Artificial Neural Networks

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Some Additional Online References

Neural Networks (+ Deep Learning)

- Michael Nielson's online book http://neuralnetworksanddeeplearning.com/chap1.html

- Deep Learning by Ian Goodfellow, Y. Bengio, and A. Courville

Backpropagation:

Step by Step example by Matt Mazur: https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/

Activation functions:

- http://cs231n.github.io/neural-networks-1/#actfun

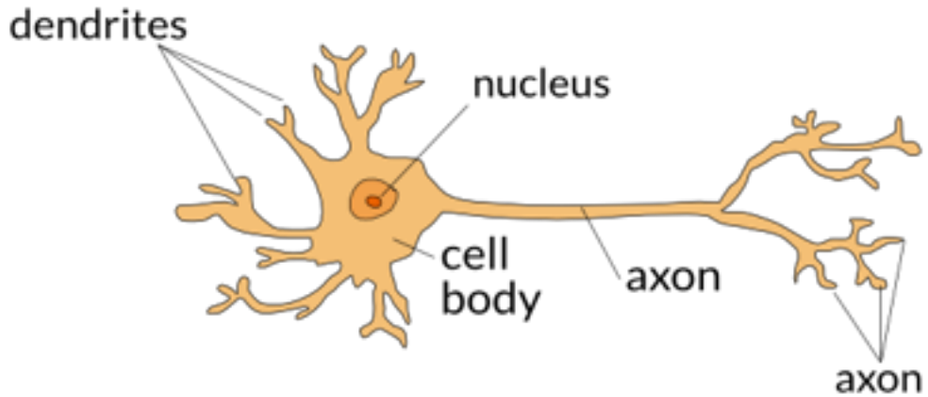
The Human Brain

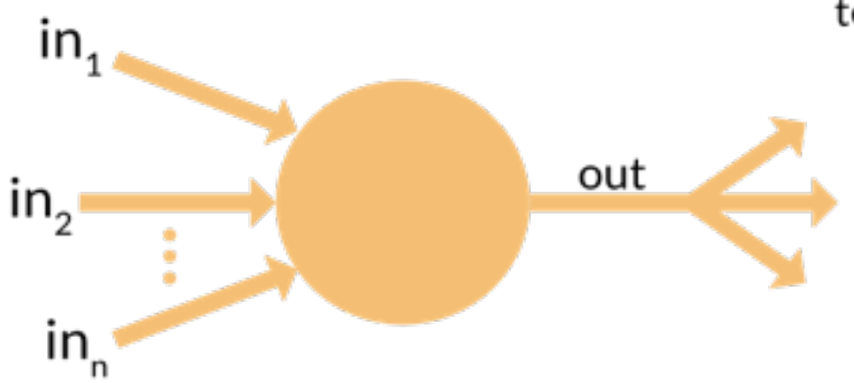
- Highly complex, non-linear, and parallel "computer"
- Structural constituents: neurons
- The structure of the brain is extremely complex and not fully understood
- Billions of nerve cells (neurons) and trillions of interconnections in the human brain
- Scientists tried to mimic the brain's behaviour in proposing the artificial neural network (ANN)
- The human brain is the inspiration for ANNs though we cannot say ANNs actually replicate the brain's behaviour very well, they are extremely simplified

The Neuron

- The basic ingredient of any ANN is the artificial neuron
- They are named and modelled after their biological counterparts - the neurons in the human brain
- input from the dendrites
- output from the axons

biological neuron





artificial neuron

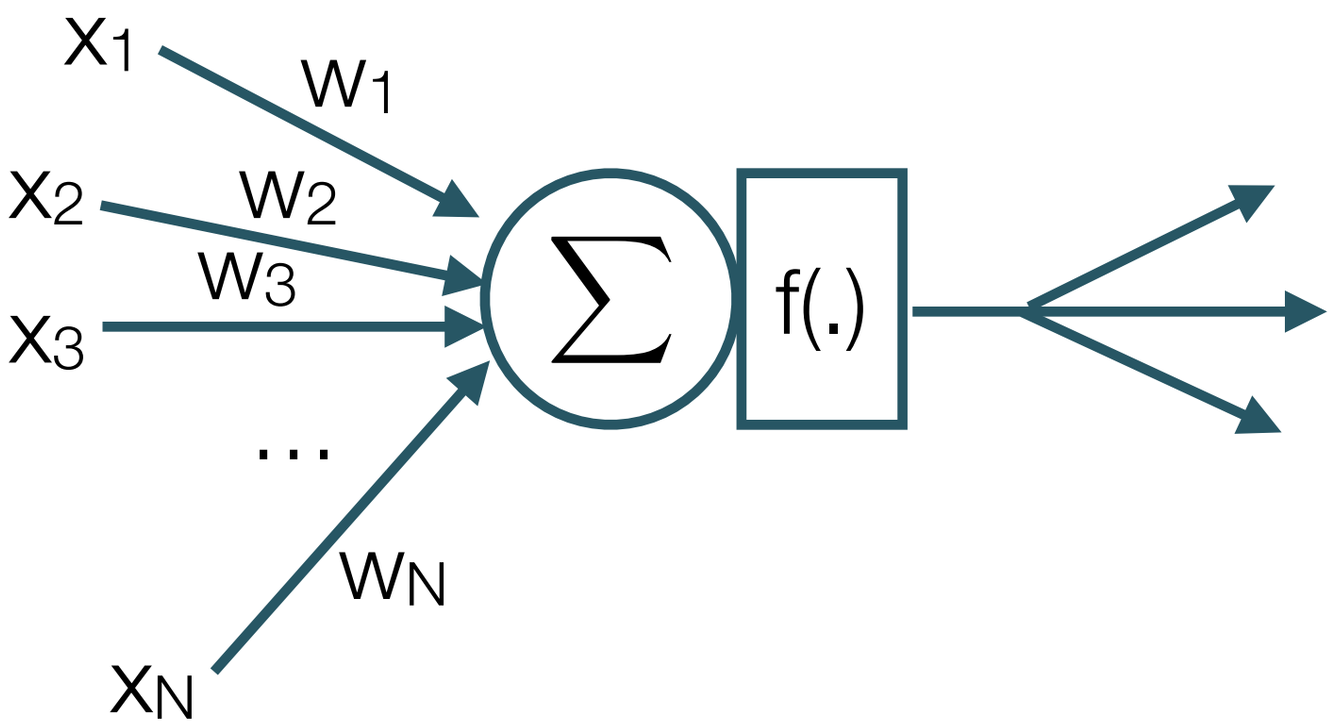
The Artificial Neuron

- The basic unit that builds up ANNs has N inputs that are connected to the neuron with varying strengths of connection that we represent as weights, $w_1 \ldots w_N$

- The signal that goes into the neuron is

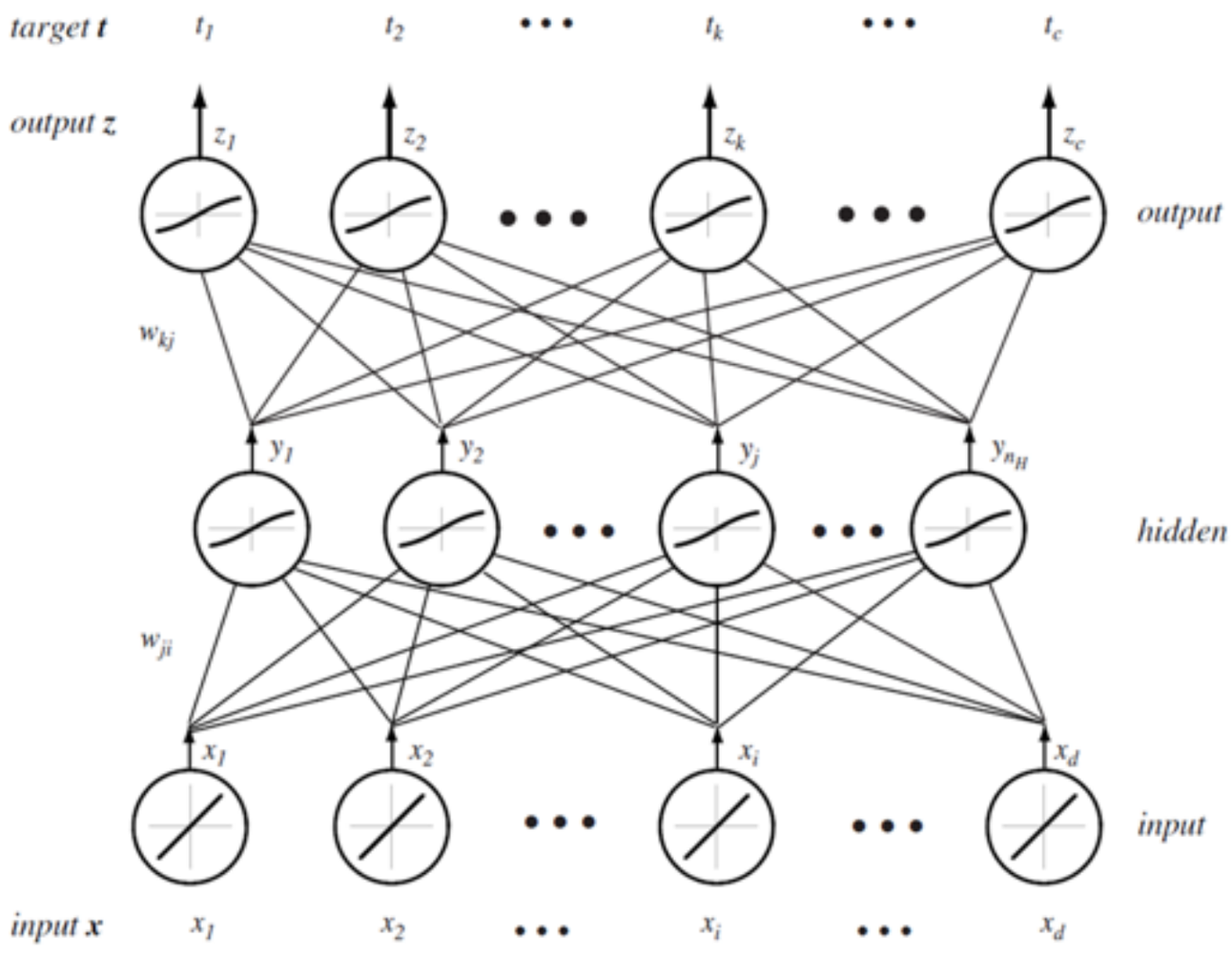
$$x_1 \cdot w_1 + x_2 \cdot w_2 + ...x_N \cdot w_N$$

