ARISTOTLE UNIVERSITY OF THESSALONIKI

FACULTY OF ENGINEERING

Pattern Recognition & Machine Learning

Neural Networks

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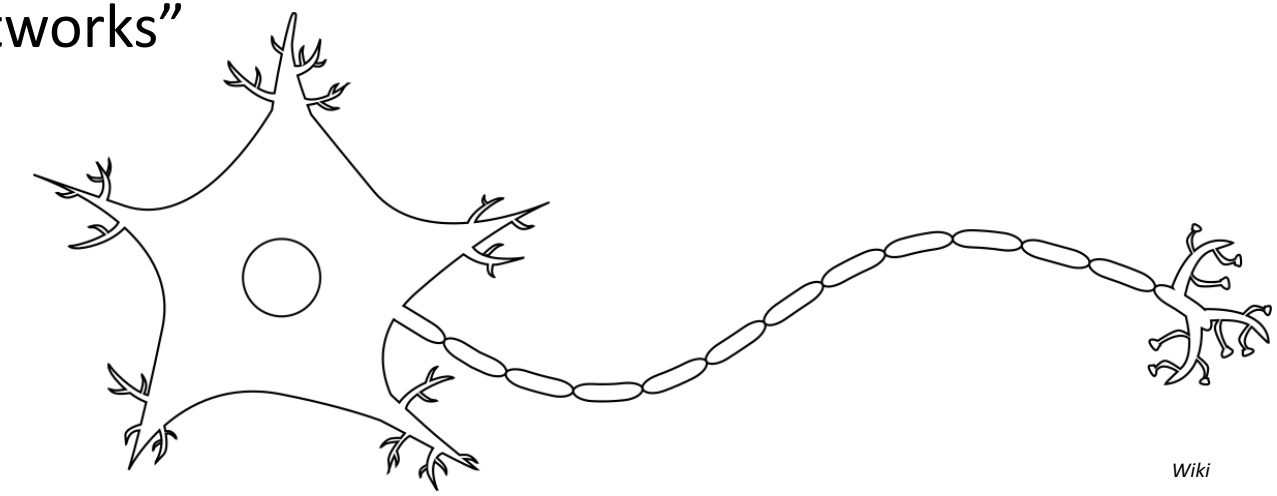
Until now…

- Dataset: inputs $\boldsymbol{X} = (\boldsymbol{x}_1, \dots, \boldsymbol{x}_N)$ and targets $\boldsymbol{t} = (t_1, \dots, t_N)$, where $\boldsymbol{x}_n \in \mathbb{R}^D$
- Fixed features: $\boldsymbol{\varphi}(\boldsymbol{x}) = \big(\varphi_0(\boldsymbol{x}), \dots, \varphi_M(\boldsymbol{x})\big)$, where $\varphi_0 = 1$
- Classification: $y(\boldsymbol{x}, \boldsymbol{w}) = f(\boldsymbol{w}^T \boldsymbol{\varphi}(\boldsymbol{x}))$
  - f: nonlinear activation function (e.g., logistic sigmoid)
- In the SVM case we had basis functions centered on training samples and then selecting a number of them to define the decision rule (support vectors)
  - convex objective function
  - again fixed features $\boldsymbol{\varphi}(\boldsymbol{x})$
- What if we want adaptive basis functions?
  - Neural Networks!

Neural Network

- Artificial “Neuron” and “Neural Networks”
  - Mathematical interpretation of information processing in the brain.
  - McCulloch and Pitts (1943)
  - Widrow and Hoff (1960)
  - Rosenblatt (1962)
  - Rumelhart et al. (1986)
  - etc. etc.



Wiki

- A vast variety of different implementations and algorithms regarding the above mentioned mathematical interpretation.
  - Biological plausibility

- Here we will talk for a class of NN that are of great practical value:
  - Multilayer Perceptrons (MLP)!

Perceptron

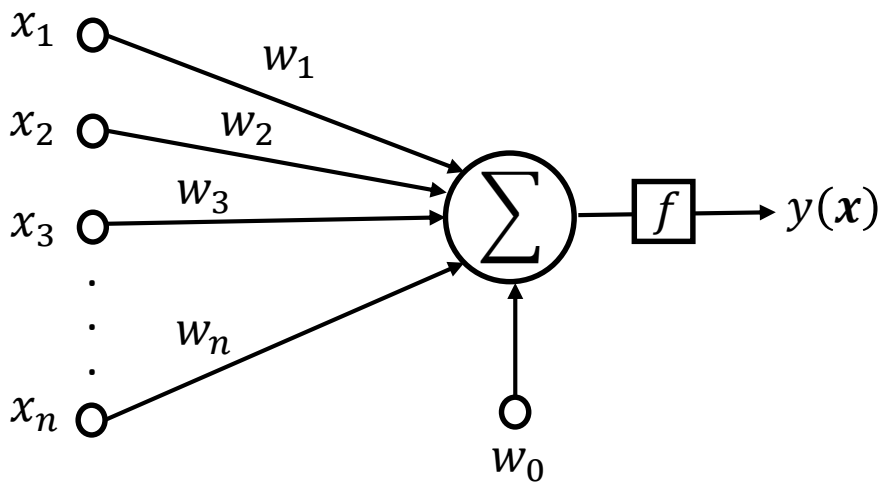
$$y(\boldsymbol{x}) = f(\boldsymbol{w}^t \boldsymbol{x} + w_0)$$

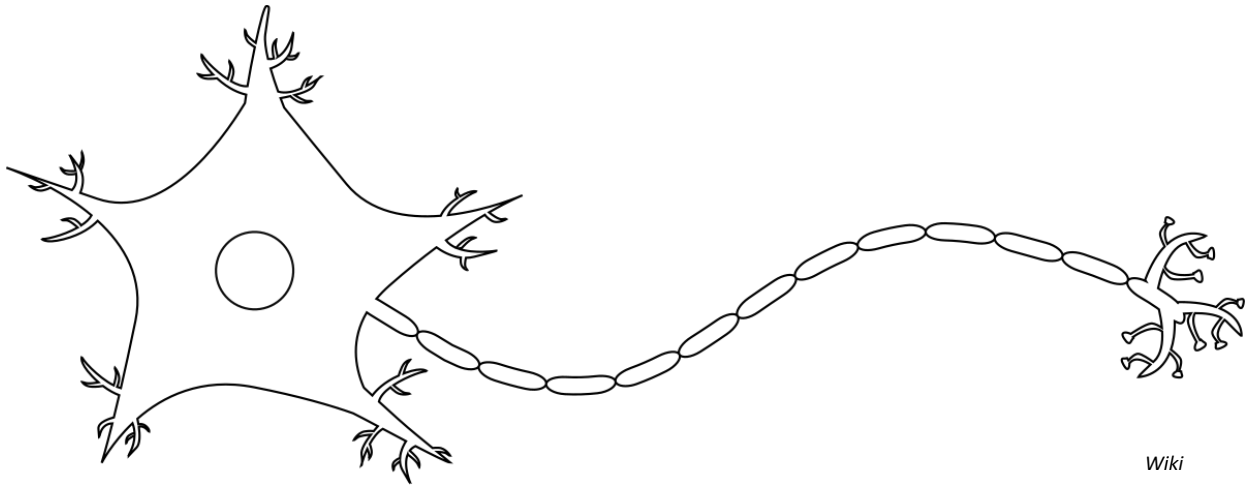
If we incorporate w_0:

$$y(\boldsymbol{x}) = f(\boldsymbol{w}^t \boldsymbol{x})$$

In the general case:

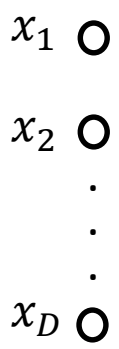
$$y(\boldsymbol{x}) = f(\boldsymbol{w}^t \boldsymbol{\varphi}(\boldsymbol{x}))$$





Wiki

From a single perceptron to a MLP



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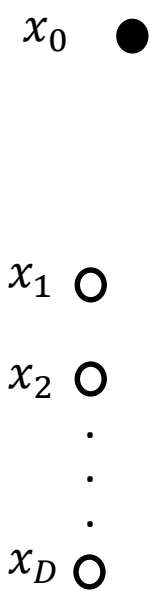

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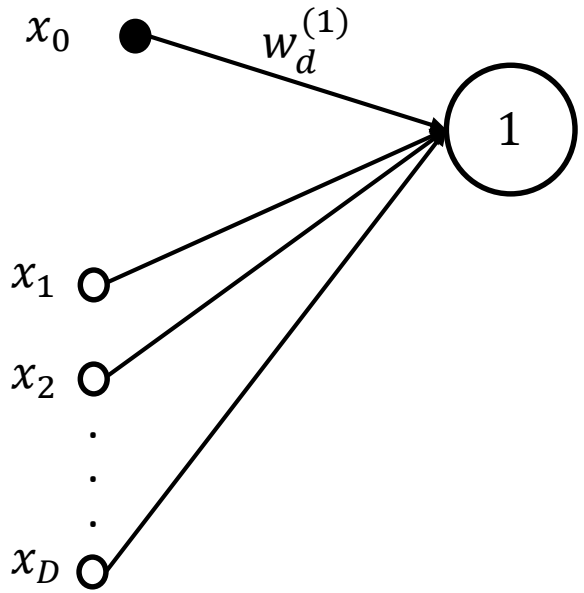

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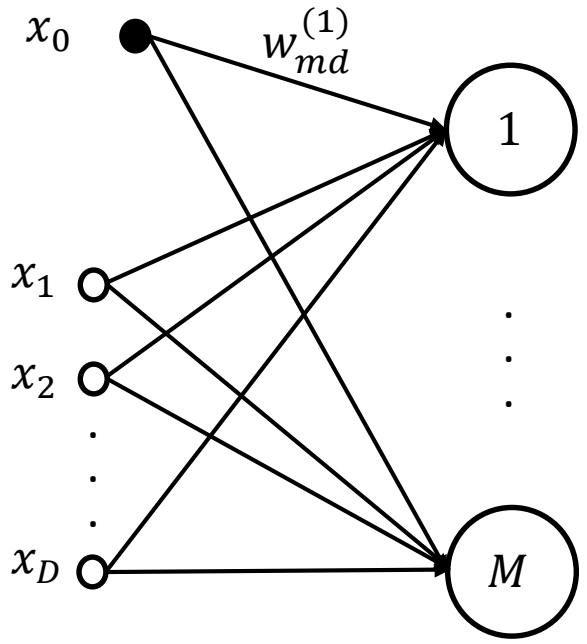

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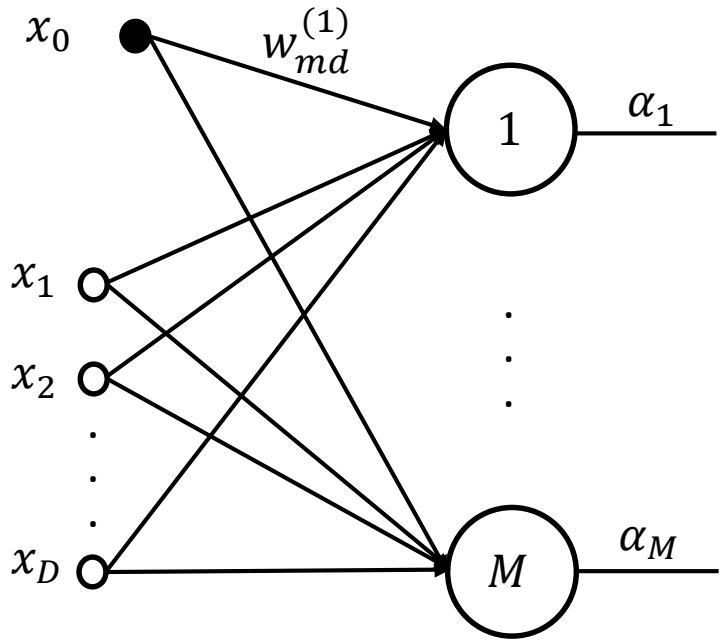

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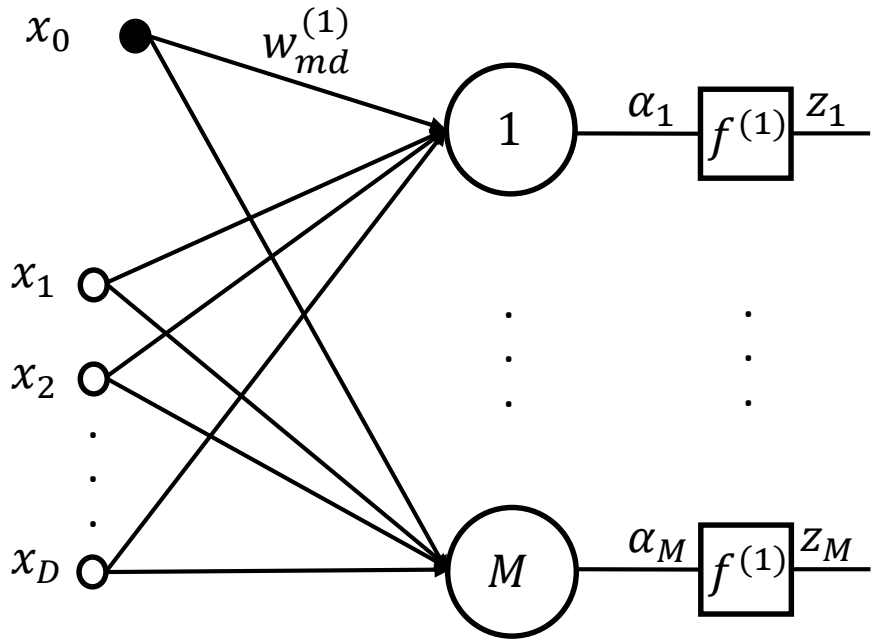
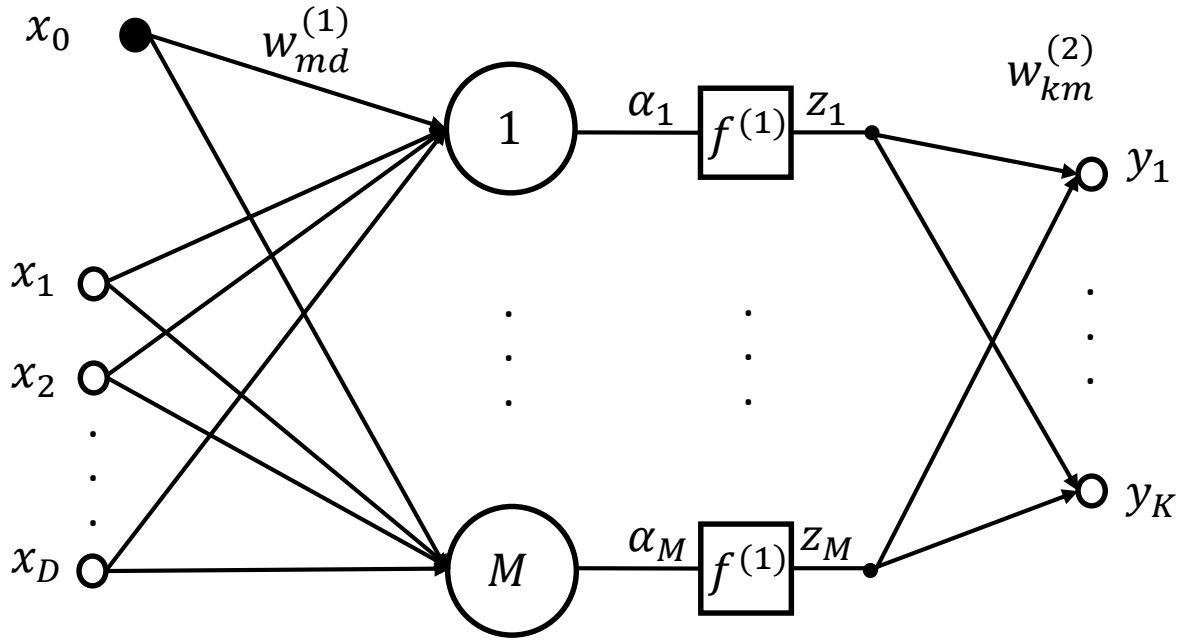


Two layer-Perceptron



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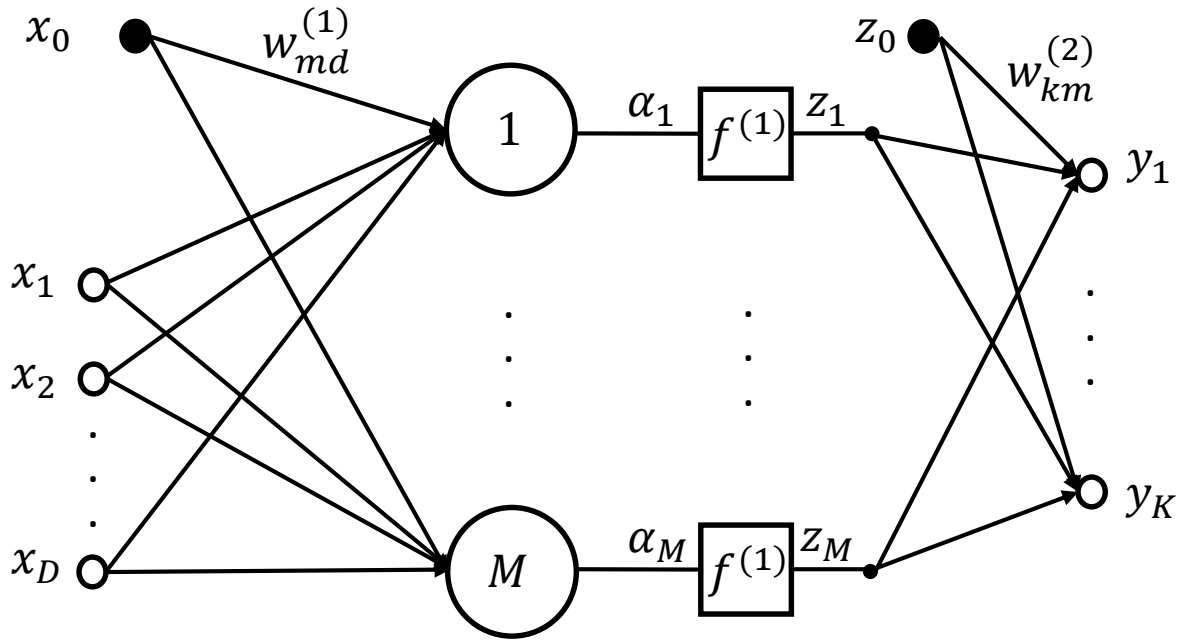

