Introduction to Neural Networks

Inspired from Prof. Xiangliang Zhang (KAUST)

---

by Dr. Rishikesh Yadav (Postdoctoral Research Fellow)

HEC Montréal, McGill University, Canada

Table of contents

References

- Christopher M. Bishop (2007). Pattern Recognition and Machine Learning
- Chollet, F., & Allaire, J. J. (2018). *Deep Learning with R*.
- There are some really good Coursera courses for machine learning and deep learning.

Goal

- The objectives of this short-course are:
  - Understanding and learning regression using gradient descent algorithm
  - Understand the basics of Neural Networks.
  - Build and train simple feed-forward Neural Networks within R from scratch and also using the R package `neuralnet`.

Background

Linear Regression (1)

- **Linear Regression** is a statistical method for modeling the relationship between a dependent variable and one or more independent variables.
- The relationship is modeled using a linear predictor function whose unknown parameters are estimated from the data.
- In its simplest form, with one dependent variable y and one independent variable x, the linear regression model is:

$$y = w_0 + w_1 x + \epsilon.$$

where:

  - y is the dependent variable (response variable).
  - x is the independent variable (predictor variable).
  - w_0 is the intercept term, which represents the expected value of y when $x = 0$.
  - w_1 is the slope term, which represents the change in y for a one-unit change in x.
  - ϵ is the error term, which accounts for the variability in y that cannot be explained by the linear relationship with x.

Linear Regression (2)

- The parameters w_0 and w_1 are estimated from the data using methods such as **Ordinary Least Squares (OLS)**, which minimizes the sum of the squared differences between the observed values and the predicted values.
- The **OLS** estimate of the parameters can be obtained by solving the following normal equations:

$$\begin{pmatrix} \hat{w}_0 \\ \hat{w}_1 \end{pmatrix} = (X^T X)^{-1} X^T y.$$

  where:
  - X is the design matrix, including a column of ones for the intercept and a column of the predictor variable values.
  - y is the vector of observed values of the dependent variable.
- Linear regression can be extended to include multiple independent variables, resulting in **Multiple Linear Regression**:

$$y = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_p x_p + \epsilon.$$

  where $x_1, x_2, \ldots, x_p$ are the predictor variables.

Gradient Descent Algorithm (1)

Gradient Descent Algorithm is an optimization technique used to minimize a loss function by iteratively moving towards the minimum of the function.

The main components of the gradient descent algorithm are:

- **Loss Function**:
  - The loss function measures the error or difference between the predicted values and the actual values. That means it measures how well the model's predictions match the actual data.
  - The goal of gradient descent is to minimize this loss function to improve the accuracy of the model.
  - Examples of loss functions include **Mean Squared Error (MSE)** for regression problems and **Cross-Entropy Loss** for classification problems.
  - Mathematically, for a set of predictions $\hat{y}$ and actual values y, the Mean Squared Error is given by:

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2.$$

Gradient Descent Algorithm (2)

- **Gradient**:
  - The gradient is a vector of partial derivatives of the loss function with respect to all the parameters of the model.
  - It points in the direction of the steepest ascent of the function.
  - In gradient descent, we move in the opposite direction of the gradient to find the minimum of the loss function.
  - For a parameter w, the gradient of the loss function L with respect to w is given by:

$$\nabla_w L = \left(\frac{\partial L}{\partial w_0}, \frac{\partial L}{\partial w_1}, \ldots, \frac{\partial L}{\partial w_p} \right).$$

- **Update Rule**:
  - In each iteration of gradient descent, the model parameters are updated using the gradient and the learning rate.
  - The update rule for a parameter w is given by:

$$w := w - \eta \nabla_w L,$$

where η is the learning rate and $\nabla_w L$ is the gradient of the loss function with respect to w.

Gradient Descent Algorithm (3)

- **Learning Rate** η:
  - The learning rate is a hyperparameter that determines the size of the steps taken towards the minimum of the loss function.
  - A smaller learning rate means smaller steps, leading to more accurate convergence but slower progress.
  - A larger learning rate can speed up the process but risks overshooting the minimum and potentially diverging.
  - It is important to choose an appropriate learning rate to ensure efficient and effective training of the model.
- **Convergence**:
  - The algorithm iteratively updates the parameters until the loss function converges to a minimum value.
  - Convergence can be determined by setting a threshold for the change in the loss function or by specifying a maximum number of iterations.

Gradient Descent Algorithm: Algorithm Steps

- **Initialize**: Start with an initial guess for the parameters.
- **Compute Gradient**: Calculate the gradient of the loss function with respect to each parameter.
- **Update Parameters**: Adjust the parameters by moving them in the direction opposite to the gradient, scaled by the learning rate.
- **Iterate**: Repeat the process until the parameters converge to the minimum or a stopping criterion is met.

Example 1: Gradient Descent for Linear Regression[1]

- **Loss Function** (Mean Squared Error, MSE):

$$\text{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y_i - (w_0 + w_1 x_i))^2.$$

- **Gradients**:

$$\frac{\partial \text{MSE}}{\partial w_1} = -\frac{2}{N}\sum_{i=1}^{N} x_i(y_i - (w_0 + w_1 x_i)),$$

$$\frac{\partial \text{MSE}}{\partial w_0} = -\frac{2}{N}\sum_{i=1}^{N}(y_i - (w_0 + w_1 x_i)).$$

- **Parameter Updates**:

$$w_1 \leftarrow w_1 - \eta\frac{\partial \text{MSE}}{\partial w_1},$$

$$w_0 \leftarrow w_0 - \eta\frac{\partial \text{MSE}}{\partial w_0}.$$

[1] See the R code gradient-descent-LM.R

Example 2: Gradient Descent for Polynomial Regression[2]

- **Polynomial Regression** is a form of regression analysis in which the relationship between the independent variable x and the dependent variable y is modeled as an Mth degree polynomial.

$$y = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M + \epsilon.$$

- **The loss function** for polynomial regression is similar to linear regression, typically using **Mean Squared Error (MSE)**.