- We want a decision out of the neuron (e.g. 1 or 0), therefore there must be a non-linear unit after the summation before outputting from the neuron



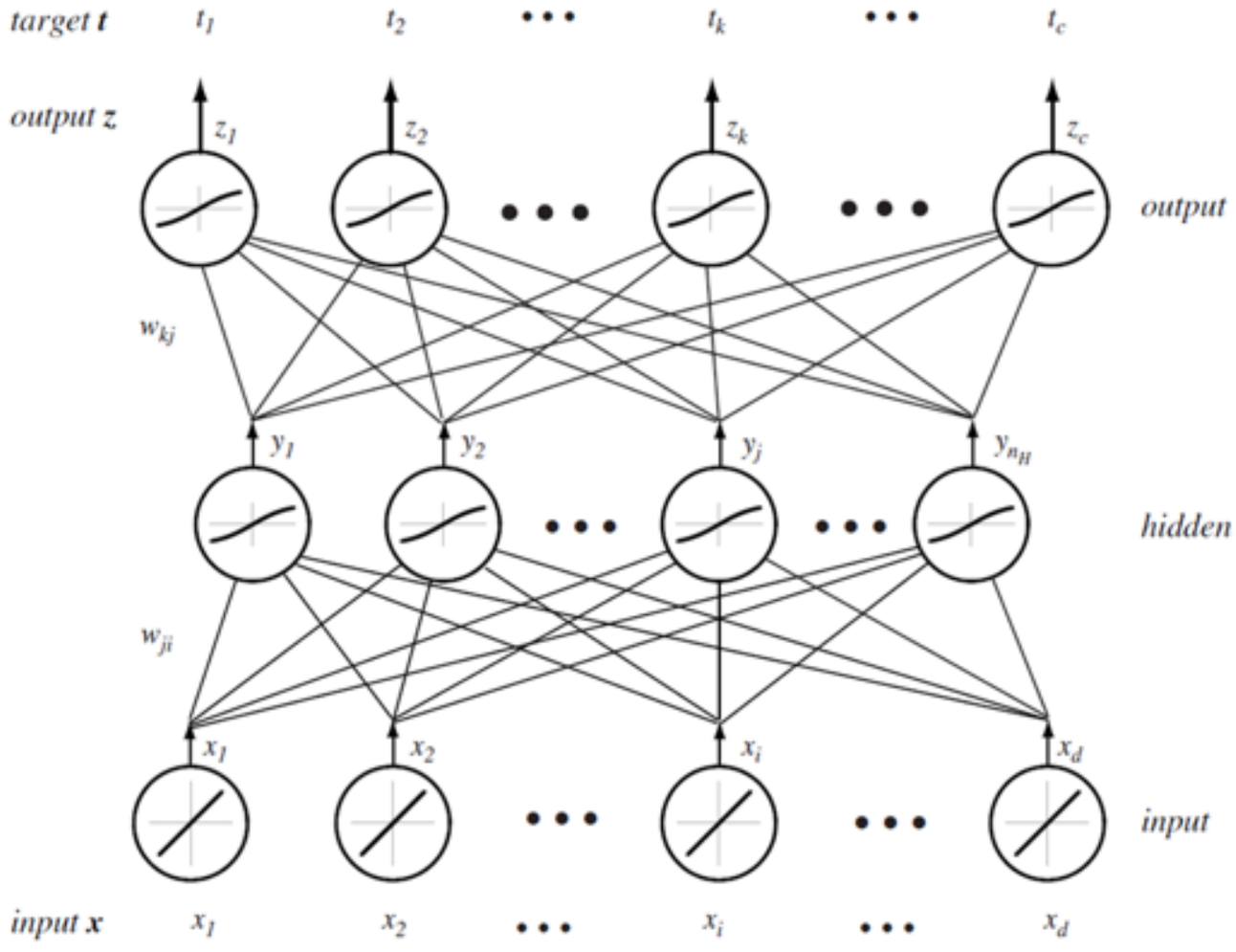
The Multilayer Perceptron - Architecture

- MLP is a class of *feedforward* artificial neural networks (ANNs)
- MLPs are fully connected
- MLPs consist of three or more layers of nodes
- 1 input layer, 1 output layer, 1 or more hidden layers
- d-n_H-c fully connected three-layer network



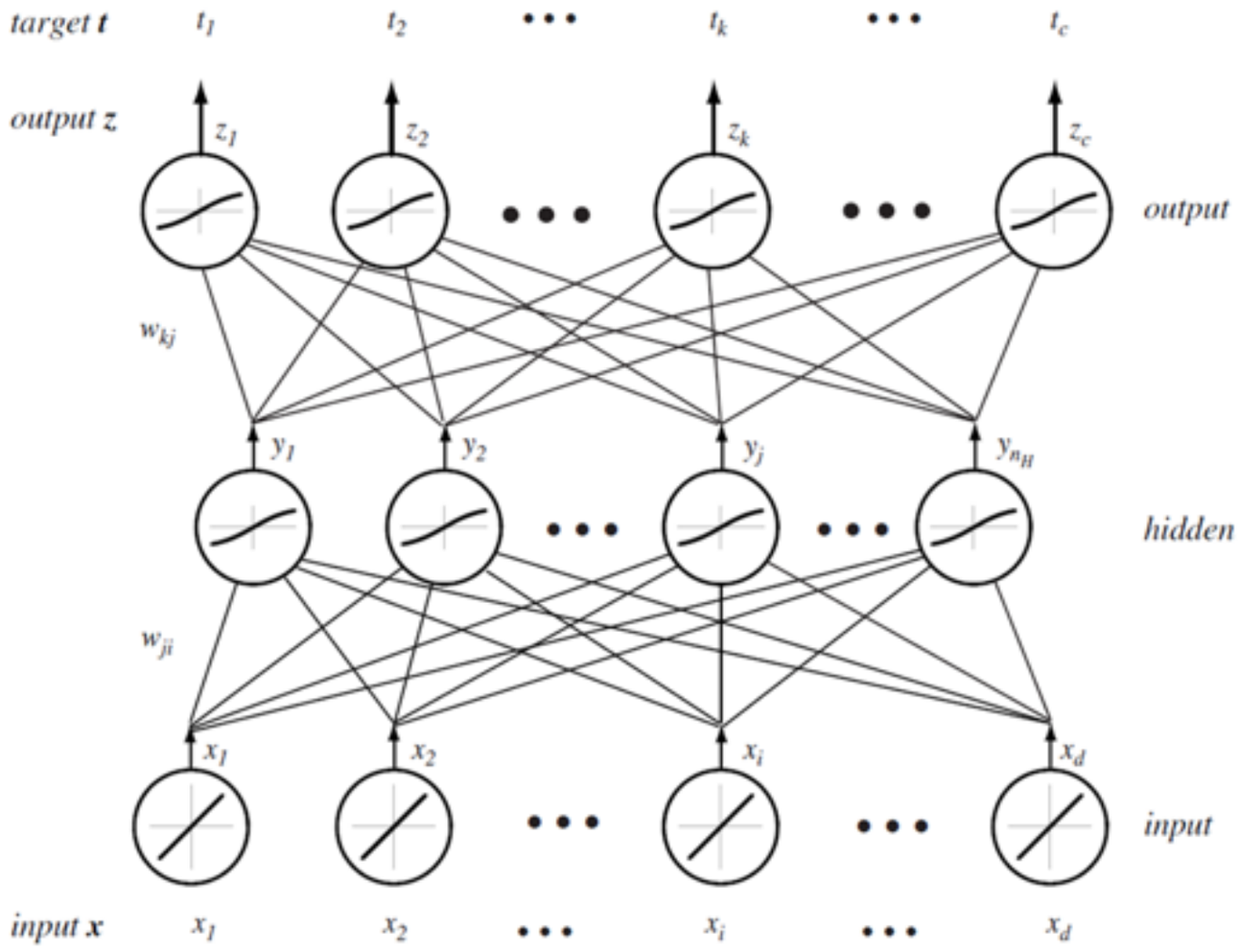
The Multilayer Perceptron - Input Layer

- d-dimensional input **x**
- no neurons at the input layer - "input units"
- each input unit simply emits the input x_i



