# Neural Networks: Basic Structure, Representation Power

Machine Learning Course - CS-433
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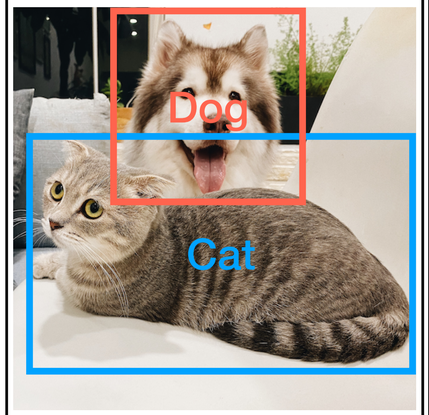
EPFL

# Deep Learning: ML Breakthrough

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

## Object Detection




NN

## Translation

elle est très intelligente

NN

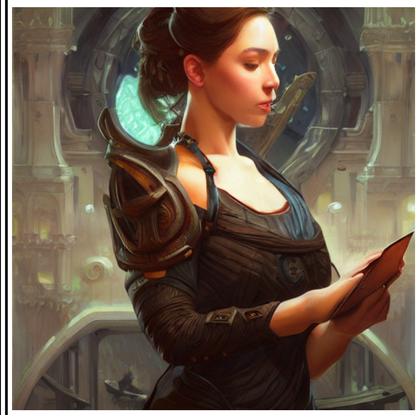
she is very smart

## Speech to Text

hey Siri next song

NN

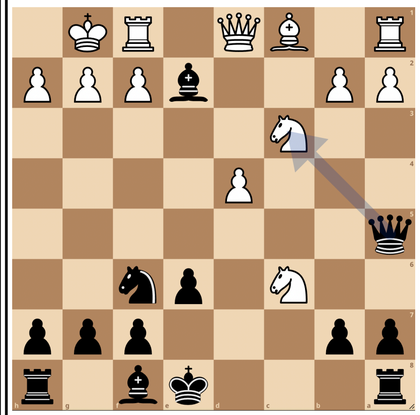
## Image Generation



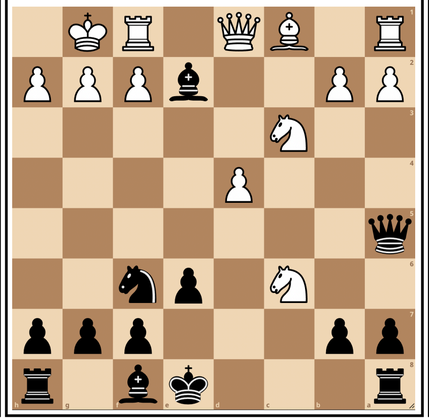
NN

student studying machine learning

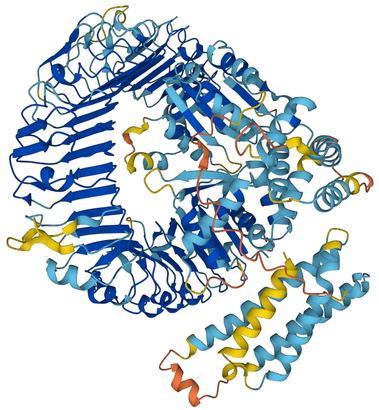
## Playing Chess



NN



## Protein Folding



NN

MAGELVSFAVNKLWDLLSHEYTLFQGVEDQ
VAELKSDLNLLKSFLKDADAKKHTSALVRY
CVEEIKDIVYDAEDVLETFVQKEKLGTTSGIR
KHIKRLTCIVPDRREIALYIGHVSKRITRVIRD
MQSFGVQQMIVDDYMHPLRNREREIRRTF
PKDNESGFVALEENVKKLVGYFVEEDNYQV
VSITGMGGLGKTTLARQVFNHDMVTKKFD
KLAWVSVSQDFTLKNVWQNILGDLKPKEEE
TKEEEKKILEMTEYTLQRELYQLLEMSKSLI
VLDDIWKKEDWEVIKPIFPPTKGWKLLLTSR
NESIVAPTNTKYFNFKPECLKTDDSWKLFQ
RIAFPINDASEFEIDEEMEKLGEKMIEHCGG
LPLAIKVLGGMLAEKYTSHDWRRLSENIGS
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 $\mathcal{X} \to \mathcal{Y}$ 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

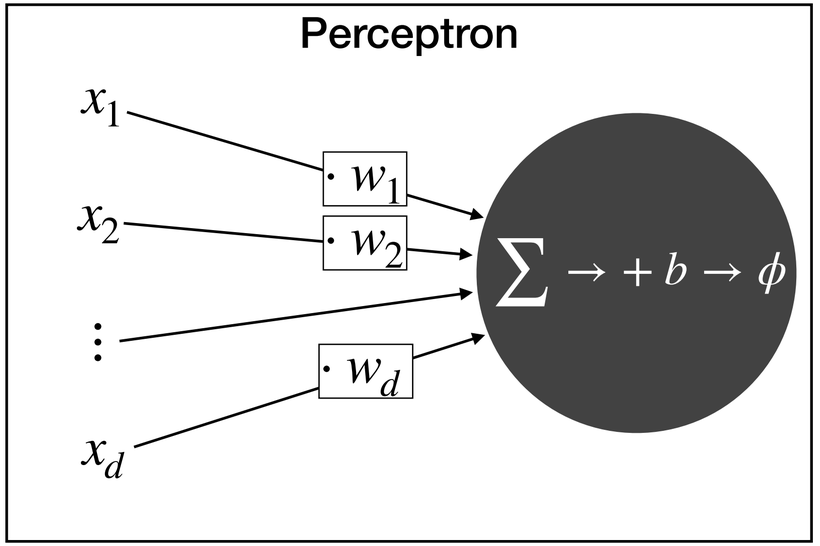
# The Basic Structure of Neural Networks

# Neurons and Logistic Regression

Recap - Logistic Regression:

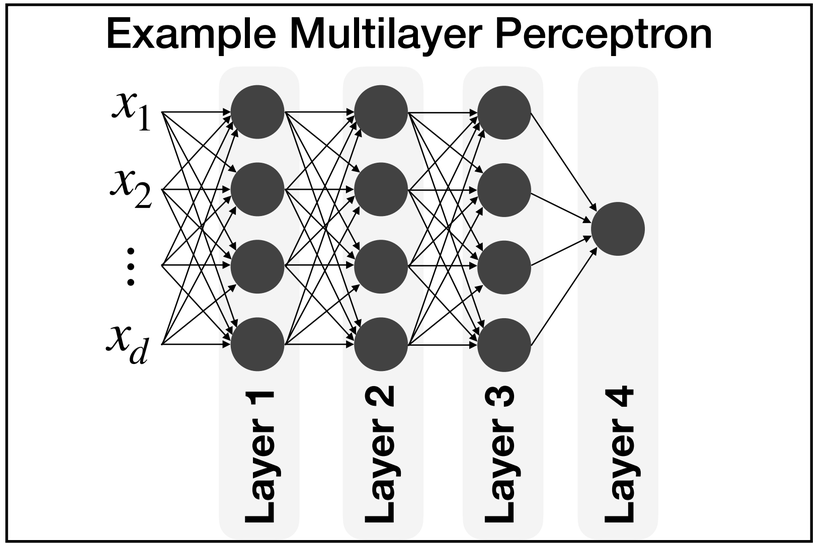
$$f_{LR}(x) = p(1 \mid x) = \sigma(x^\top w + b) = \sigma\left(\sum_{i=1}^{d} x_i w_i + b\right)$$

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




Perceptron:

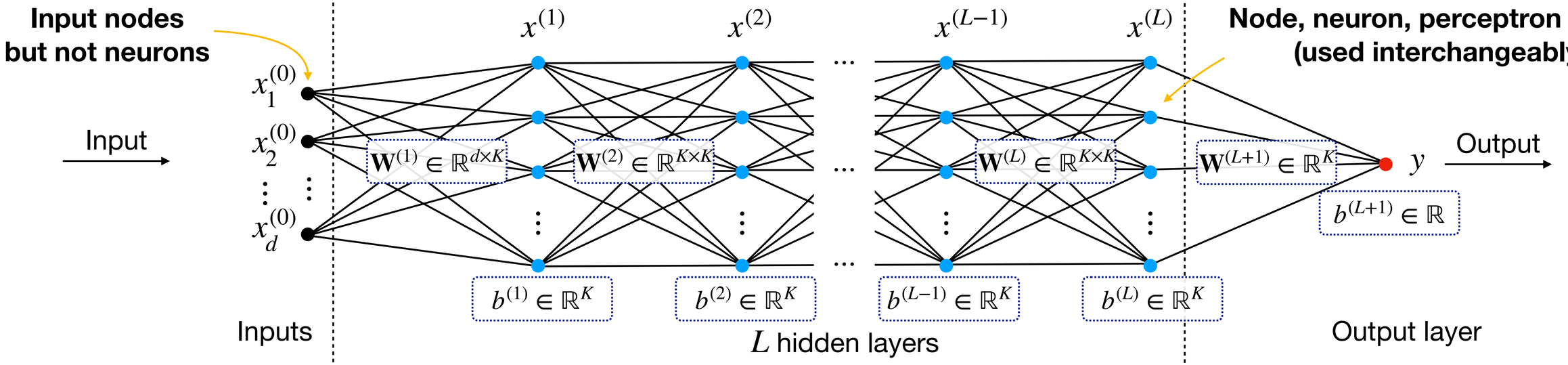
- A simple model of biological neurons
- Activation function $\phi$
- Equivalent to $f_{LR}$ when $\phi = \sigma$