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2, \quad \hat{y}_i = w_0 + w_1 x_i + w_2 x_i^2 + \ldots + w_M x_i^M.$$

- The update rule is similar but applied to all polynomial coefficients.

$$w_j := w_j - \alpha \frac{\partial}{\partial w_j} MSE,$$

$$\frac{\partial}{\partial w_j} MSE = -\frac{2}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)x_i^j, \qquad j = 0, \ldots, M.$$

[2]See the R code gradient-descent-polynomial.R

Implementing Gradient Descent in R for Linear Regression

- See the code gradient-descent-LM.R for fitting a linear regression using the gradient decent algorithm
- See the code gradient-descent-polynomial.R for fitting for fitting a non-linear regression using the gradient decent algorithm

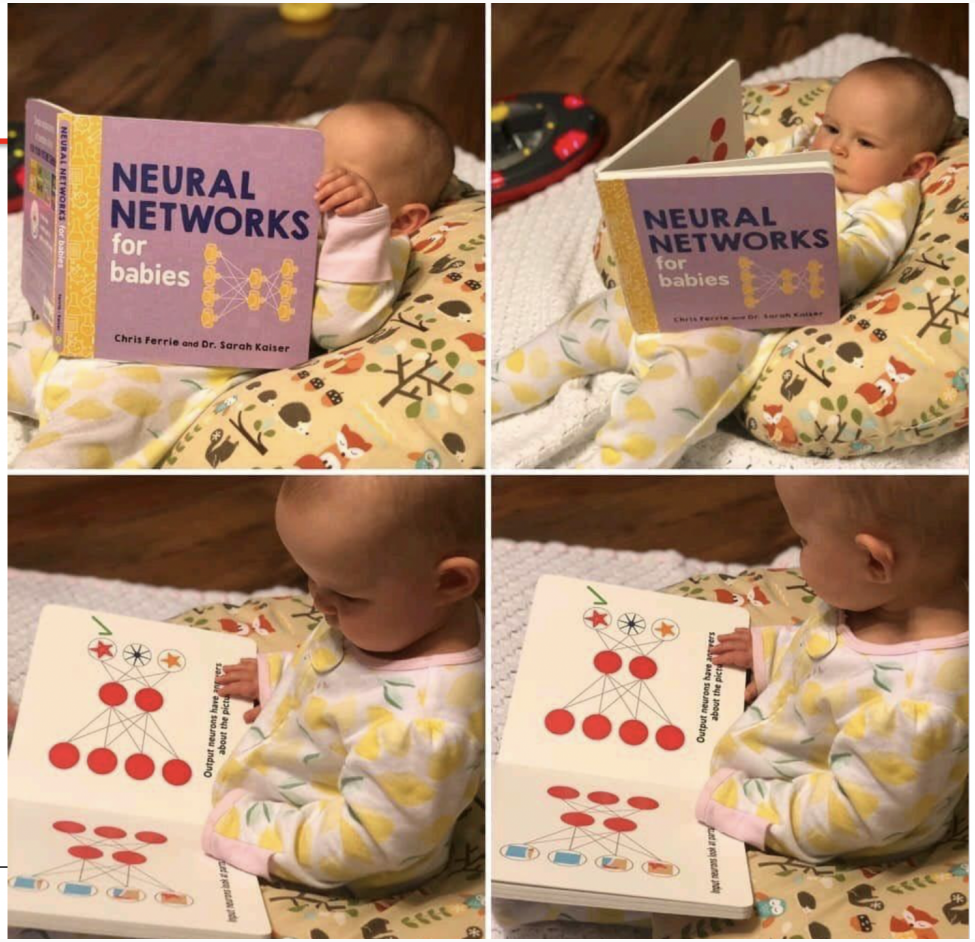
Exercise

- Try changing the learning rate parameter. What did you notice in the learning loss function?
- Try increasing the order of the polynomials to lets say of order 20. What did you notice? Do you still recover the parameters estimates? How the learning rates reacts?