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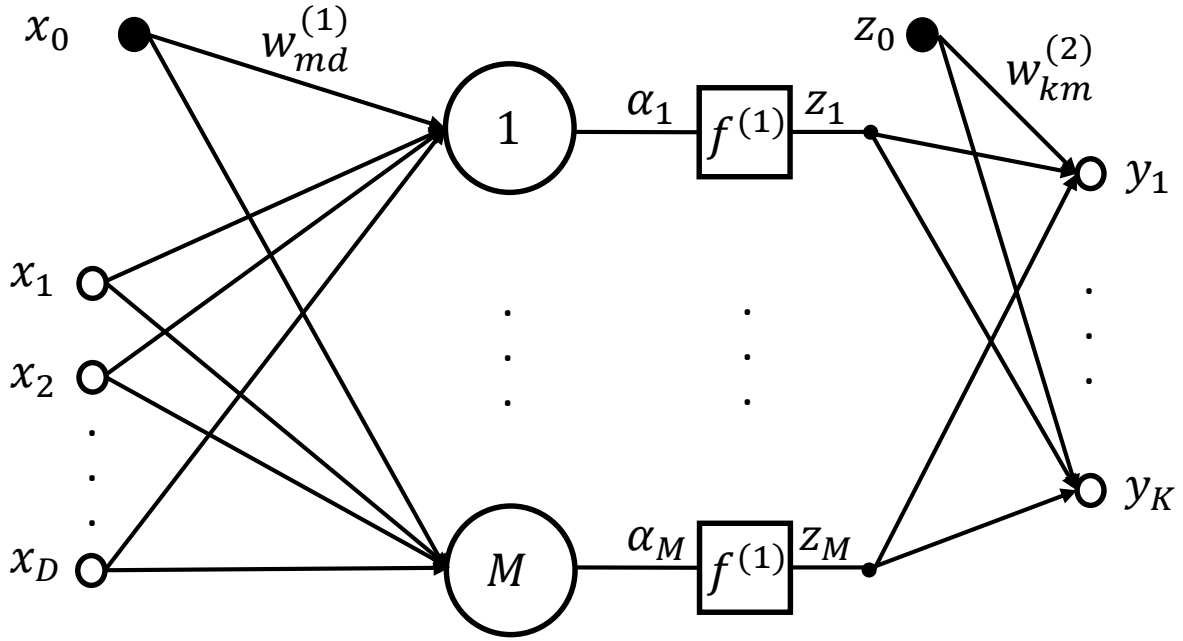
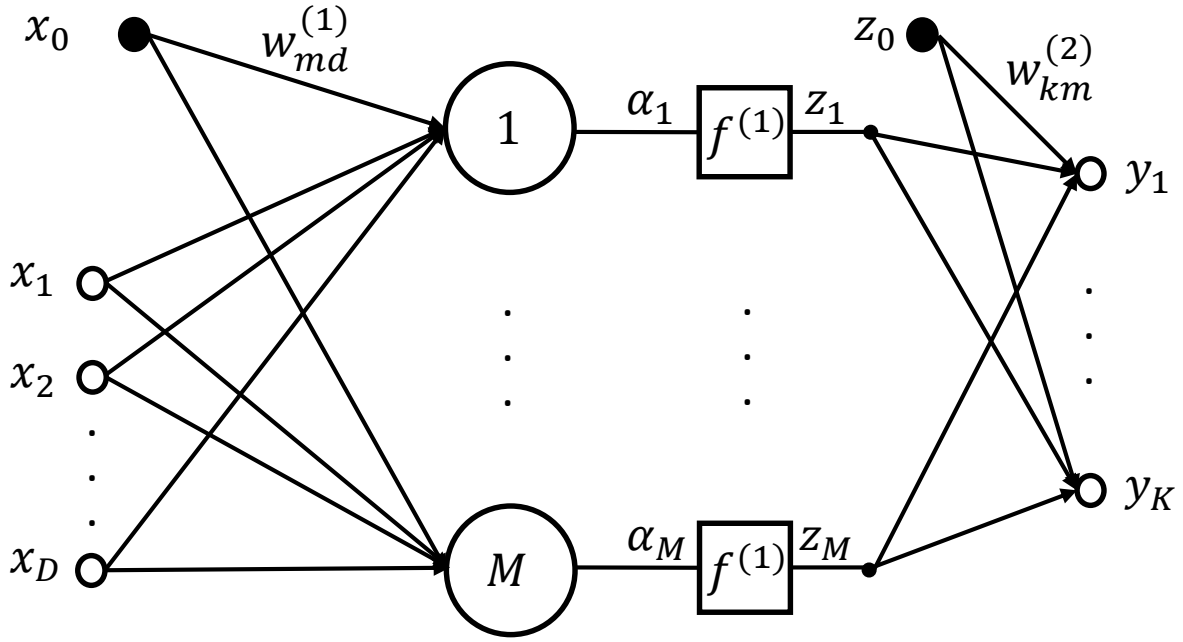


Two layer-Perceptron

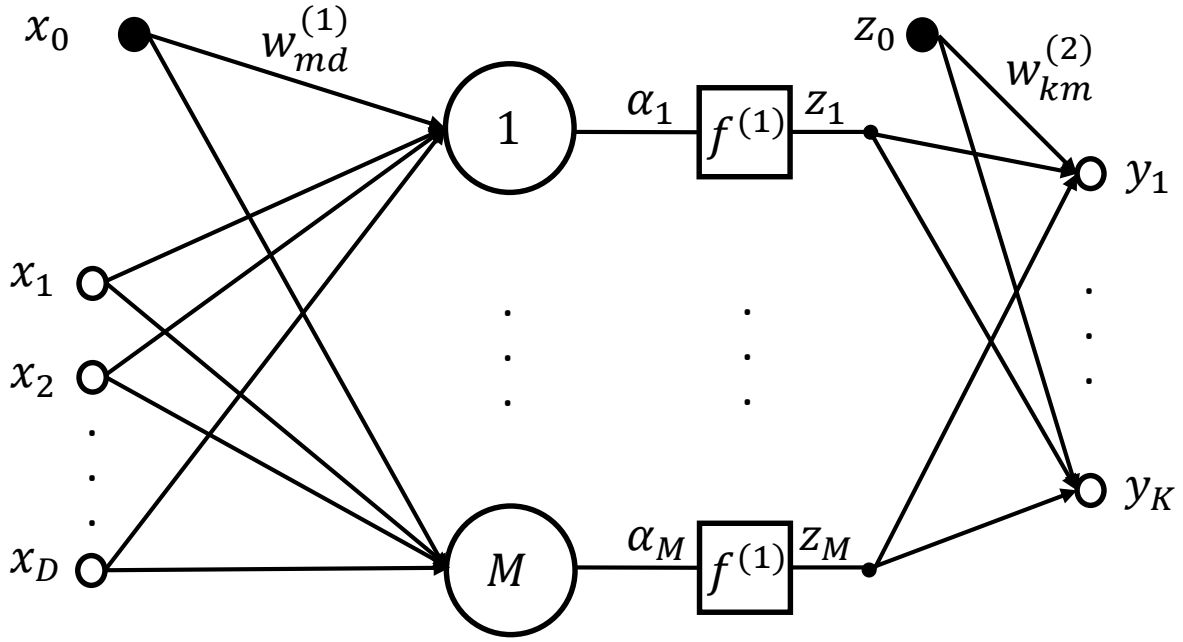
$$y_k = \sum_{m=0}^{M} w_{km}^{(2)} z_m$$



Two layer-Perceptron

$$y_k = \sum_{m=0}^{M} w_{km}^{(2)} z_m$$

$$y_k = \sum_{m=0}^{M} w_{km}^{(2)} f^{(1)}(\alpha_m)$$



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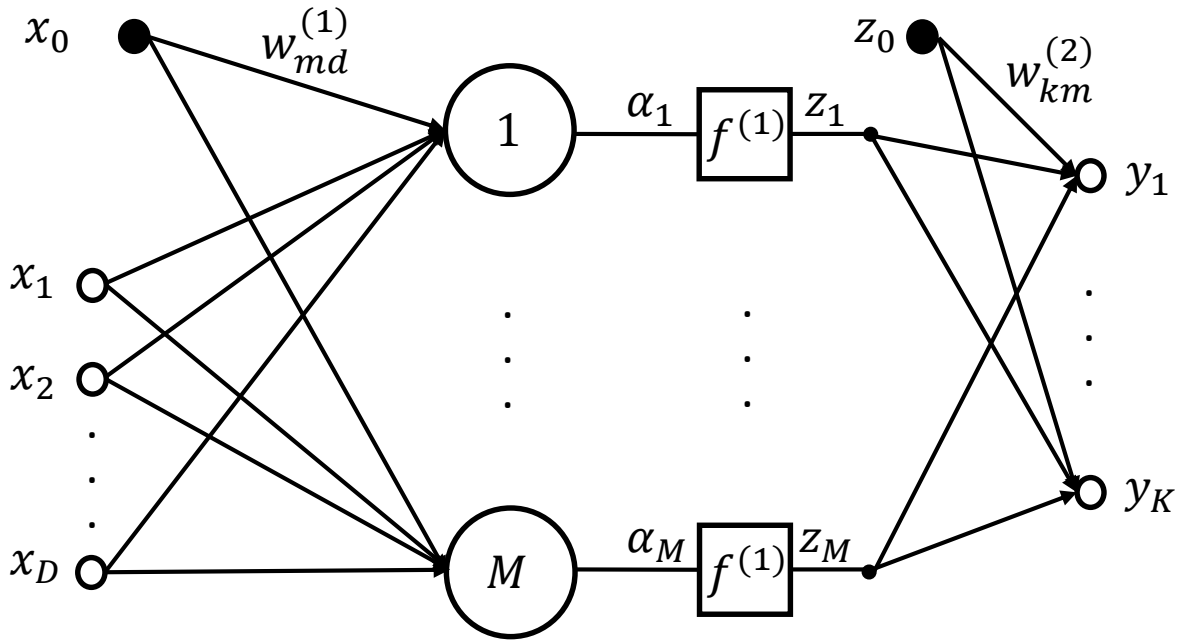
$$y_k = \sum_{m=0}^{M} w_{km}^{(2)} f^{(1)}\left(\sum_{d=0}^{D} w_{md}^{(1)} x_d\right)$$



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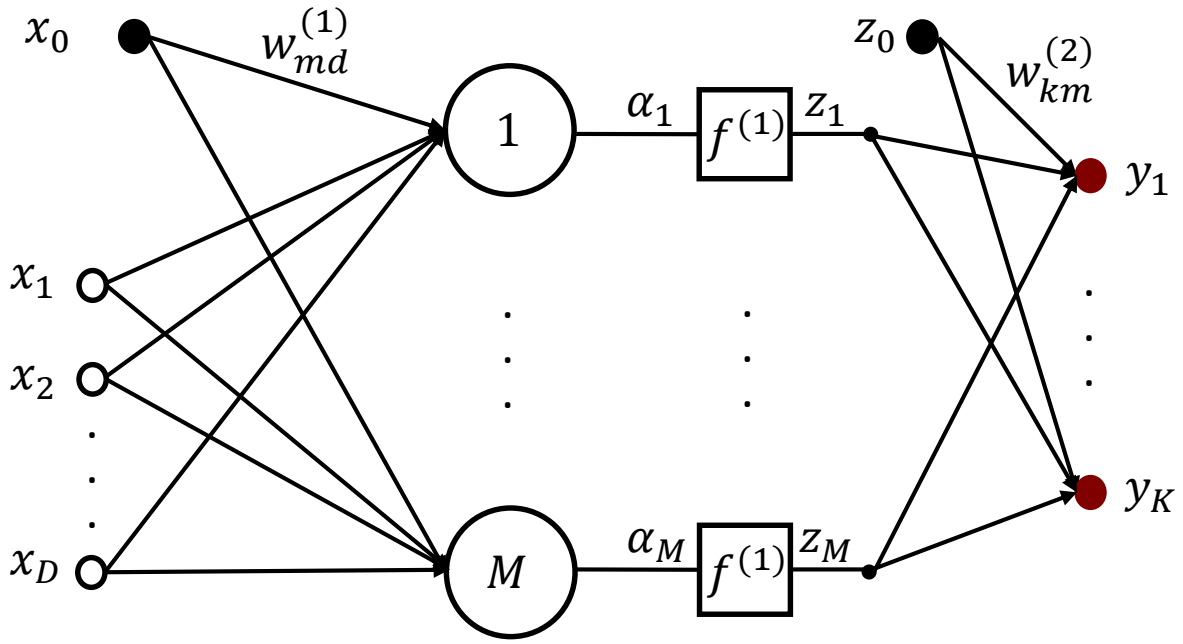

Usually: $y_k = f^{(2)}\left(\sum_{m=0}^{M} w_{km}^{(2)} f^{(1)}\left(\sum_{d=0}^{D} w_{md}^{(1)} x_d\right)\right)$

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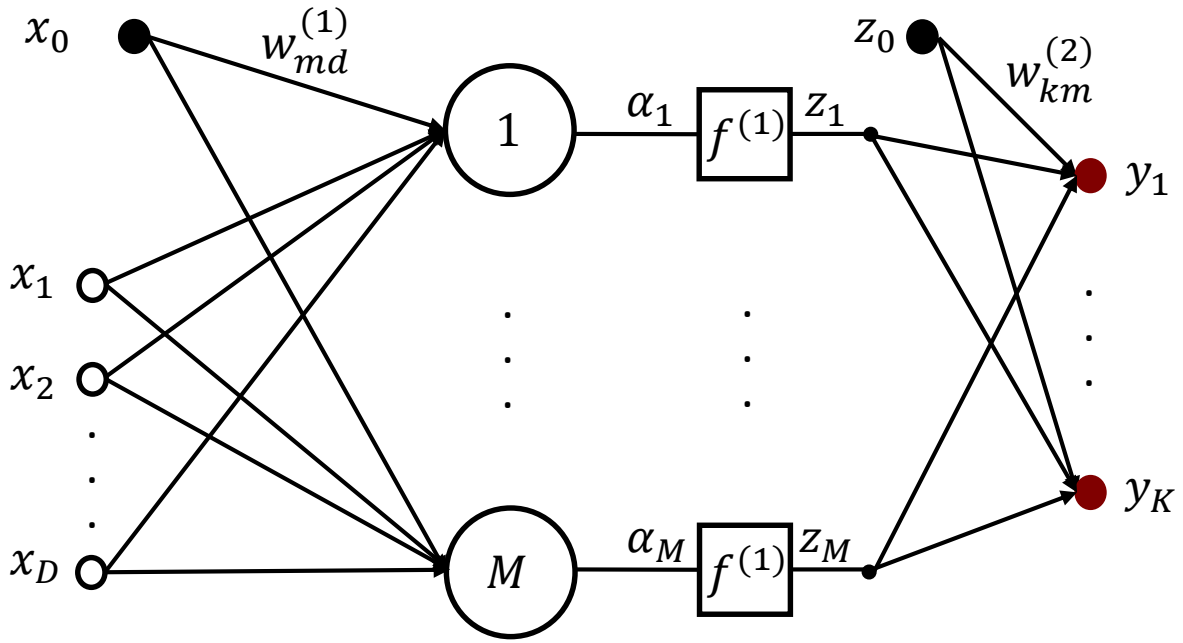
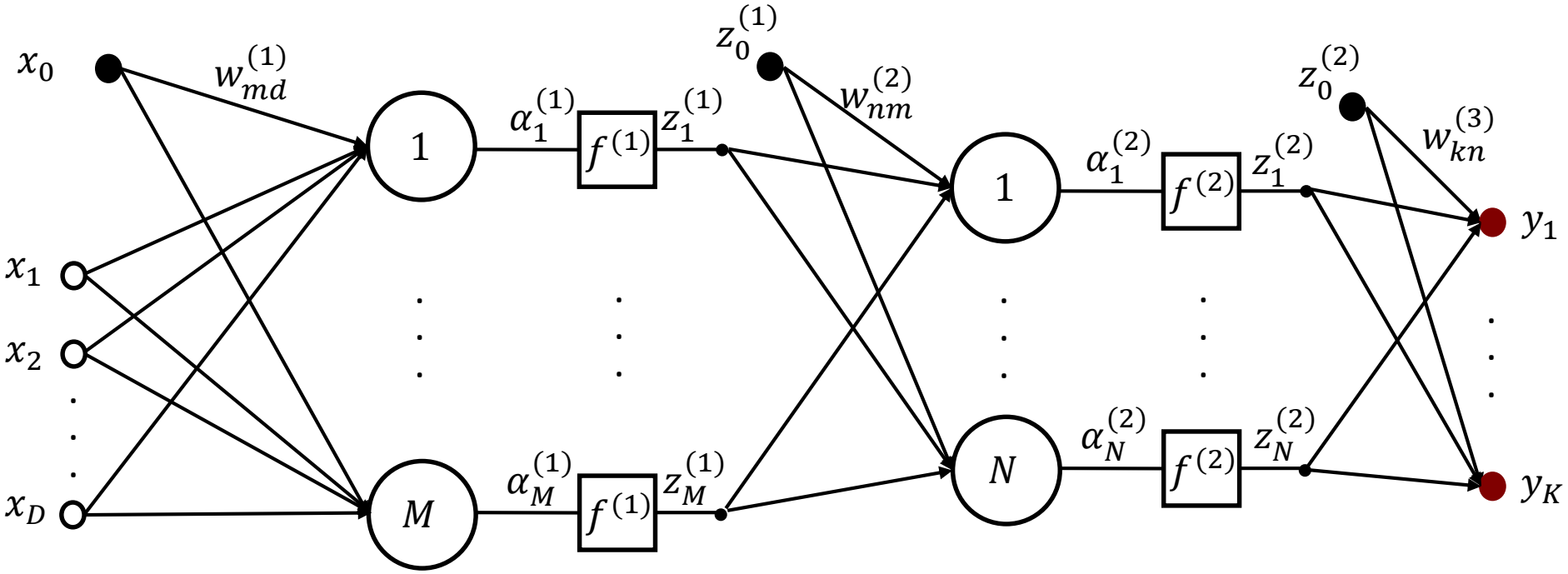


