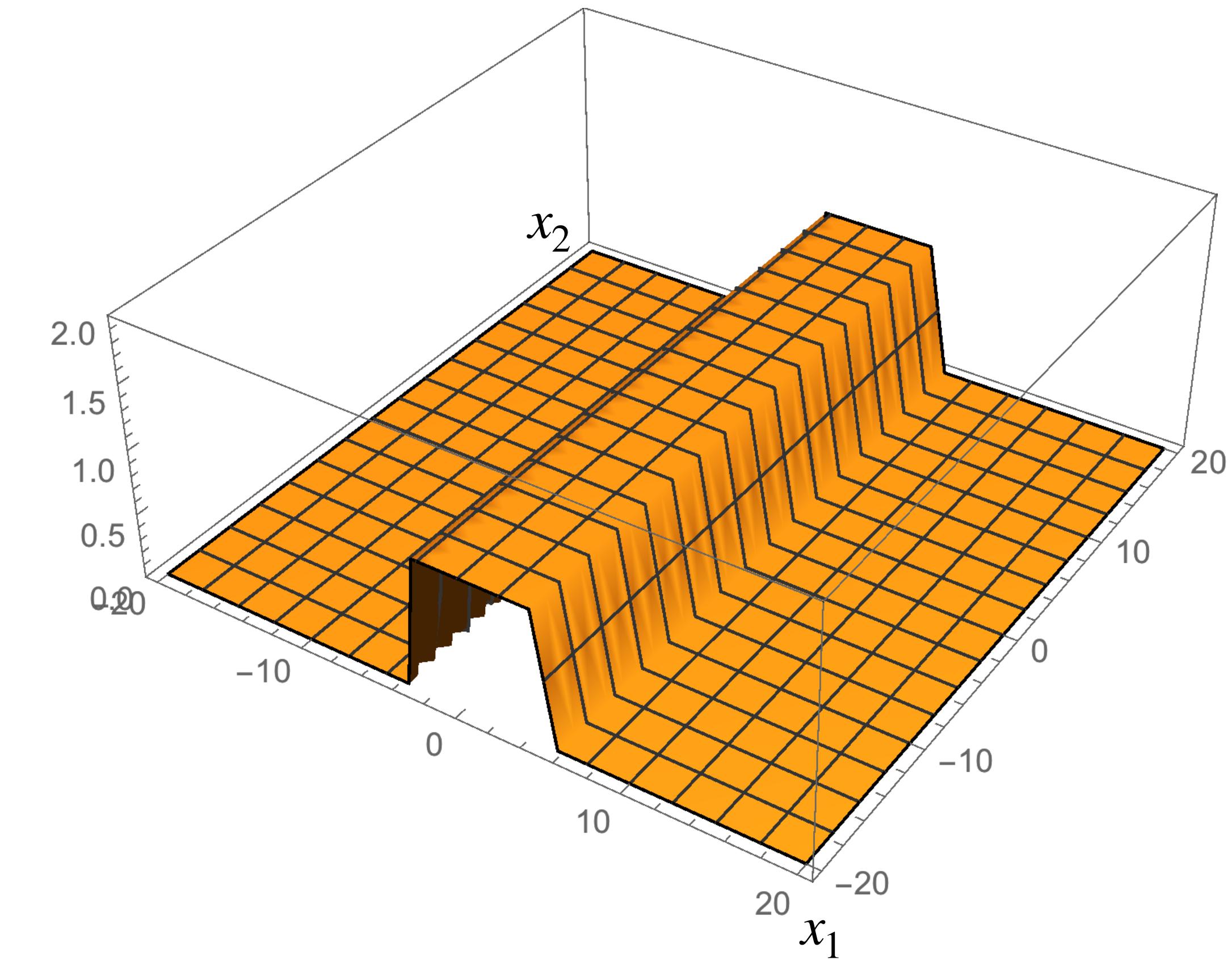
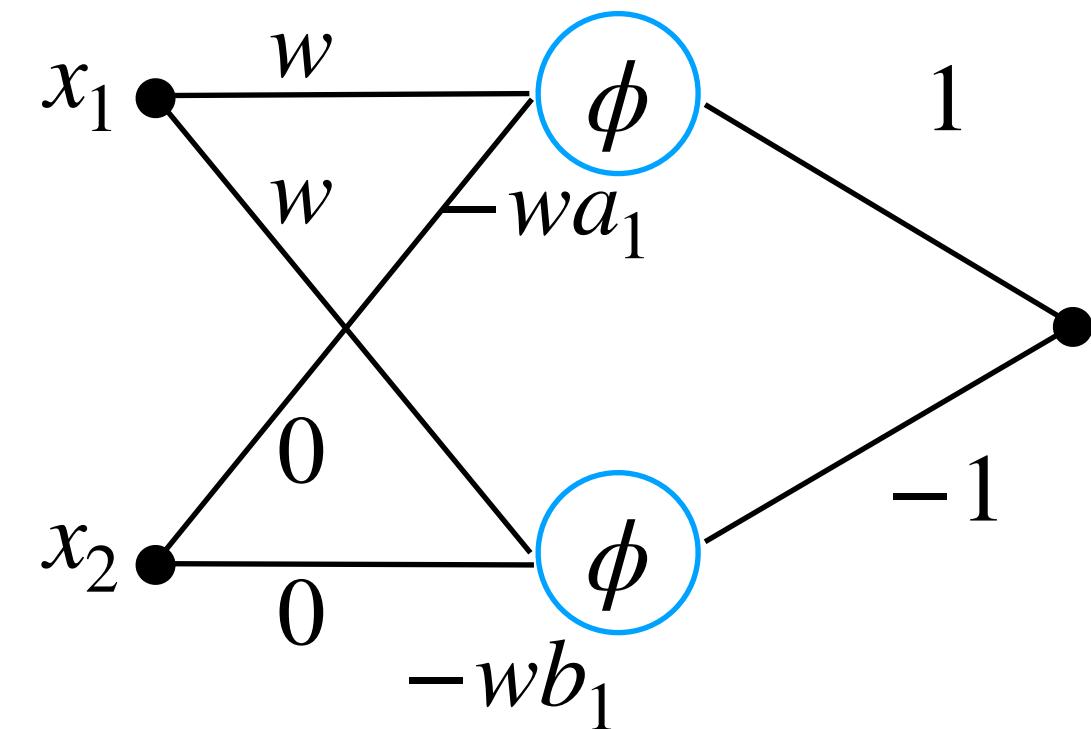


Two sigmoids can approximate an infinite rectangle

$$(x_1, x_2) \mapsto \phi(w(x_1 - a_1)) - \phi(w(x_1 - b_1))$$

Rectangle:

- going from a_1 to b_1 in the x_1 direction
- unbounded in the x_2 direction

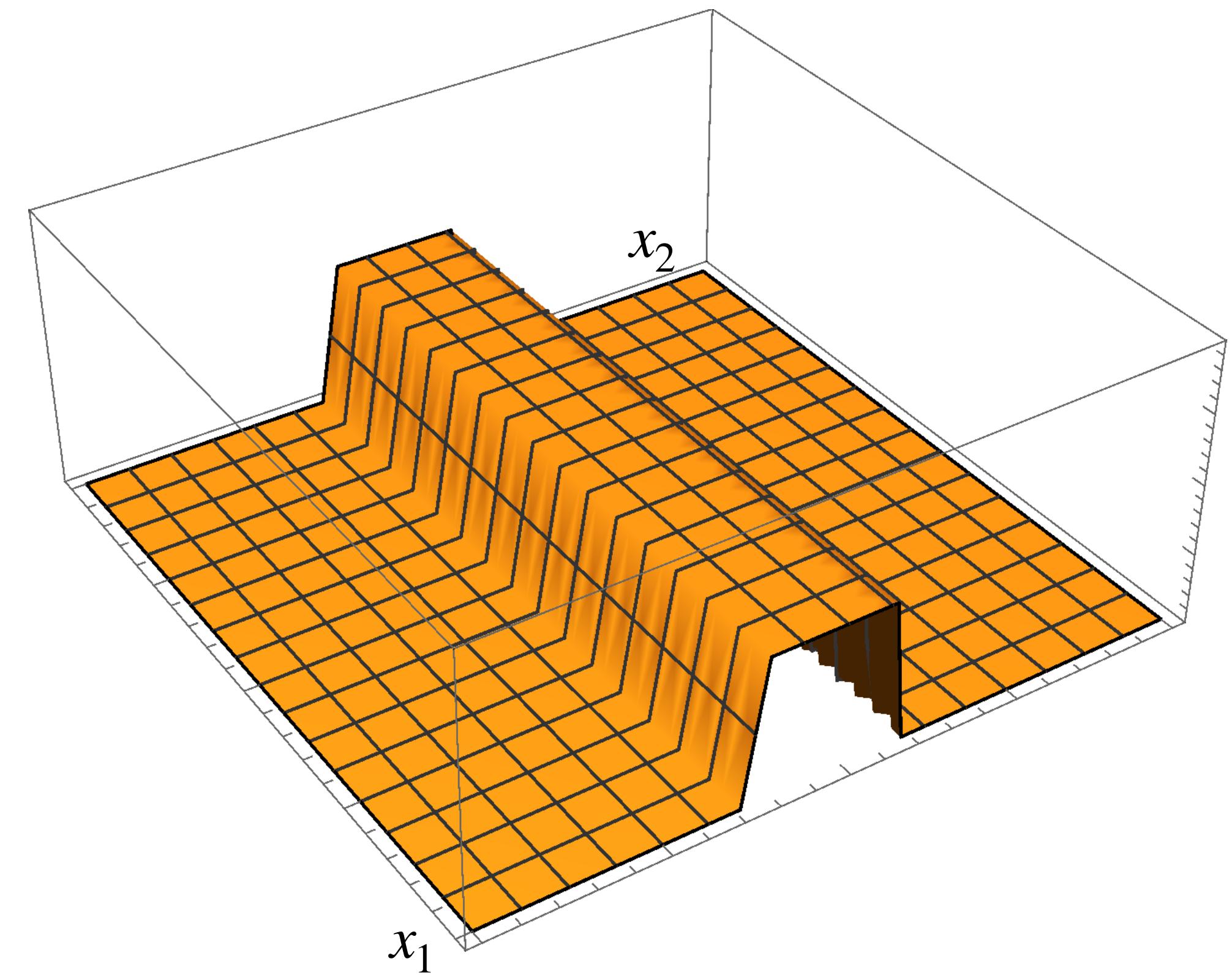
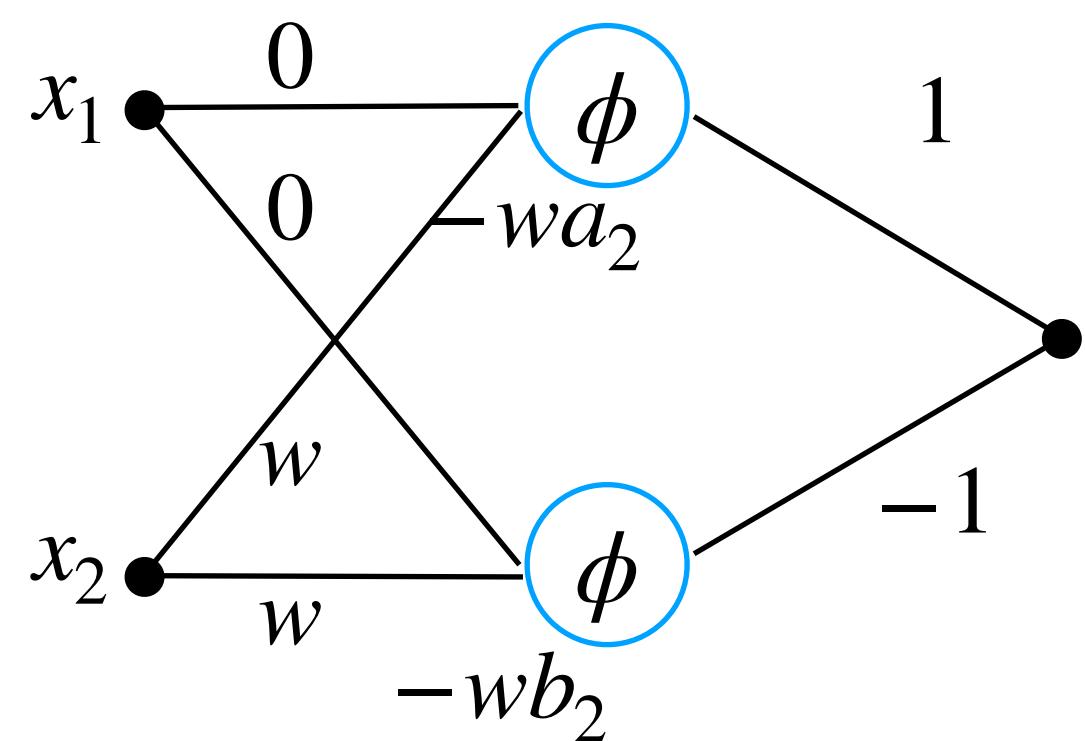


Two sigmoids can approximate an infinite rectangle

$$(x_1, x_2) \mapsto \phi(w(x_2 - a_2)) - \phi(w(x_2 - b_2))$$

Rectangle:

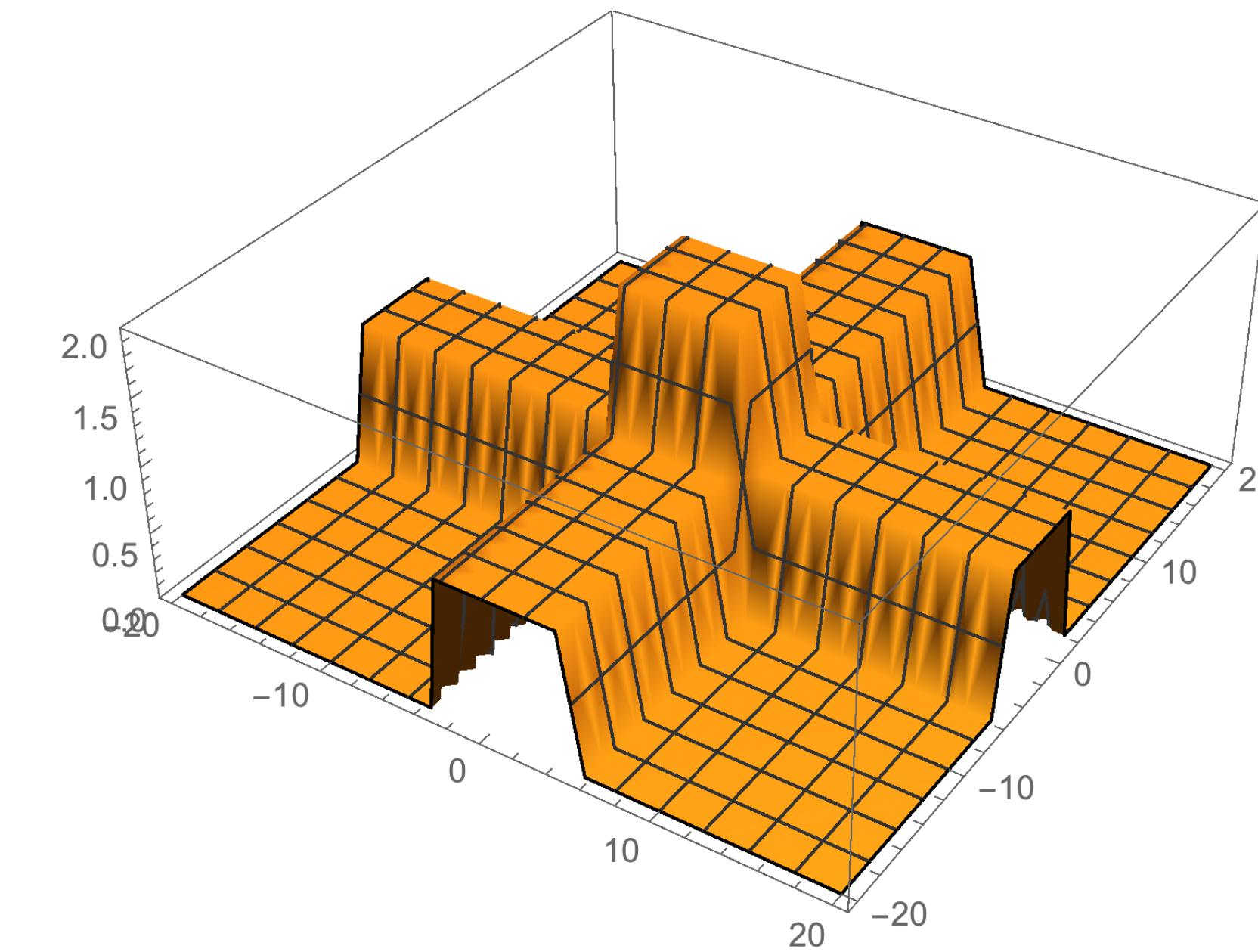
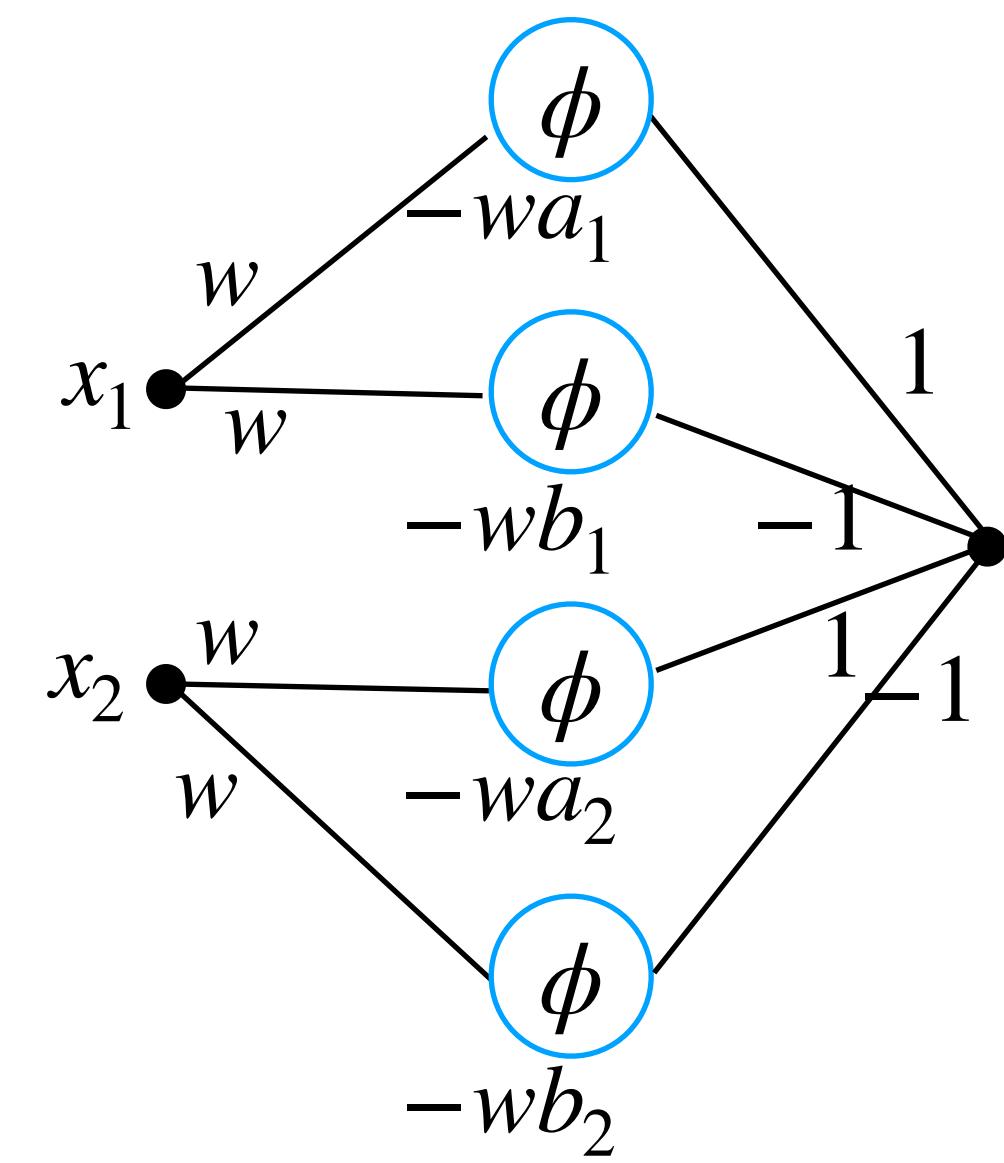
- going from a_2 to b_2 in the x_2 direction
- unbounded in the x_1 direction



Four sigmoids can approximate a cross

$$(x_1, x_2) \mapsto \phi(w(x_1 - a_1)) - \phi(w(x_1 - b_1)) + \phi(w(x_2 - a_2)) - \phi(w(x_2 - b_2))$$

→ close to what we want with the exception of the two infinite “arms”