Neural Networks

Everybody is learning

Never too late



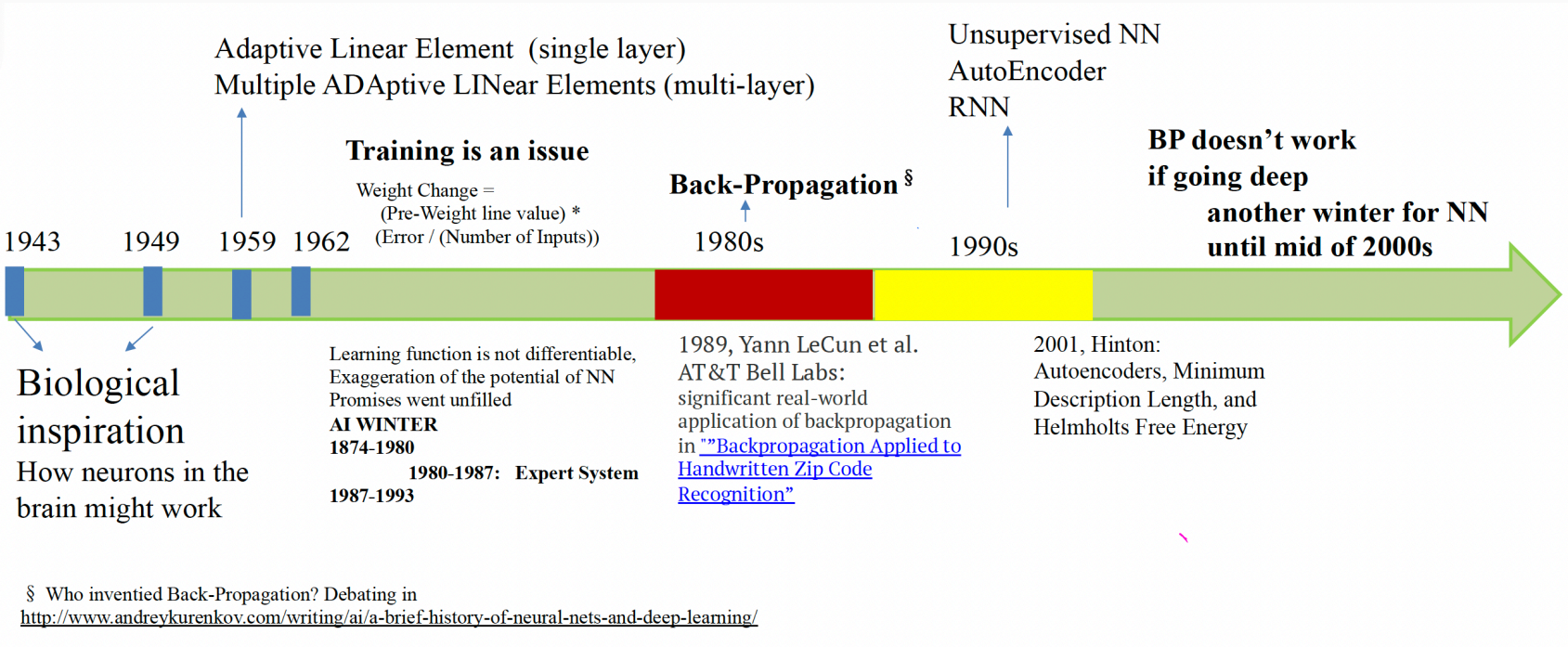
[3]

[3]CS 229: Prof. Xiangliang Zhang (KAUST)

What is a Neural Network?

- A **Neural Network** is a computational model inspired by the way biological neural networks in the human brain process information.
- It consists of **layers** of interconnected **nodes**, or **neurons**, which work together to solve complex problems.
- Similarly, brain activity occurs when a **stimulus** enters the system; information is processed through the network via neurons that extract relevant information, and this information is passed to another area.
- Neural networks can **learn** from data through **training**, making them powerful tools for **pattern recognition** and **predictive modeling**.

History of NNs



4

[4] CS 229: Prof. Xiangliang Zhang (KAUST)