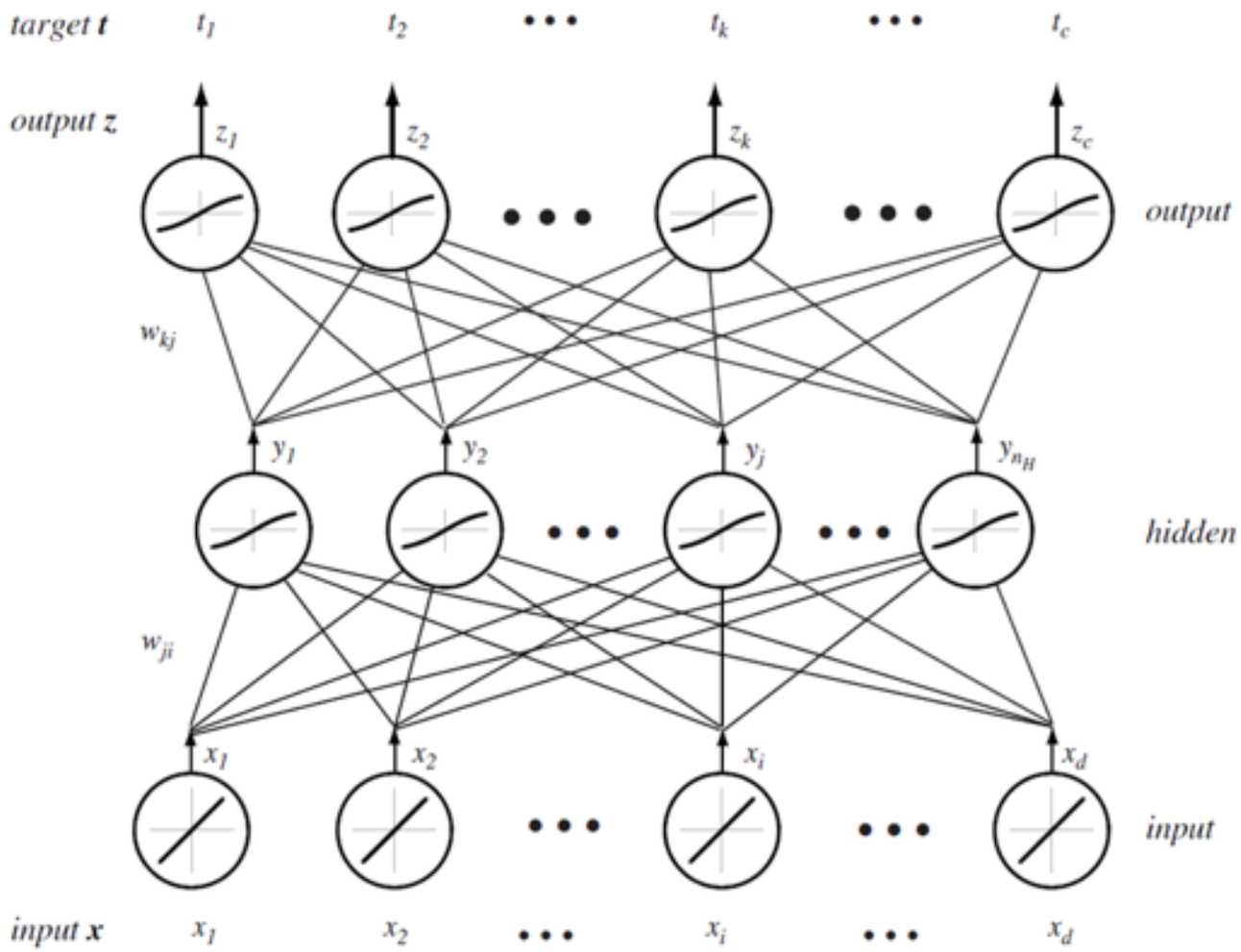
The Multilayer Perceptron - Hidden Layer

- n_H neurons in the hidden layer
- each neuron in the hidden layer uses a non-linear activation function
- Weight w_{ji} denotes the input-to-hidden layer weights at the hidden unit j

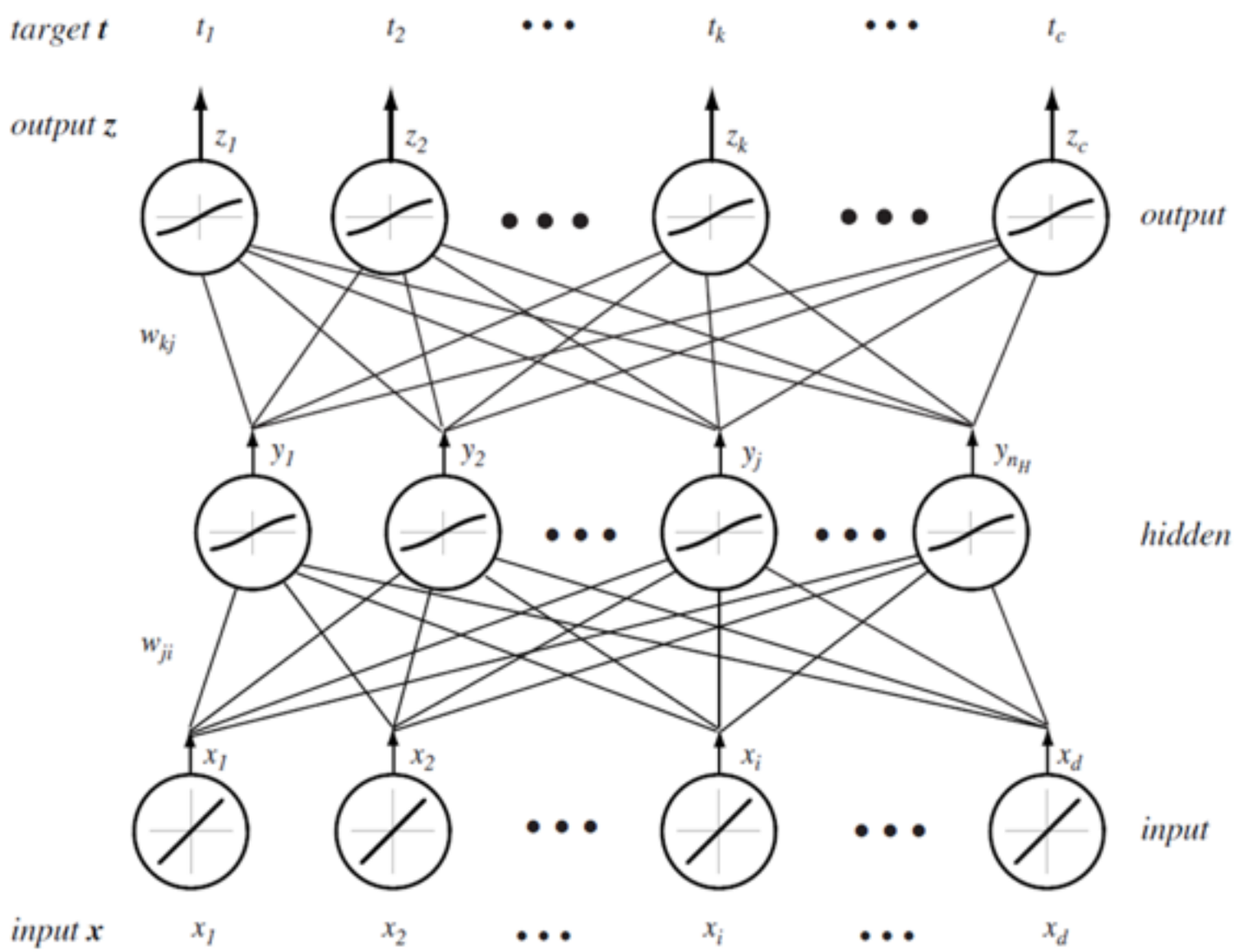


The Multilayer Perceptron - Output Layer

- c neurons in the output layer
- each neuron in the output layer also uses a non-linear activation function
- c and the activation function at the output layer related to the problem you are trying to solve - more details later

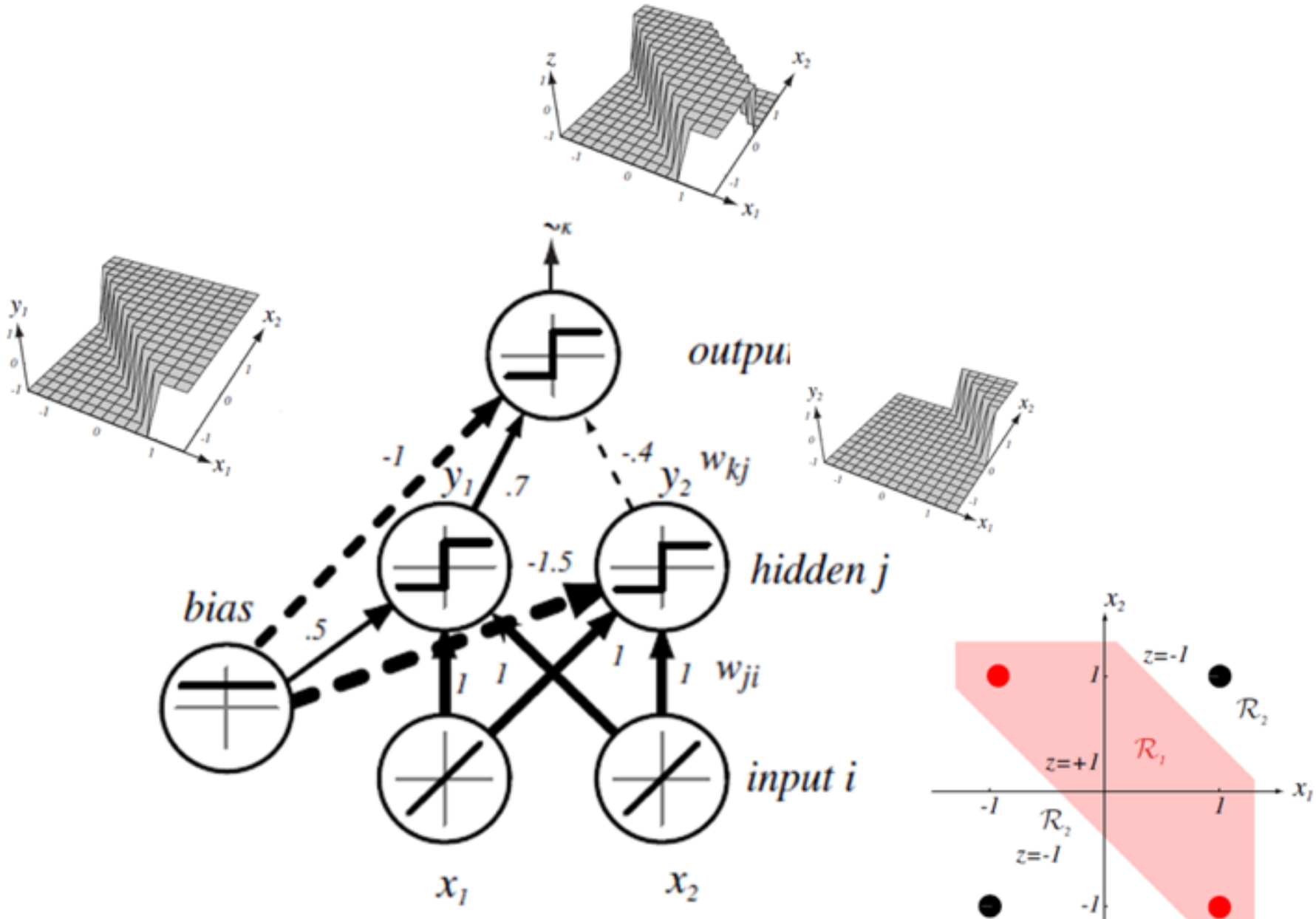


The Multilayer Perceptron - Output Layer



$$g_k(\mathbf{x}) = f(\sum_{j=1}^{n_H} w_{jk} f(\sum_{i=1}^{d} w_{ji} x_i + w_{j0}) + w_{k0})$$