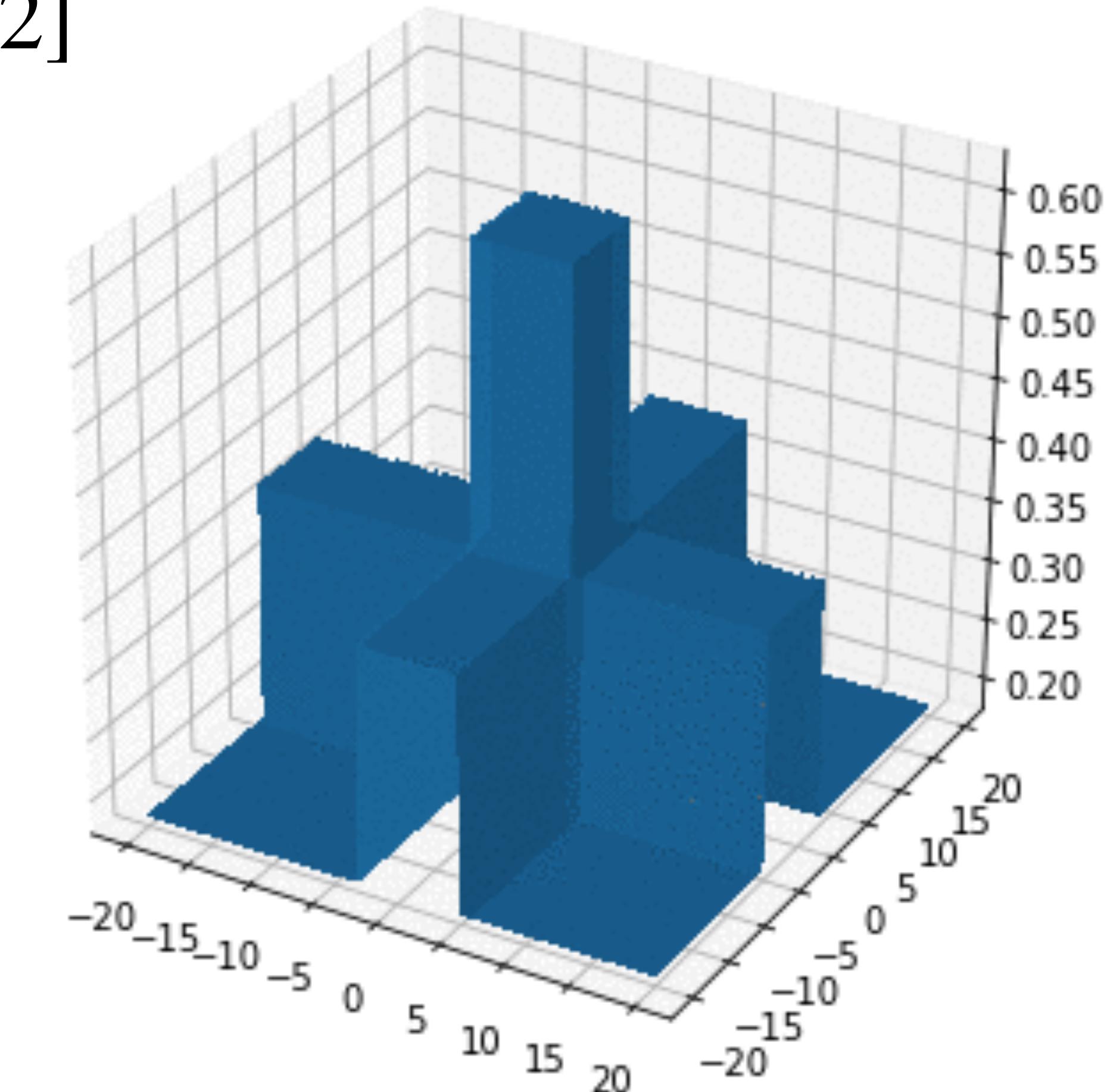
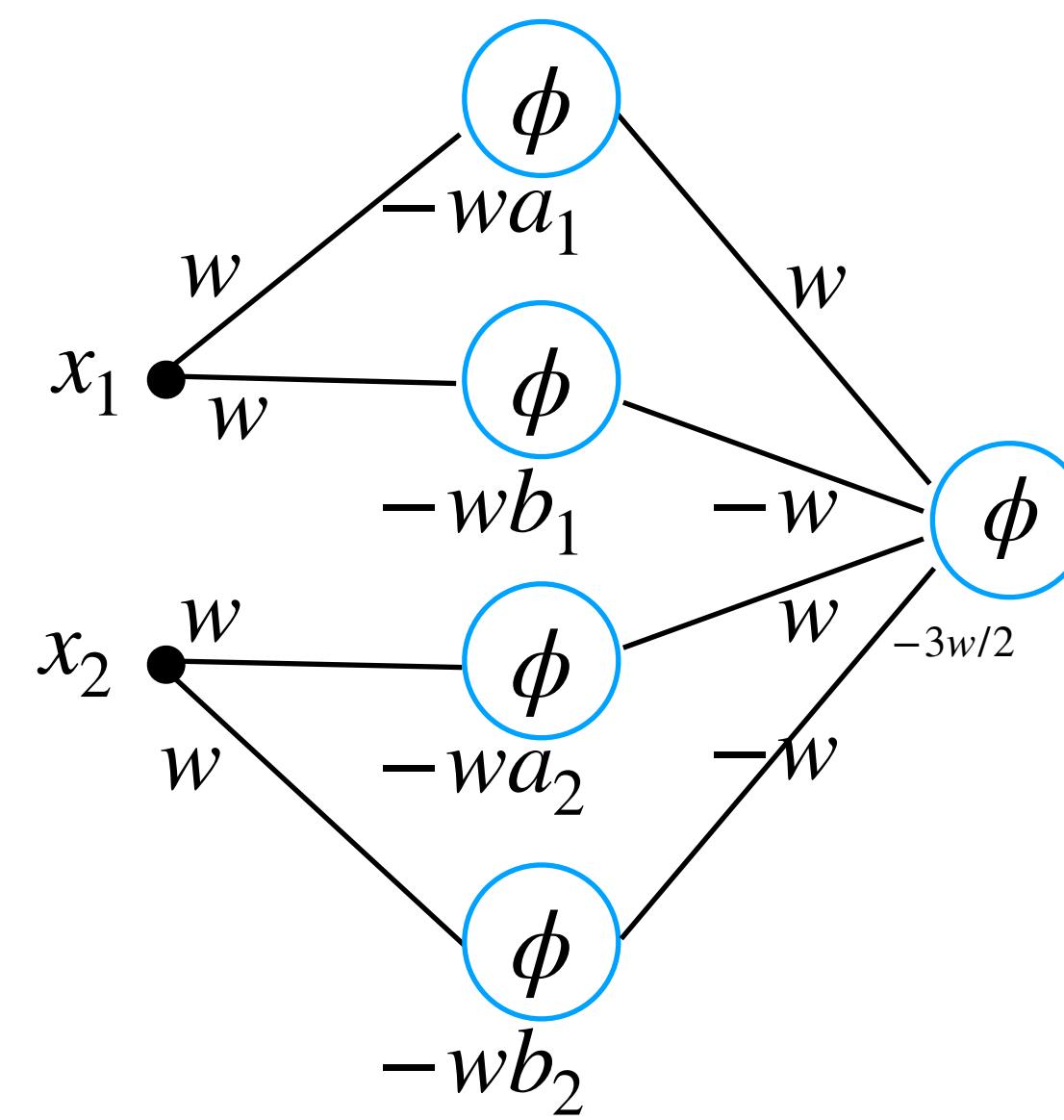
How to get rid of the crossed arms?

The sigmoid can threshold the unwanted infinite arms

Threshold the function value would remove the arms

It is equivalent to compose it with $1_{y \geq c}$ for $c \in (1,2]$

- approximate $1_{y \geq c}$ by a sigmoid with large weight w and appropriate bias (e.g., $3w/2$)



Point-wise approximations

Def: piecewise linear (PWL) function:

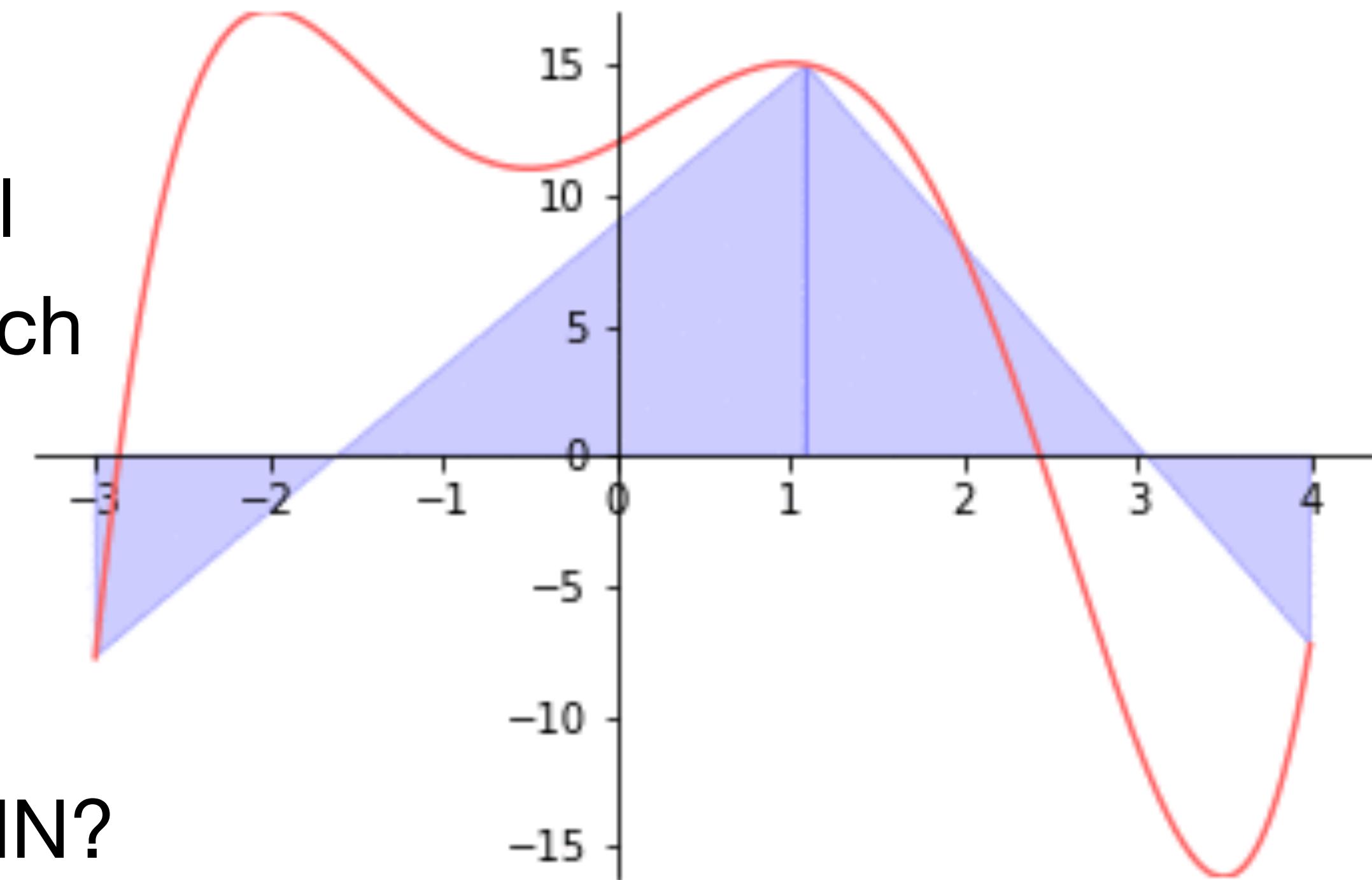
$$q(x) = \sum_{i=1}^m (a_i x + b_i) \mathbf{1}_{r_{i-1} \leq x < r_i} \text{ with } a_i r_i + b_i = a_{i+1} r_i + b_{i+1}$$