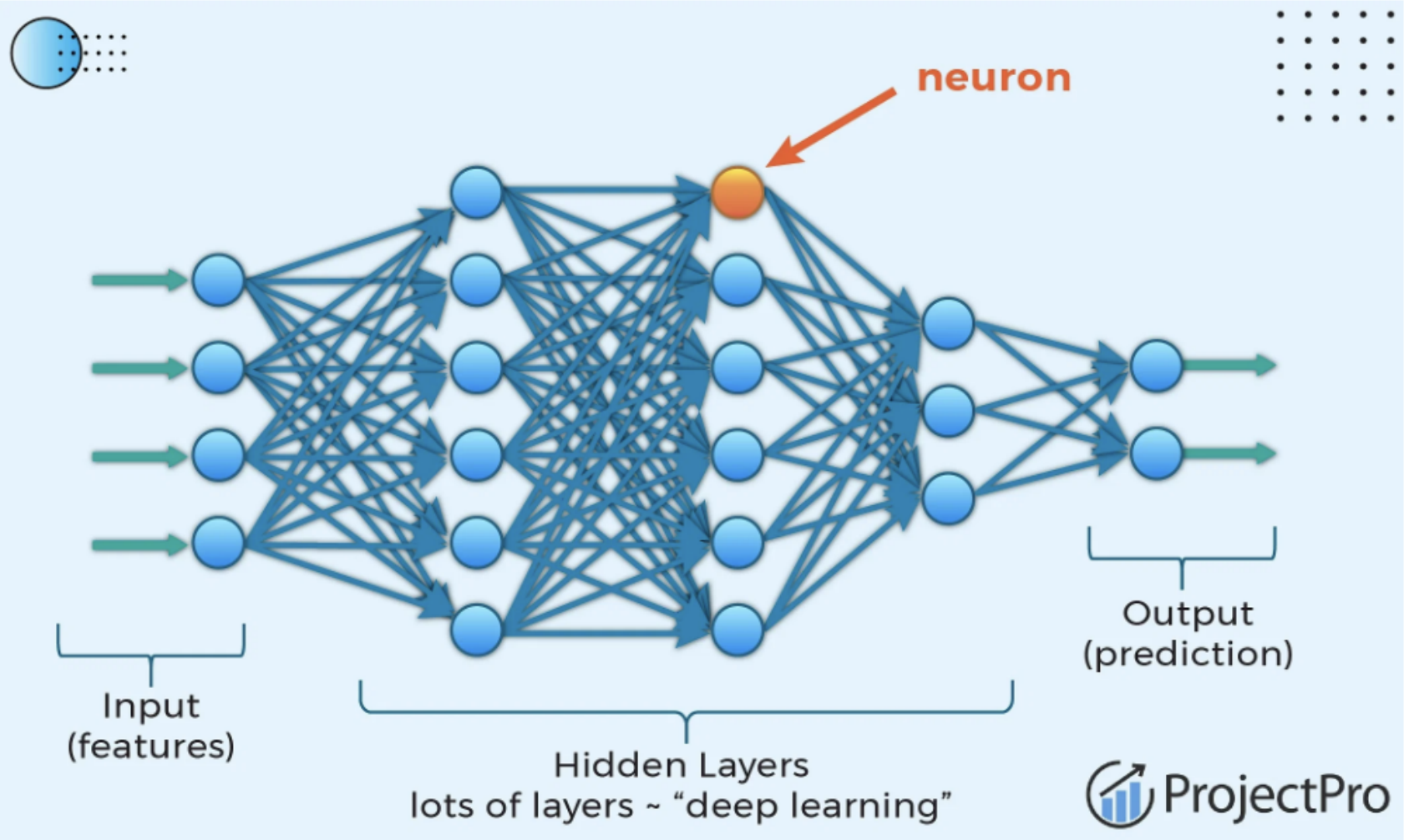
Components of Neural Networks

- Layers
- Neurons
- Weights
- Bias
- Activation Functions
- Forward Propagation
- Loss Function
- Backpropagation
- Learning Rate
- Training Data
- Validation and Test Data

A Basic Architectures of Neural Networks (1)

- A neural network consists of several key components:
- **Input Layer:** Each input represents a single predictor variable, which can be a scalar value, a sequence, an image, or even a sequence of images.
- **Output Layer:** For prediction or classification tasks, this layer typically has a single node. For Conditional Density Estimation (CDE), it contains multiple nodes.
- **Hidden Layers:** These layers, often more than one, perform calculations at each node. Each hidden layer's computations are parameterized by weights and biases.
- The calculations within a layer can vary in type, including standard, convolutional, and recurrent layers.
- The structure of a neural network, referred to as its **architecture**, defines the arrangement and connectivity of these layers.

A Basic Architectures of Neural Networks (2)



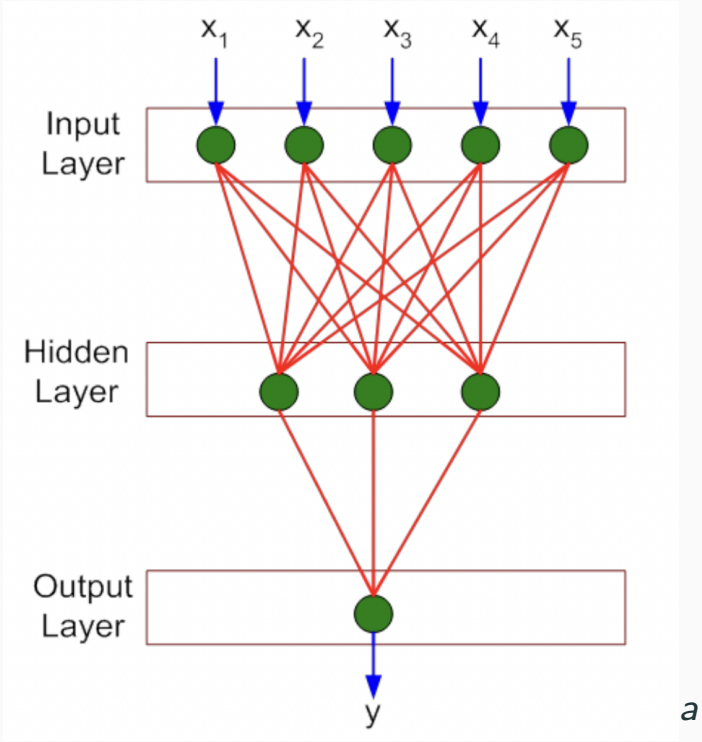
[5]

[5] ProjectPro

Layers

Neural computing requires a number of neurons, to be connected together into a neural network. Neurons are arranged in layers.

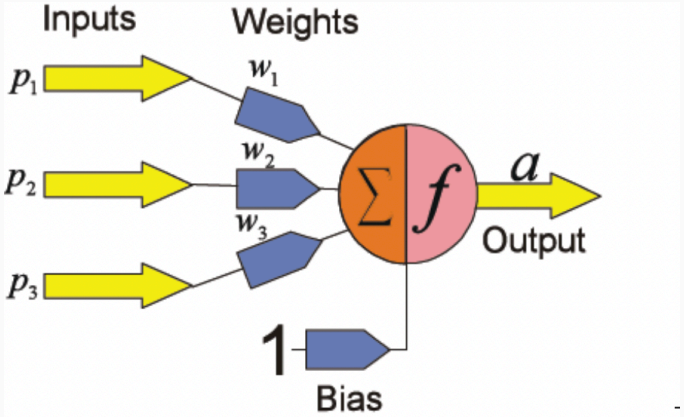
- **Input Layer**
  - First layer of neurons.
  - Receives raw data directly from the input features.
- **Hidden Layers**
  - Layers between the input and output layers.
  - Perform computations.
  - Can have one or many hidden layers.
- **Output Layer**
  - Final layer.
  - Produces the network's output.
  - Structure depends on the specific task (e.g., classification, regression).