XOR Using a MLP



XOR using MLP with sign function as activation

- Weighted sum of inputs - net activation

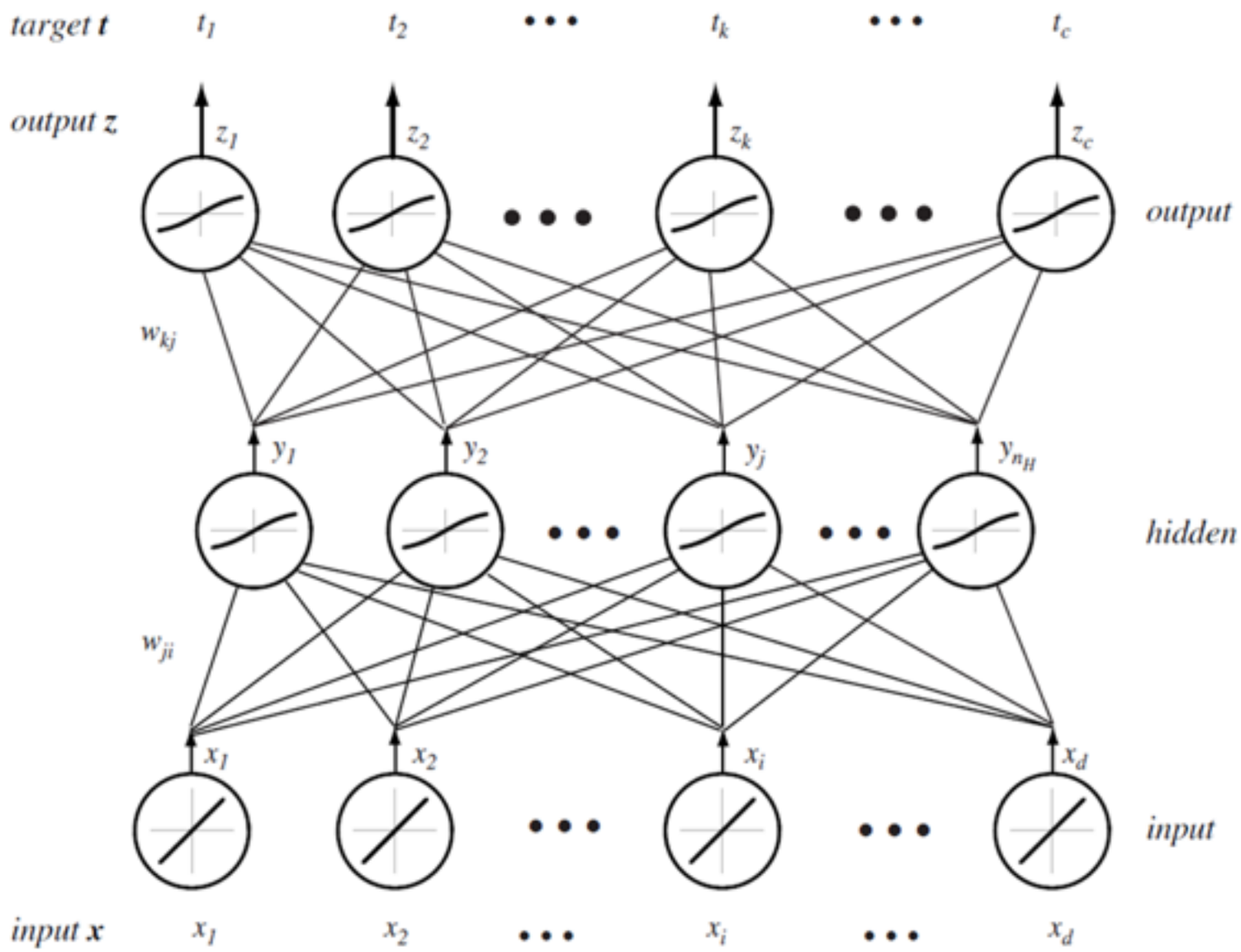
$$net_j = \sum_{i=1}^{d} x_i w_{ji} + w_{j0}$$

- index i indexes the units of the input layer

- index j indexes the units in the hidden layer

- Squashed by a nonlinearity $y_j = f(net_j)$

The Multilayer Perceptron

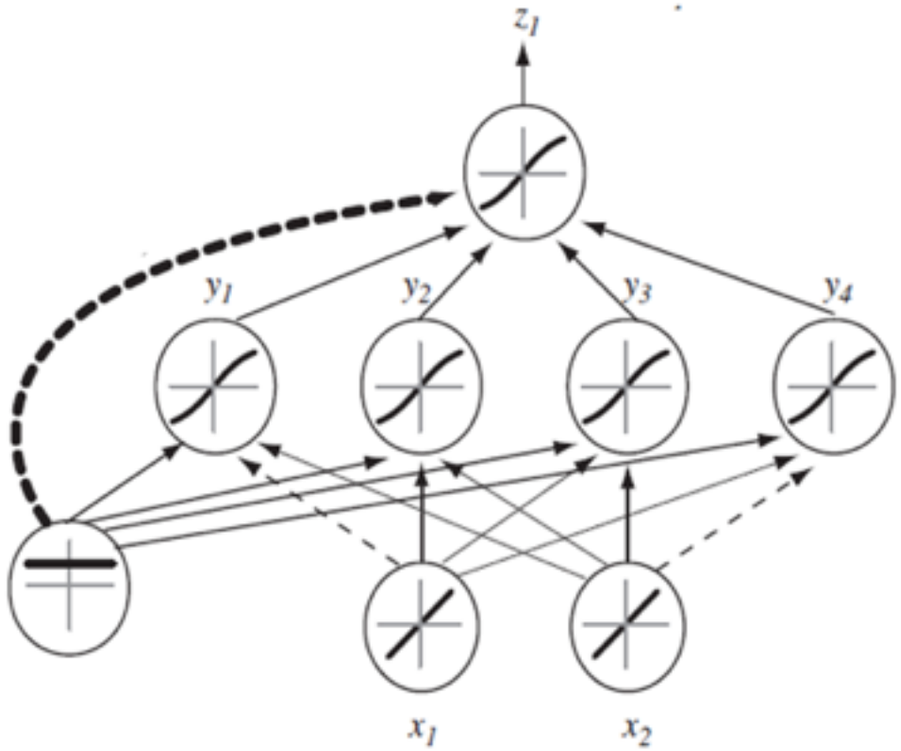


$$g_k(\mathbf{x}) = f(\sum_{j=1}^{n_H} w_{jk} f(\sum_{i=1}^{d} w_{ji} x_i + w_{j0}) + w_{k0})$$

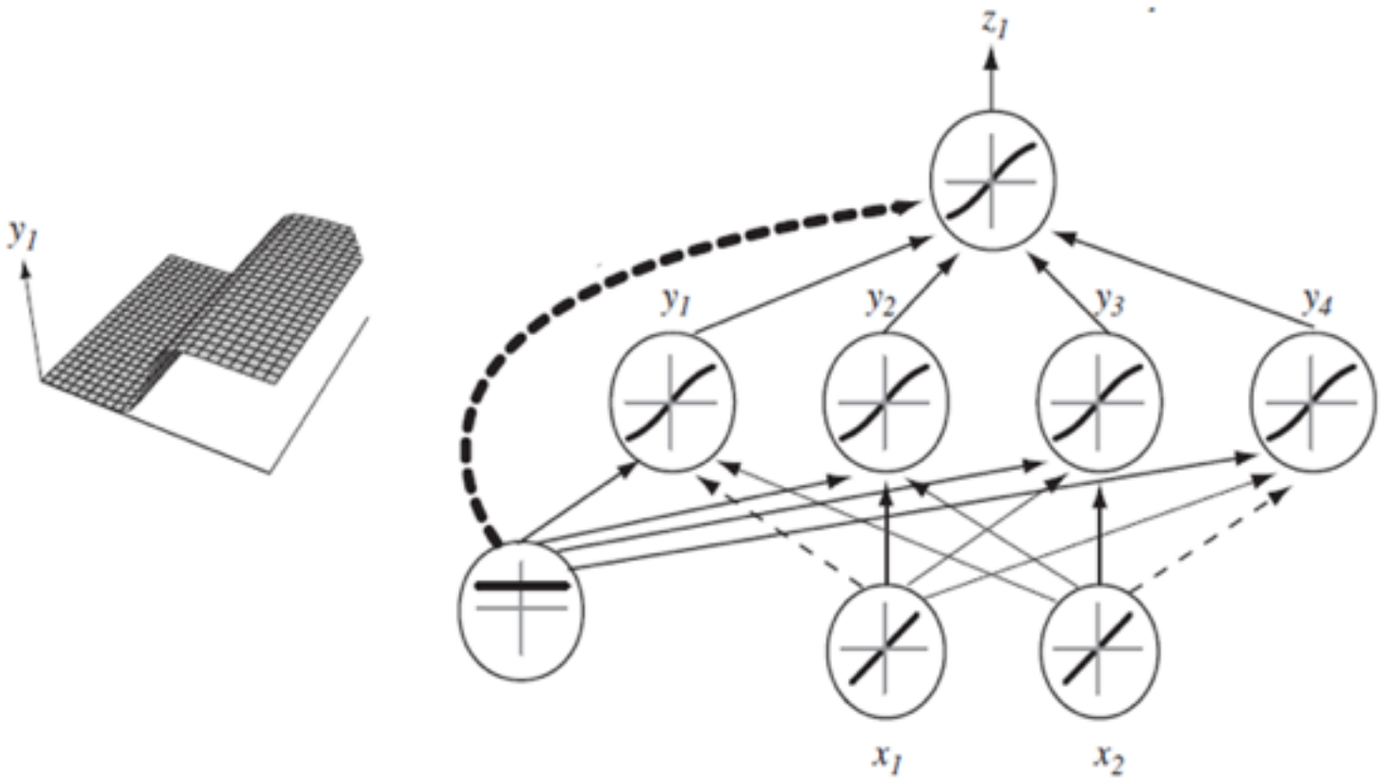
Expressive Power of Multilayer Networks

- Any continuous function from input to output can be implemented in a three-layer network, given sufficient number of hidden units n_H, proper nonlinearities, and weights.