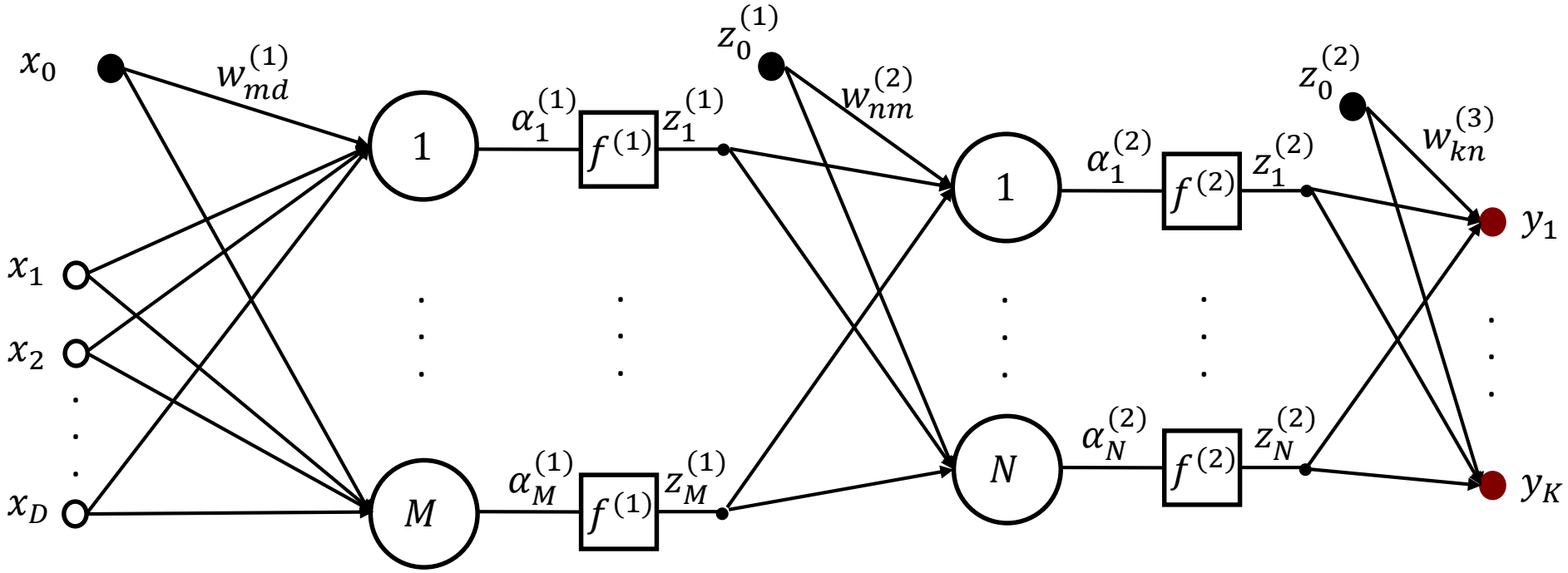
Usually: $y_k = f^{(2)}\left(\sum_{m=0}^{M} w_{km}^{(2)} f^{(1)}\left(\sum_{d=0}^{D} w_{md}^{(1)} x_d\right)\right) = f^{(2)}\left(\sum_{m=0}^{M} w_{km}^{(2)} \varphi(\boldsymbol{x})\right)$

- Thus we use parametric forms of basis functions in advance and allow them to be *adaptive!*
- Adaptive: learn through training!

Three-layer Perceptron

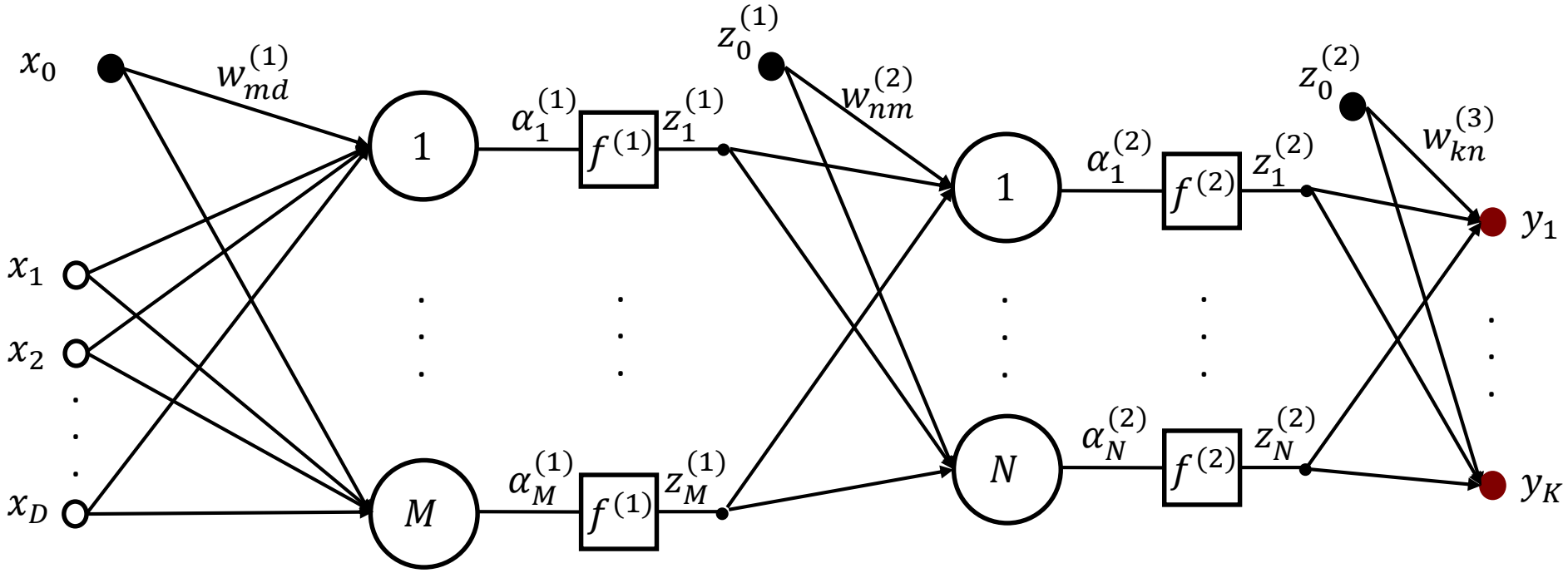


Three-layer Perceptron



$$y_k = f^{(3)}\left(\sum_{n=0}^{N} w_{kn}^{(3)} f^{(2)}\left(\sum_{m=0}^{M} w_{nm}^{(2)} f^{(1)}\left(\sum_{d=0}^{D} w_{md} x_d\right)\right)\right)$$

Three-layer Perceptron



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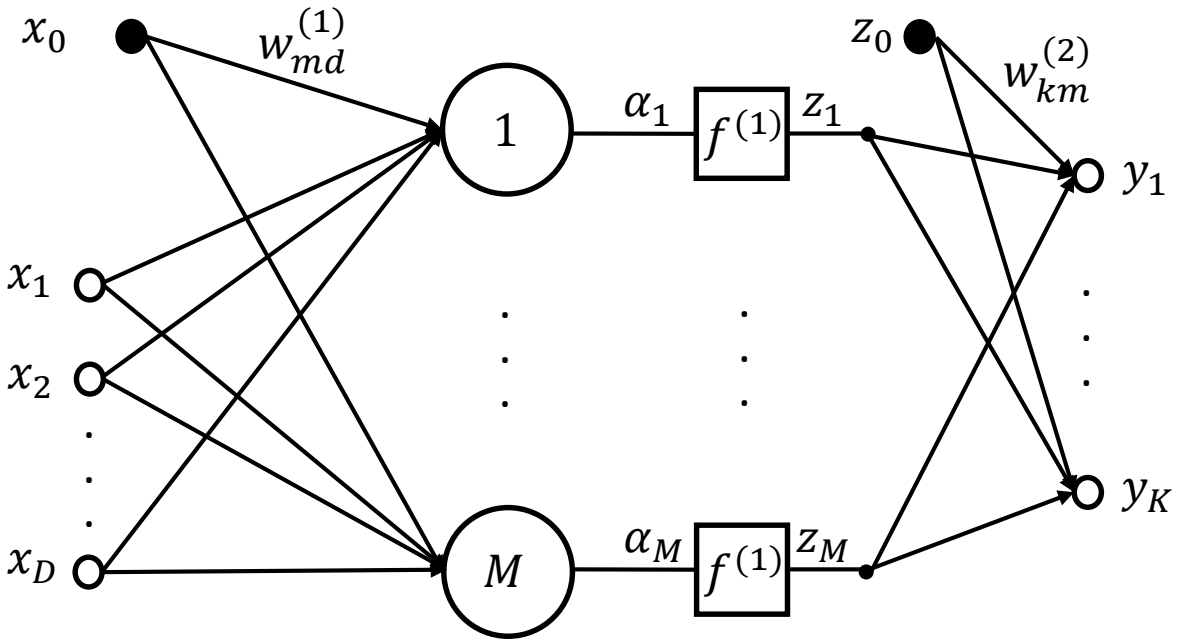
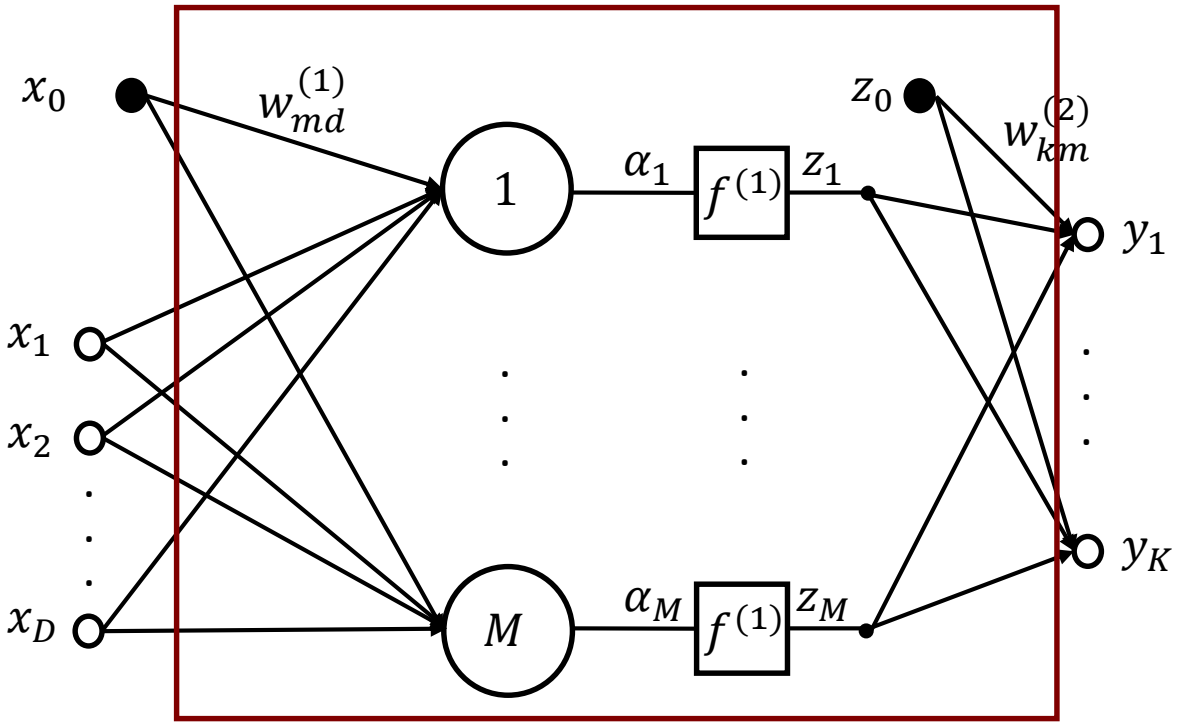
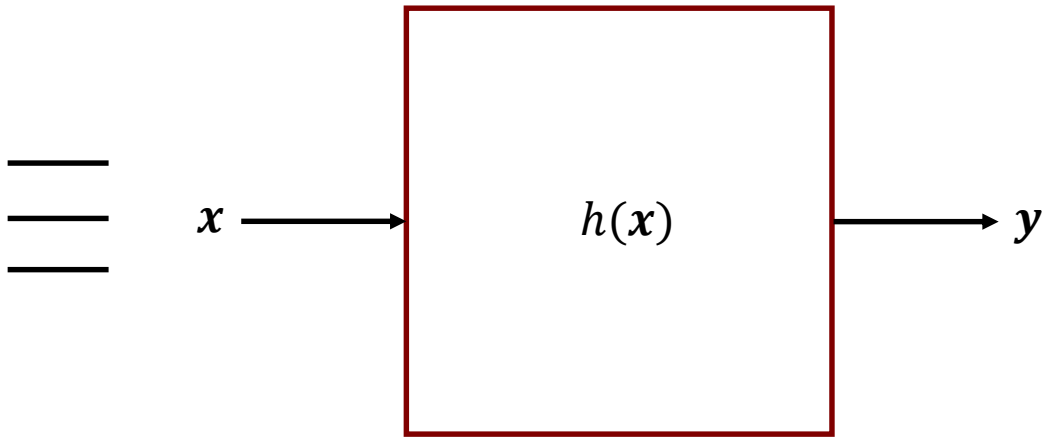
- Very complicated basis functions as functions of $\boldsymbol{x}$ (sequential mapping from layer to layer)

Function Approximators



Function Approximators





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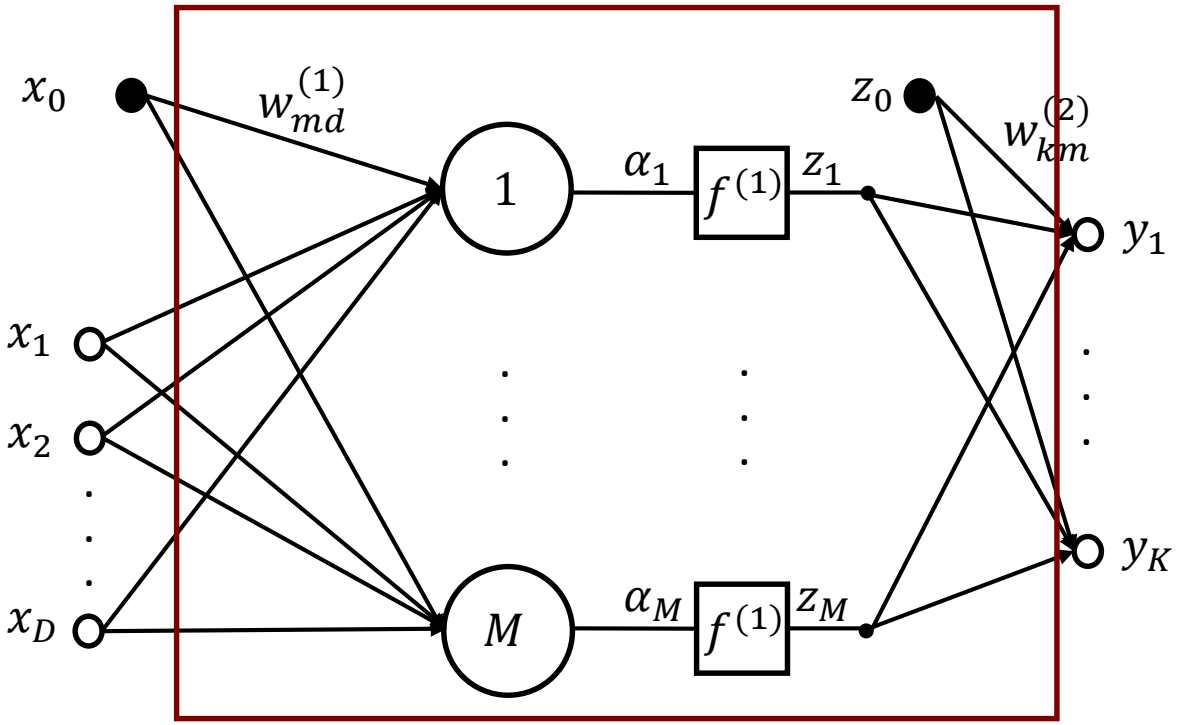
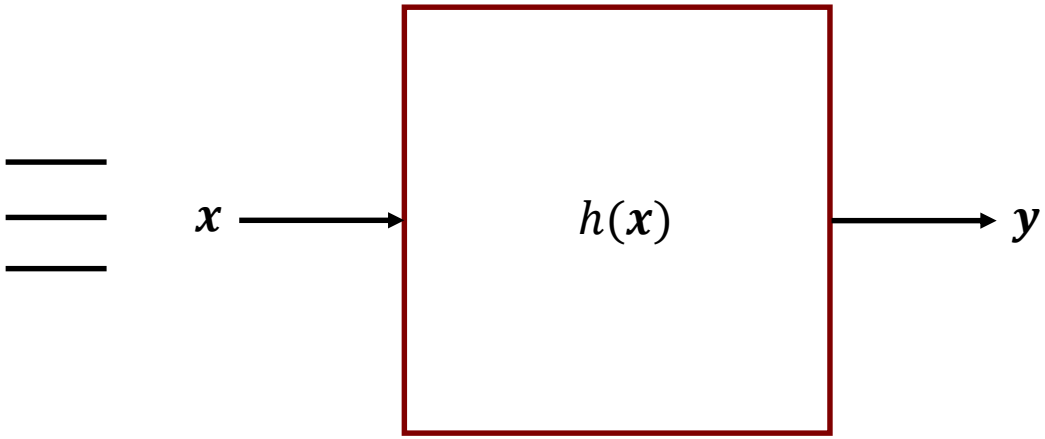
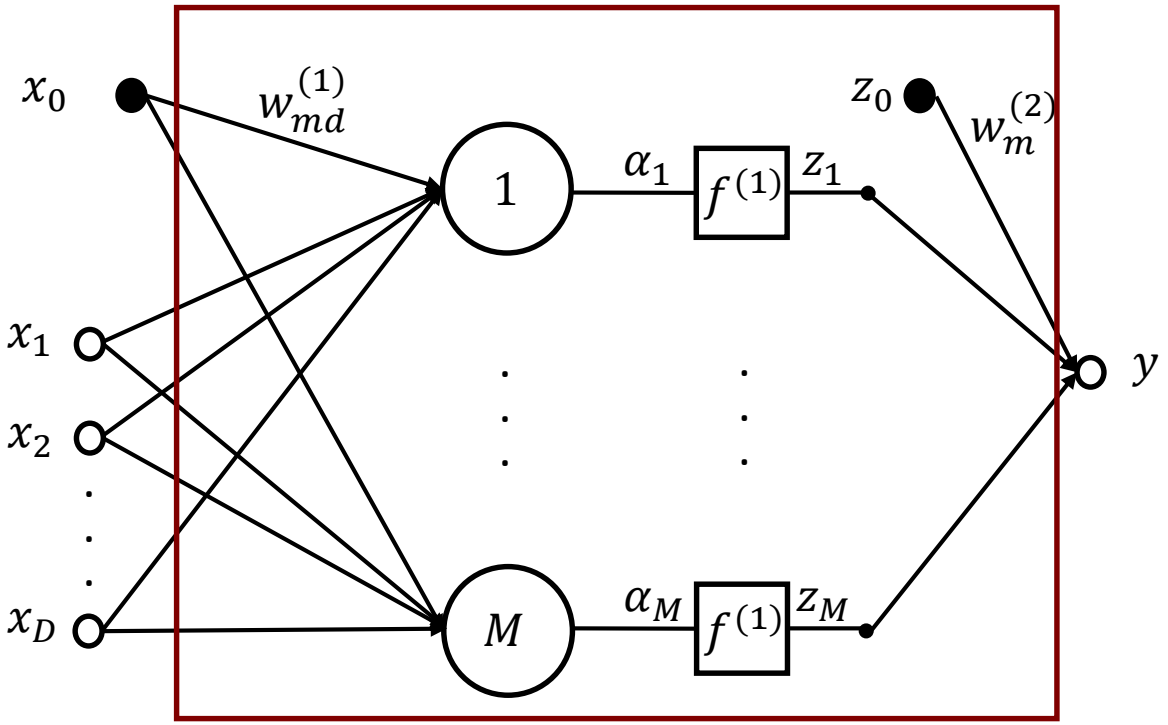
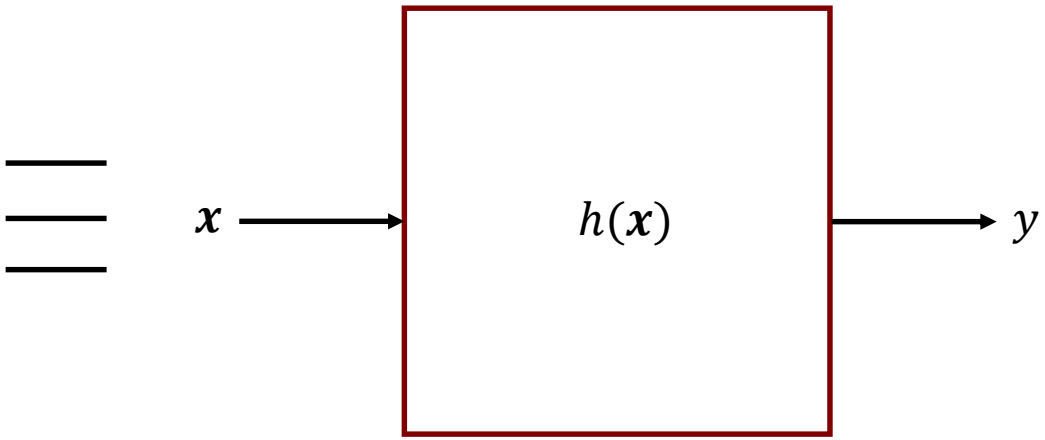