ℓ_∞ -approximation result (Shektman, 1982):

Let f be a continuous function on $[0,1]$. For all $\varepsilon > 0$, it exists a piecewise linear function q such that:

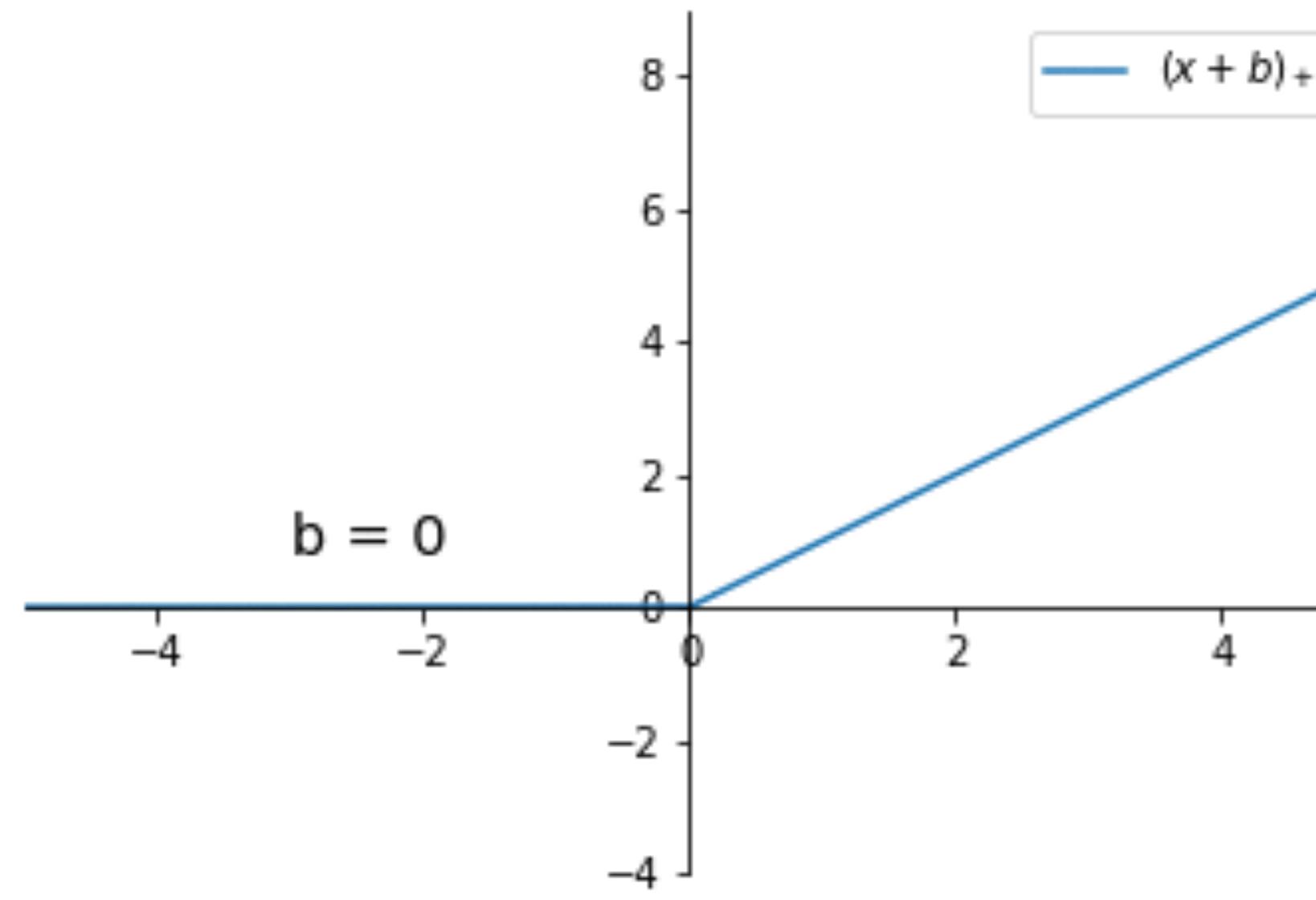
$$\sup_{x \in [0,1]} |f(x) - q(x)| \leq \varepsilon$$

→ How to approximate PWL functions with a NN?