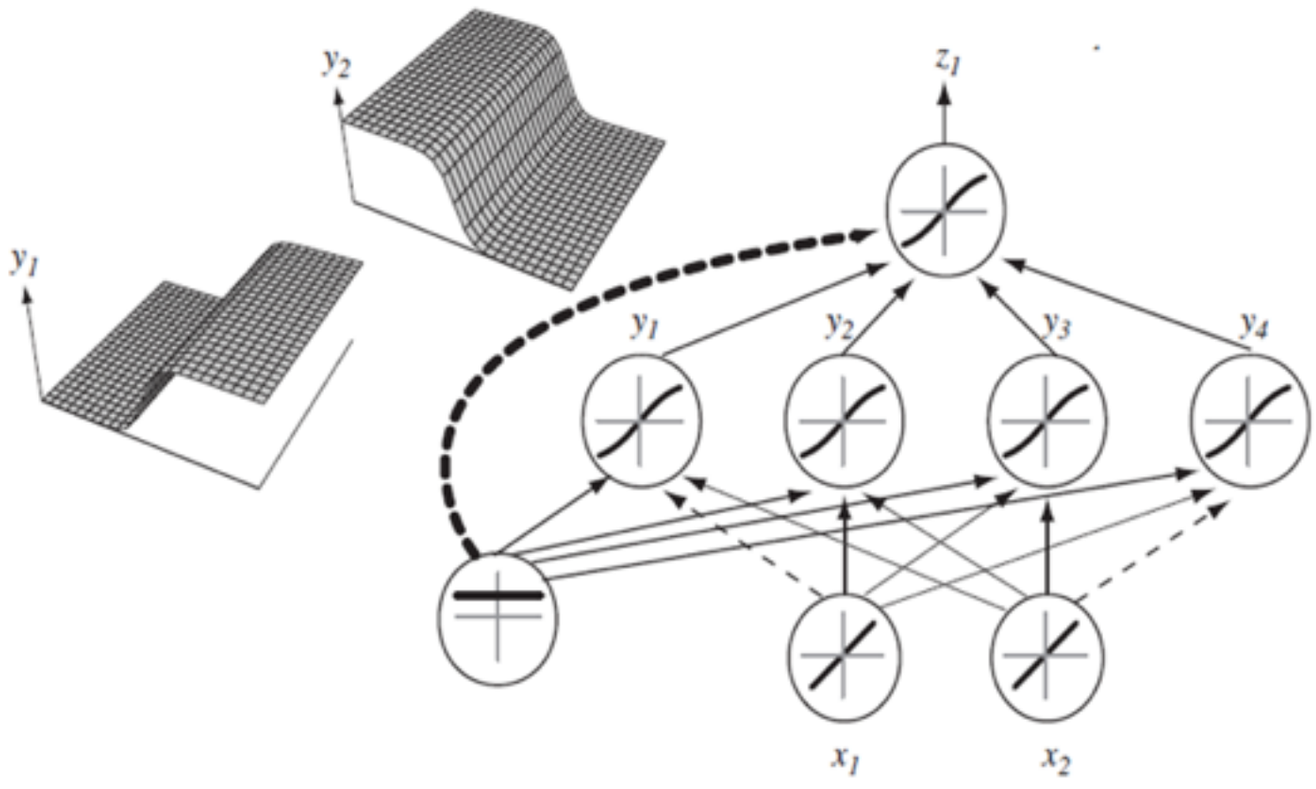
MLP Constructing Complex Functions



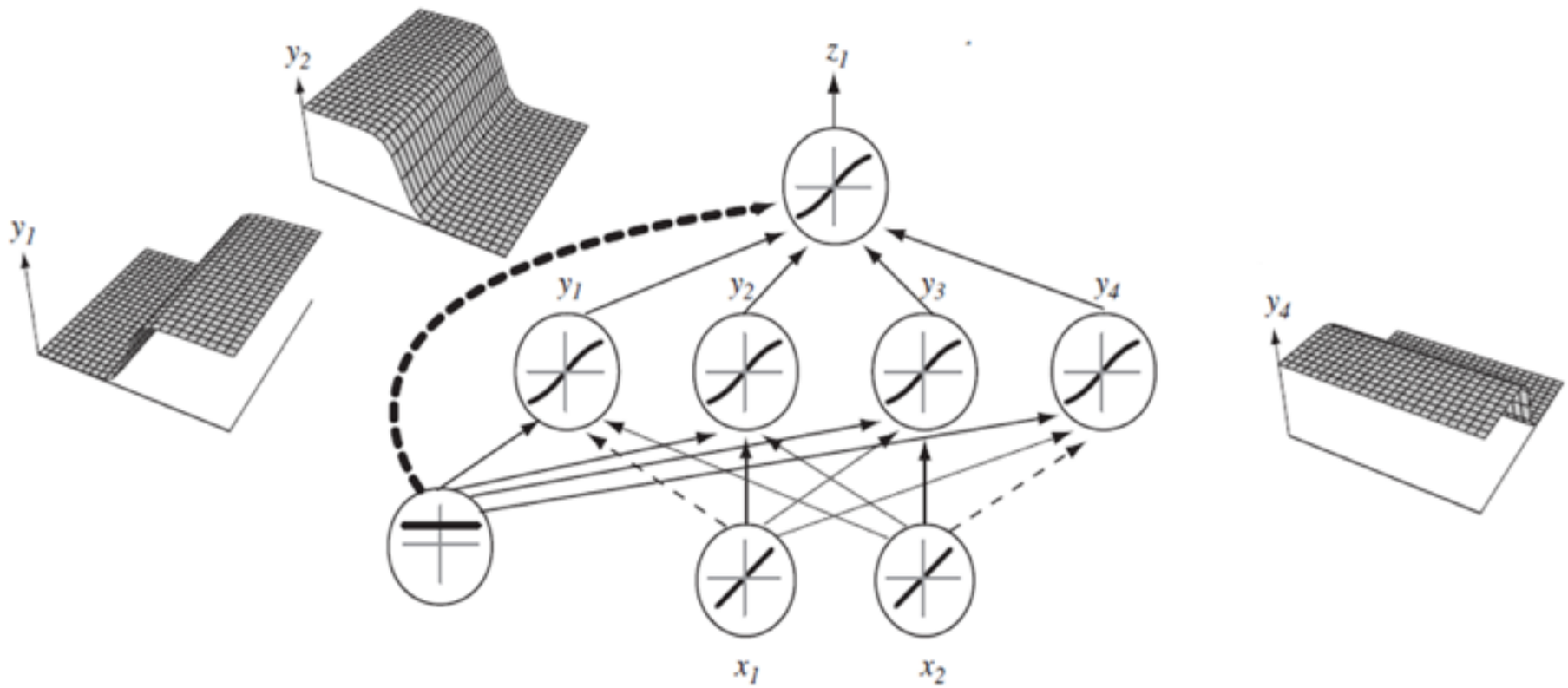
MLP Constructing Complex Functions



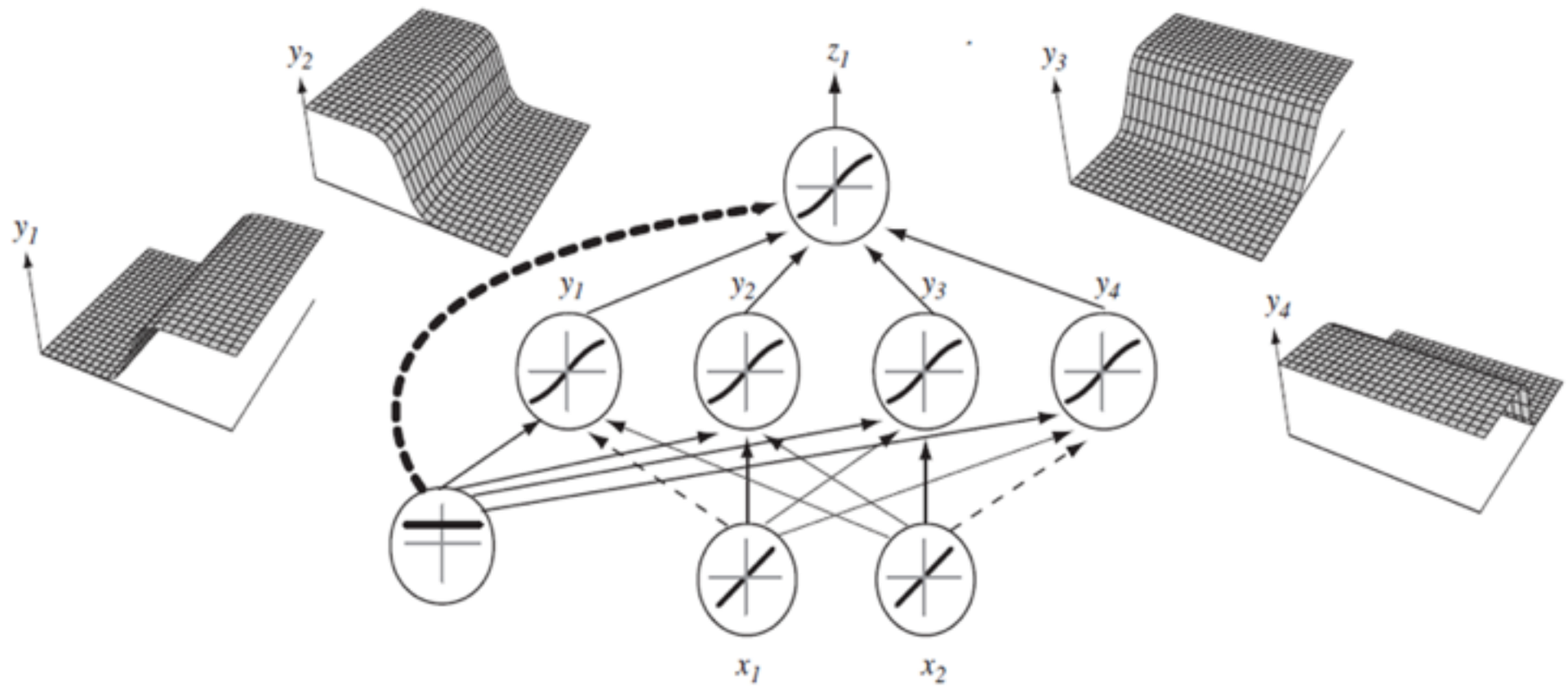
MLP Constructing Complex Functions



MLP Constructing Complex Functions



MLP Constructing Complex Functions



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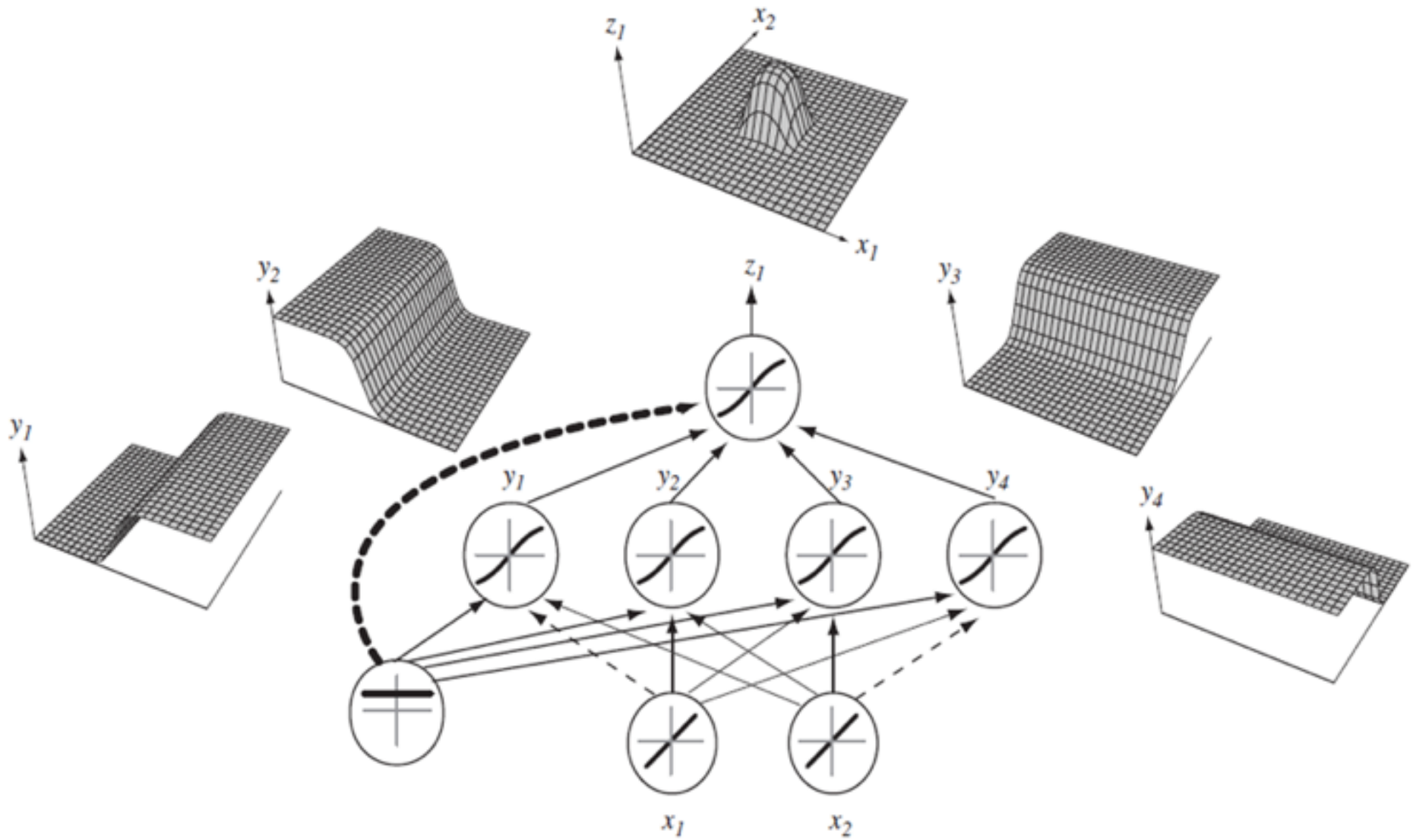


Activation Functions

- The activation function in a neural network is a function used to transform the activation level of a unit (neuron) into an output signal.

- The activation function essentially divides the original space into typically two partitions, having a "squashing" effect.

- The activation function is usually required to be a non-linear function.