[a] CS 229: Prof. Xiangliang Zhang (KAUST)

Neurons, Weights, and Biases

- **Neurons**:
  - Basic units of a neural network.
  - Receive input, process it, and pass it to other neurons.
  - Apply a mathematical function to generate an output.
- **Weights**:
  - Parameters that transform input data within the network.
  - Each connection between neurons has an associated weight.
- **Biases**:
  - Additional parameters in a neuron that allow to fit the data better.
  - Provide ability to each neuron have output not 0 when inputs are 0.



$$a = f(p_1 w_1 + p_2 w_2 + p_3 w_3 + b) = f\left(\sum p_i w_i + b\right)$$ [6]

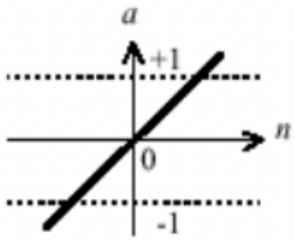
[6] CS 229: Prof. Xiangliang Zhang (KAUST)

Activation function

- The activation function defines the **output of the node**. There is two different functions that we can use, but it must satisfy bwlow two properties
  - **Nonlinear**: If all node has linear activation functions, this is just a linear regression model.
  - **Continuously differentiable:** Needed for gradient based optimization

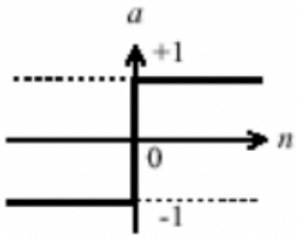
For example, we can think of this activation functions as link function in generalized linear model. In fact a single layered NN is simply a generalized linear model.

Some Examples of Activation Function



$a = purelin(n)$

Linear Transfer Function

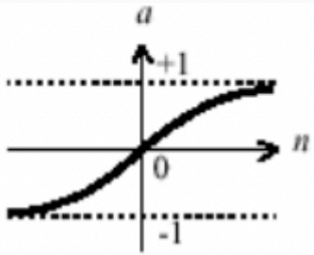


$a = hardlims(n)$

Symmetric Hard Limit Trans. Funct.

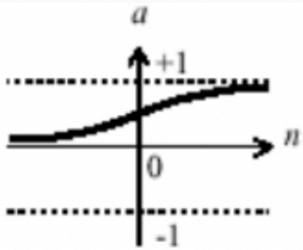
ReLU function

[7]



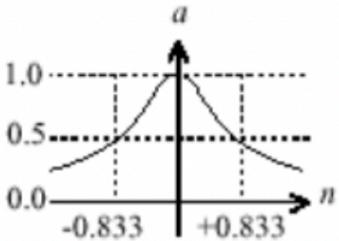
$a = tansig(n)$

Tan-Sigmoid Transfer Function



$a = logsig(n)$

Log-Sigmoid Transfer Function



$a = radbas(n)$

Radial Basis Function

[7] CS 229: Prof. Xiangliang Zhang (KAUST)

Rectified Linear Unit (ReLu) Activation Function

- Older neural networks relied on sigmoid or tanh activation functions that suffsred from vanishing gradient problems which restrict going to deep
- ReLu[8] somewhat solve this issue and turn out to be a huge help
- ReLu has the following forms

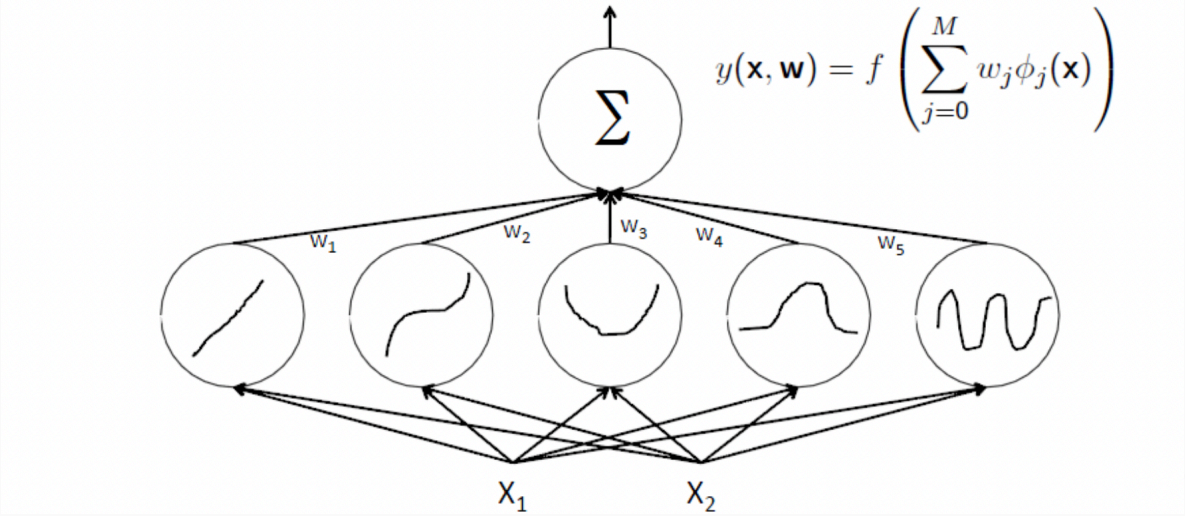
$$a(x) = \max\{0, x\}.$$

That means

- The neuron **activates** only when enough information passes through
- One drawbacks: Not differentiable at zero.