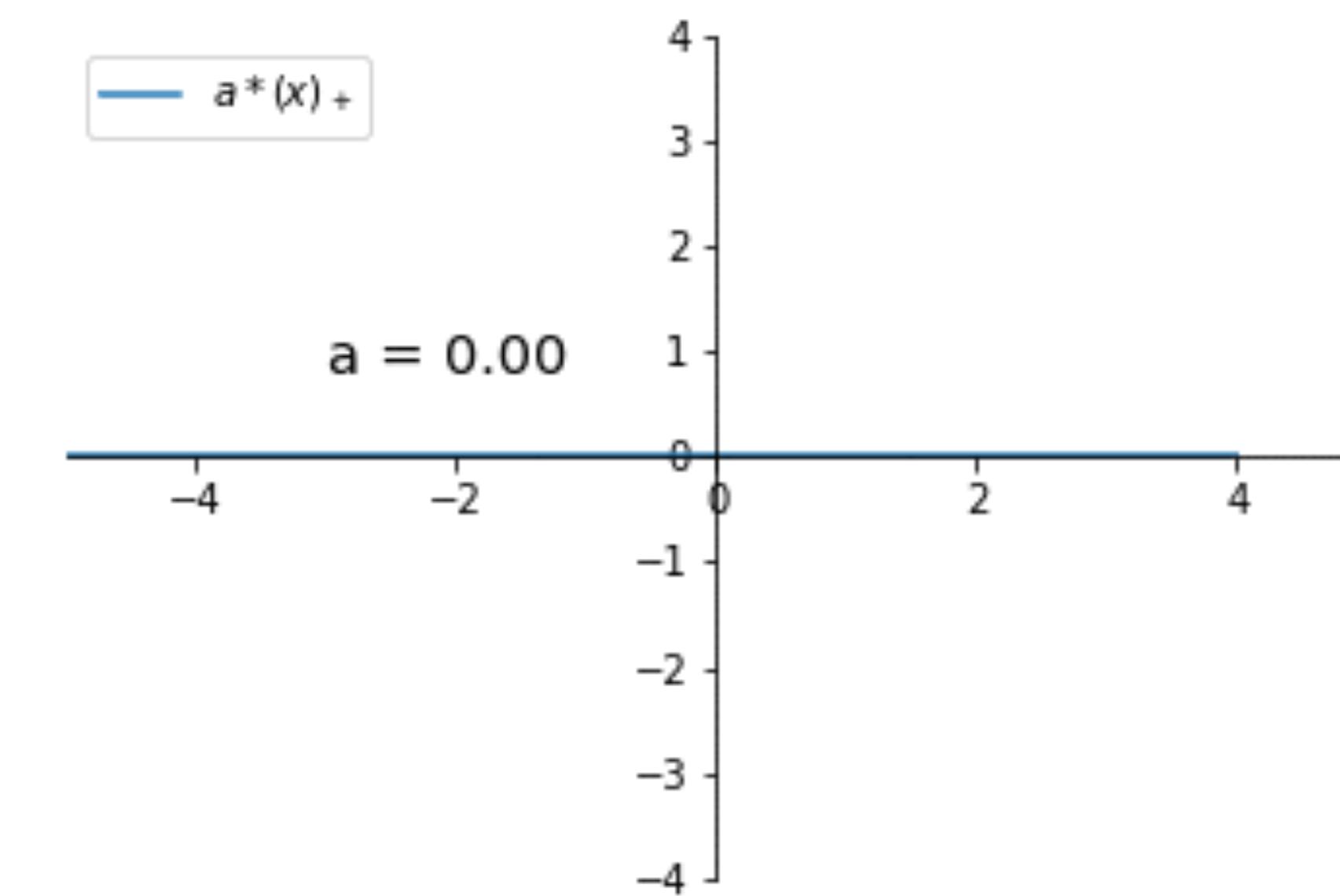


Rectified linear unit - RELU

$$(x)_+ = \max \{0, x\}$$



The bias b determines where the kink is



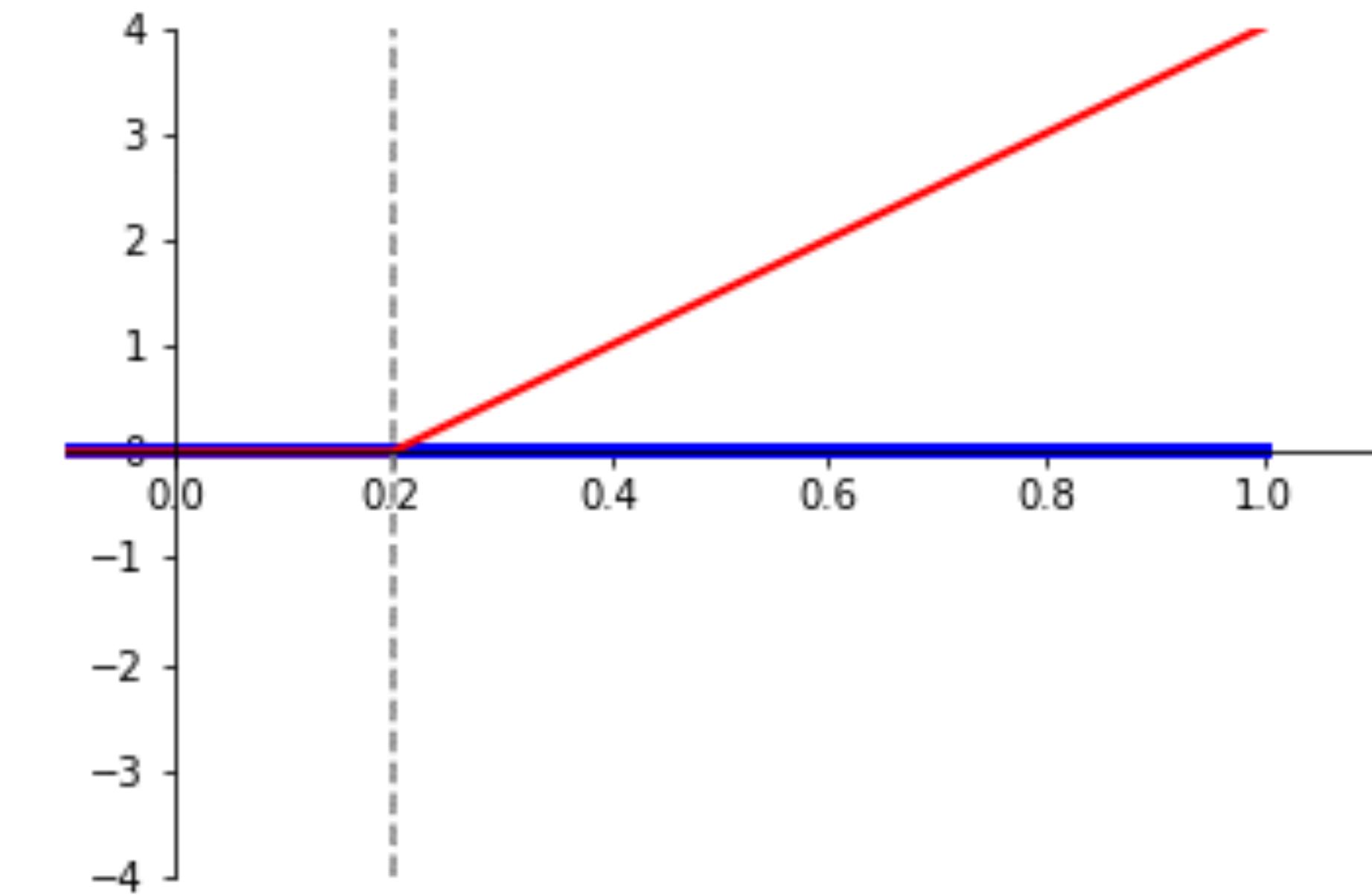
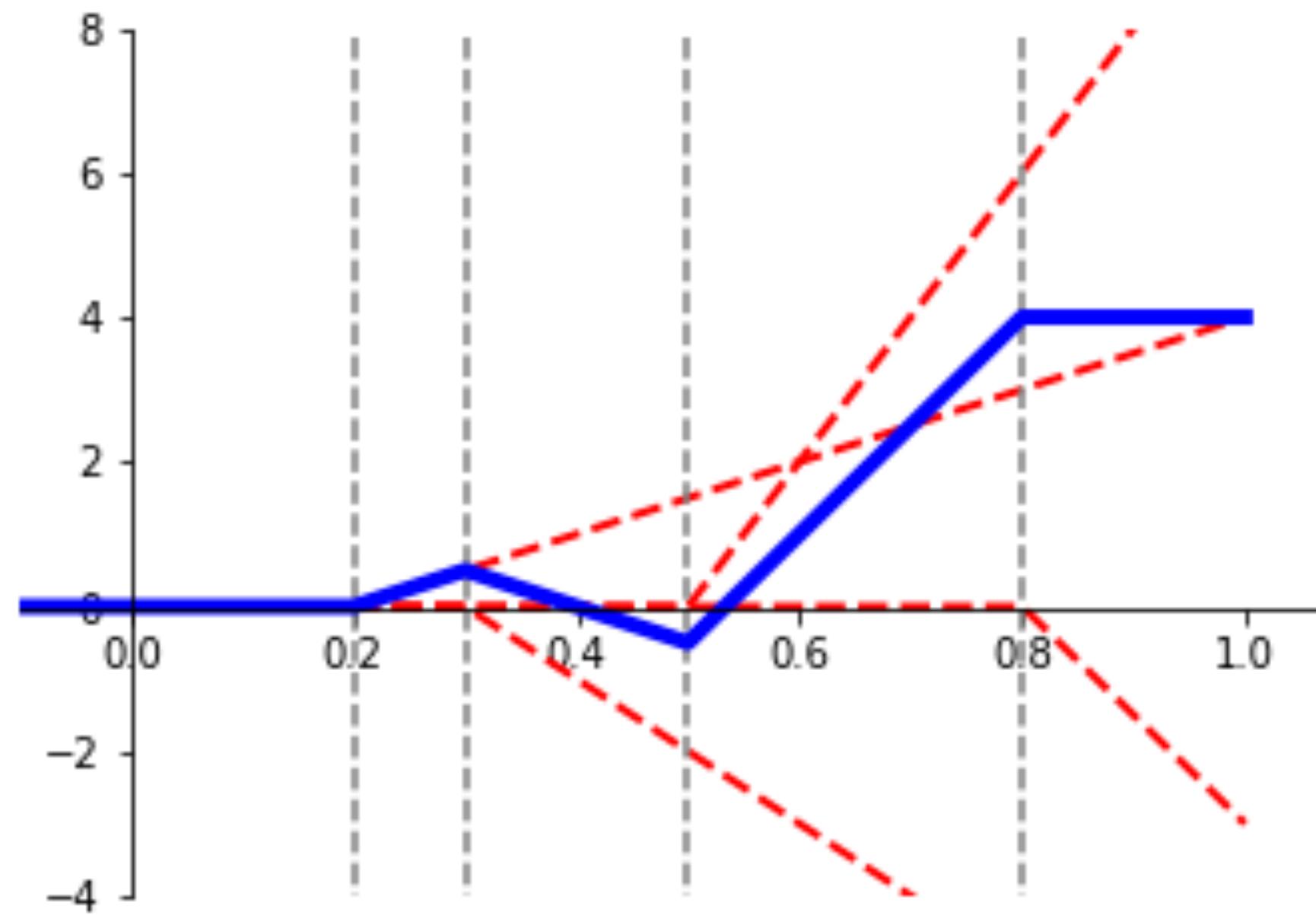
The weight a determines the slope

Linear combinations of RELUs are PWL functions

$\sum_{i=1}^m \tilde{a}_i(x - \tilde{b}_i)_+$ is a piecewise linear function

How do we get a new segment with slope a starting at $r > \max_i(\tilde{b}_i)$?