- The input space is mapped to a different space in the output.

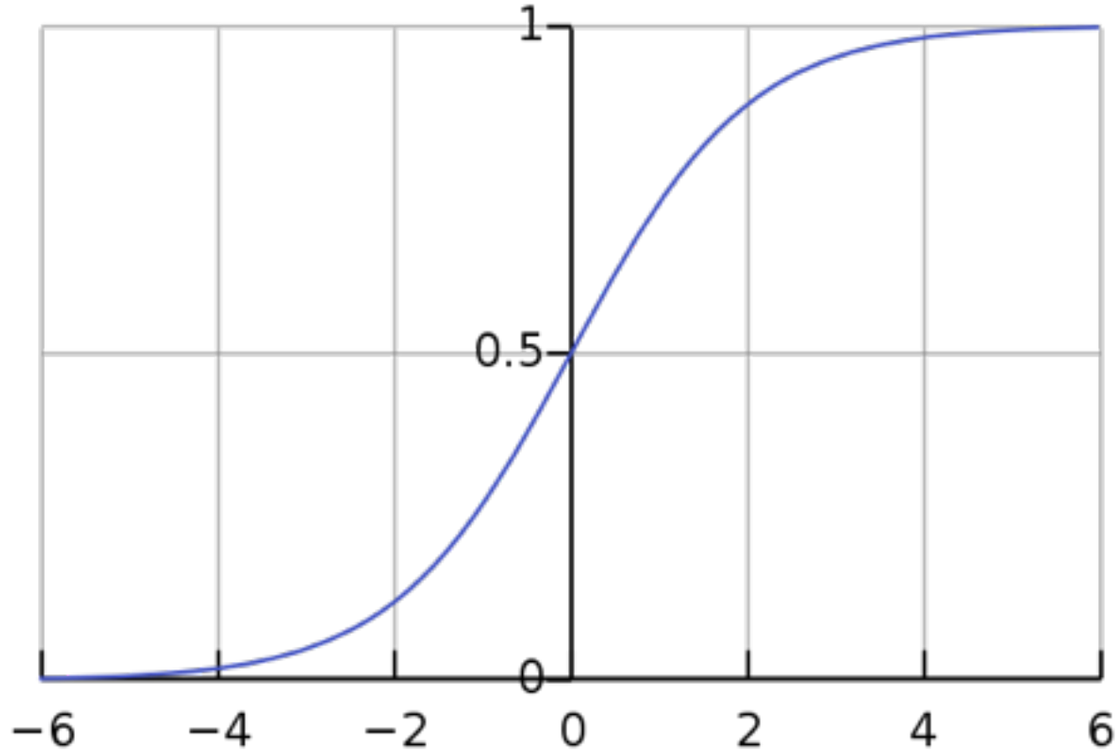
- There have been many kinds of activation functions proposed over the years (640+), however, the most commonly used are the **Sigmoid**, **Tanh**, ReLU, and Softmax.

The Logistic (or Sigmoid) Activation Function

- The sigmoid function is a special case of a logistic function given by f(x) and the plot below

$$f(x) = \frac{1}{1 + e^{-x}}$$

- non-linear (slope varies)
- continuously differentiable
- monotonically increasing
- NB: e is the natural logarithm



Sigmoid Function - Derivative

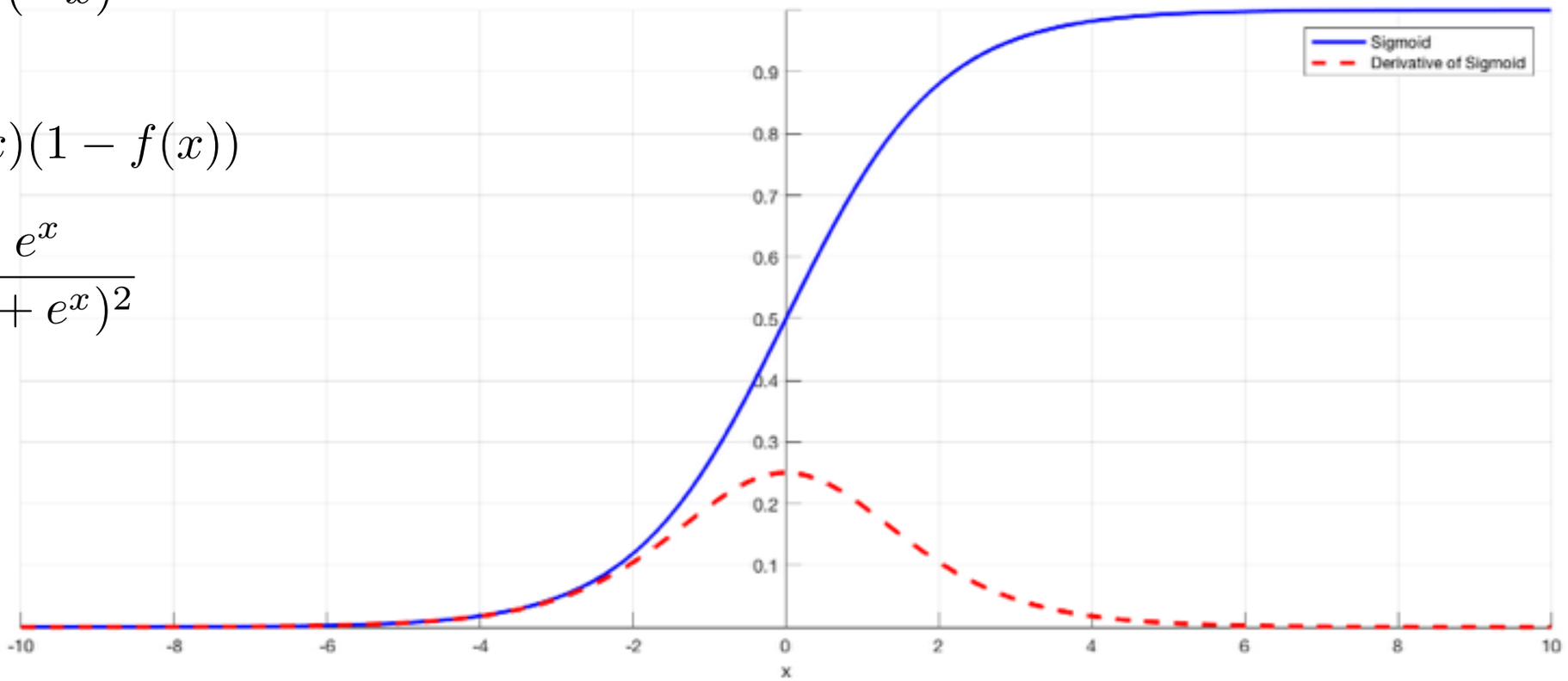
- The sigmoid function has an easily calculated derivative which is used in the back propagation algorithm