$$\boldsymbol{y}\left(\boldsymbol{x}, \boldsymbol{W}^{(1)}, \boldsymbol{W}^{(2)}\right) = \sum_{m=0}^{M} w_{km}^{(2)} f^{(1)}\left(\sum_{d=0}^{D} w_{md}^{(1)} x_d\right) = \sum_{m=0}^{M} w_{km}^{(2)} \varphi_m(\boldsymbol{x})$$

Function Approximators



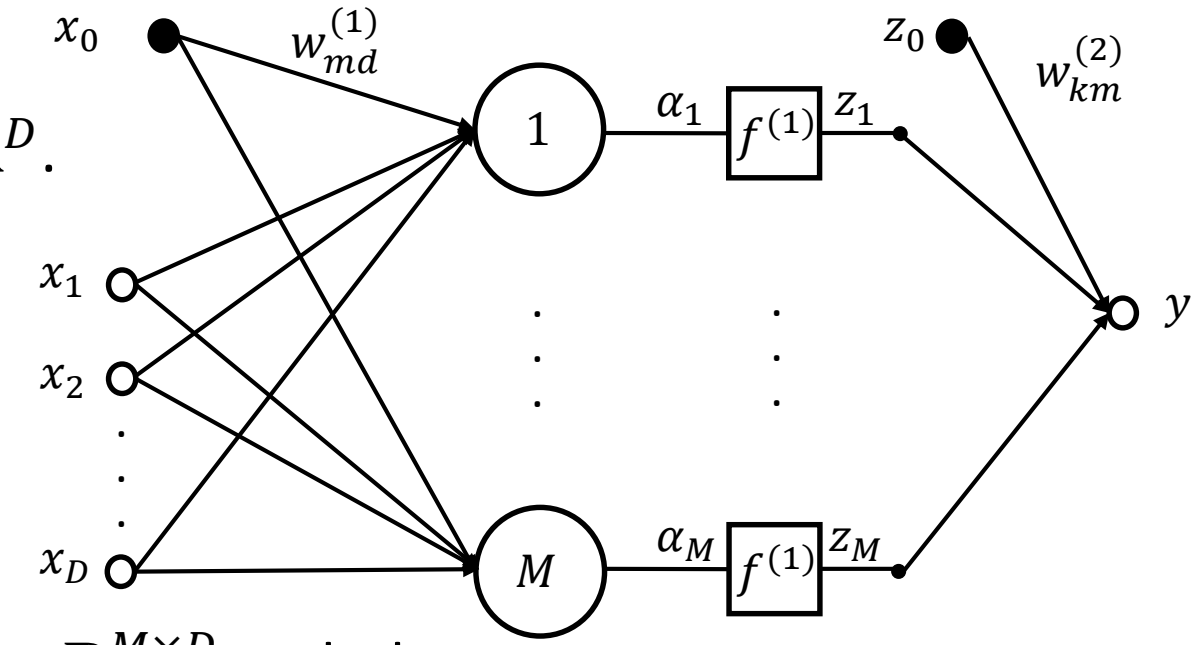


$$y\left(\boldsymbol{x}, \boldsymbol{W}^{(1)}, \boldsymbol{w}^{(2)}\right) = \sum_{m=0}^{M} w_m^{(2)} f^{(1)} \left(\sum_{d=0}^{D} w_{md}^{(2)} x_d \right) = \sum_{m=0}^{M} w_m^{(2)} \varphi_m(\boldsymbol{x})$$

Universal approximators

Theorem:

- Let $h(.)$ be a continuous function on $\mathbb{R}^D$.
- Let $f(.)$ be a fixed analytic function which is **not** polynomial.
- Given any small number $\varepsilon > 0$,we can find a number M, $\boldsymbol{w}^{(2)} \in \mathbb{R}^M$ and $\boldsymbol{W}^{(1)} \in \mathbb{R}^{M\times D}$ such that:



$$\left|h(x) - y\left(\boldsymbol{x}, \boldsymbol{W}^{(1)}, \boldsymbol{w}^{(2)}\right)\right| < \varepsilon$$

Note: For smaller ε we usually need larger M.

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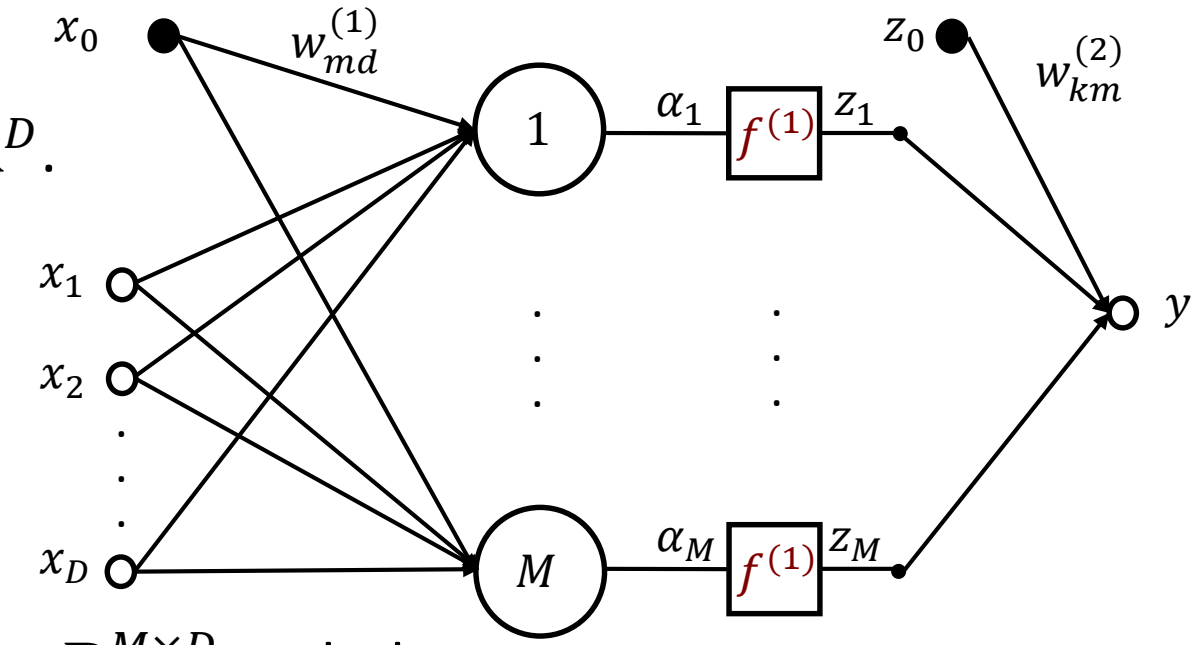

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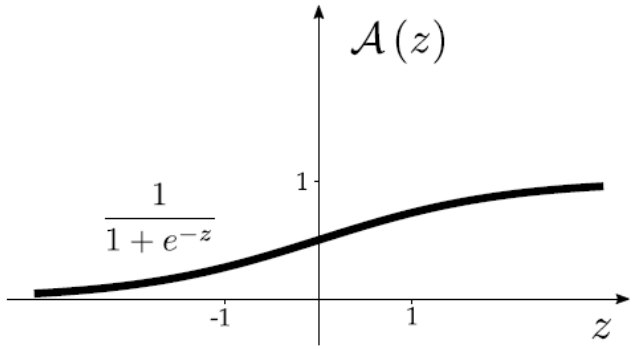
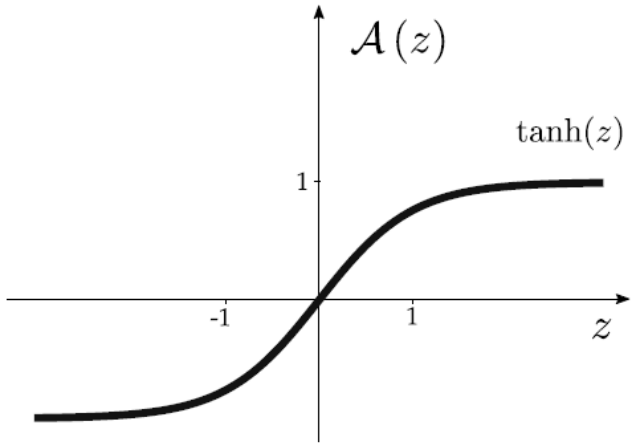
Activation Functions

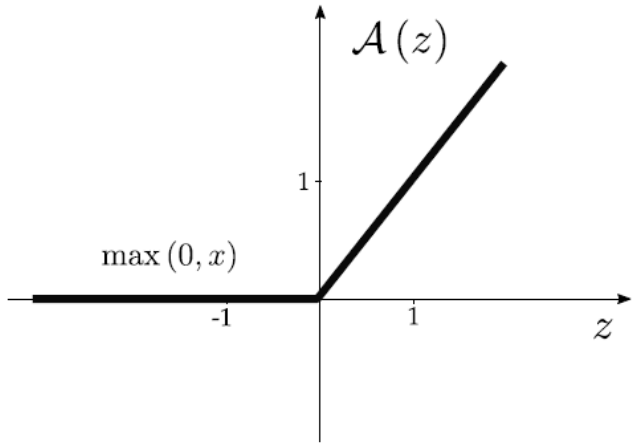
Logistic sigmoid



Tanh



Rectified Linear Unit (RELU)



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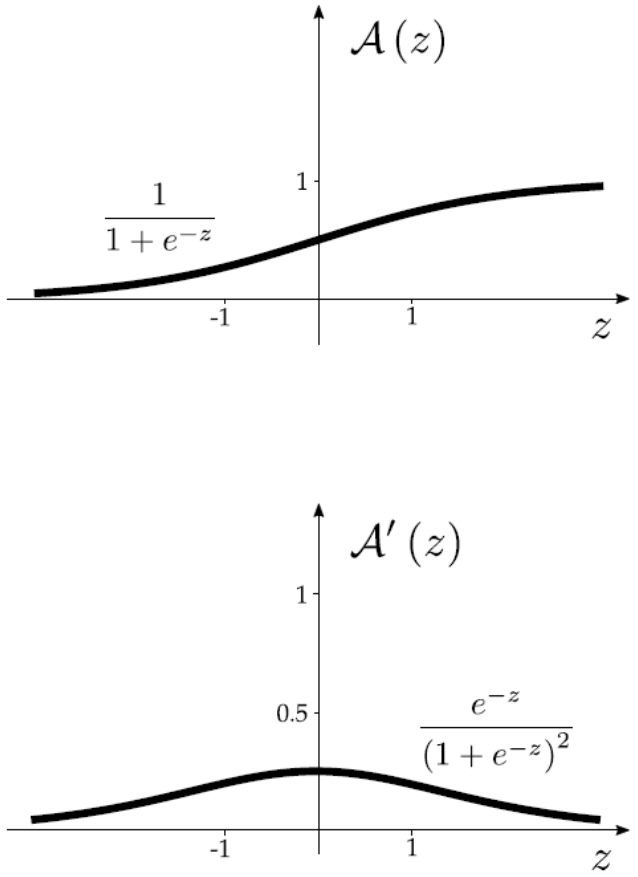

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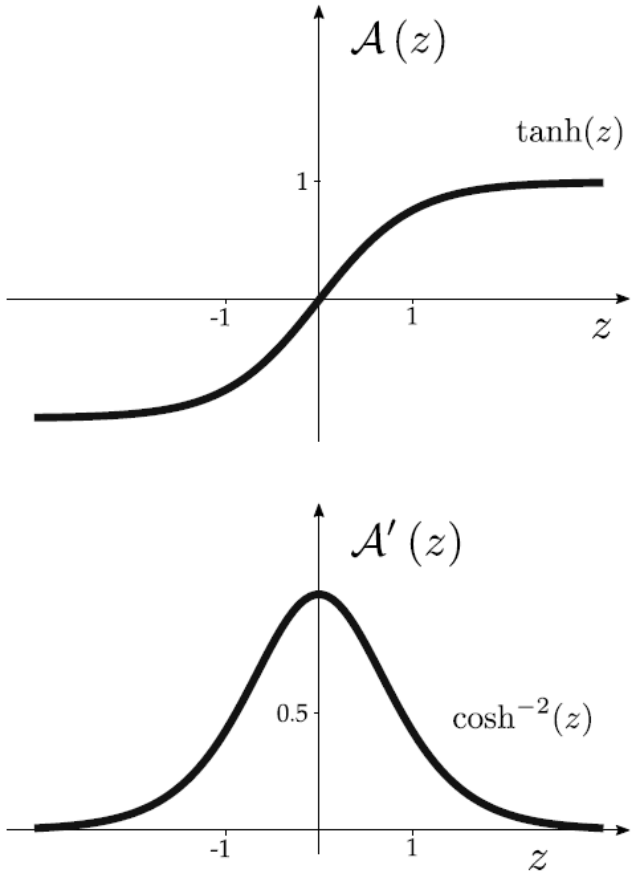