Multilayer Perceptron (MLP):

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

# Fully Connected Neural Networks




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

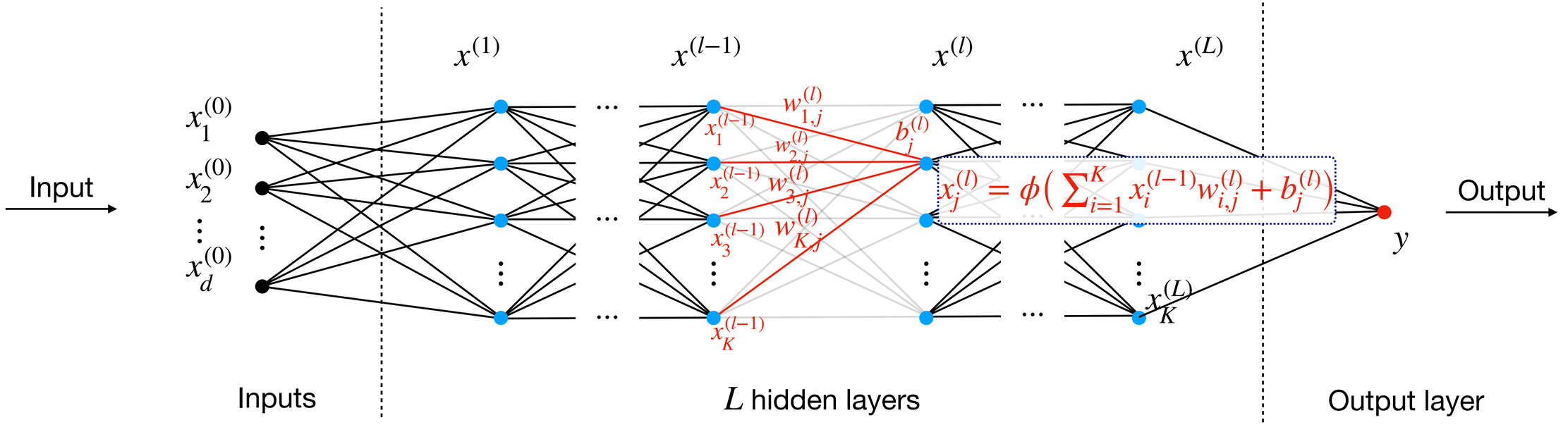
Outputs of hidden layer $l$ given by vector: $x^{(l)} = f^{(l)}(x^{(l-1)}) := \phi\left((\mathbf{W}^{(l)})^\top x^{(l-1)} + b^{(l)}\right)$

**Elementwise**

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

— 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: $\phi$ is non-linear otherwise we can only represent linear functions

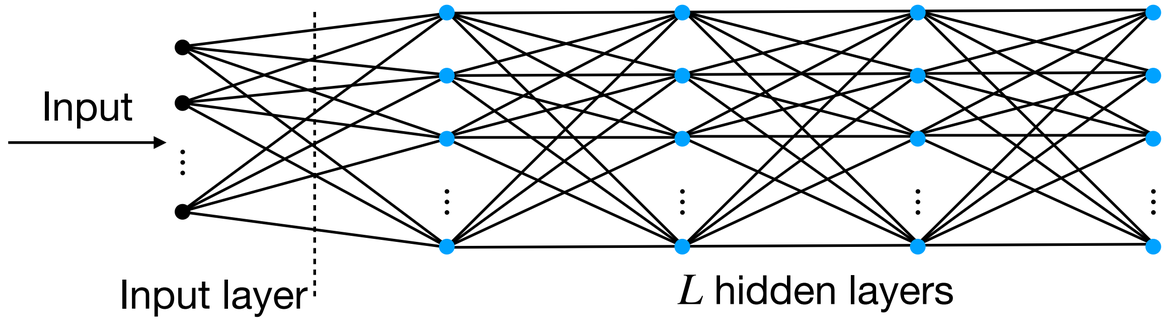
**weight of the edge going from node $i$ in layer $l-1$ to node $j$ in layer $l$**

**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 $\mathbb{R}^K$:




$$\Longleftrightarrow$$

$$\mathbb{R}^d \to \mathbb{R}^K$$

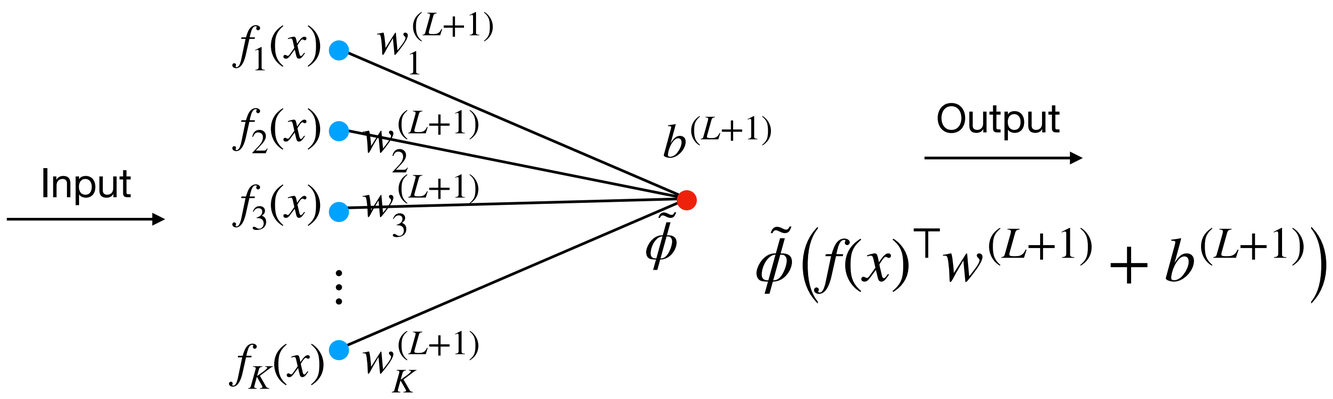
$$f: \quad x \mapsto \begin{pmatrix} f_1(x) \\ \vdots \\ f_K(x) \end{pmatrix}$$

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 $\phi$ we pick

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

# The last layer performs the desired ML task




**Regression** $\tilde{\phi} = I$

$$y = f(x)^\top w^{(L+1)} + b^{(L+1)}$$

**Classification** $\tilde{\phi}$ **:sigmoid**

$$y = \tilde{\phi}\left(f(x)^\top w^{(L+1)} + b^{(L+1)}\right)$$

Data representation

Linear prediction

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 $f : \mathbb{R}^d \to \mathbb{R}$ 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