$$f(x) = \frac{1}{1+e^{-x}} = \frac{e^x}{1+e^x} = \frac{1}{2} + \frac{1}{2}tanh(\frac{x}{2})$$

$$1 - f(x) = f(-x)$$

$$\frac{d}{dx}f(x) = f(x)(1-f(x))$$

$$= \frac{e^x}{(1+e^x)^2}$$

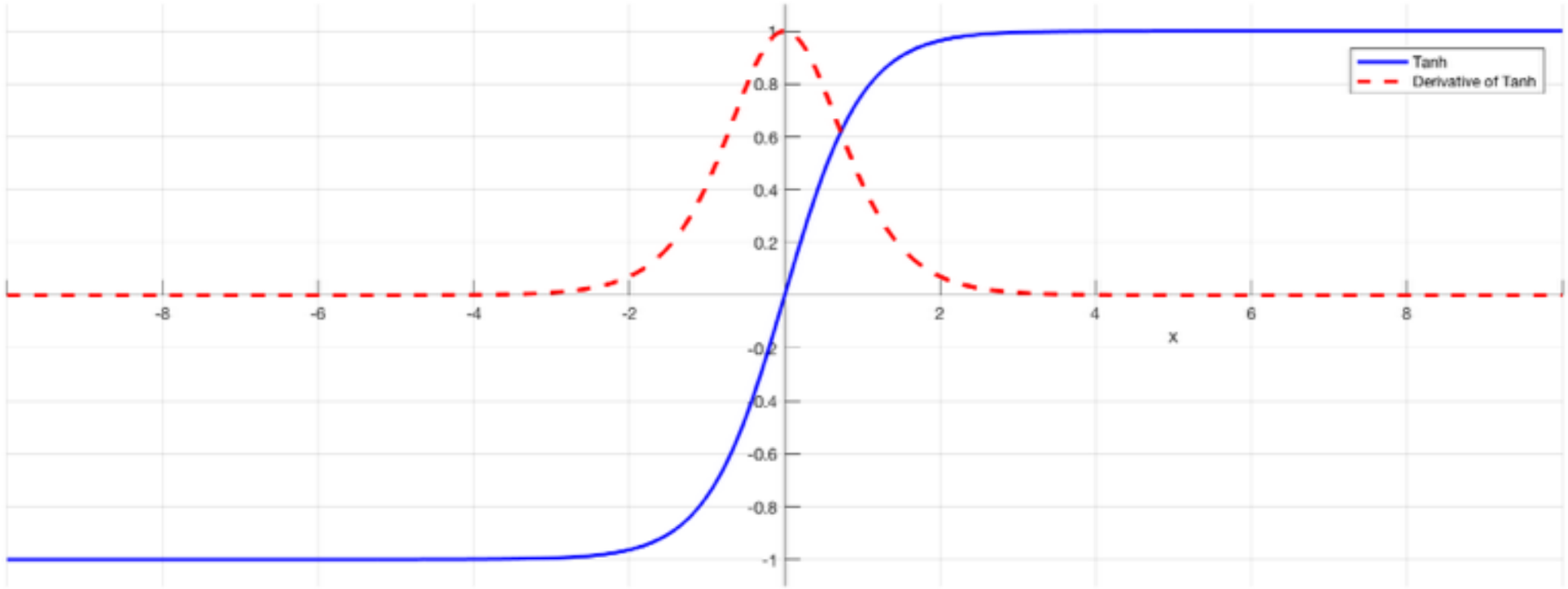


Reference: https://isaacchanghau.github.io/2017/05/22/Activation-Functions-in-Artificial-Neural-Networks/

The Hyperbolic Tangent Activation Function

- The tanh function is also "s"-shaped like the sigmoidal function, but the output range is (-1, 1)

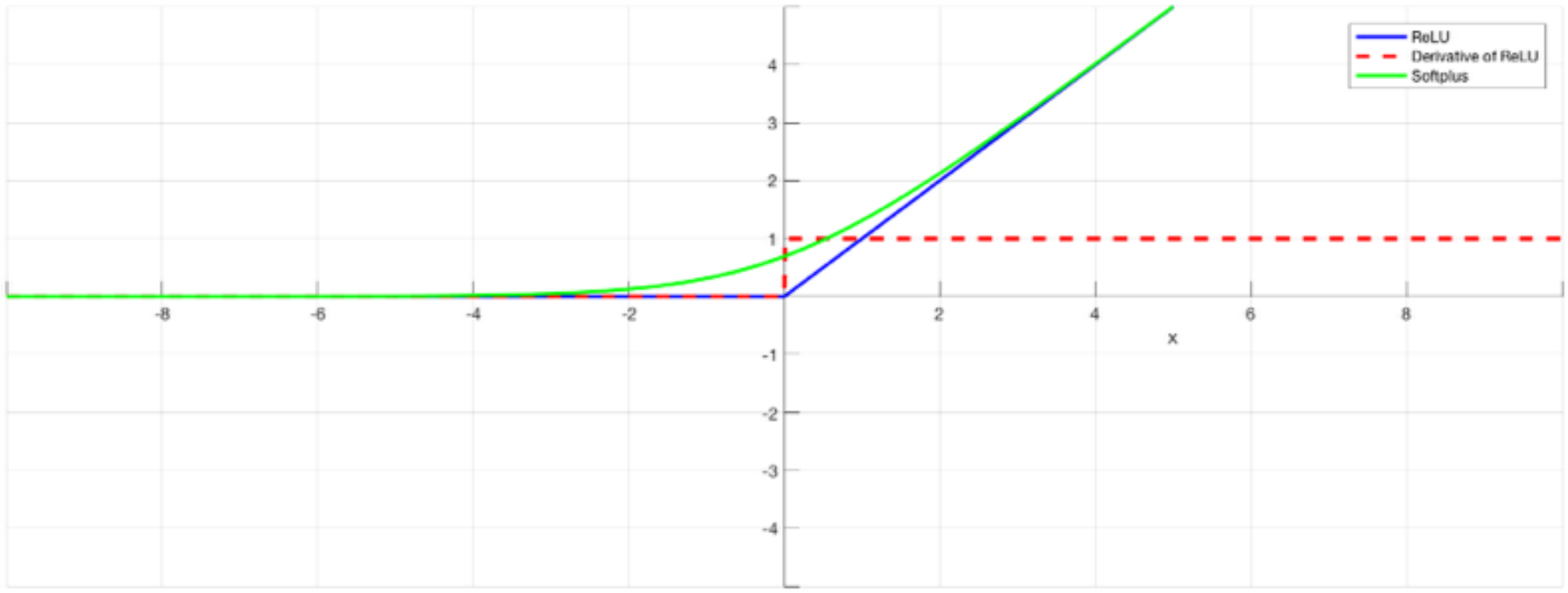
$$tanh(x) = \frac{1 - e^{-2x}}{1 + e^{-2x}} \qquad tanh'(x) = 1 - tanh^2(x)$$



Reference: https://isaacchanghau.github.io/2017/05/22/Activation-Functions-in-Artificial-Neural-Networks/

Rectified Linear Units (ReLU)

- The ReLU (used for the hidden layer neurons) is defined as $$f(x) = max(0, x)$$
- The range of the ReLU is between 0 to ∞



Multi-class Problems

- Binary classification - either 1 or 2 neurons in the output layer depending on what activation function you choose (1 neuron - tanh or sigmoid, 2 neurons - softmax)

- Multiclass classification - Number of neurons in the output layer, K, corresponds to the number of classes in your dataset - K neurons with softmax activation function

Softmax Function

- Used in the output layer of a neural network-based classifier

- Generalization of the logistic function that "squashes" a K-dimensional vector **z** of arbitrary real values to a K-dimensional vector σ(z) of real values in the range [0,1] that add up to 1

$$\sigma(z)_j = \frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_j}} \quad \text{for j = 1, ..., K}$$

Questions from last time

- Softmax not used in the hidden layers of a neural network, it is only used in the output layer

- Vanishing gradient problem is always an issue with neural networks, particularly with deep networks

- Error functions - the cross entropy error function (cost function) is often used with softmax at the output layer

- How to know which error function to use?

