

Graph Neural Networks in Biology: Glossary

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OUTLINE

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Deep Learning

Neural Network

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Depth

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Optimizer

Backpropagation

OUTLINE

Graph Neural Networks

Graph

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Adjacency matrix

Attributes

Neighbours

Invariance

Equivariance

Graph neural network

DISCLAIMER

This glossary is intended to help you have an **overview** of deep learning and graph neural network concepts that will be needed for this seminar.

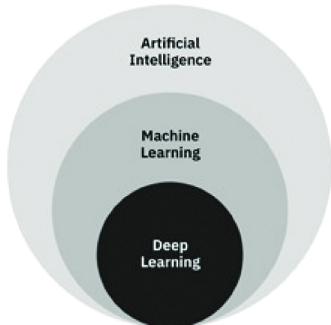
The provided definitions are not mathematically formal, but are purposefully **discursive** for the sake of those who are not very familiar with this field. Links attached in each slide contain additional resources and more formal contents.

Neural networks

DEEP LEARNING

Definition:

Deep learning is a subset of machine learning focusing on artificial neural networks. “Deep” refers to the many layers constituting neural networks

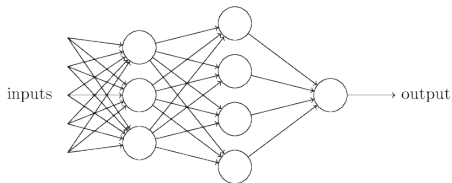


- ▶ <https://www.ibm.com/topics/deep-learning>
- ▶ <https://uk.mathworks.com/discovery/deep-learning.html>

NEURAL NETWORK

Definition:

A neural network is a nonlinear, parameterized function with restricted output range

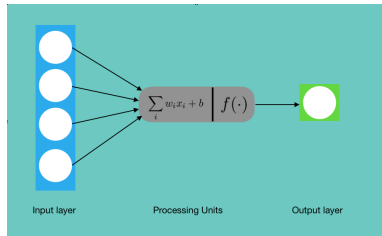


- ▶ https://diposit.ub.edu/dspace/bitstream/2445/180441/2/tfm_lichtner_bajjaoui_aisha.pdf (pages 5 and 6)

NEURONS

Definition:

A neuron is a composition of an activation function with a linear function; it is the basic processing unit of a neural network

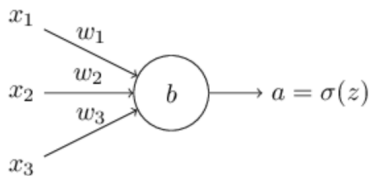


► https://en.wikipedia.org/wiki/Neural_circuit

WEIGHTS

Definition:

Weights are real numbers associated to each connection between neurons in a neural network and represent the strength of the connection or influence that a neuron has on another. Weights are the parameters that are adjusted during the training of neural network to improve its prediction performance



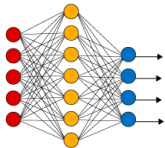
- ▶ <https://deepai.org/machine-learning-glossary-and-terms/weight-artificial-neural-network>

WIDTH

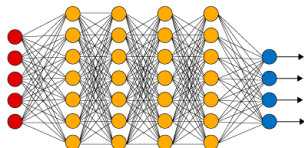
Definition:

The width is the number of neurons in a hidden layer of a neural network

Simple Neural Network



Deep Learning Neural Network



● Input Layer

● Hidden Layer

● Output Layer

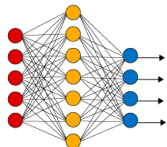
- ▶ https://proceedings.neurips.cc/paper_files/paper/2017/file/32cbf687880eb1674a07bf717761dd3a-Paper.pdf

DEPTH

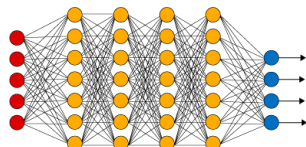
Definition:

The depth is the number of layers in a neural network

Simple Neural Network



Deep Learning Neural Network



● Input Layer

● Hidden Layer

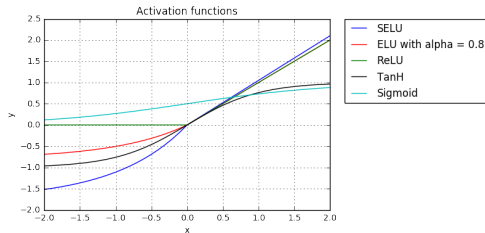
● Output Layer

- ▶ https://proceedings.neurips.cc/paper_files/paper/2017/file/32cbf687880eb1674a07bf717761dd3a-Paper.pdf

ACTIVATION FUNCTION

Definition:

Also called "nonlinearity", the activation function of a node in a neural network is a nonlinear function that calculates the output of the node based on its individual inputs and their weights