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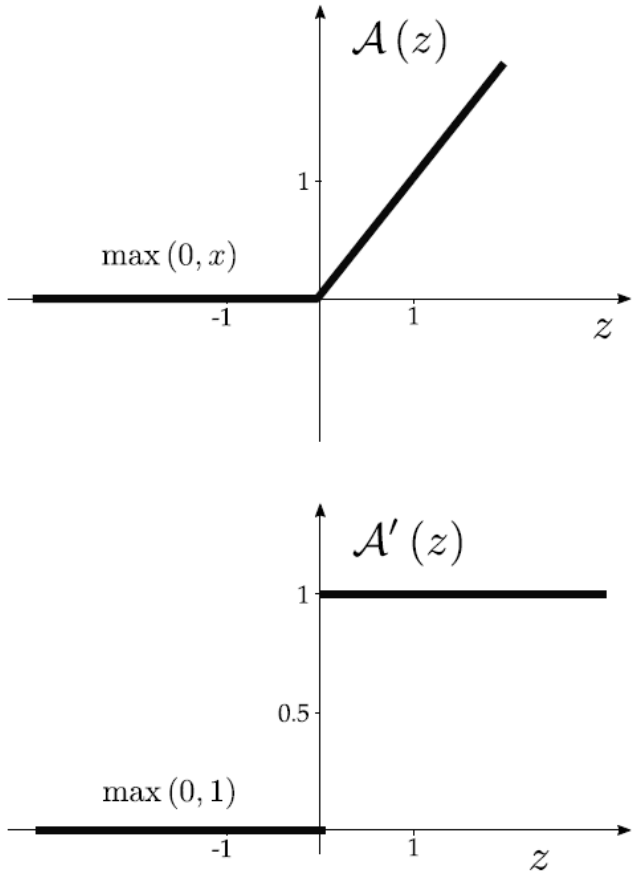
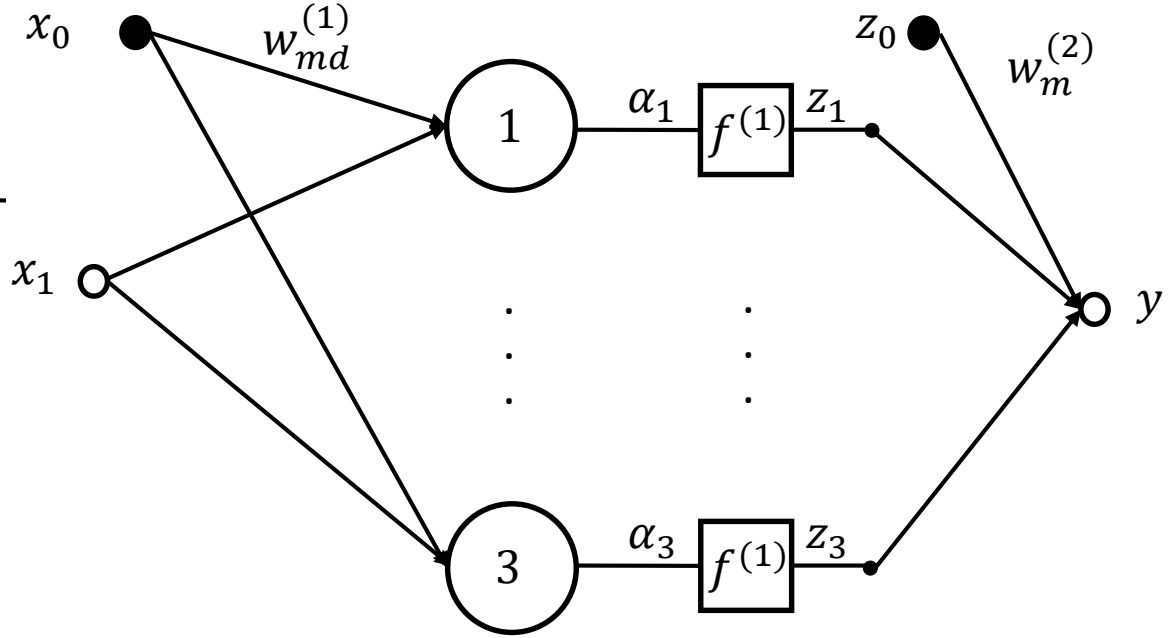


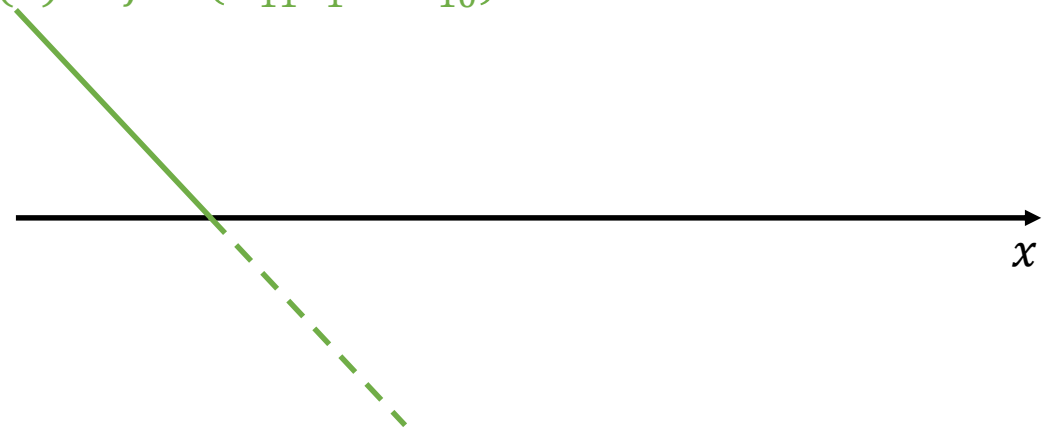
Masi et al. 2020

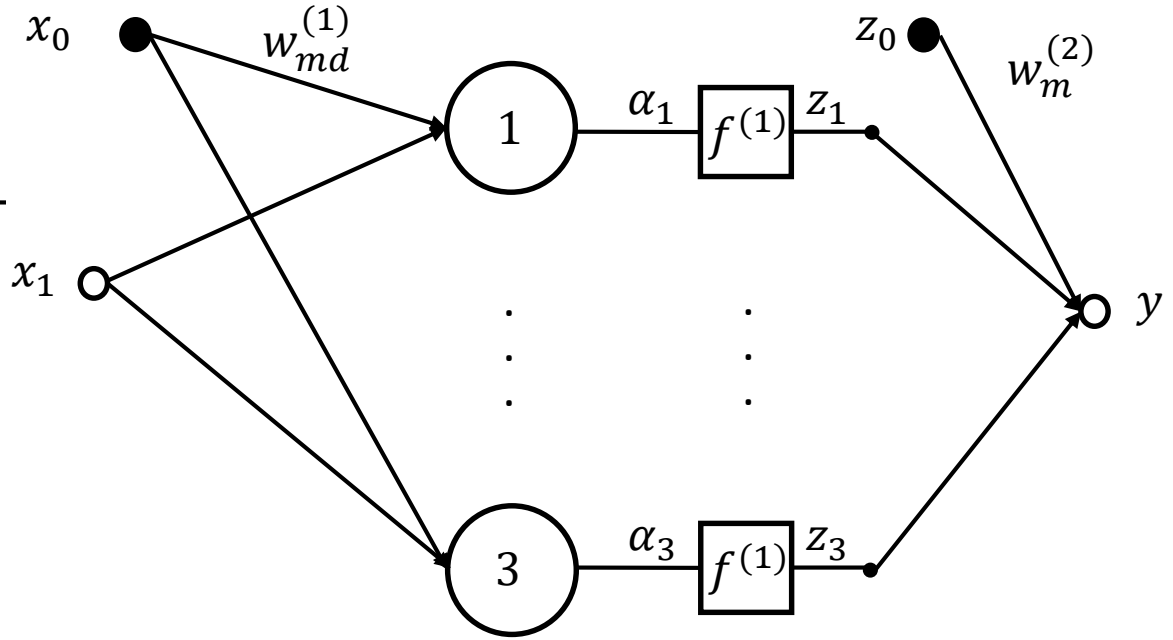
NN with ReLU



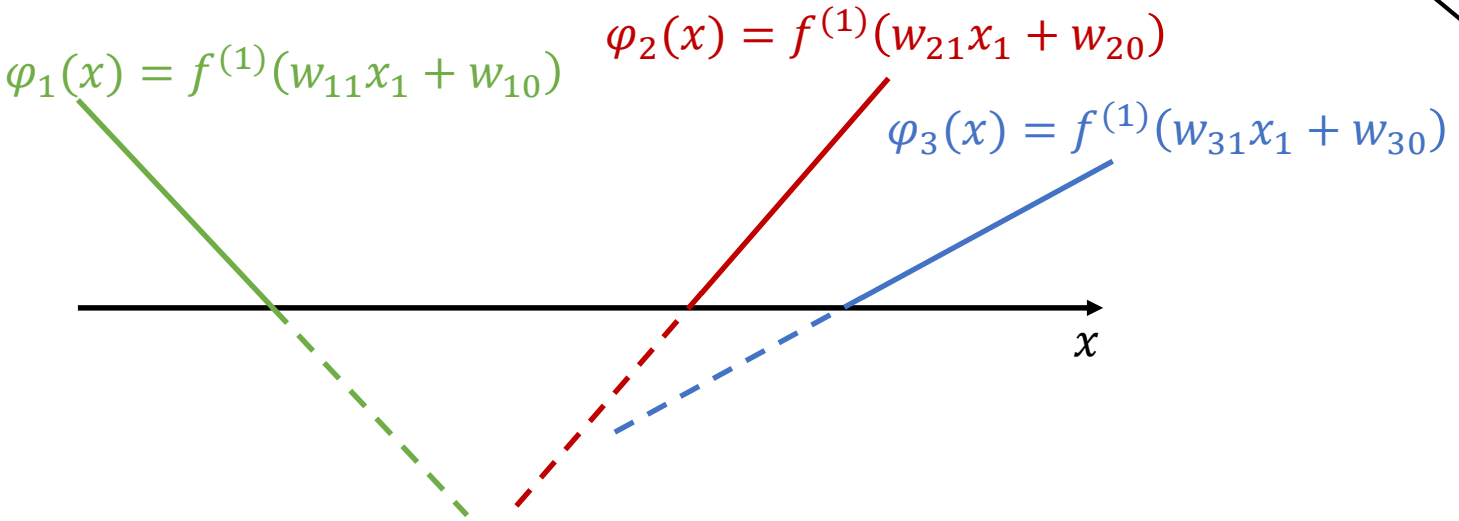
NN with ReLU

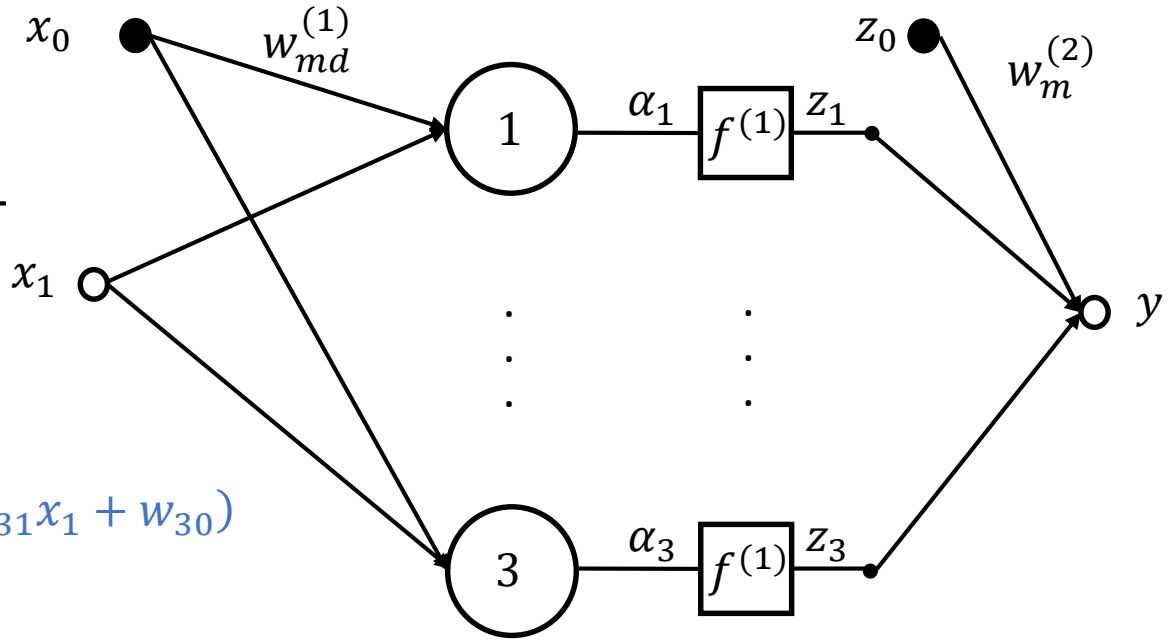
$z_1 = \varphi_1(x) = f^{(1)}(w_{11}x_1 + w_{10})$



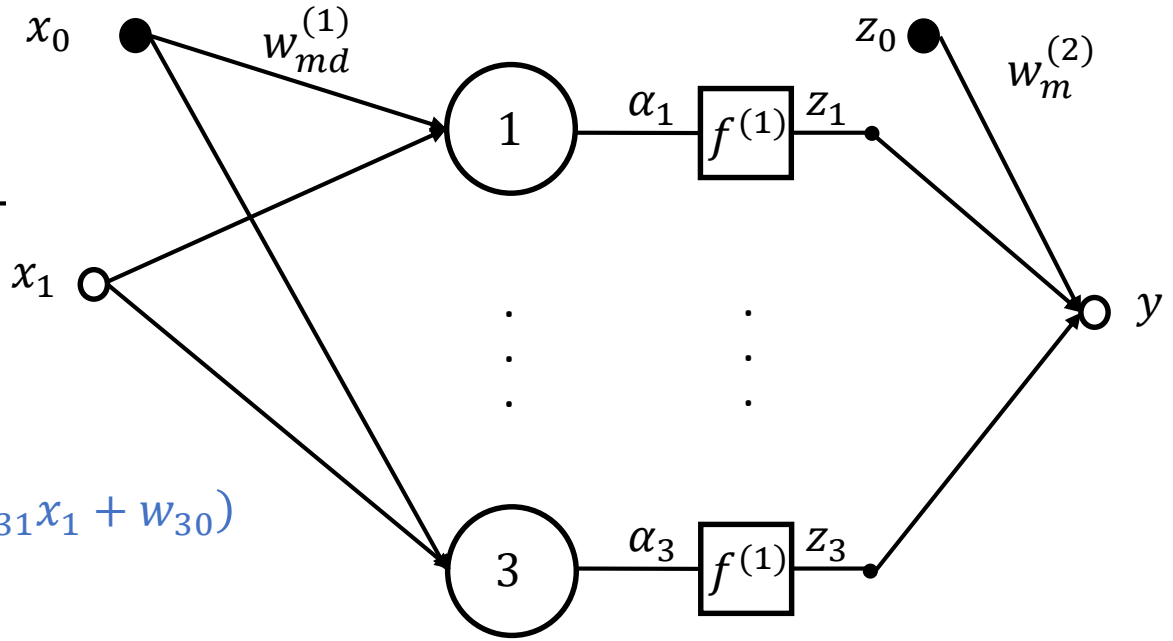


NN with ReLU


$\varphi_1(x) = f^{(1)}(w_{11}x_1 + w_{10})$
$\varphi_2(x) = f^{(1)}(w_{21}x_1 + w_{20})$
$\varphi_3(x) = f^{(1)}(w_{31}x_1 + w_{30})$
x


x_0
$w_{md}^{(1)}$
x_1
1
3
α_1
α_3
$f^{(1)}$
$f^{(1)}$
z_1
z_3
z_0
$w_m^{(2)}$
y

NN with ReLU



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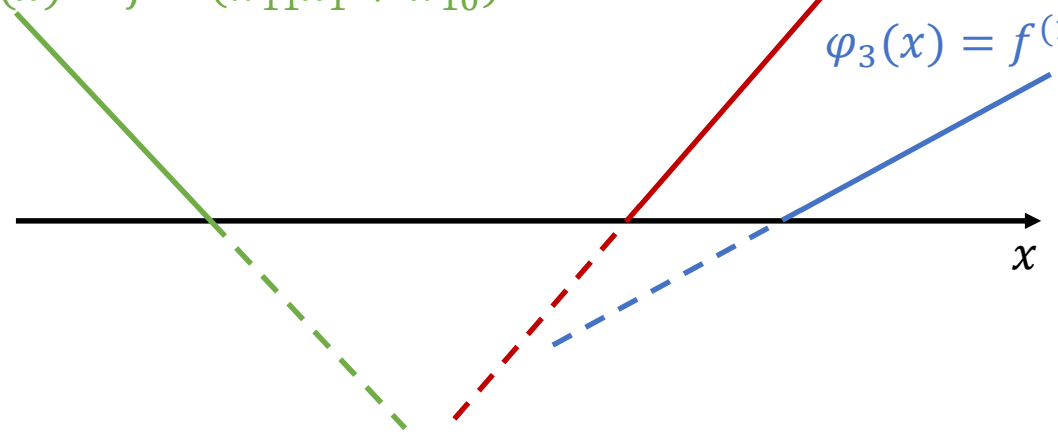
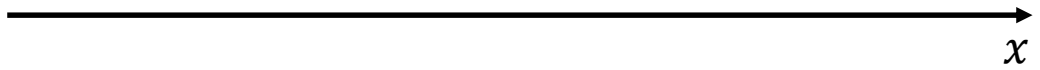
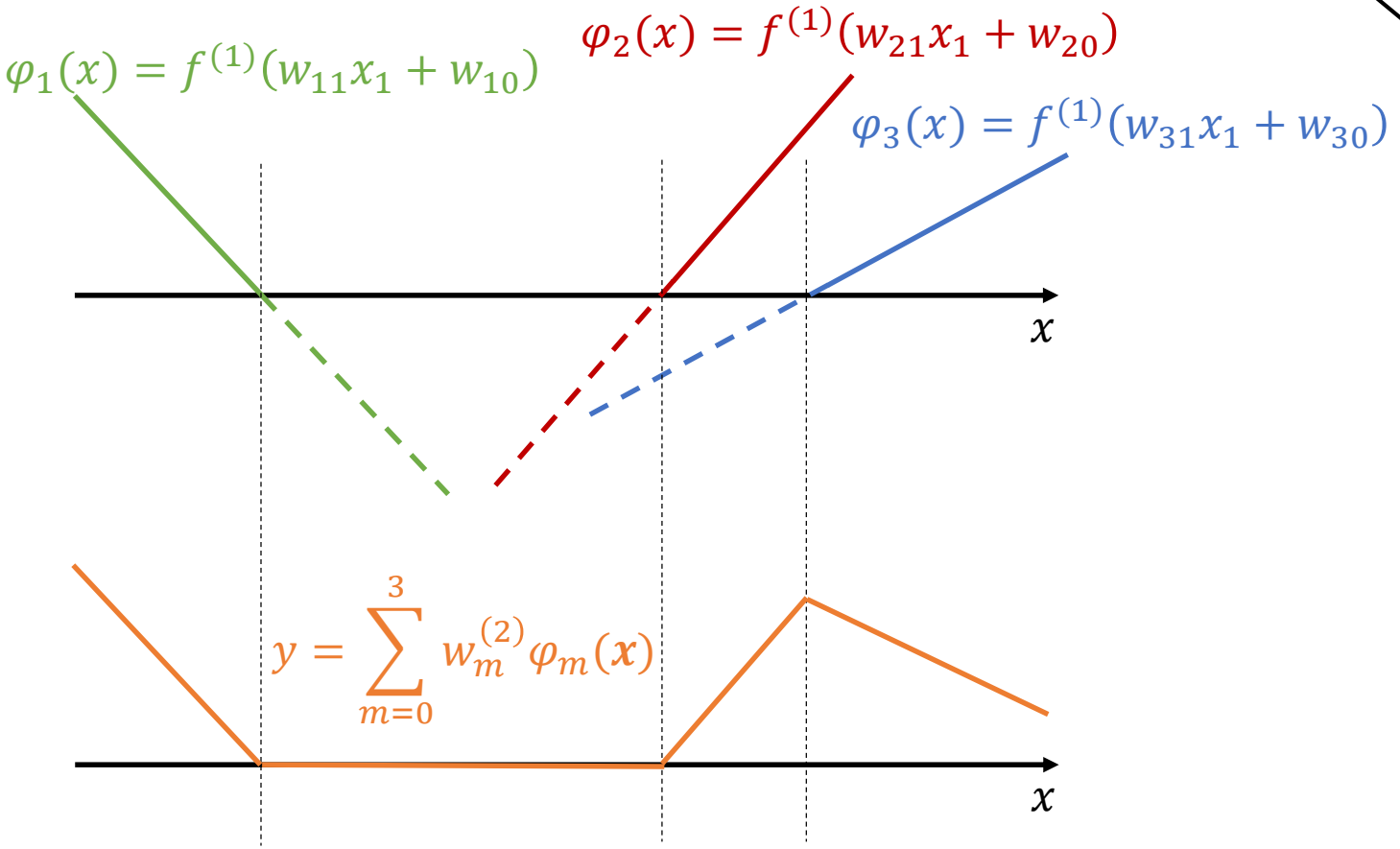
$\varphi_3(x) = f^{(1)}(w_{31}x_1 + w_{30})$