[8] https://machinelearningmastery.com/rectified-linear-activation-function-for-deep-learning-neural-networks/

Linear Regression as Neural Networks



$f(\cdot)$ [9]

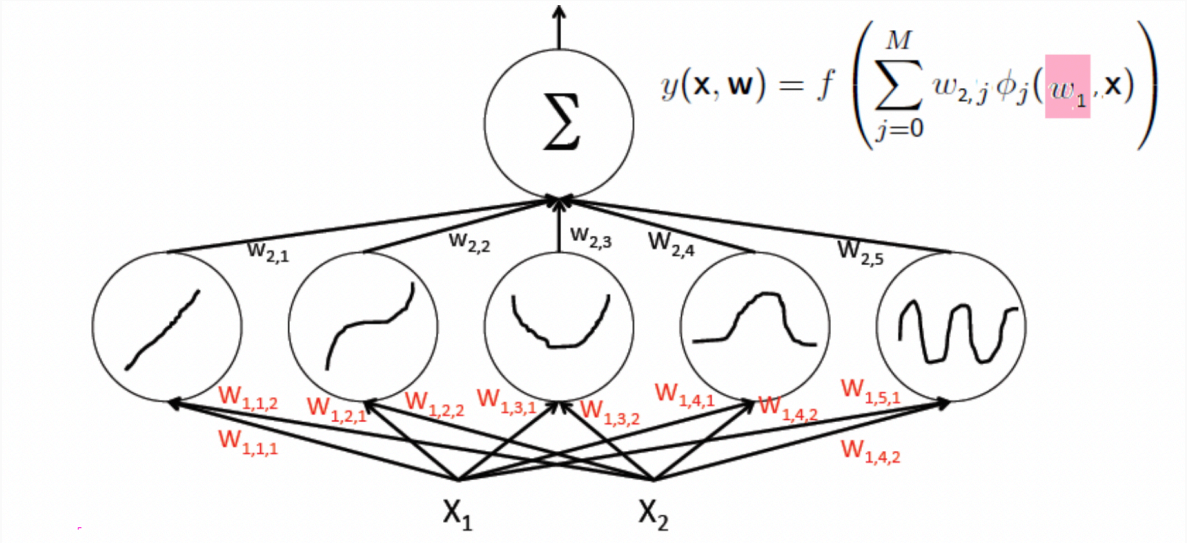
- The identity function in the case of regression.
- A nonlinear activation function in the case of classification.

Learning object:

- Learn w's so the function fits the data well.
- The basis functions are fixed functions of X.

[9] CS 229: Prof. Xiangliang Zhang (KAUST)

Non Linear Regression as Neural Networks

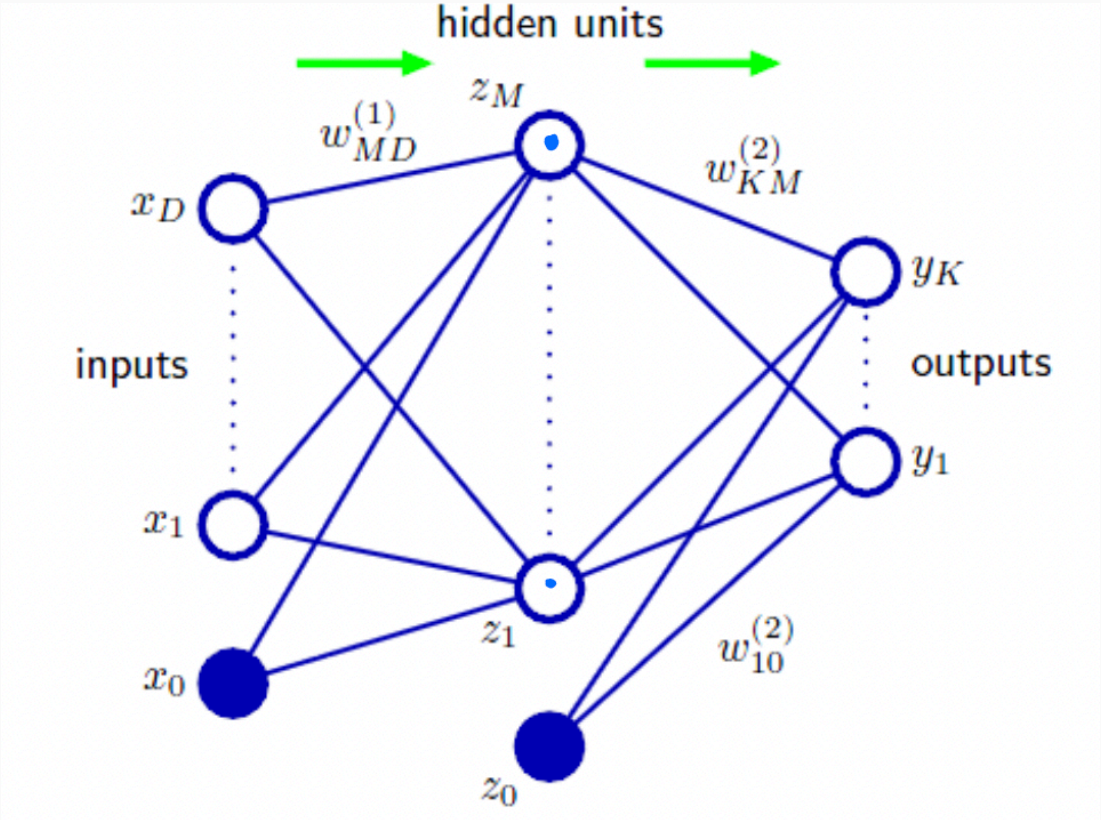


[10]