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

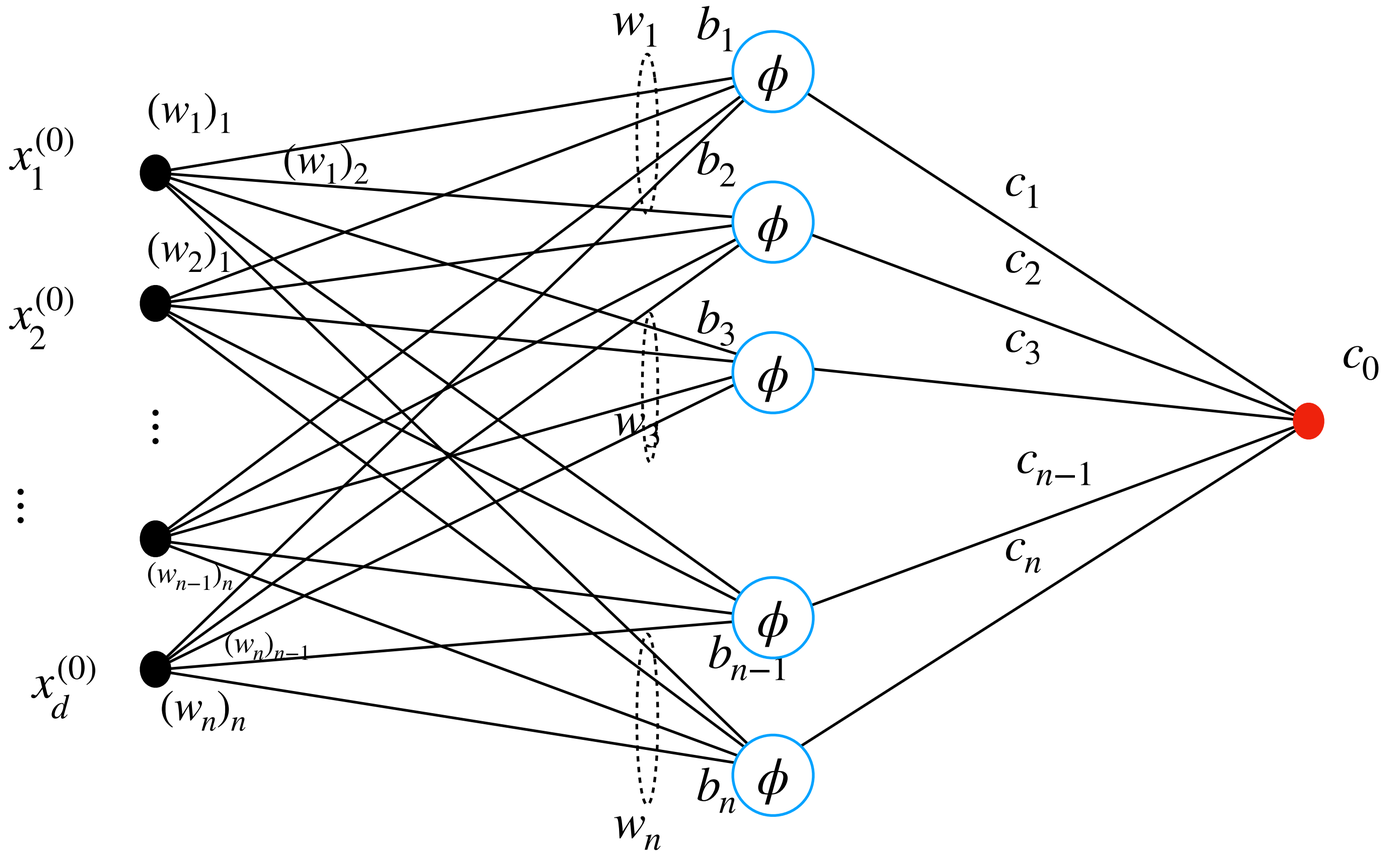
# All sufficiently smooth function can be approximated by a one-hidden-layer NN

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

- 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 $\ell_2$-norm)
- For any “sigmoid-like” activation function

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

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

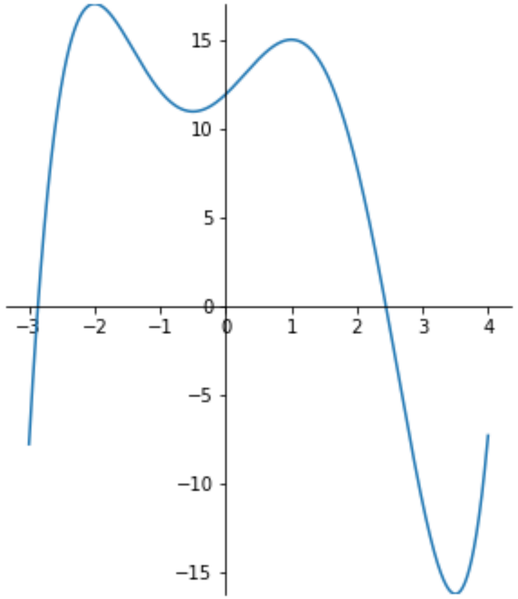


# $L_1$ Approximation: Proof by picture

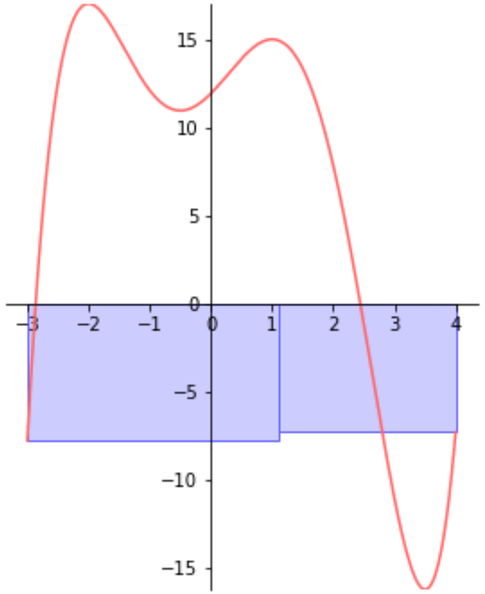
Simple and intuitive explanation of a slightly different result:

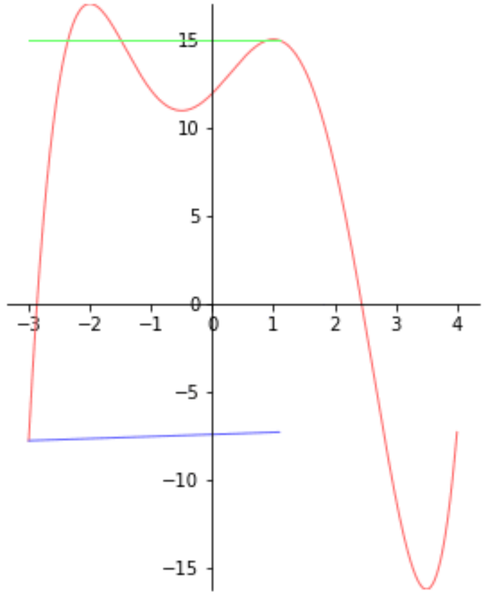
"A NN with sigmoid activation and at most two hidden layers can approximate well a smooth function in average, i.e, in $\ell_1$-norm"

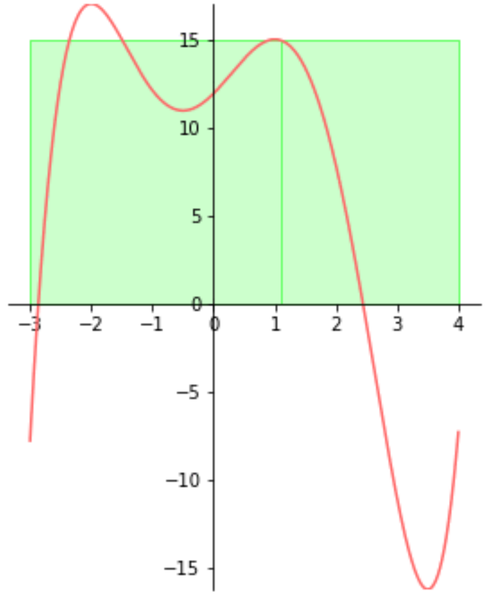
Consider a function $f : \mathbb{R} \to \mathbb{R}$ on a bounded domain