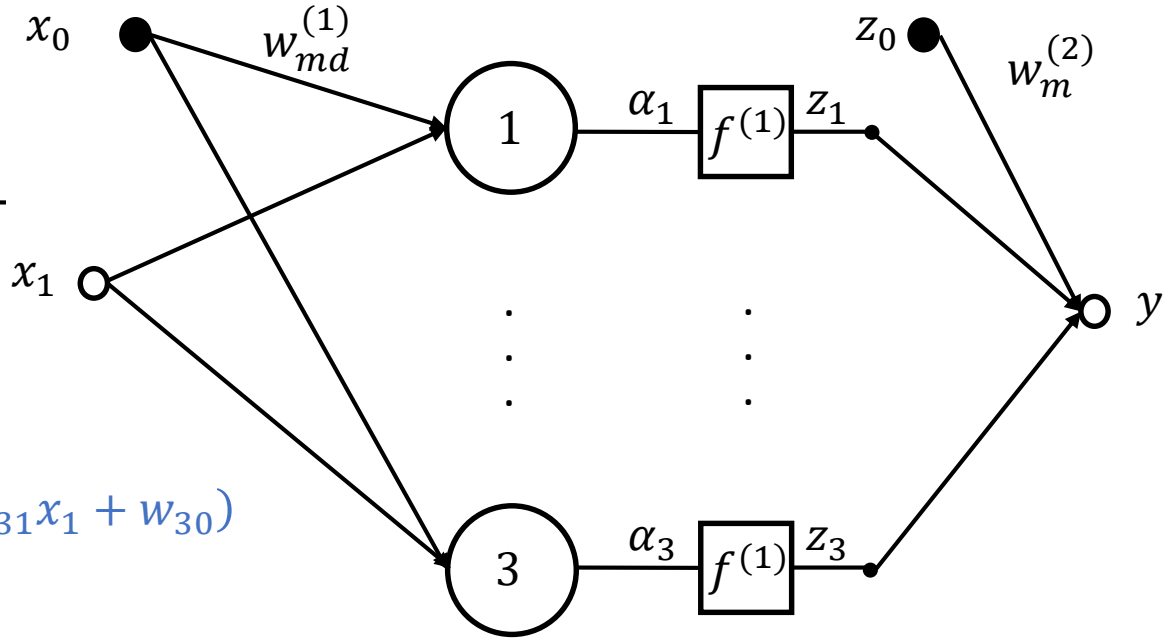


$$y = \sum_{m=0}^{3} w_m^{(2)} \varphi_m(\boldsymbol{x})$$

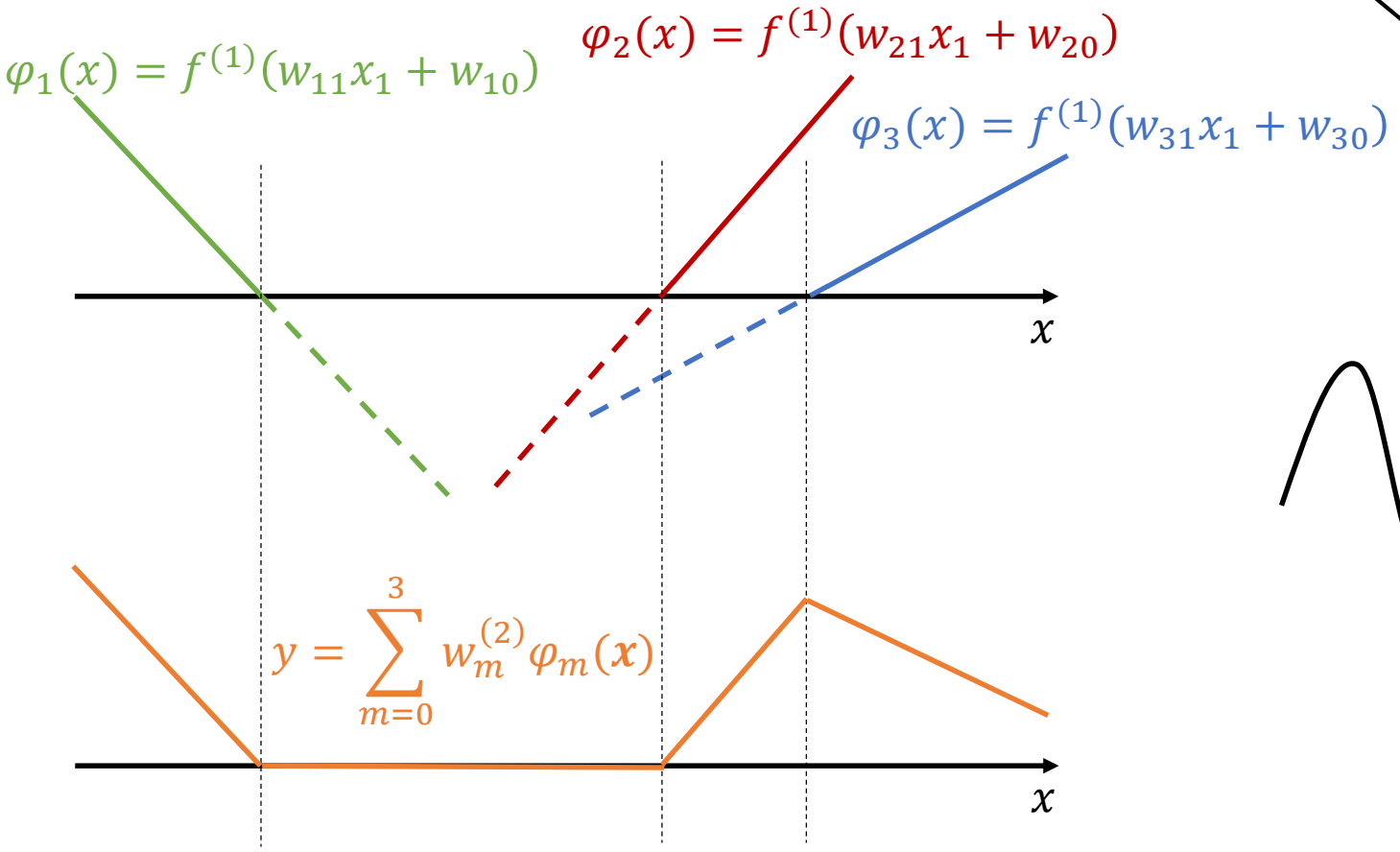


NN with ReLU


$\varphi_1(x) = f^{(1)}(w_{11}x_1 + w_{10})$
$\varphi_2(x) = f^{(1)}(w_{21}x_1 + w_{20})$
$\varphi_3(x) = f^{(1)}(w_{31}x_1 + w_{30})$
x
$y = \sum_{m=0}^{3} w_m^{(2)} \varphi_m(\boldsymbol{x})$
x


x_0
$w_{md}^{(1)}$
z_0
$w_m^{(2)}$
1
α_1
$f^{(1)}$
z_1
x_1
y
3
α_3
$f^{(1)}$
z_3

NN with ReLU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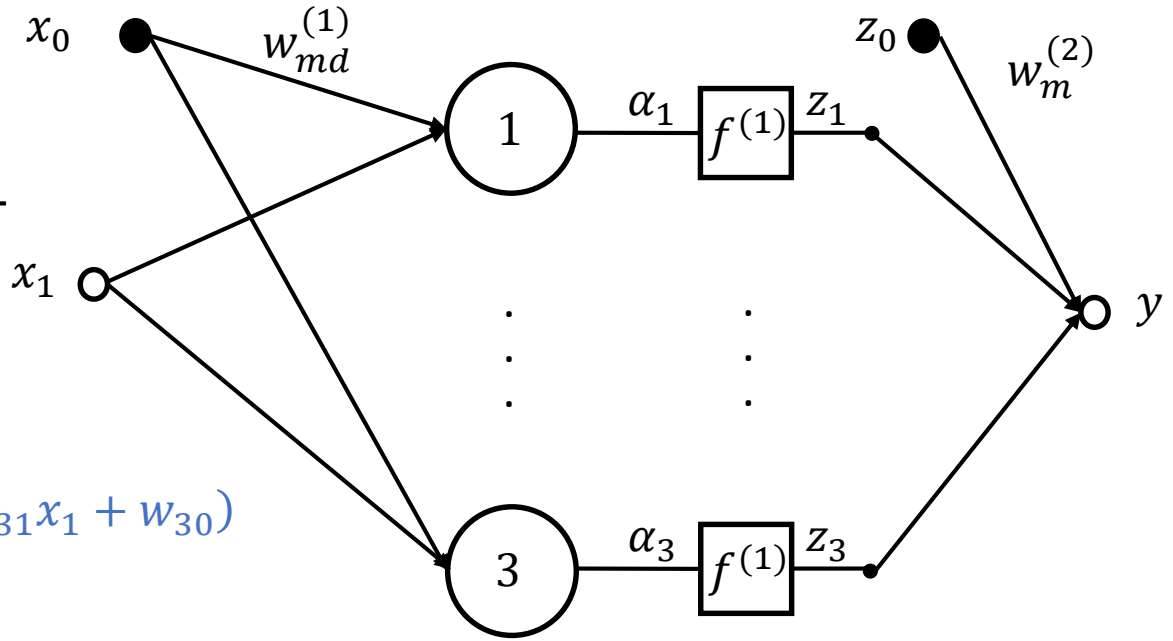
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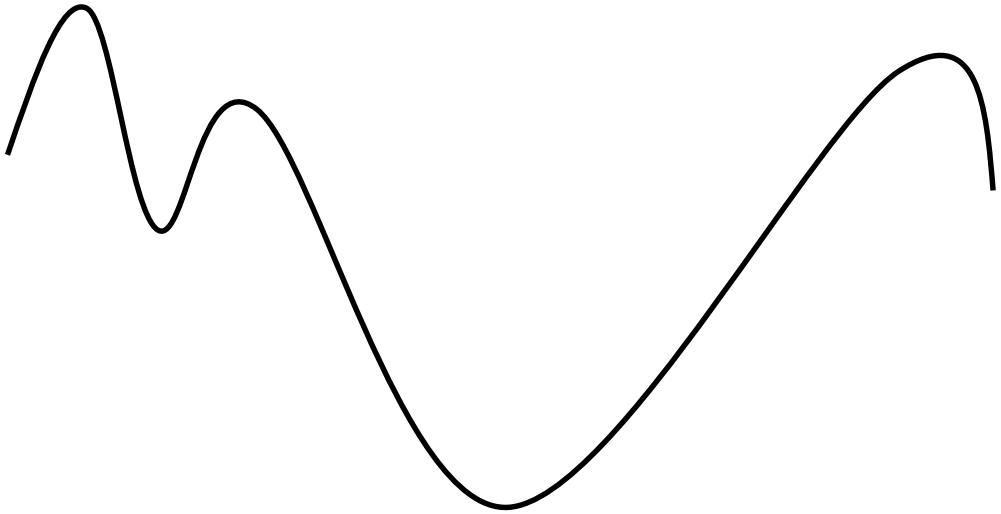
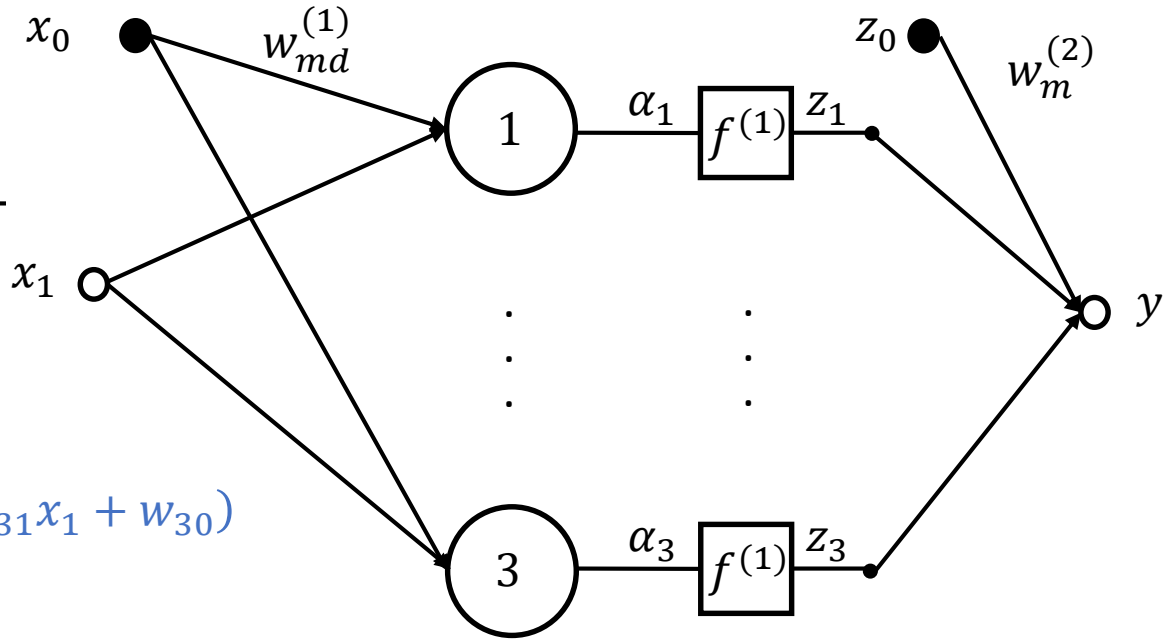