Intuition: Get the kink at r by setting $\tilde{b}_{i+1} = r$ and slope by additionally canceling existing slope i.e. $\tilde{a}_{i+1} = a - \sum_i \tilde{a}_i$



Formal: Piecewise linear functions can be written as combination of RELU

Claim 1: q can be rewritten as

$$q(x) = \tilde{a}_1 x + \tilde{b}_1 + \sum_{i=2}^m \tilde{a}_i (x - \tilde{b}_i)_+$$

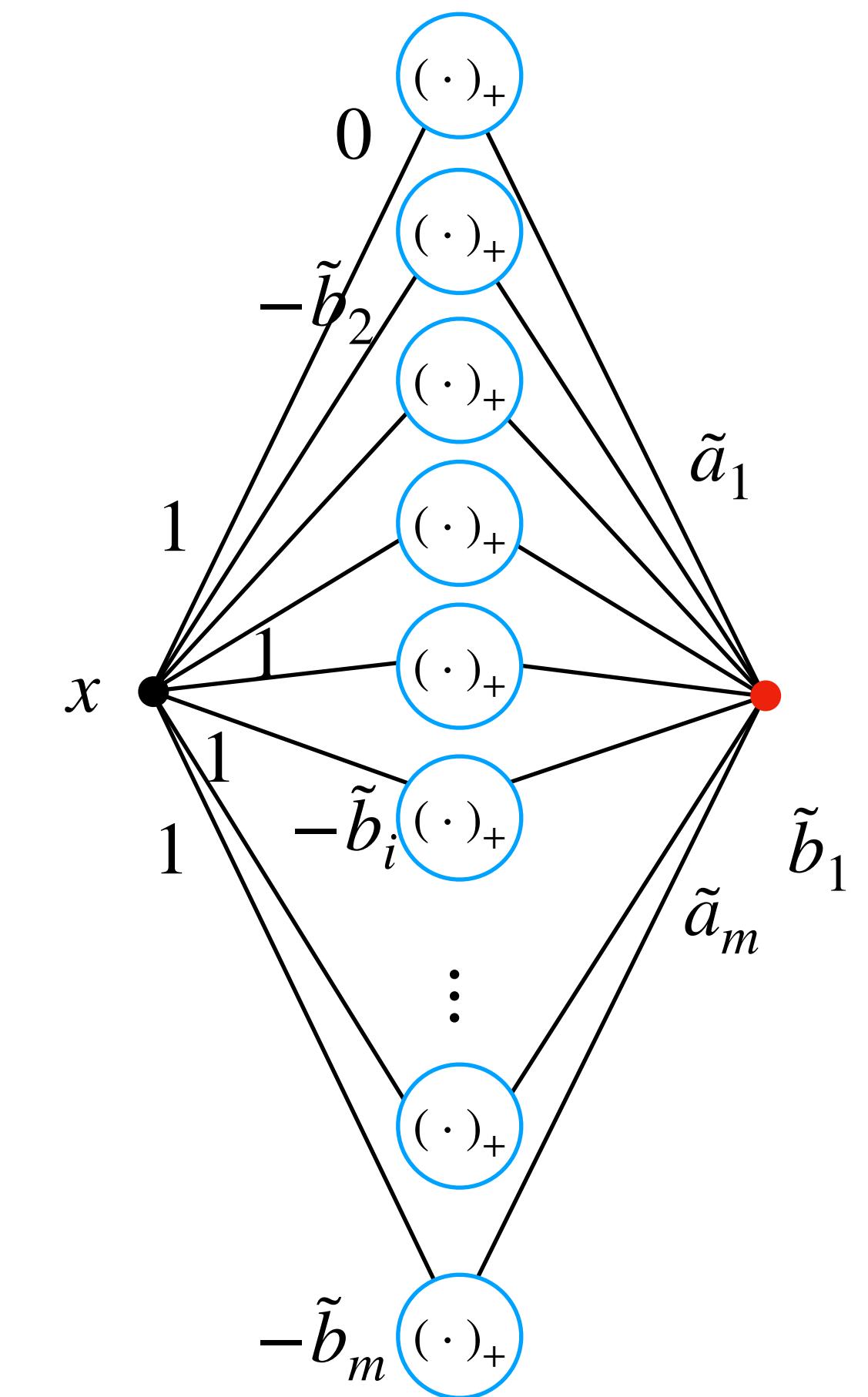
where $\tilde{a}_1 = a_1$, $\tilde{b}_1 = b_1$, $a_i = \sum_{j=1}^i \tilde{a}_j$ and $\tilde{b}_i = r_{i-1}$

Claim 2: q can be implemented as a one-hidden-layer NN with RELU activation. Each term corresponds to one node:

- Bias $-\tilde{b}_i$
- Output weight \tilde{a}_i

The term $\tilde{a}_1 x + \tilde{b}_1$ also corresponds to one node:

- Bias \tilde{b}_1 : bias of the output node
- Term $\tilde{a}_1 x = \tilde{a}_1 (x)_+$ since $x \in [0,1]$



Proof of the equivalent formulation

$$q(x) = \sum_{i=1}^m (a_i x + b_i) 1_{r_{i-1} \leq x < r_i} \quad r(x) = \tilde{a}_1 x + \tilde{b}_1 + \sum_{i=2}^m \tilde{a}_i (x - \tilde{b}_i)_+$$

$$\tilde{a}_1 = a_1, \tilde{b}_1 = b_1 \text{ and } a_i = \sum_{j=1}^i \tilde{a}_j \text{ and } \tilde{b}_i = r_{i-1}$$

- For $x \in [0, r_1]$
 $(\tilde{a}_1, \tilde{b}_1) = (a_1, b_1) \implies q(x) = a_1 x + b_1 = \tilde{a}_1 x + \tilde{b}_1 = r(x)$ because $\tilde{b}_2 = r_1$
- For $x \in [r_1, r_2]$,
$$\begin{aligned} r(x) &= \tilde{a}_1 x + \tilde{b}_1 + (a_2 - a_1)(x - r_1)_+ \\ &= a_1 x + b_1 + (a_2 - a_1)(x - r_1) = a_2 x + b_1 - (a_2 - a_1)r_1 \end{aligned}$$

 $r'(x) = a_2$ and $r(r_1) = q(r_1)$ as shown above
 $\implies r(x) = q(x)$ for $x \in [r_1, r_2]$