# Approximation of the function by a sum of rectangles



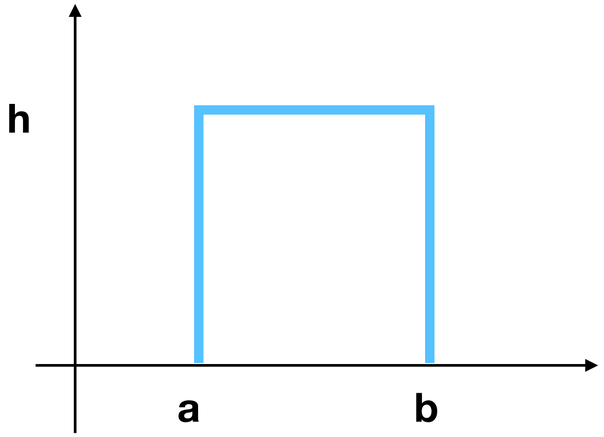




**From below**

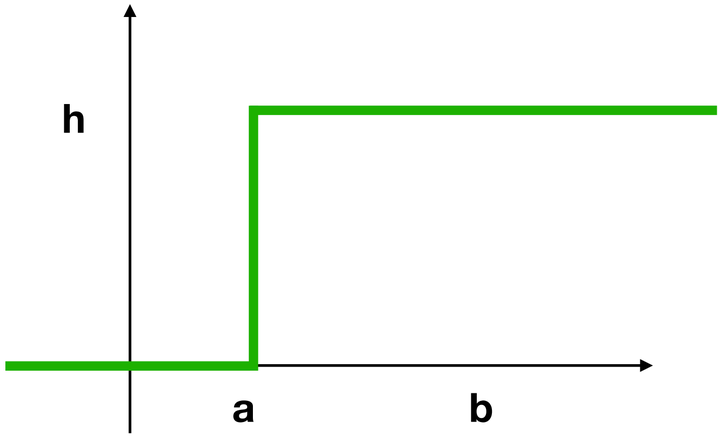
**From above**

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

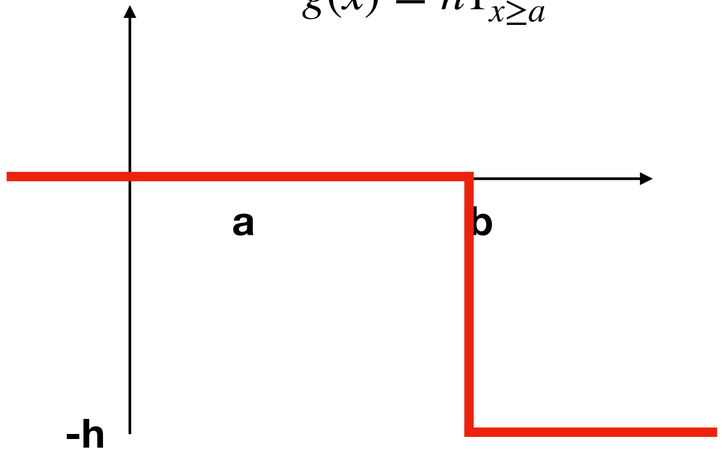
# A rectangle is equal to the sum of two step functions



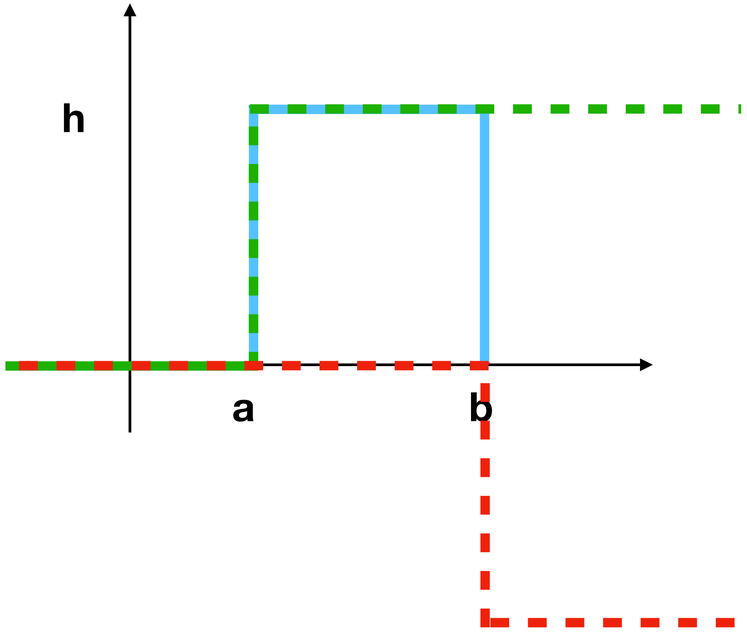

$$f(x) = h1_{x\in[a,b]}$$




$$g(x) = h1_{x\geq a}$$




$$h(x) = -h1_{x\geq b}$$




$$f(x) = g(x) + h(x)$$

# Approximate a step function with a sigmoid

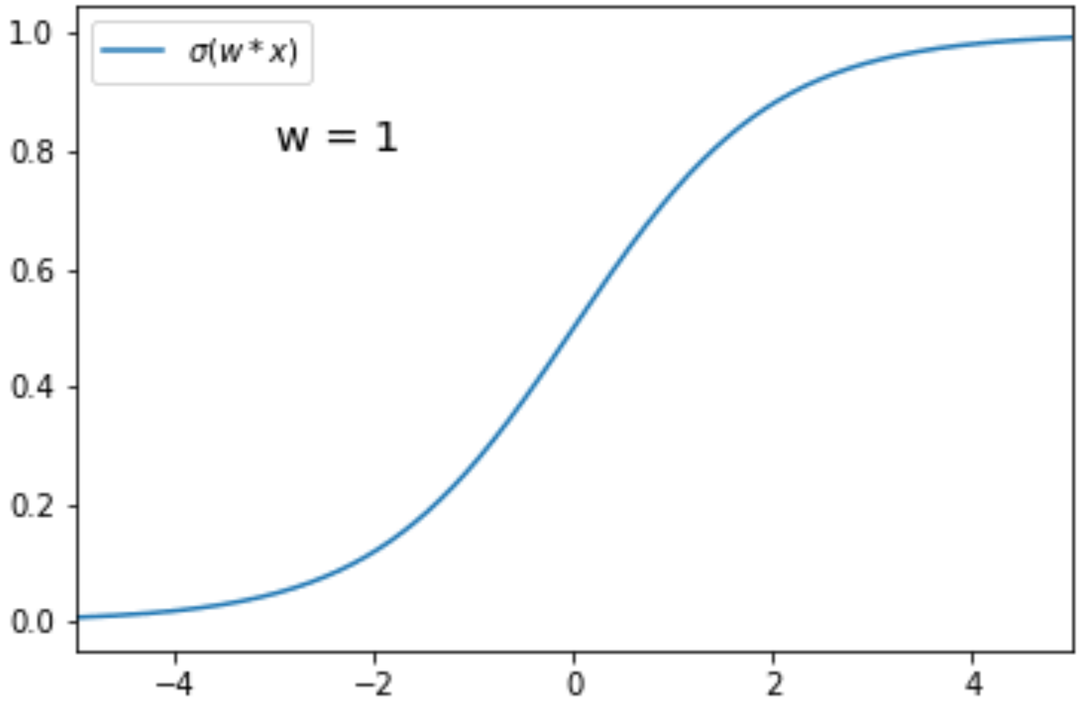
$$\tilde{\phi}(x) = \sigma\big(w(x-b)\big)$$

By setting:

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

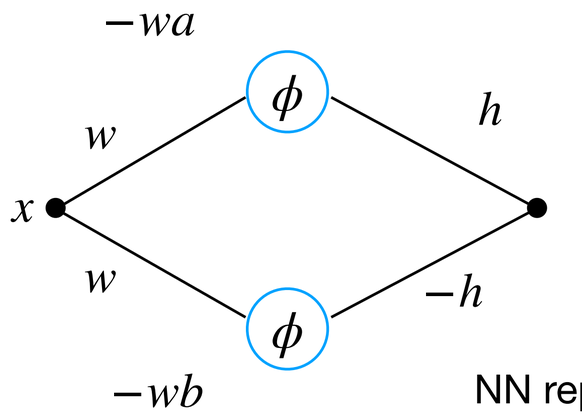
Derivative: $\tilde{\phi}'(b) = w/4$

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



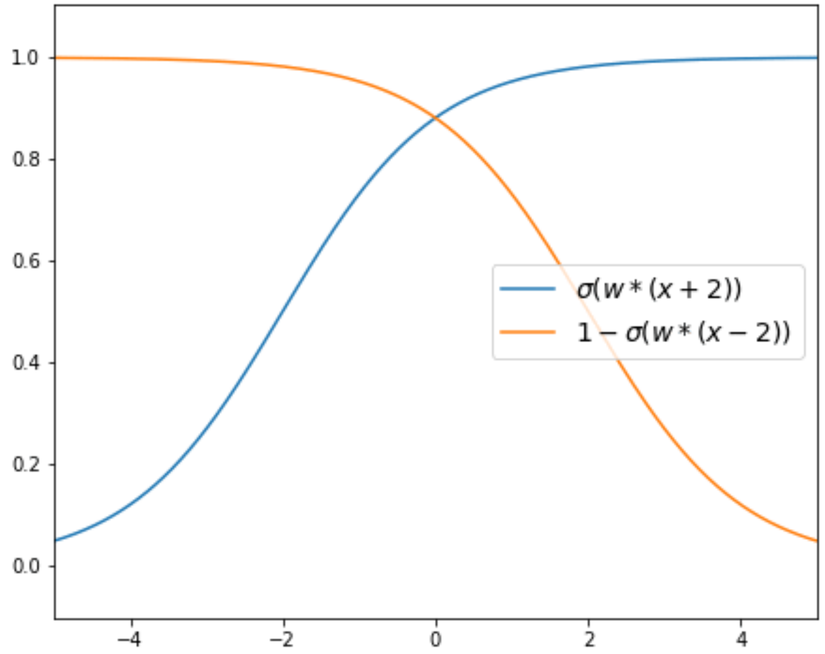
# Approximation of the rectangle

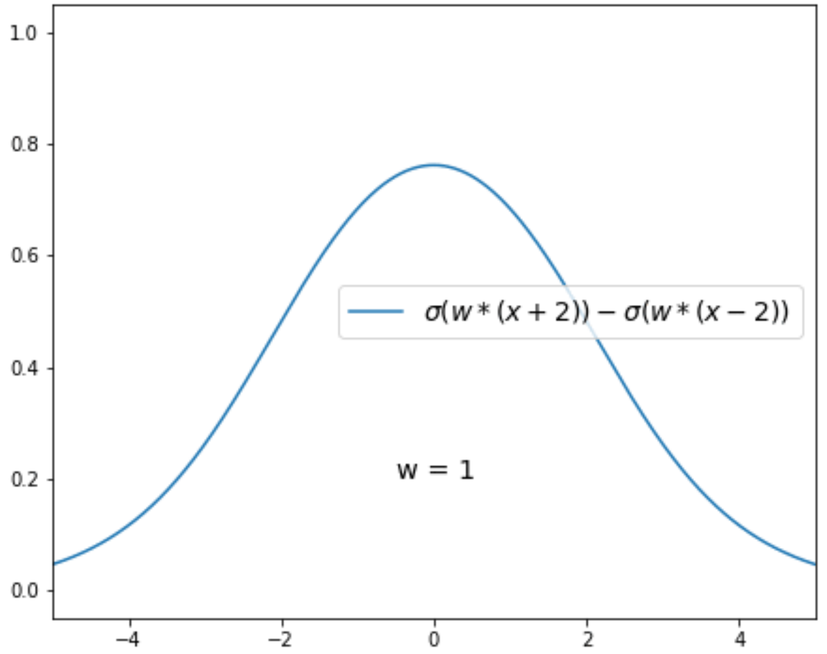
$$h\big(\phi(w(x-a)) - \phi(w(x-b))\big)$$




NN representation

$a = -2$
$b = 2$
$h = 1$

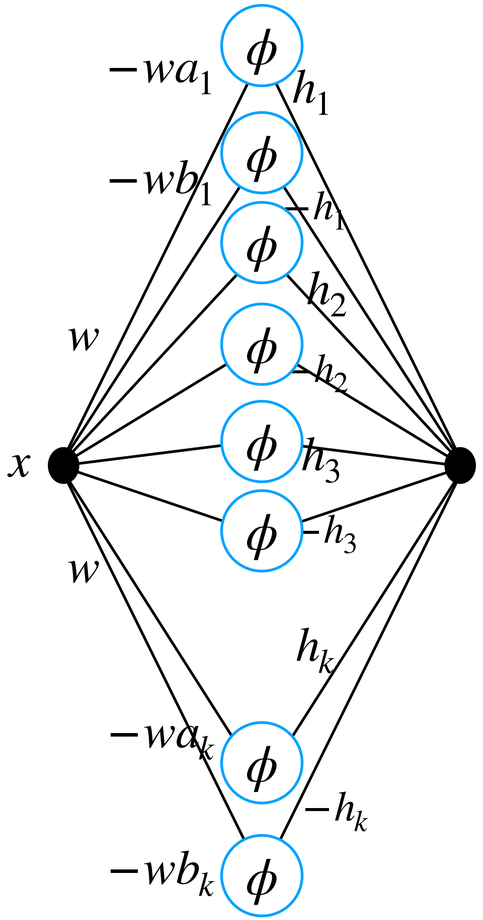


# Conclusion in the 1D case

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



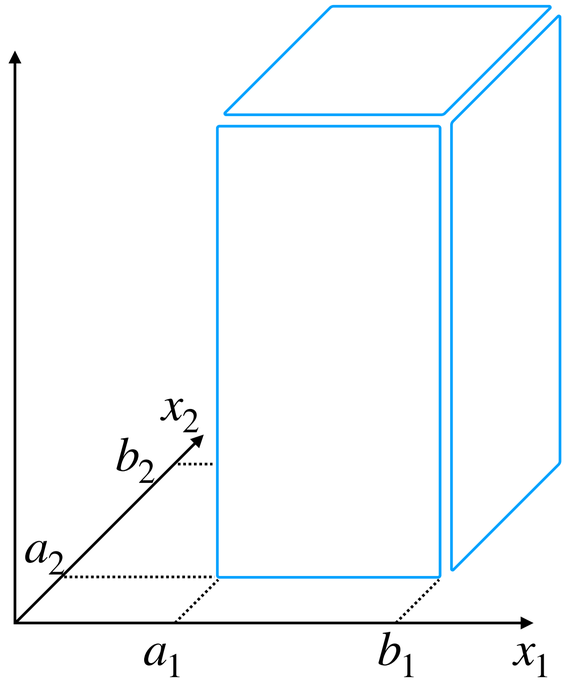

<u>Remarks:</u>

- 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

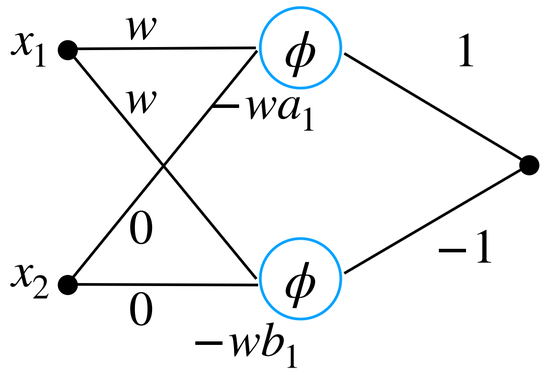


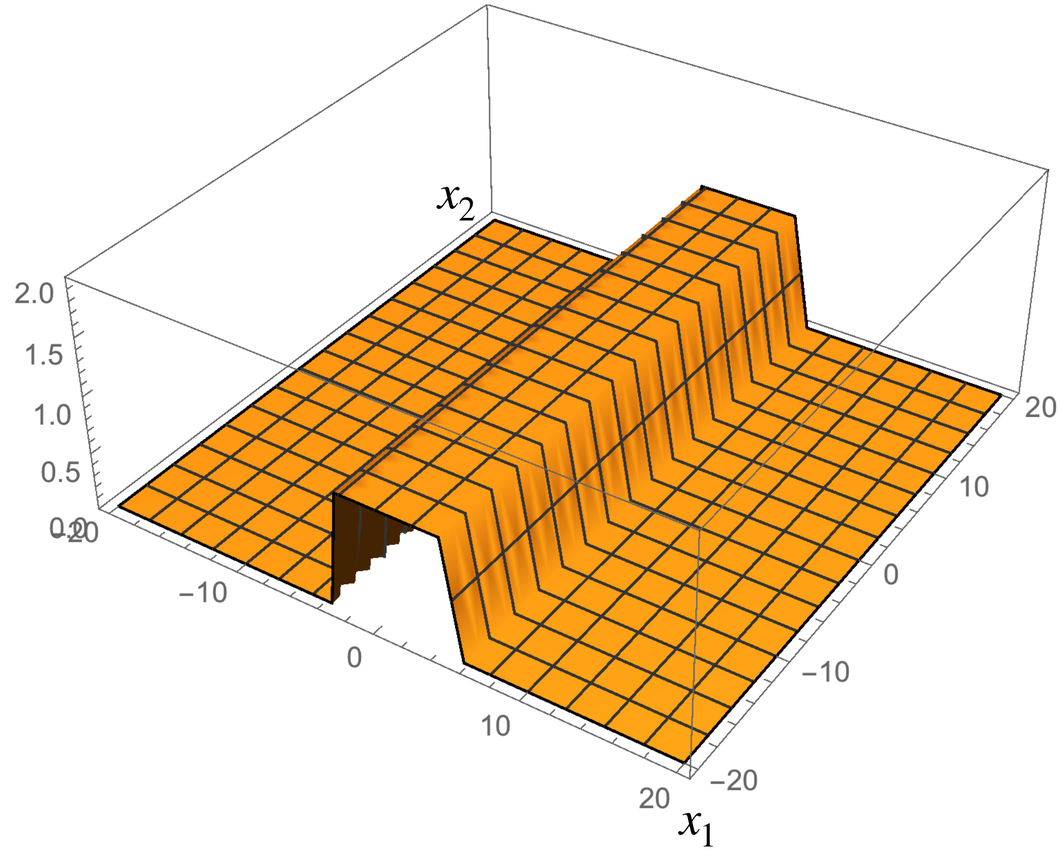
# Two sigmoids can approximate an infinite rectangle

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

Rectangle:

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



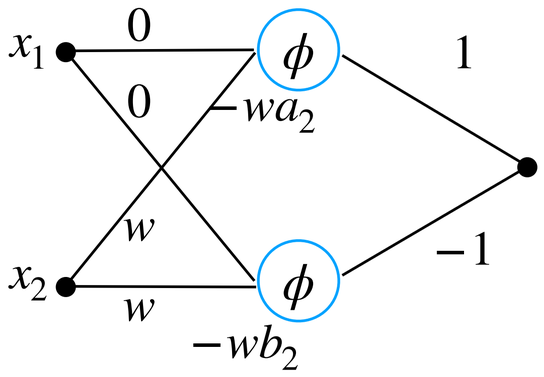



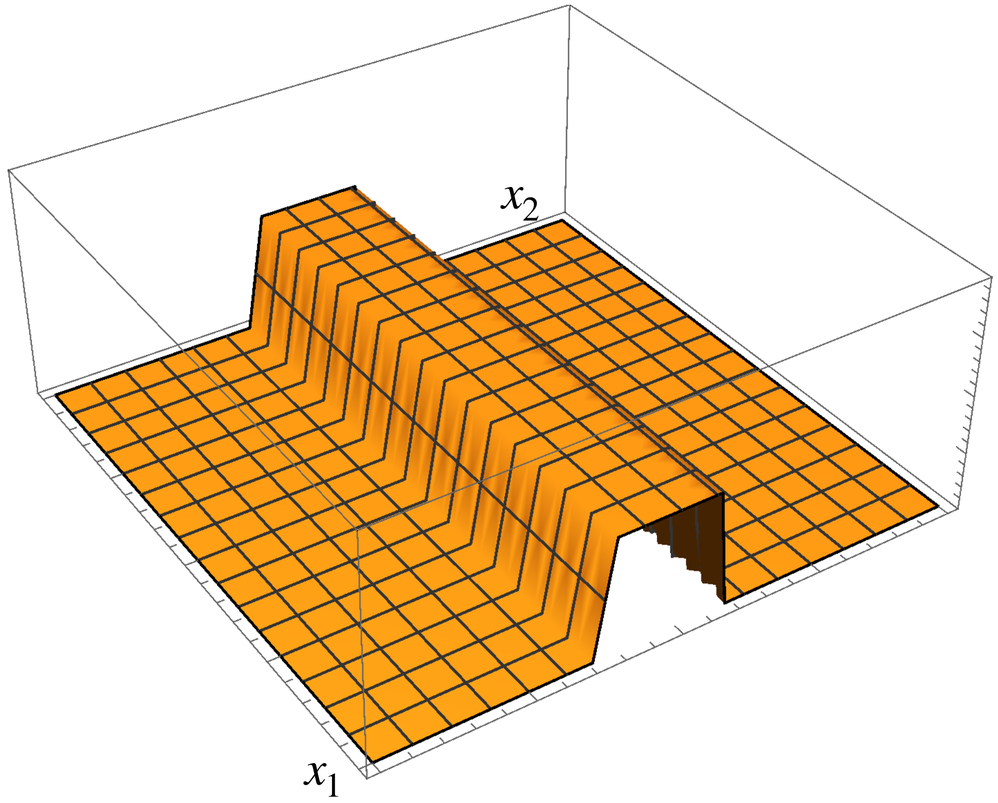
# Two sigmoids can approximate an infinite rectangle

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

Rectangle:

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

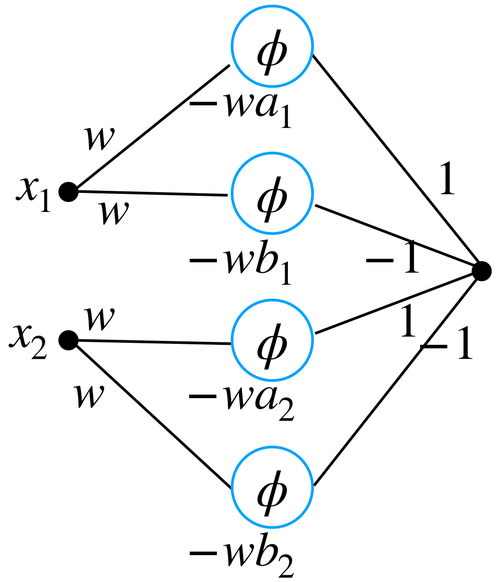


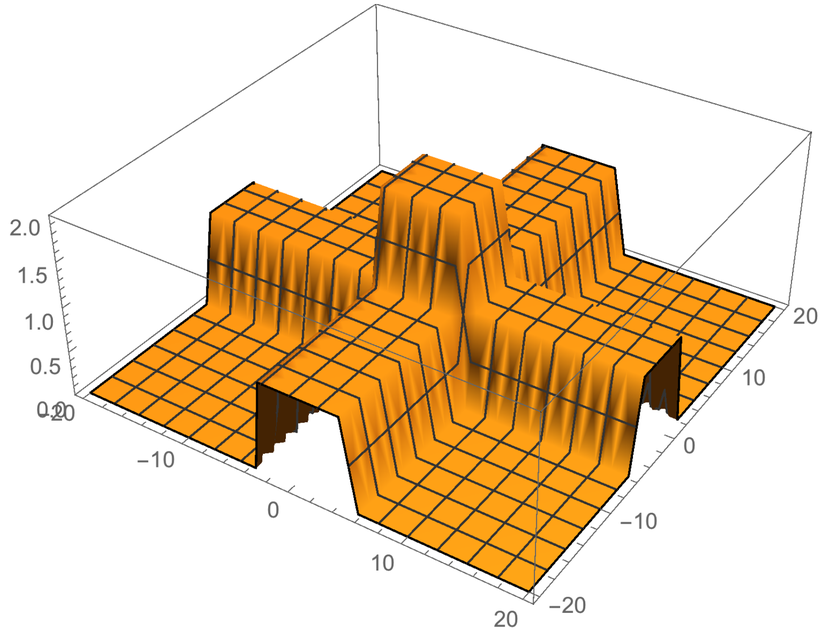



# Four sigmoids can approximate a cross

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

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



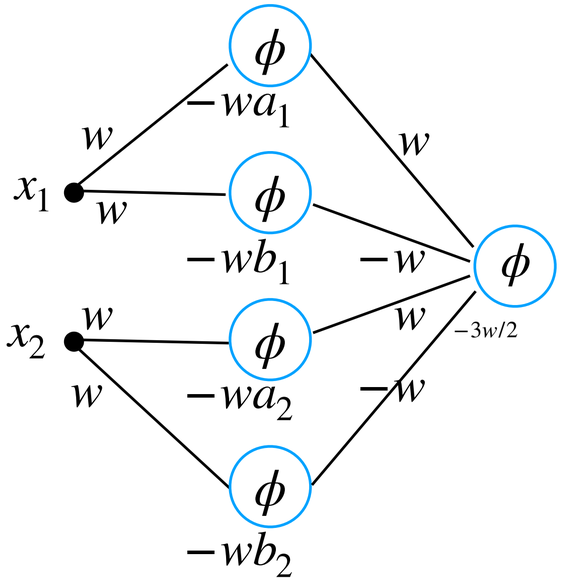

How to get rid of the crossed arms?

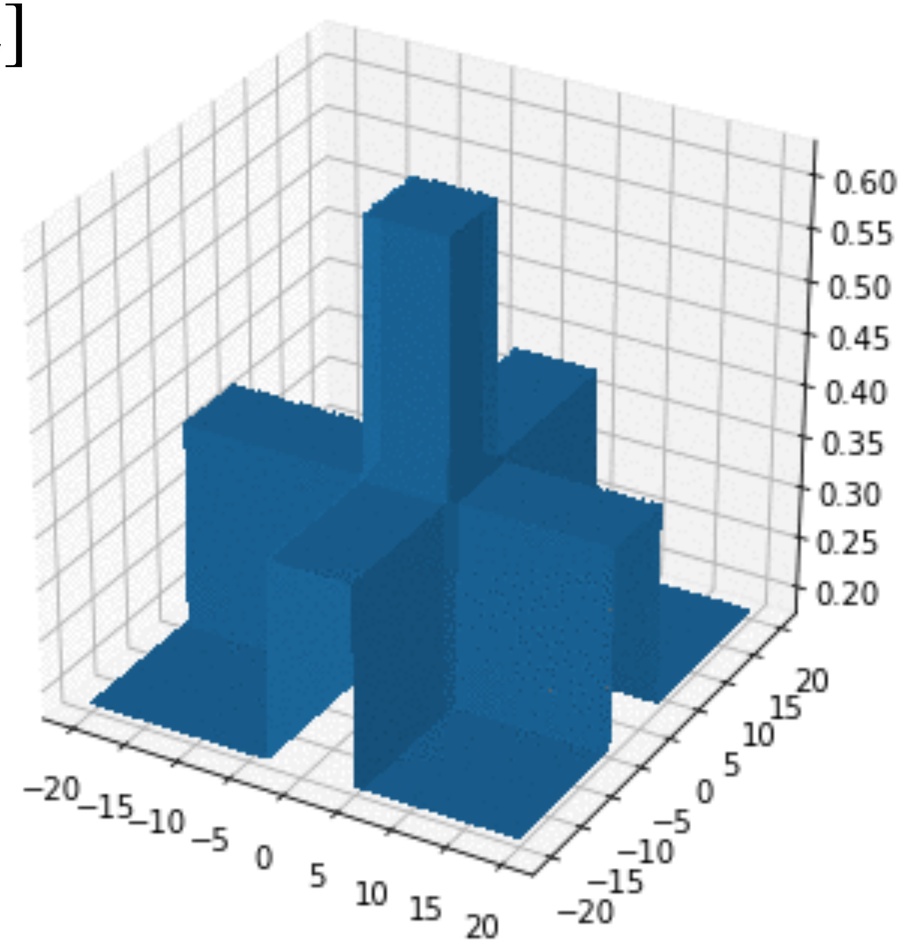
# The sigmoid can threshold the unwanted infinite arms