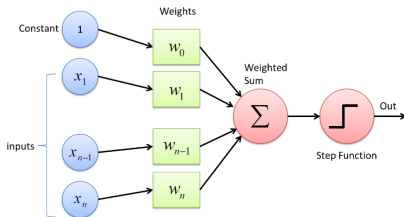


► https://en.wikipedia.org/wiki/Activation_function

PERCEPTRON

Definition:

A perceptron is an algorithm that performs linear binary classification. A perceptron can solve the AND gate problem but not the XOR gate problem



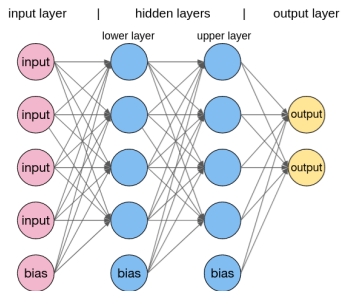
Source

- ▶ <https://brilliant.org/wiki/perceptron/>
- ▶ <https://sefiks.com/2020/01/04/a-step-by-step-perceptron-example/>

MULTI-LAYER PERCEPTRON

Definition:

A multi-layer perceptron can be constructed by combining multiple single-layer perceptrons and can thus perform nonlinear classification. A MLP can solve the XOR problem



- ▶ <https://towardsdatascience.com/perceptrons-logical-functions-and-the-xor-problem-37ca5025790a>
- ▶ <https://www.deeplearningbook.org/contents/mlp.html> (pages 167-172)

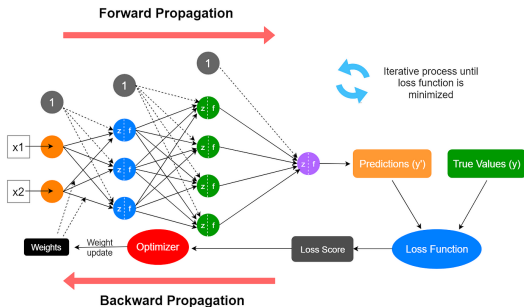
TRAINING A NEURAL NETWORK

Definition:

Training a neural network means to update the weights of the network so as to have better predictions.

Ingredients needed:

- Data
- Loss function
- Optimizer
- Backpropagation



- <https://medium.com/data-science-365/overview-of-a-neural-networks-learning-process-61690a502fa>

DATA

What type of data?

Data used for deep learning can be of many various types: images, sequences, graphs, etc.

- ▶ `https://uk.mathworks.com/discovery/deep-learning.html`

LOSS FUNCTION

Definition:

A loss function is a criterion according to which we can evaluate the quality of the predictions that a neural networks makes

- ▶ Mean squared error loss function

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n \left(Y_i - \hat{Y}_i \right)^2$$

- ▶ Cross-entropy loss function

$$H(p, q) = -E_p [\log q]$$

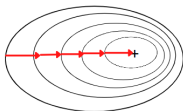
- ▶ https://en.wikipedia.org/wiki/Loss_function
- ▶ https://en.wikipedia.org/wiki/Mean_squared_error
- ▶ <https://en.wikipedia.org/wiki/Cross-entropy>

OPTIMIZER

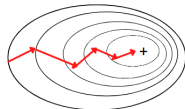
Definition:

An optimizer is a strategy to optimize the training of a neural network. The most frequently used one is called stochastic gradient descent

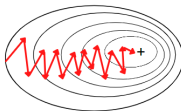
Batch Gradient Descent



Mini-Batch Gradient Descent



Stochastic Gradient Descent

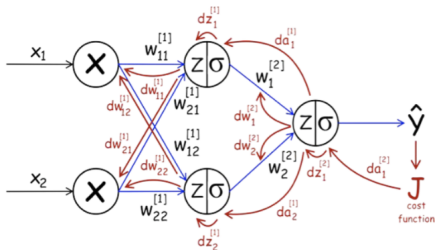


- ▶ https://en.wikipedia.org/wiki/Stochastic_gradient_descent

BACKPROPAGATION

Definition:

Backpropagation is the mechanism through which we can propagate backwards the error signal obtained during training by a deep neural network to update its weights and in turn improve predictions



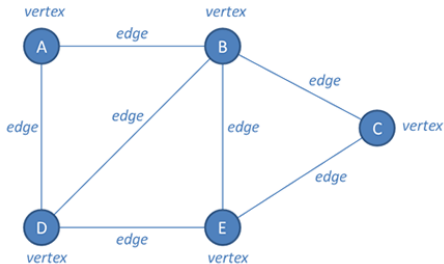
- ▶ <https://towardsdatascience.com/understanding-backpropagation-algorithm-7bb3aa2f95fd>
- ▶ <https://analyticsarora.com/8-unique-machine-learning-interview-questions-on-backpropagation/>