NN with ReLU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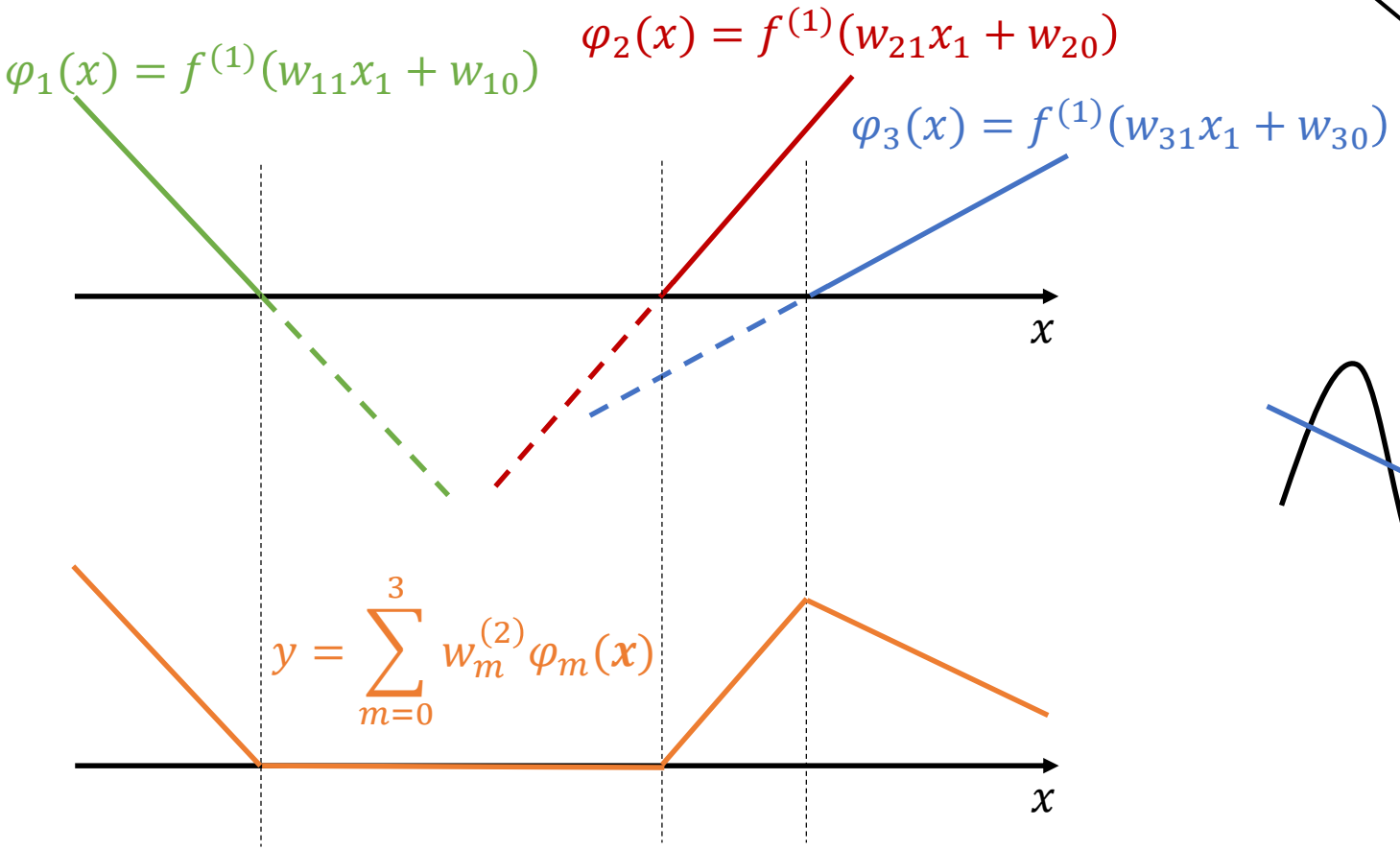
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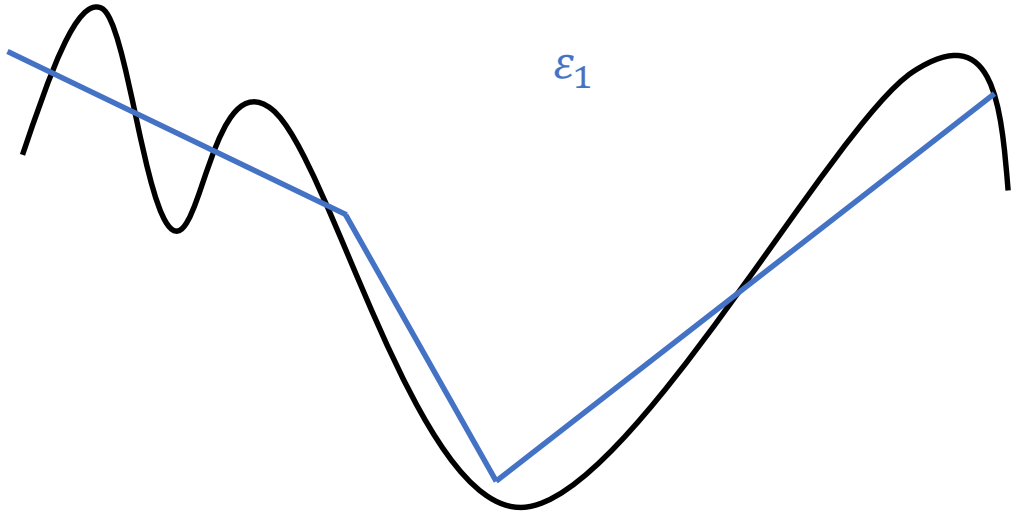
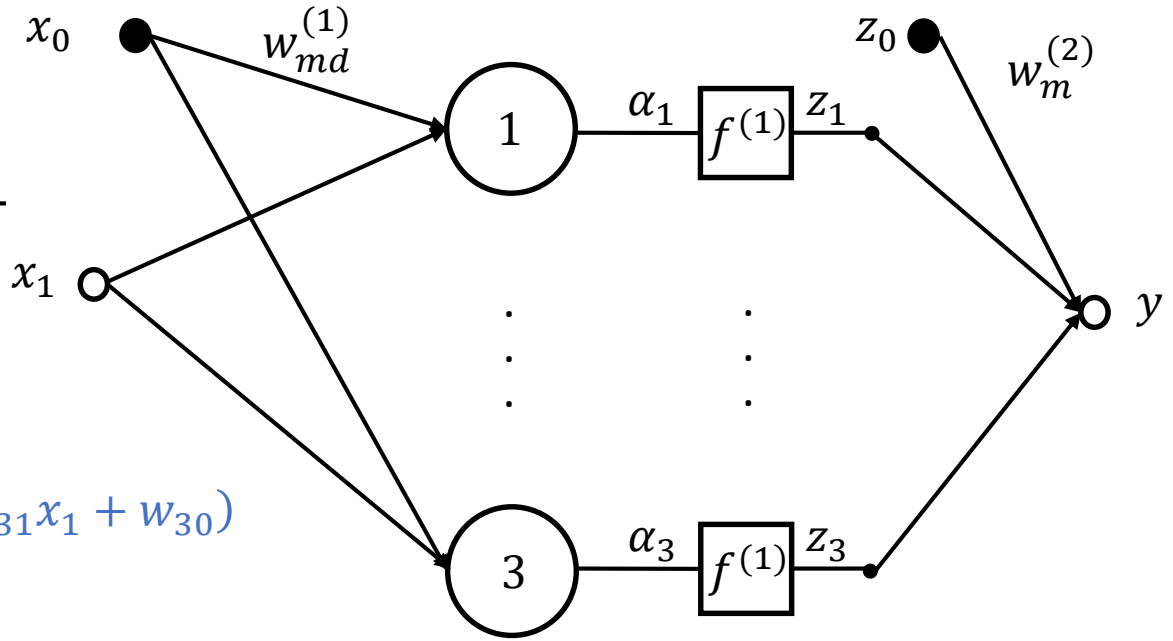

ε_1

NN with ReLU


x_0
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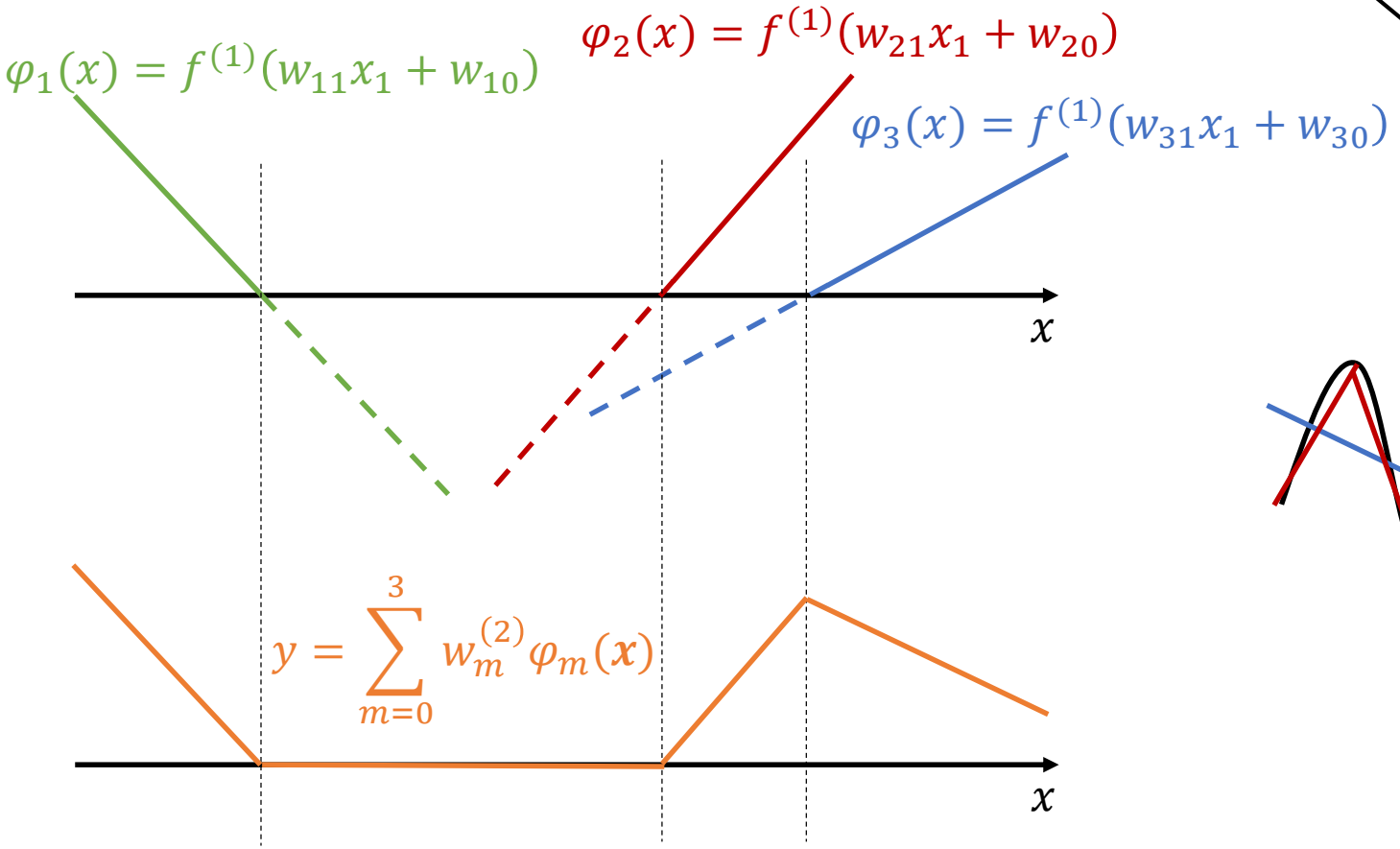
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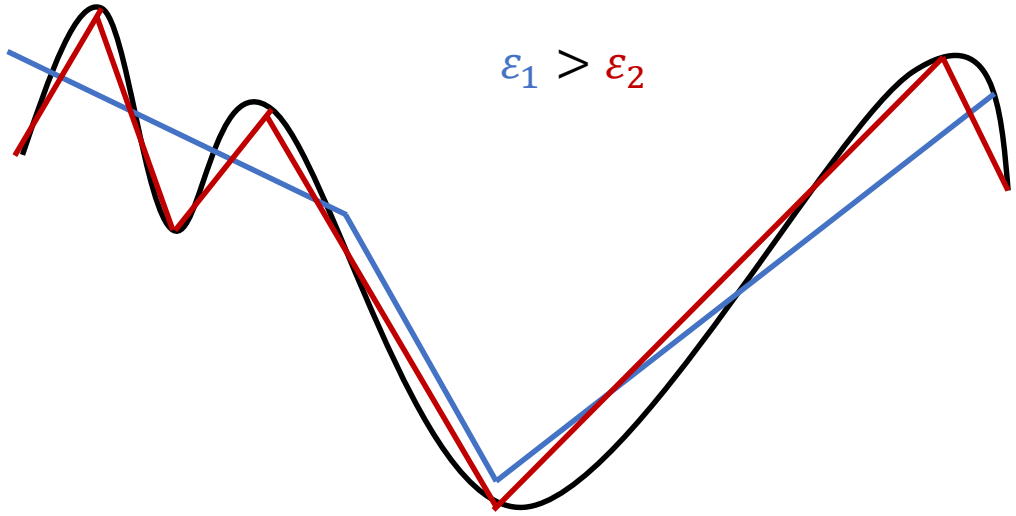

$\varepsilon_1 > \varepsilon_2$

Expressive power of ReLU Networks

- The expressive power of ReLU-DNN networks is represented by the number of linear regions (see the example in the previous slide).
- In particular:

$$\#linear\ regions = width^{depth \times D}$$

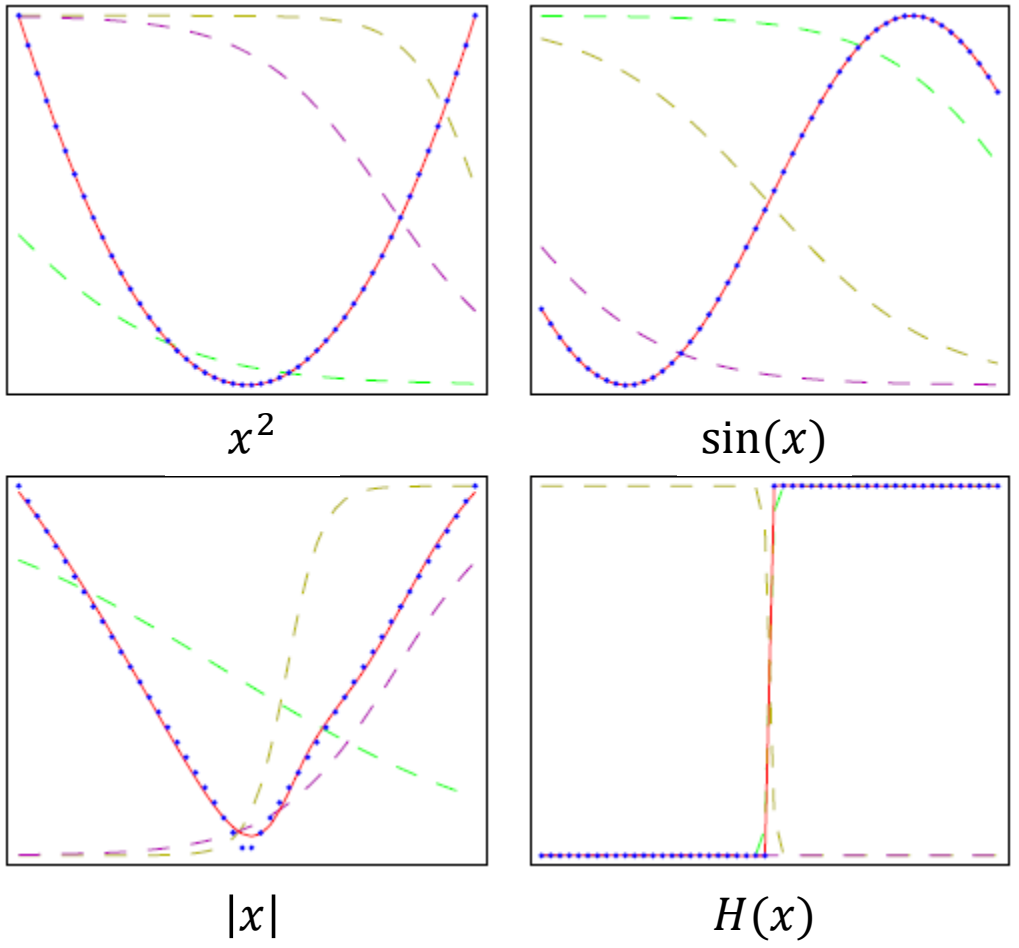
- Thus the expressive power is polynomial in width but exponential in depth.
- With fixed network capacity:

$$\#parameters = width^2 \times depth$$

- Most expressive power is gained by going deeper instead of making wider networks (per layer) and staying shallow!

Examples: Function Approximations

- $N = 50$
- $\#layers = 2$
- $M = 3$ (hidden units)
- Activation function: $\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$
- One linear output unit
- Dashed curves: Hidden units output



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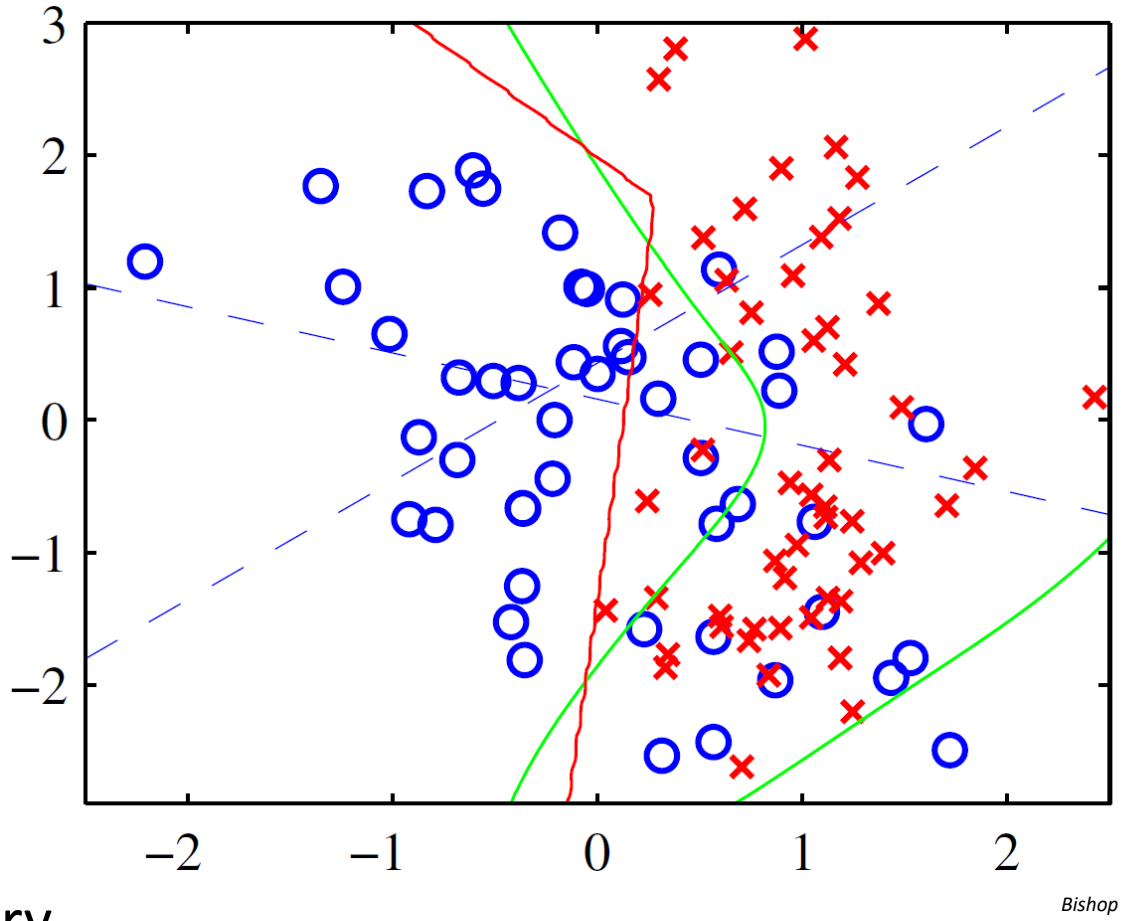
Example: Classification

- $\#layers = 2$
- $M = 2$ (hidden units)
- Activation function: $\tanh(x)$
- One output unit with sigmoid activation
- Red line: 2-LP decision boundary
- Green line: optimal decision boundary



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Thus far…

- We have defined:
  - Number of inputs
  - Hidden layers
  - Output layers
  - Activation functions (of hidden layers)
- We will use now a probabilistic interpretation of the network outputs to choose:
  - Number of outputs
  - Output activation function
  - Loss function!