- Model selection, Regularization, discussed in more detail later

Backpropagation Algorithm

- Error $$J(\mathbf{w}) = \frac{1}{2}\sum_{k=1}^{c}(t_k - z_k)^2$$
$$= \frac{1}{2}||\mathbf{t} - \mathbf{z}||^2$$

- Change in weight for gradient descent $$\Delta\mathbf{w} = -\eta\frac{\partial J}{\partial \mathbf{w}}$$

- Gradient descent update $$\mathbf{w}(m+1) = \mathbf{w}(m) + \Delta\mathbf{w}(m)$$

Error Backpropagation Algorithm

- Hidden to Output Layer Weights $$\frac{\partial J}{\partial w_{kj}} = \frac{\partial J}{\partial net_k}\frac{\partial net_k}{\partial w_{kj}}$$
$$= -\delta_k \frac{\partial net_k}{\partial w_{kj}}$$

where, change in error with respect to the activation of the unit,

$$\delta_k = -\frac{\partial J}{\partial net_k}$$

Easy form for δ_k,

$$\delta_k = -\frac{\partial J}{\partial net_k} = -\frac{\partial J}{\partial z_k}\frac{\partial z_k}{\partial net_k} = (t_k - z_k) f^{'}(net_k)$$

Error at output x slope of nonlinearity

Also with respect to weights net is differentiated easily $\frac{\partial net_k}{\partial w_{kj}} = y_j$

Error Backpropagation (cont'd)

- Units internal to the network have no explicit error signal

- Chain rule of differentiation helps!

$$\frac{\partial J}{\partial w_{ji}} = \frac{\partial J}{\partial y_j}\frac{\partial y_j}{\partial net_j}\frac{\partial net_j}{\partial w_{ji}}$$

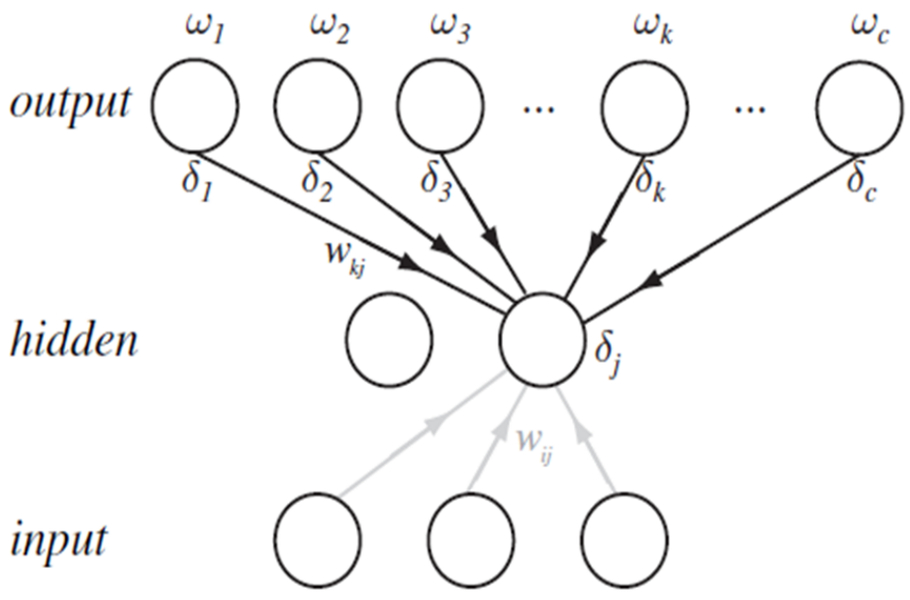
$$\begin{aligned}
\frac{\partial J}{\partial y_j} &= \frac{\partial}{\partial y_j}[\frac{1}{2}\sum_{k=1}^{c}(t_k - z_k)^2] \\
&= -\sum_{k=1}^{c}(t_k - z_k)\frac{\partial z_k}{\partial y_j} \\
&= -\sum_{k=1}^{c}(t_k - z_k)\frac{\partial z_k}{\partial net_k}\frac{\partial net_k}{\partial y_j} \\
&= -\sum_{k=1}^{c}(t_k - z_k)f^{'}(net_k)w_{kj}
\end{aligned}$$

Error propagation (cont'd)

$$\delta_j \;=\; f'(\mathrm{net}_j) \sum_{k=1}^{c} w_{kj}\, \delta_k$$

and the update rule

$$\delta w_{ji} = \eta\, x_i\, \delta_j \;=\; \eta \left[\sum_{k=1}^{c} w_{kj}\delta_k\right] \; f'(\mathrm{net}_j)\, x_i$$



- Signal y_j propagates forward
- δ_j's propagate backwards

Gradient Descent with Momentum

- Allows the network to learn more quickly than standard gradient descent

- Learning with momentum reduces the variation in overall gradient directions to speed learning

- Learning with momentum is given by

$$w(m+1) = w(m) + (1-\alpha)\Delta w_{bp}(m) + \alpha \Delta w(m-1)$$

$$\Delta w(m) = w(m) - w(m-1)$$

where $\Delta w_{bp}(m)$ is the the change in weight given by the backpropagation algorithm and $\alpha = 0.9$ is a robust value

Practical Considerations - Initializing Weights

- All of the weights should be randomly initialized to a small random number, close to zero but not identically zero.

- If they're all set to zero, they will all undergo the exact same parameter updates during backprop - there will be no source of asymmetry if the weights are all initialized to be the same

- Calibrating the variances to 1/sqrt(n) ensures that all neurons in the network initially have approximately the same output distribution and empirically improves the rate of convergence.

- It is common to initialize all of the biases to zero or a small number such as 0.01.

Practical Considerations - Learning Rates

- Plot the cost function J as a function of iterations (epochs)
- J should decrease after every iteration on your training data!
- If J is increasing then something is wrong, it is likely that the learning rate is too high
- Standard test for convergence, $\Delta J < Th$ where $Th = 10^{-3}$
- Note, it is difficult to choose a threshold. Looking at the overall plot of the cost function vs. iterations on data is always most informative.

Practical Considerations - Model Selection

- Split your dataset D into 3 sets
    - training set serves to train a model (70%)
    - validation set to select hyper-parameters (15%)
    - test set to estimate the generalization performance (error) (15%)
- The success of the algorithm is how well your model predicts on the test set (unseen data)!

Practical Considerations - Model Selection

- To search for the best configuration of the hyper-parameters:
- You can perform a **grid search:**
  - specify a set of values you want to test for each hyper-parameter
  - try all possible configurations of these values
- You can also perform a **random search:**
  - specify the distribution over the values of each hyper-parameter
  - sample independently each hyper-parameter to get a configuration, and repeat as many times as wanted

Reference: Hugo Larochelle Neural Networks

Training Protocols - Stochastic Gradient Descent

- Patterns are chosen randomly from the training set, and the network weights are updated for each pattern presentation.

- One epoch corresponds to a single presentation of all patterns in the training set.

Algorithm 1. (Stochastic Backpropagation)

begin initialize $n_{hidden}, w, criterion\ \theta, \eta, m \leftarrow 0$

  do $m \leftarrow m + 1$

    $x^m \leftarrow$ randomly chosen pattern

    $w_{ji} \leftarrow w_{ji} + \eta \delta_j x_i; \quad w_{kj} \leftarrow w_{kj} + \eta \delta_k y_j$

  until E(w) < θ

return w

end

Training Protocols - Batch Gradient Descent

- All patterns are presented to the network before learning takes place.

Algorithm 2. (True gradient Backpropagation)

begin initialize $n_{hidden}, w, criterion\ \theta, \eta, r \leftarrow 0$

do $r \leftarrow r + 1$ (increment epoch)

$m \leftarrow 0;\ \ \Delta w_{ji} \leftarrow 0;\ \ \Delta w_{kj} \leftarrow 0$

do $m \leftarrow m + 1$

$x^{m} \leftarrow$ selected pattern

$\Delta w_{ji} \leftarrow \Delta w_{ji} + \eta \delta_j x_i;\ \ \Delta w_{kj} \leftarrow \Delta w_{kj} + \eta \delta_k y_j$

until $m = n$

$w_{ji} \leftarrow w_{ji} + \Delta w_{ji};\ \ w_{kj} \leftarrow w_{kj} + \Delta w_{kj}$

until $E(w) < \theta$

return w

end

Stochastic Gradient Descent - Advantages and Disadvantages

✓ The **frequent updates** immediately give an insight into the performance of the model

✓ The noisy update process can allow the model to avoid local minima

- Updating the model so frequently is more computationally expensive, **taking significantly longer to train models on large datasets**

- The frequent updates can result in a noisy gradient signal, which may cause the model parameters and in turn the model error to jump around

- The noisy learning process down the error gradient can also make it hard for the algorithm to settle on an error minimum for the model

Batch Gradient Descent - Advantages and Disadvantages

✓ Fewer updates to the model means this variant of gradient descent is more computationally efficient

✓ The decreased update frequency results in a **more stable error gradient** and may result in a more stable convergence

✓ The separation of the calculation of prediction errors and the model update lends the algorithm to parallel processing based implementations

- The more stable error gradient may result in premature convergence of the model to a less optimal set of parameters

- The updates at the end of the training epoch require the additional complexity of accumulating prediction errors across all training examples

- Commonly, batch gradient descent is implemented in such a way that it requires the entire training dataset in memory and available to the algorithm

- **Model updates, and in turn training speed, may become very slow for large datasets**

Mini-Batch Gradient Descent

- Mini-batch gradient descent is a variation of the gradient descent algorithm that splits the training dataset into small batches that are used to calculate model error and update model coefficients.

- Implementations may choose to sum the gradient over the mini-batch or take the average of the gradient which further reduces the variance of the gradient.

- Mini-batch gradient descent seeks to find a balance between the robustness of stochastic gradient descent and the efficiency of batch gradient descent. It is the most common implementation of gradient descent used in the field of deep learning.

Mini-Batch - Advantages and Disadvantages

- ✓ The model update frequency is higher than batch gradient descent which allows for a more robust convergence, avoiding local minima

- ✓ The batched updates provide a computationally more efficient process than stochastic gradient descent

- ✓ The batching allows both the efficiency of not having all training data in memory and algorithm implementations

- \- Mini-batch requires the configuration of an additional “mini-batch size” hyperparameter for the learning algorithm

- \- Error information must be accumulated across mini-batches of training examples like batch gradient descent

Practical Considerations - Regularization

- **L2 regularization** is the most common form of regularization.

- It is implemented by penalizing the squared magnitude of all parameters directly in the objective. For every weight in the network, we add the term $\frac{1}{2}\lambda w^2$, where λ is the regularization strength.

- L2 regularization has the property of encouraging the network to use all of its inputs a little rather that some of its inputs a lot.

Practical Considerations - Regularization

- **L1 regularization** is another common form of regularization.

- For every weight w in the network, we add the term $\lambda|w|$, to the objective.

- L1 regularization leads to the weight vectors becoming sparse during optimization.

- L1 can be seen as doing feature selection.

- In practice, L2 regularization gives superior performance.