Graph neural networks

GRAPH

Definition:

A graph is a pair $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, where \mathcal{V} is a set of vertices and \mathcal{E} is a set of edges



- ▶ <https://distill.pub/2021/gnn-intro/>
- ▶ https://en.wikipedia.org/wiki/Glossary_of_graph_theory

NODES

Definition:

A node (also frequently called “vertex”) is an abstract representation of an entity in a graph

- ▶ [https://en.wikipedia.org/wiki/Vertex_\(graph_theory\)](https://en.wikipedia.org/wiki/Vertex_(graph_theory))

EDGES

Definition:

An edge is an abstract representation of a relationship between nodes in a graph. Edges can be undirected or directed

- ▶ https://en.wikipedia.org/wiki/Glossary_of_graph_theory#edge

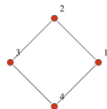
ADJACENCY MATRIX

Definition:

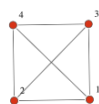
The adjacency matrix is the most convenient way of storing and representing a graph. It has as many rows and as many columns as the number of nodes in the graph. An entry of the matrix is 1 if there is an edge between the two nodes under consideration, otherwise it is 0



$$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$



$$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$



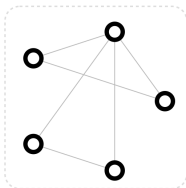
$$\begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

► <https://mathworld.wolfram.com/AdjacencyMatrix.html>

ATTRIBUTES

Definition:

Attributes are information that a node, edge or entire graph can carry



V Vertex (or node) attributes
e.g., node identity, number of neighbors

E Edge (or link) attributes and directions
e.g., edge identity, edge weight

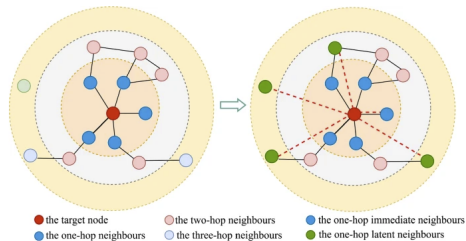
U Global (or master node) attributes
e.g., number of nodes, longest path

▶ <https://distill.pub/2021/gnn-intro/>

NEIGHBOURS

Definition:
Said of nodes,
neighbours indicate
adjacent vertices

Fig. 1

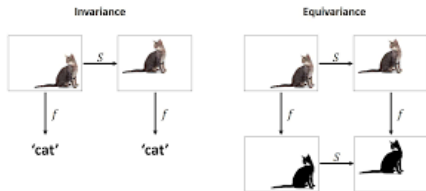


► <https://link.springer.com/article/10.1007/s10115-023-01963-x>

(PERMUTATION) INVARIANCE

Definition:

Permutation invariance is the concept indicating that the permutation of the nodes of the input graph does not affect the output

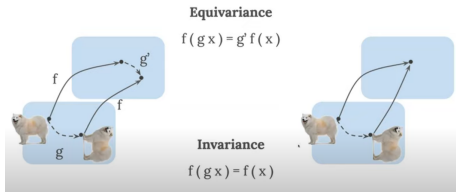


- ▶ https://proceedings.neurips.cc/paper_files/paper/2019/file/ea9268cb43f55d1d12380fb6ea5bf572-Paper.pdf
- ▶ <https://www.doc.ic.ac.uk/~bkainz/teaching/DL/notes/equivariance.pdf>

(PERMUTATION) EQUIVARIANCE

Definition:

Permutation equivariance is the concept indicating that the permutation of the input permutes in turn the output

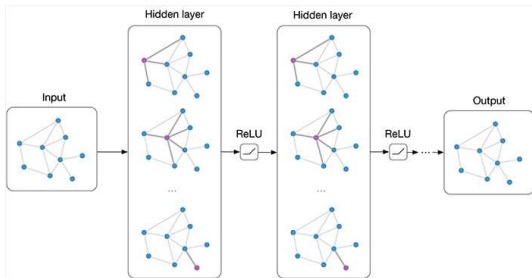


- ▶ https://proceedings.neurips.cc/paper_files/paper/2019/file/ea9268cb43f55d1d12380fb6ea5bf572-Paper.pdf
- ▶ <https://datascience.stackexchange.com/questions/16060/what-is-the-difference-between-equivariant-to-translation-and-invariant-to-tr>

GRAPH NEURAL NETWORK

Definition:

A graph neural network (GNN) is a particular type of neural network that can handle graph structured objects by design



- ▶ <https://distill.pub/2021/gnn-intro/>
- ▶ https://theaisummer.com/Graph_Neural_Networks/

Happy learning!