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

Let $f$ be a continuous function on $[0,1]$

Different $\ell_\infty$-approximation results exist:

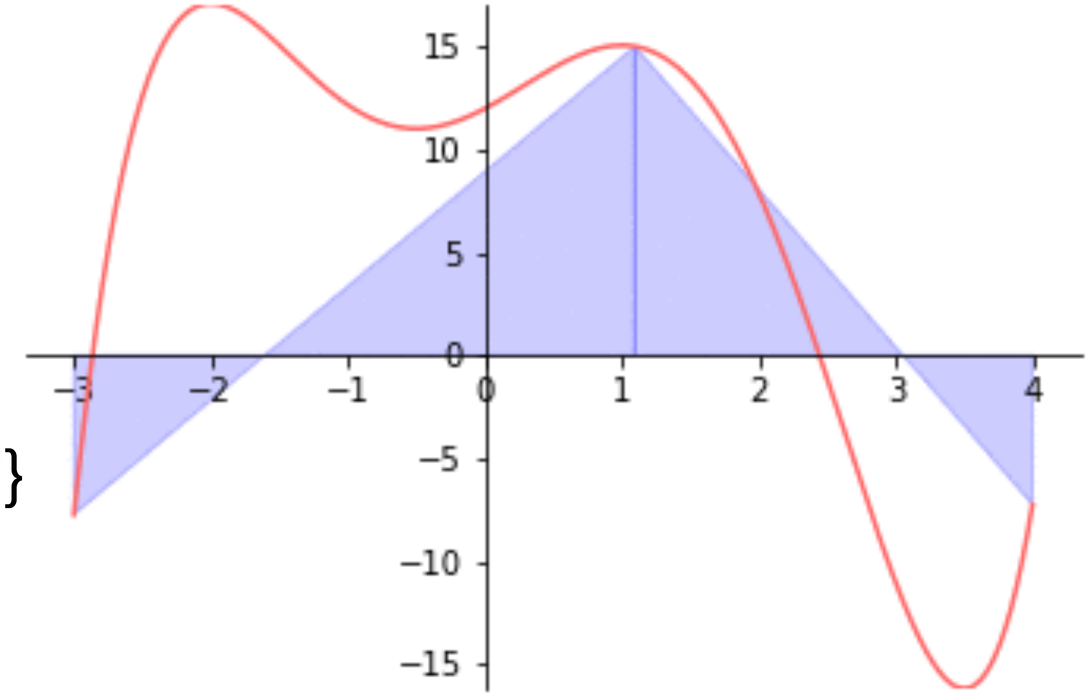
- Polynomials: Stone Weierstrass theorem:

$$\forall \varepsilon > 0,\ \exists p \in \mathbb{R}[X],$$
$$\sup_{x \in [0,1]} |f(x) - p(x)| \leq \varepsilon$$

- Piecewise linear function (Shektman, 1982}

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

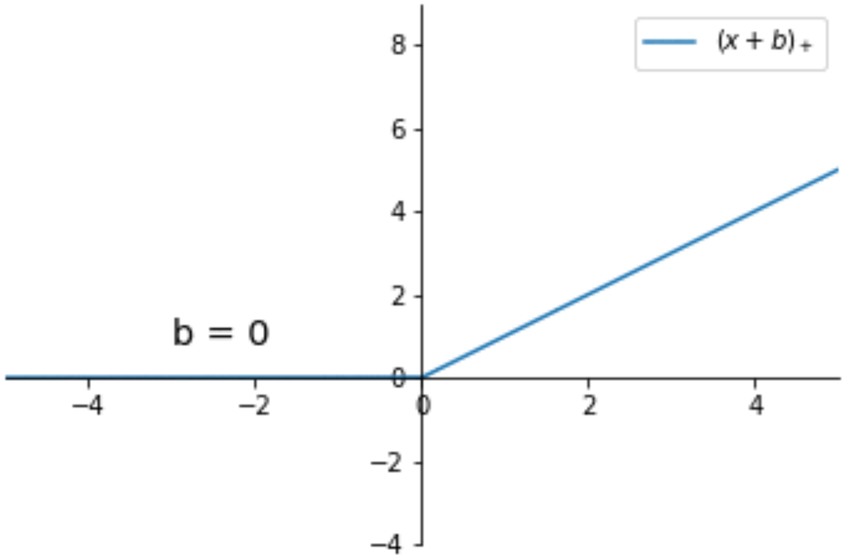
with $a_i r_i + b_i = a_{i+1} r_i + b_{i+1}$



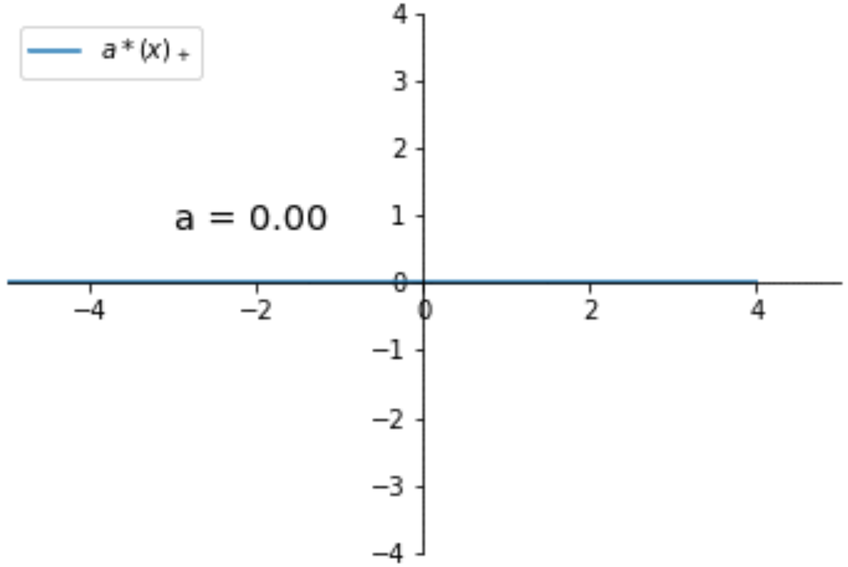

➡ How to approximate PWL functions with a NN?