Proof by induction

Let's assume that $r(x) = q(x)$ for $x \in [0, r_{i-1}]$

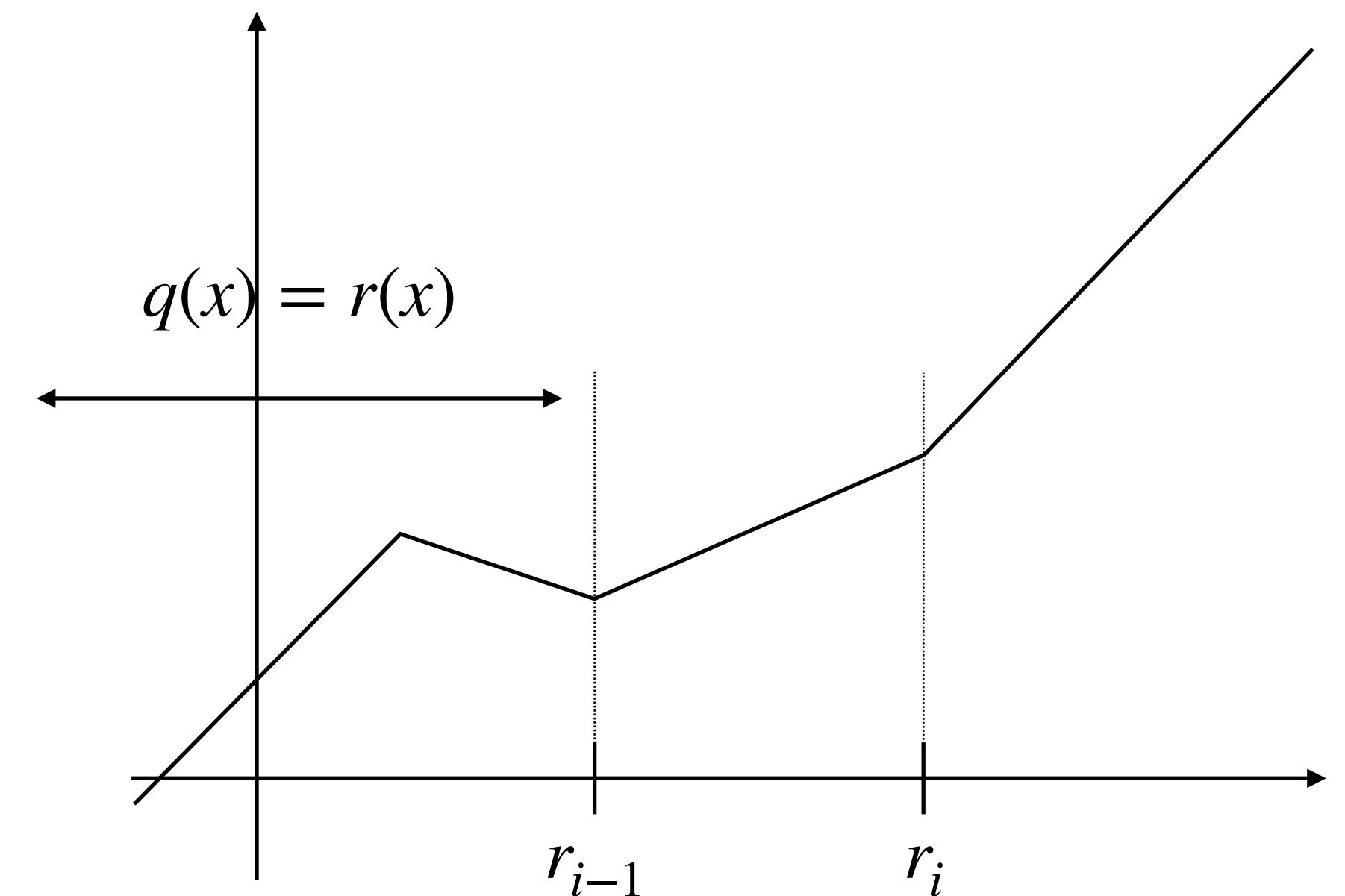
For $x \in [r_{i-1}, r_i]$

$$\begin{aligned} r(x) &= \tilde{a}_1 x + \tilde{b}_1 + \sum_{j=2}^m \tilde{a}_j (x - \tilde{b}_j)_+ \\ &= \tilde{a}_1 x + \tilde{b}_1 + \sum_{j=2}^i \tilde{a}_j (x - \tilde{b}_j) \\ &= \sum_{j=1}^i \tilde{a}_j x + \tilde{b}_1 - \sum_{j=2}^i \tilde{a}_j \tilde{b}_j \end{aligned}$$

Thus

- $r'(x) = \sum_{j=1}^i \tilde{a}_j = a_i$ good slope
- $r(r_{i-1}) = q(r_{i-1})$ good starting point

$$\implies r(x) = q(x) \text{ for } x \in [r_{i-1}, r_i]$$



Why: two affine functions with the same starting point and the same slope are equal

Proof by induction - bis

Let's assume that $r(x) = q(x)$ for $x \in [0, r_{i-1}]$

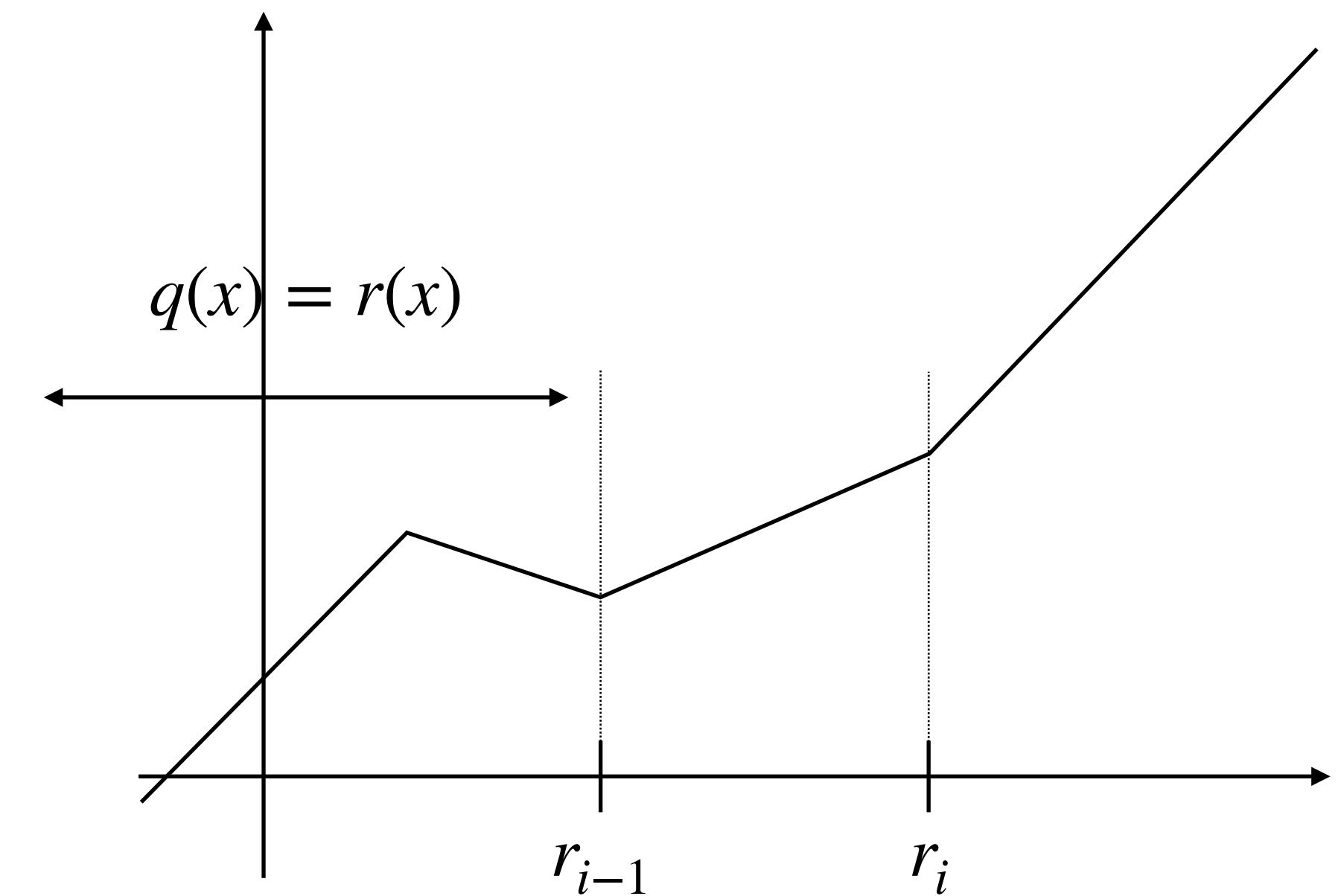
For $x \in [r_{i-1}, r_i]$

$$\begin{aligned} r(x) &= \tilde{a}_1 x + \tilde{b}_1 + \sum_{j=2}^m \tilde{a}_j (x - \tilde{b}_j)_+ \\ &= \underbrace{\tilde{a}_1 x + \tilde{b}_1 + \sum_{j=2}^{i-1} \tilde{a}_j (x - \tilde{b}_j)_+}_{= q(x), x \in [r_{i-2}, r_{i-1}] \text{ by induction}} + \tilde{a}_i (x - \tilde{b}_i) \\ &= a_{i-1} x + b_{i-1} + \tilde{a}_i (x - \tilde{b}_i) \end{aligned}$$

Thus

- $r'(x) = a_{i-1} + \tilde{a}_i = a_i$ good slope
- $r(r_{i-1}) = q(r_{i-1})$ good starting point

$$\implies r(x) = q(x) \text{ for } x \in [r_{i-1}, r_i]$$



Why: two affine functions with the same starting point and the same slope are equal

Conclusion: representation power

- f smooth (condition on its Fourier coefficients)
- Bounded domain
- Condition on the activation function
- Average approximation in ℓ_2 -norm but also point-wise approximation in ℓ_∞ -norm