Binary classification

- Data: inputs $\boldsymbol{X} = (\boldsymbol{x}_1, \dots, \boldsymbol{x}_N)$, targets $\boldsymbol{t} = (t_1, \dots, t_N)$, where $\boldsymbol{x}_n \in \mathbb{R}^D, t \in [0,1]$.

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$$p(t = 1|\boldsymbol{x}) = y(\boldsymbol{x}, \boldsymbol{w})$$ (output of the NN)

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- In general:

$$p(t|\boldsymbol{x}, \boldsymbol{w}) = y(\boldsymbol{x}, \boldsymbol{w})^t \big(1 - y(\boldsymbol{x}, \boldsymbol{w})\big)^{1-t} \text{ (Bernoulli distribution)}$$

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- Thus, we have a single output unit: $y(\boldsymbol{x}, \boldsymbol{w}) = f^L(a^{out}) = \sigma(a^{out}) \in [0,1]$.
- Maximum likelihood or Minimum Negative log likelihood:

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$$E(\boldsymbol{w}) = -\sum_{n=1}^{N} t_n \ln\big(y(\boldsymbol{x}_n, \boldsymbol{w})\big) + (1 - t_n) \ln\big(1 - y(\boldsymbol{x}_n, \boldsymbol{w})\big) \text{ (Cross Entropy Loss)}$$

Classification with c classes

- Data: inputs $\boldsymbol{X} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$, targets $\boldsymbol{T} = (\boldsymbol{t}_1, \ldots, \boldsymbol{t}_N)$, where $\boldsymbol{x}_n \in \mathbb{R}^D$, $and\ \boldsymbol{t}_n = [t_{n1}, \ldots, t_{nc}]$ (one hot encoding).

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- For multi-class classification we define c output units and we assume target distribution:

$$p(\boldsymbol{t}_n|\boldsymbol{x}_n, \boldsymbol{w}) = \prod_{i=1}^{c} y_i(\boldsymbol{x}_n, \boldsymbol{w})^{t_{ni}}$$ (Generalized Bernoulli)

where

$$y_i(\boldsymbol{x}_n, \boldsymbol{w}) = p(\omega_i|\boldsymbol{x}_n, \boldsymbol{w})$$(output of the NN)

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- Maximum likelihood or Minimum Negative log likelihood:

$$E(\boldsymbol{w}) = -\sum_{n=1}^{N}\sum_{i=1}^{c} t_{ni} \ln(y_i(\boldsymbol{x}_n, \boldsymbol{w}))$$(Cross Entropy Loss)

Regression

- Data: inputs $\boldsymbol{X} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$, targets $\boldsymbol{t} = (t_1, \ldots, t_N)$, where $\boldsymbol{x}_n \in \mathbb{R}^D, t_n \in \mathbb{R}$.

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- We adopt a single output NN. In particular, $y(\boldsymbol{x}_n, \boldsymbol{w}) = f^L(a^{out})$.
- Because the outputs are real valued we assume an identity output activation function:$y(\boldsymbol{x}_n, \boldsymbol{w}) = f^L(a^{out}) = a^{out}$.

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- Maximum likelihood or Minimum Negative log likelihood:

$$E(\boldsymbol{w}) = -\ln p(\boldsymbol{t}|\boldsymbol{X}, \boldsymbol{w}) = \frac{\beta}{2}\sum_{n=1}^{N}(y(\boldsymbol{x}_n, \boldsymbol{w}) - t_n)^2 - \frac{N}{2}\ln\beta + \frac{N}{2}\ln 2\pi$$

- In essence: $E(\boldsymbol{w}) = \sum_{n=1}^{N}(y(\boldsymbol{x}_n, \boldsymbol{w}) - t_n)^2$

Losses overview

- Binary classification:
  - Assumed Bernoulli target distribution
  - NN makes prediction of the probability of class ω_1
  - Output activation is logistic sigmoid
  - Minimize cross entropy loss
- Multi-class classification
  - Assumed generalized Bernoulli target distribution
  - NN makes prediction of the probability of each class
  - Output activation is softmax function
  - Minimize (multi-class) cross entropy loss.
- Regression
  - Assumed gaussian target distribution
  - NN makes prediction for the mean
  - Output activation function is the identity function
  - Minimize least squares.

Training

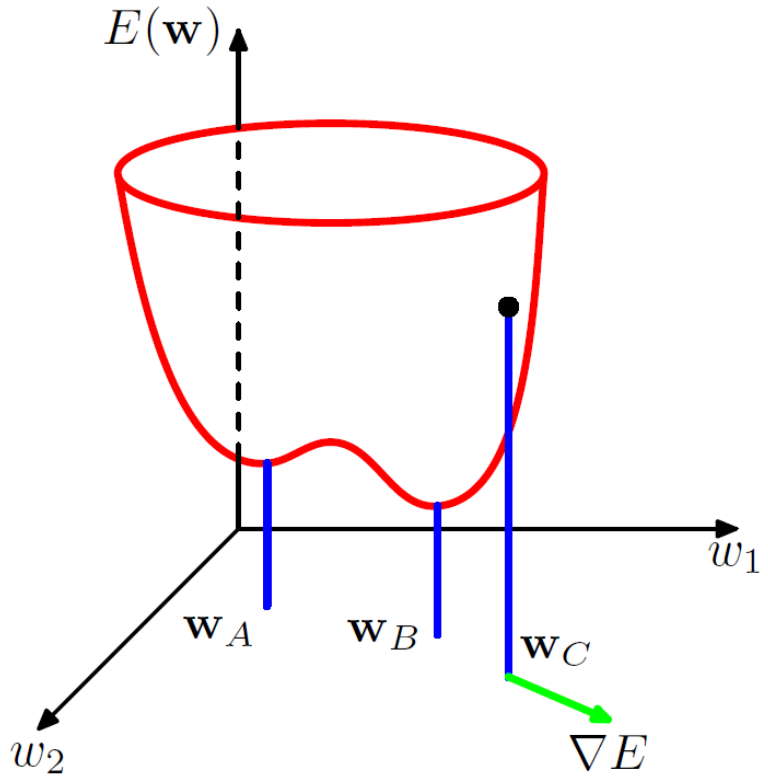
- Thus far:
  - Structure
  - different components of the NNs
  - activation functions
  - loss functions

- Next:

  Training: How can I adjust $\boldsymbol{w}$ in order to approximate the function I am interested in.

Optimization

- For each task I have a different loss function $E(\boldsymbol{w})$ that I want to minimize.
- Parameter optimization: $\boldsymbol{w_{opt}} = \underset{\boldsymbol{w}}{\operatorname{argmin}}\, E(\boldsymbol{w})$
- A big problem: $E(\boldsymbol{w})$ is not convex in $\boldsymbol{w}$, thus several local optimal exist!
- How to reach a global minimum?



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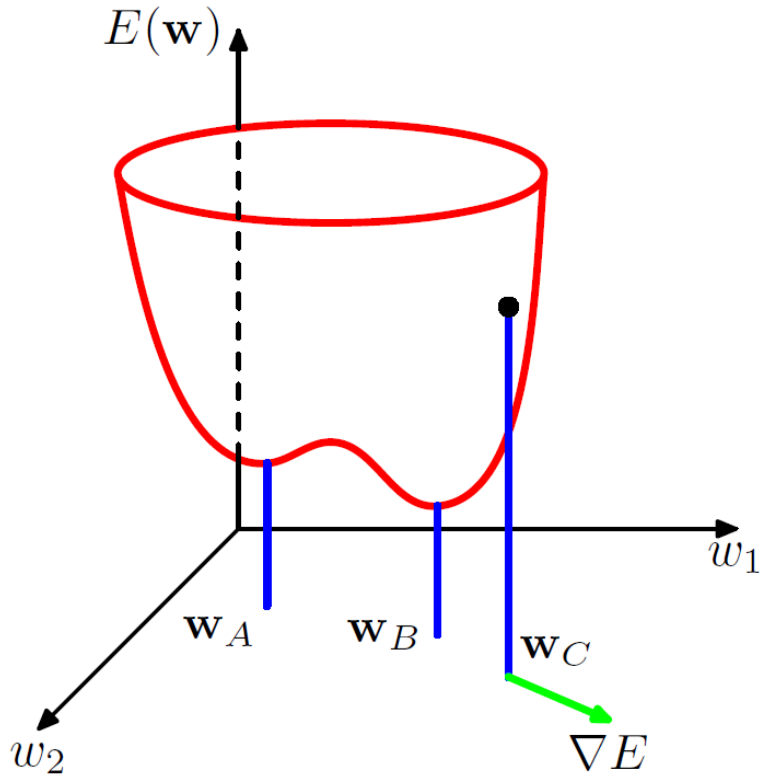
Stochastic Gradient Descent



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Stochastic gradient descent

- Gradient descent: $\boldsymbol{w}^{i+1} = \boldsymbol{w}^{i} - \eta \nabla E(\boldsymbol{w}^{i})$

  where $E(\boldsymbol{w}^{i}) = \sum_{n=1}^{N} E_n(\boldsymbol{w}^{i})$

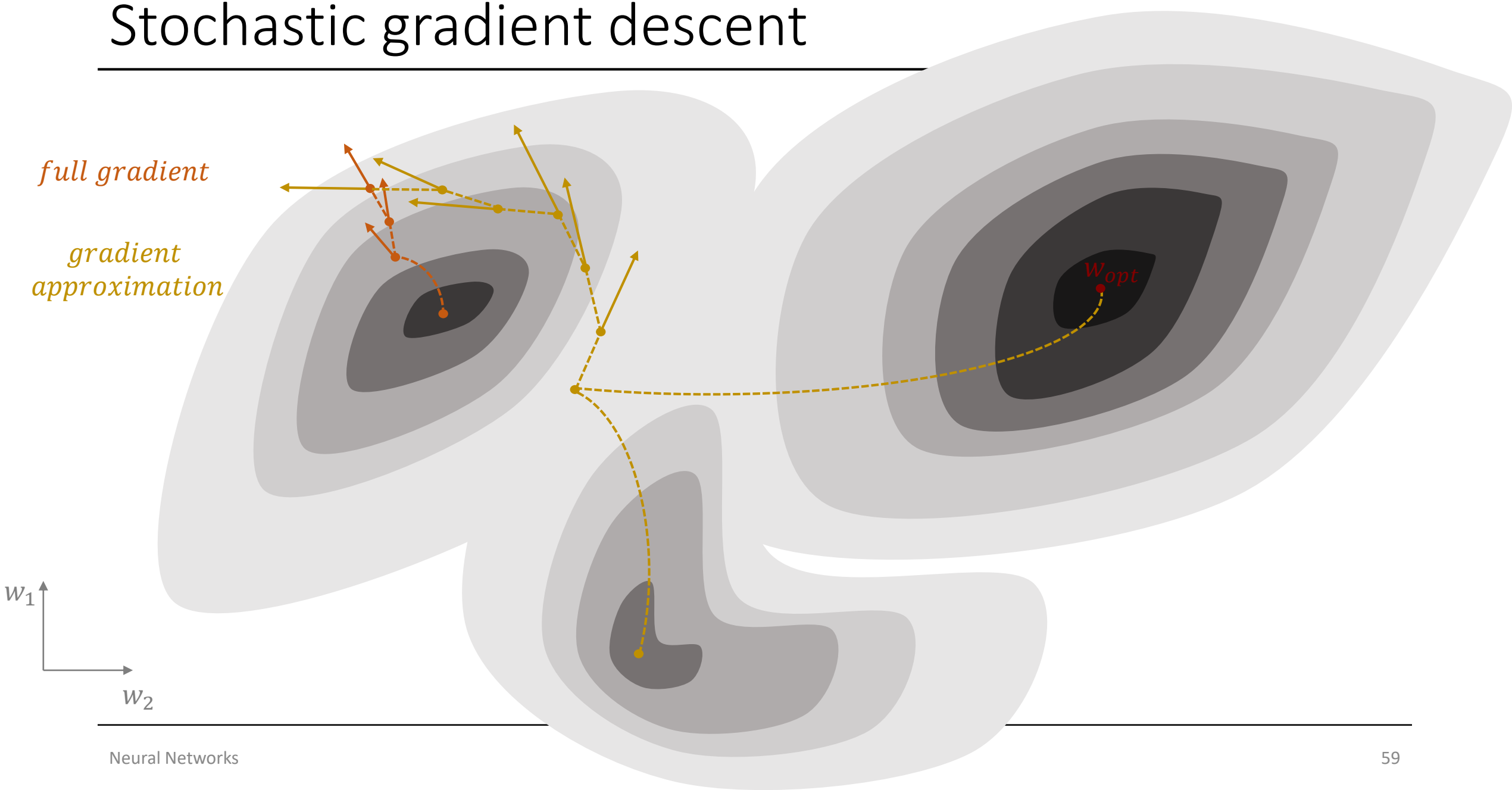
- By incorporating Stochasticity:

$$\boldsymbol{w}^{i+1} = \boldsymbol{w}^{i} - \eta \nabla E_n(\boldsymbol{w}^{i})$$

or

$$\boldsymbol{w}^{i+1} = \boldsymbol{w}^{i} - \eta \nabla \sum_{l=1}^{L} E_l(\boldsymbol{w}^{i}) \textit{ (minibatch)}$$

Stochastic gradient descent



Comments on SGD

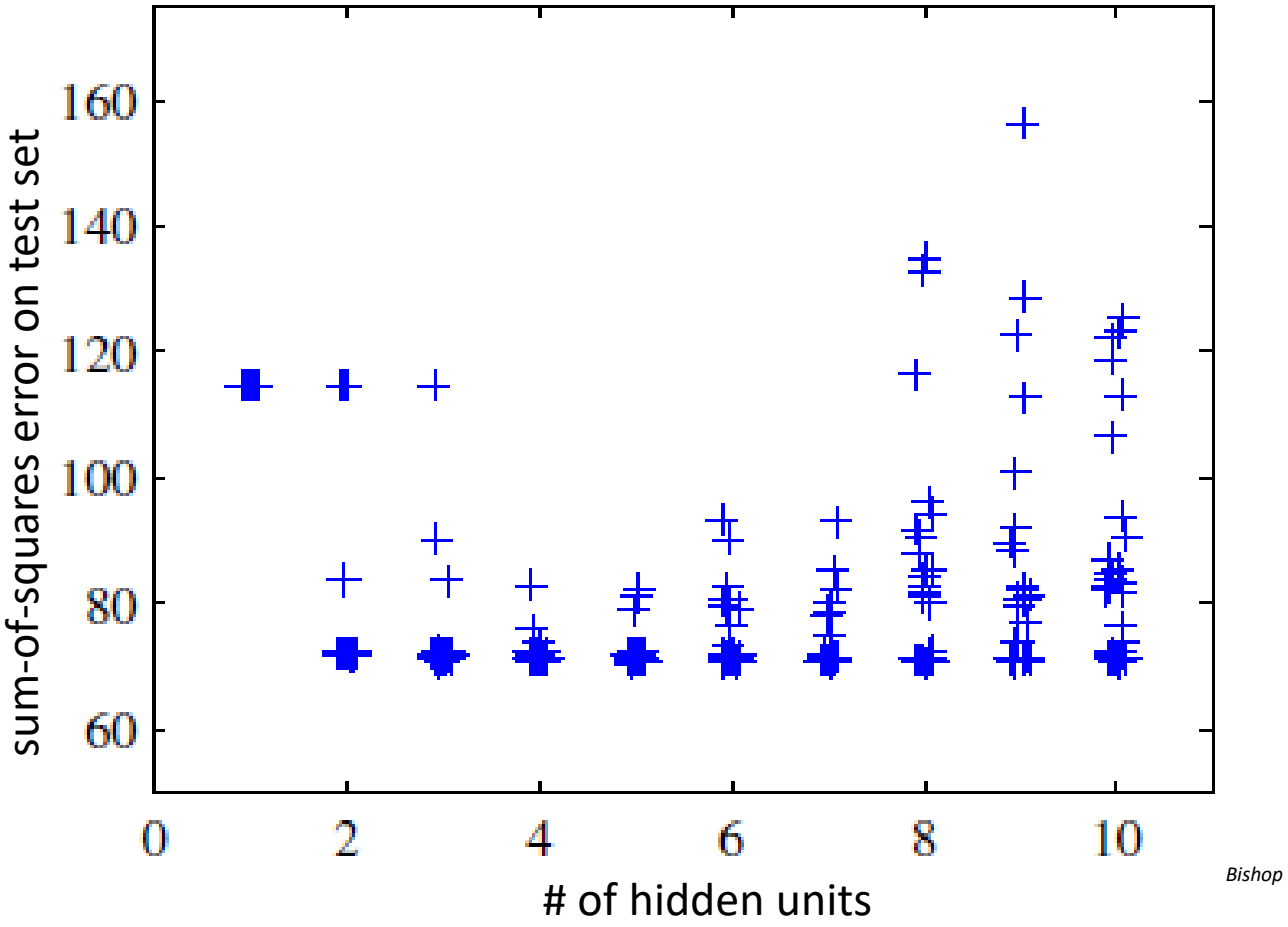
- Learning rate η too small: slow convergence
- Learning rate η too large: oscillations (no convergence)
- We most often use rate scheduling with smaller and smaller rates over time.
- SGD is more likely to escape a local minimum as:

$$\nabla E(\boldsymbol{w}) = \mathbf{0} \text{ does not necessarily imply } \nabla E_n(\boldsymbol{w}) = \mathbf{0}!$$

- As the number of hidden units increases the landscape becomes more complex and thus more initializations are needed to prove the robustness of the network

Comments on SGD

- Try several initialization of $\boldsymbol{w}$ to test uncertainty on performance



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ARISTOTLE UNIVERSITY OF THESSALONIKI

FACULTY OF ENGINEERING

Questions?

Pattern Recognition & Machine Learning

Neural Networks