# Rectified linear unit - RELU

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




The bias $b$ determines where the kink is



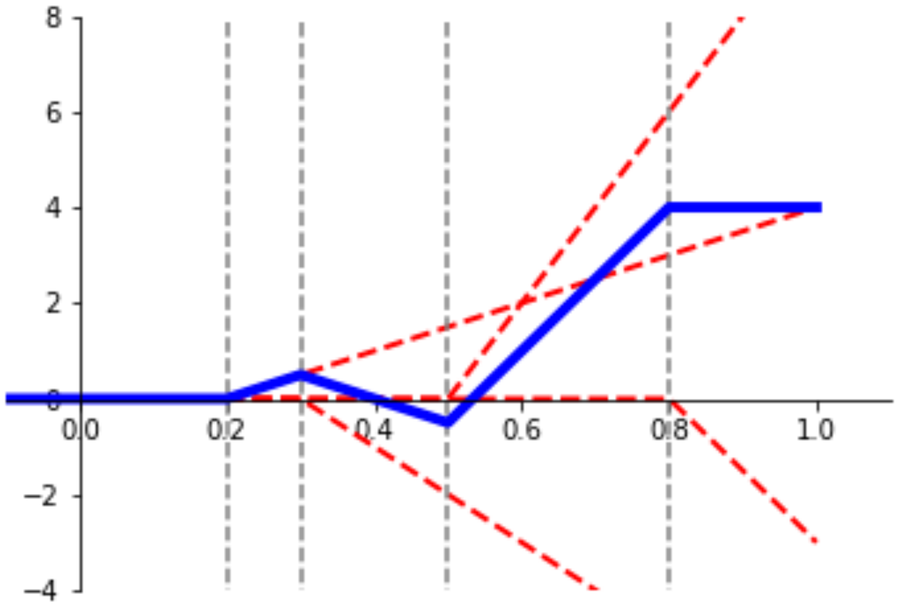

The weight $a$ determines the slope

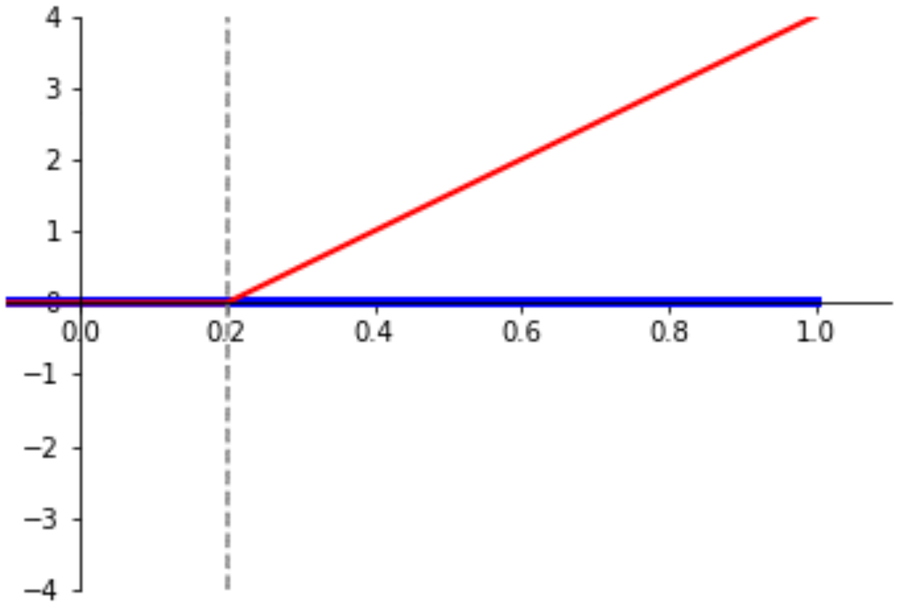
# Linear combinations of RELUs are PWL functions

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

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

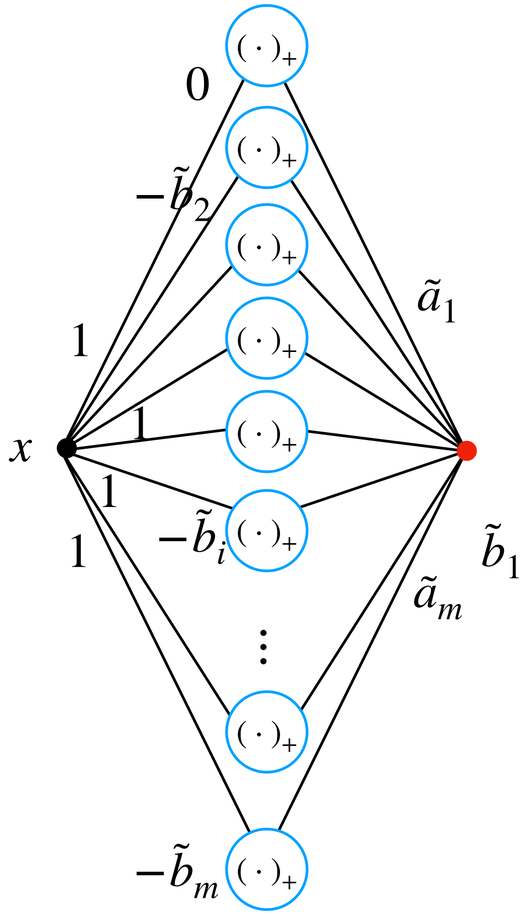
where $\tilde{a}_1 = a_1, \tilde{b}_1 = b_1, \; a_i = \sum_{j=1}^{i} \tilde{a}_i$ and $\tilde{b}_i = r_{i-1}$

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

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

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

- 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 $x \in [r_1, r_2]$, $r(x) = \tilde{a}_1 x + \tilde{b}_1 + (a_2 - a_1)(x - r_1)_+$

  $= a_1 x + b_1 + (a_2 - a_1)(x - r_1) = a_2 x + b_1 - (a_2 - a_1) r_1$

  $r'(x) = a_2$ and $r(r_1) = q(r_1)$ as shown above

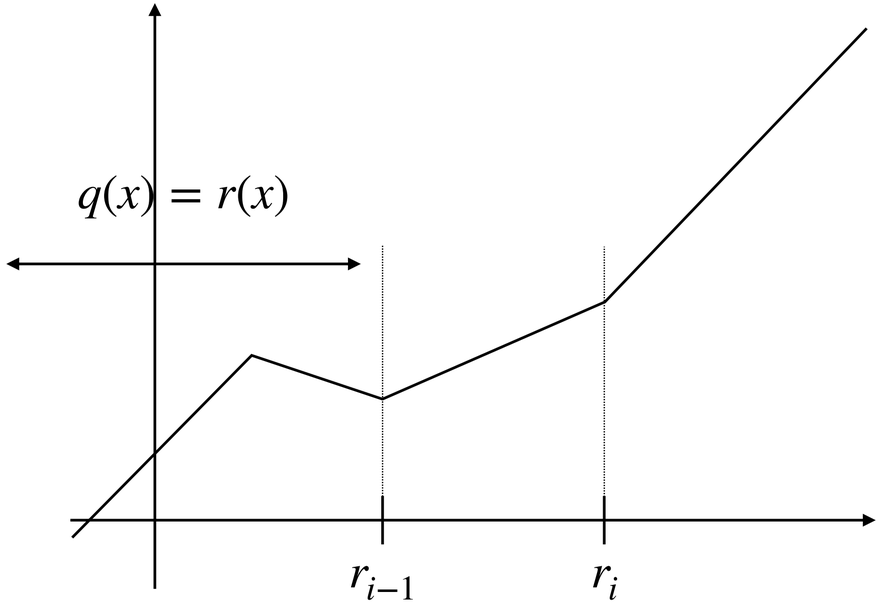
  $\implies r(x) = q(x)$ for $x \in [r_1, r_2]$

# Proof by induction

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

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

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




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

$\Longrightarrow$ $r(x) = q(x)$ for $x \in [r_{i-1}, r_1]$

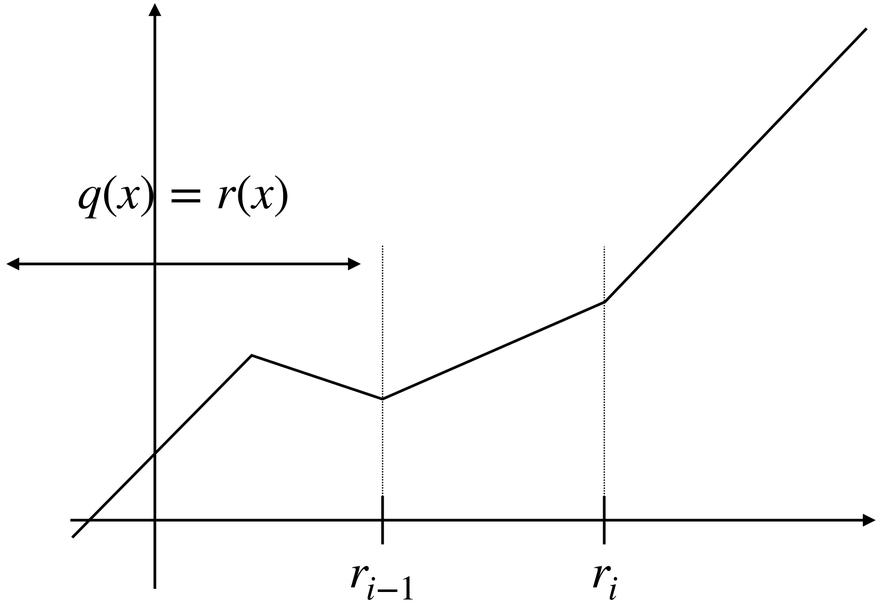
Why: two affine functions with the same starting point and the same slope are equal

# 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

$\Longrightarrow$ $r(x) = q(x)$ for $x \in [r_{i-1}, r_1]$

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