- Learning object: Learn w so the function fits the data well
- The basis functions are fixed functions of X and w_1

[10] CS 229: Prof. Xiangliang Zhang (KAUST)

A Two-Layer Neural Network (1)



- D input variables
- M hidden neurons
- K outputs
- Use the two activation function on weights sum on hidden layers and output layers

A Two-Layer Neural Network (2)

Construct M linear combinations of the inputs $x_1, \ldots, x_d$

$$a_j = \sum_{i=0}^{D} w_{ji}^{(1)} x_i, \qquad x_0 = 1.$$

- a_j are the activations, $j = 1, \ldots, M$.
- $w_{ji}^{(1)}$ are the layer one weights, $i = 1, \ldots, D$.
- $w_{j0}^{(1)}$ are the layer one biases.

Each linear combination a_j is transformed by a (non-linear differentiable) activation function

$$z_j = h(a_j).$$

A Two-Layer Neural Network (3)

The hidden output $z_j = h(a_j)$ are linearly combined in layer two:

$$a_k = \sum_{j=0}^{M} w_{kj}^{(2)} z_j, \qquad z_0 = 1.$$

- a_k are the output activations, $k = 1, \ldots, K$.
- $w_{kj}^{(2)}$ are the layer two weights, $j = 1, \ldots, M$.
- $w_{k0}^{(2)}$ are the layer one biases.

The output activations a_k are transformed by the output (non-linear differentiable) activation function

$$y_k = \sigma(a_k).$$

- y_k are the final outputs.
- $\sigma(\cdot)$ is like $h(\cdot)$, but often sigmoid function for classification and linear function for Regressions.

A Two-Layer Neural Network (4)

After substituting $y_k = \sigma(a_k)$ the definitions of a_j and a_k :

$$y_k(x, w) = \sigma\left(\sum_{i=0}^{M} w_{kj}^{(2)} h\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_i\right)\right).$$

Evaluation of this is called **forward propagation**.

- $h(\cdot)$ and $\sigma(\cdot)$ are a sigmoid functions, e.g., the logistics function.

$$s(a) = \frac{1}{1 + \exp(-a)}, \quad s(a) \in [0, 1].$$

- If $\sigma(a)$ is the identity, then a regression model is obtained.

Properties & Generalizations

- Typically, $K < D < M$. If $M < D$ or $M < K$, information may be lost at the hidden units.
- A multilayer network of linear units (where all $h(\cdot)$ are linear) is not interesting and can be simplified to a network without hidden units.
- There may be more than one layer of hidden units.
- Individual units need not be fully connected to the next layer.
- Individual links may skip over one or more subsequent layers.
- There may be symmetries in the weight space, meaning that different choices of w may define the same mapping from input to output.

Learning the Weights

- The learning rule modifies the weights according to the input patterns that it is presented with.
- In a sense, artificial neural networks (ANNs) learn by examples, similar to their biological counterparts.
- When the desired outputs are known, the process is referred to as supervised learning.
- Each weight will be changed proportional to the error gradient.

Error (Loss) Function

Training a neural network involves estimating the weights and biases by optimizing a loss function. Let N represent the number of observations of the response $t_1, t_2, \ldots, t_N$, and let the neural network predict some output $y(x_1, w), y(x_2, w), \ldots, y(x_N, w)$ (which could be a vector). We express the loss function or error here as $E(w)$.

- Regression: Sum of squared

$$E(w) = \frac{1}{2} \sum_{n=1}^{N} \{y(x_n, w) - t_n\}^2 ,$$

  where $t_n, n = 1, \ldots, N$ is the observed response. N is the total number of training samples (examples).
- Binary classification: NNs with only one output node whose activation function is a logistic sigmoid Cross-entropy error function

$$E(w) = -\frac{1}{2} \sum_{n=1}^{N} \{t_n \log y(x_n, w) + (1 - t_n) \log(1 - y(x_n, w))\} .$$

Training Process of a Neural Network

- The **loss function** is minimized using a form of **gradient descent**.
- Neural networks are trained for a finite number of **epochs** (iterations).
- Let w represent the set of all **trainable weights** and **parameters** for our neural network. For epoch i:
  1. We go **forward** through the network to compute $y(x_n, w)$ given the current state of the network. This allows us to evaluate $E(w)$.
  2. We move **back** through the network to compute $\nabla_w E(w)$ with respect to w.
  3. We update the parameters using

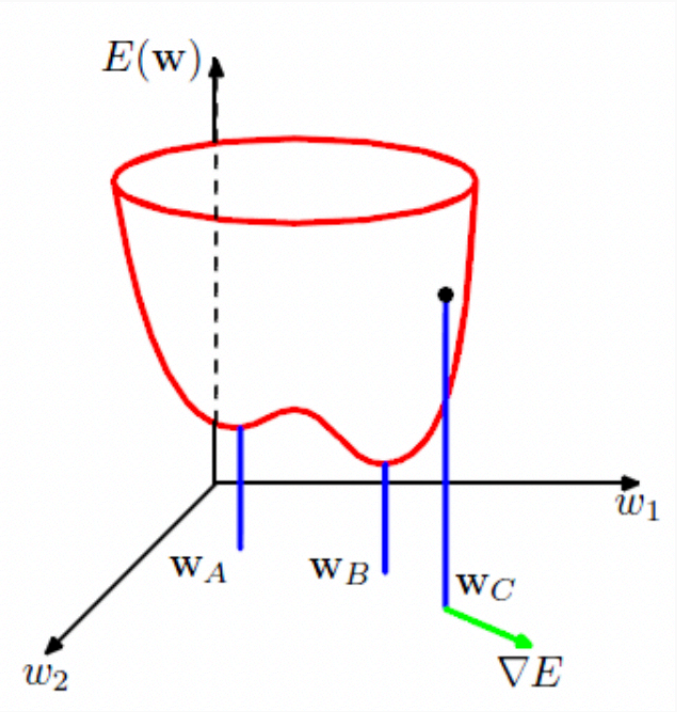
$$w^{(i+1)} = w^{(i)} - \eta^{(i)} \nabla_w E(w^{(i)}),$$

     where the product is taken componentwise and $\eta^{(i)}$ are the **learning rates** which is quite important. Large rates will cause the optimization to diverge; small rates may cause convergence to local minima.

Gradients of Error Function

- $y(x_n, w)$ is non-linear w.r.t w
- Error function $E(w)$ is non-convex
- Gradient of $E(w)$, $\nabla E(w)$
  - Direction of greatest rate of increase
  - Minima, $E(w) = 0$
  - No analytical solution
- Gradient descent: Moving through weight space in direction of $-\nabla E(w)$

$$w^{(i+1)} = w^{(i)} - \eta^{(i)} \nabla_w E(w^i).$$



Gradient Descent towards Global Minima

Learning by gradients decent algorithm: Require the evaluation of gradients wrt weight parameters.

How to Evaluate the Gradient: Backpropagation

Need an efficient techniques for evaluating the gradient $\nabla_w E$

Back Propogation Algorithm

Each iteration of the gradient decent algorithm has two stages:

- Evaluate derivatives of error w.r.t. weights
- Use derivatives to compute adjustments of the weights

Note: In statistical modelling, we often need to approximate the **partial derivatives** when optimizing particularly complicated functions. For **neural networks**, we compute $\nabla_w E(w)$ through a procedure called **backpropagation**. This involves moving **backwards** through the network and using the **chain rule** to calculate the partial derivatives at each layer. As we have constructed the neural network output as a function of **differentiable functions** with known derivatives, this process is very quick and efficient!

Backpropagatinon

- For output units

$$\delta_k = y(x_n, w) - t_k.$$

- For hidden units

$$\delta_j = \frac{\partial E}{\partial a_j} = \sum_k \frac{\partial E}{\partial a_k} \frac{\partial a_k}{\partial a_j} = h'(a_j) \sum_k w_{kj} \delta_k.$$

Summary

- Apply input x, and forward propagate to find the hidden and output activations.
- Evaluate δ_k directly for the outputs units
- Back propagate δ's to obtain a δ_j's for each hidden unit.
- Evaluate the derivatives $\frac{\partial E}{\partial a_j} = \delta_i Z_i$
- Sum these derivatives to over training cases to compute $\frac{\partial E}{\partial w_{ij}}$

Overfitting and Vanishing/Exploding Gradients Issues

- Vanishing gradient problems due to propagated error coming from the other neurons and layers
  - Use of smart activation functions solve this issue
- Overfitting due to a lot number of hidden units the number of hidden units determines the complexity of the learned function (the number of parameters $\boldsymbol{w}$)
  - We may allow regularizations
  - Drop of techniques
  - Sparse neural networks

Training/Validation/Testing

- Due to their large number of parameters, **neural networks** are prone to **overfitting**. It is necessary to use **validation/testing** to assess any overfitting.
- First, we subset the data into **training**, **validation**, and **testing** sets. The standard is 80/10/10.
- Each set has a different purpose:
  - The model is trained on the **training data**. This is used to optimize the **weights**, **biases**, and other **hyper-parameters**.
  - We then **validate** the model by getting predictions for the **validation set** and evaluating the **validation loss**. This provides insight into whether or not overfitting is occurring. Typically, the validation loss is used for **model selection**.
  - To get a truly **unbiased evaluation** of the model fit and to compare amongst different models, we should **test** the model on previously unseen data.
- Overfitting in neural networks is inevitable if a network is trained indefinitely. However, we can mitigate the risk of fitting using forms of **regularisation**.

Practical Rule of Thumb on Deciding Hidden Units

- There is no theoretical results that determines the minimum number of hidden units.
- Practical rule of thumb
  - For binary data $M = 2D$
  - For real data $M >> 2D$
- Multiple hidden layers with fewer nodes maybe trained faster for similar quality in some applications

Example: Classification Using two-Layer Neural Networks

- See the code NNs-for-classification-from-scratch.R for fitting a two layer Neural Networks from scratch for classification task
- See the code NNs-for-classification-using-neuralnet-package.R for fitting a two layer Neural Networks using the `neuralnet` R-package

Exercise

- Compare the two results that you got from the one coded from scratch and one using the `neuralnet` R-package
- Try changing the number of neurons (M) in hidden layers. How does this affect the accuracy in test and train data sets. Do you see some sort of overfitting as increasing M?
- Try changing the activation functions to linear which results in Linear regression. How accurate results you got?
- Try changing the learning rate parameter. What did you notice in the learning loss function?

Further Topics in Neural Networks

- Deep learning

Some Resources to Fit a Neural Networks and Deep Neural Networks in R

-