Graph Neural Networks in Big Data Analytics: Introduction

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Bielefeld University
October 20, 2022

Who are we?

- Research group “Genome Data Science”
  `https://gds.techfak.uni-bielefeld.de`
- Coordinates:
  Prof. Dr. Alexander Schönhuth
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Organization

Modules

- Lecture part of modules
  - *31-M-ASM2 Advanced Statistical Methods II* (graded, "benotete Prüfungsleistung")
  - *39-Inf-AB Algorithmen der Bioinformatik* (ungraded, "Studienleistung")
  - *39-Inf-SAB_a Spezielle Algorithmen der Bioinformatik* (ungraded, "Studienleistung")
  - *39-M-Inf-ABDA Advanced Big Data Analytics* (ungraded)
    - See here `https://ekvv.uni-bielefeld.de/sinfo/publ/modul/308598306`

Presentation, Papers

- Presentations:
  - Presentations individually, or in groups of 2
  - Individual presentation to last for approx. 30 minutes, followed by discussion
- Papers:
  - Papers for presentations: some already available, list will be completed
  - Papers available via Wiki:
    `https://gds.techfak.uni-bielefeld.de/teaching/2022winter/graphnet`

Schedule

- Organization and introduction: *today*
- How to present (brief): *Oct 27*
- How to write (brief): *shortly before first presentation*
- Introductory tutorial: *today, Oct 27, Nov 3, Nov 10* (yet TBD in detail, will be announced)

Schedule

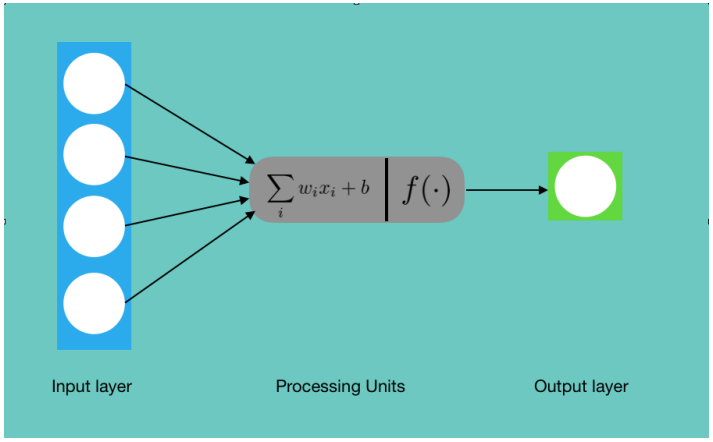
- **Presentations:** *from December 1 (earlier possible if desired)*
  - Up to two presentations per week, if that suits everyone's schedules
  - If desired/necessary, block seminar day possible as well
- **Technical Report:** *after presentation:*
  - Each report 8-15 pages
  - Optimally, report profits from feedback provided after presentation
  - Drafts can be submitted for discussion
  - Improving drafts based on feedback
  - *Submission deadline: February 28*

Graph Neural Networks: Motivation

Neural Networks

Neurons

Linear + Activation Function



$$\text{output} = a(w^T \cdot x + b)$$

Note: replace f in Figure by a!

Neuron: linear function followed by activation function

Examples

- Linear regression:

$$a = \text{Id}$$

a is identity function

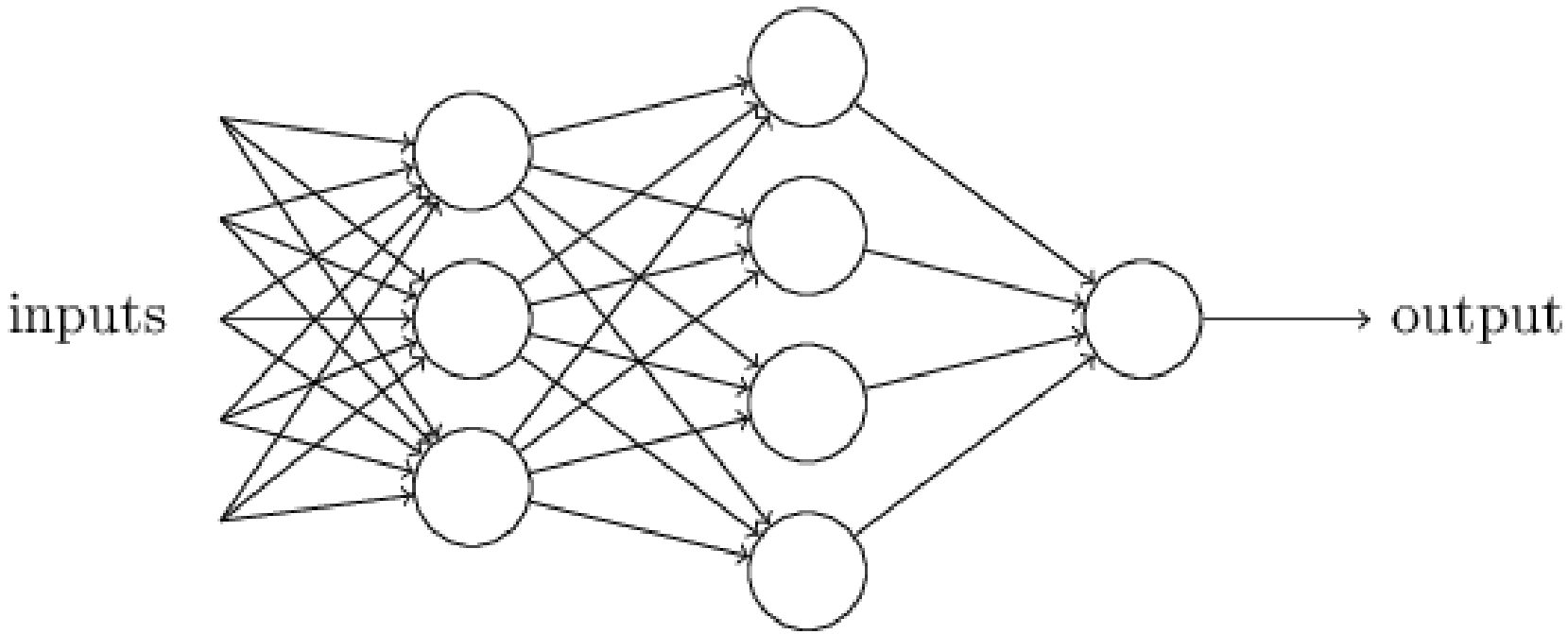
- Perceptron:

$$a(x) = \begin{cases} 1 & x \geq 0 \\ 0 & x < 0 \end{cases}$$

a is step function

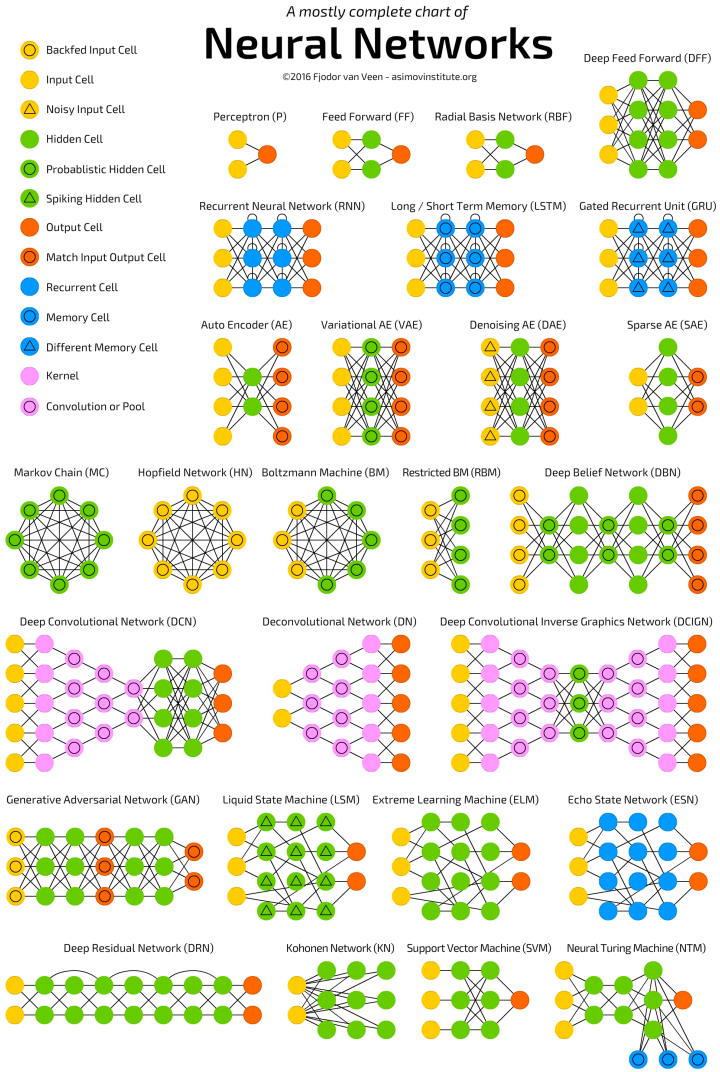
Neural Networks

Concatenating Neurons

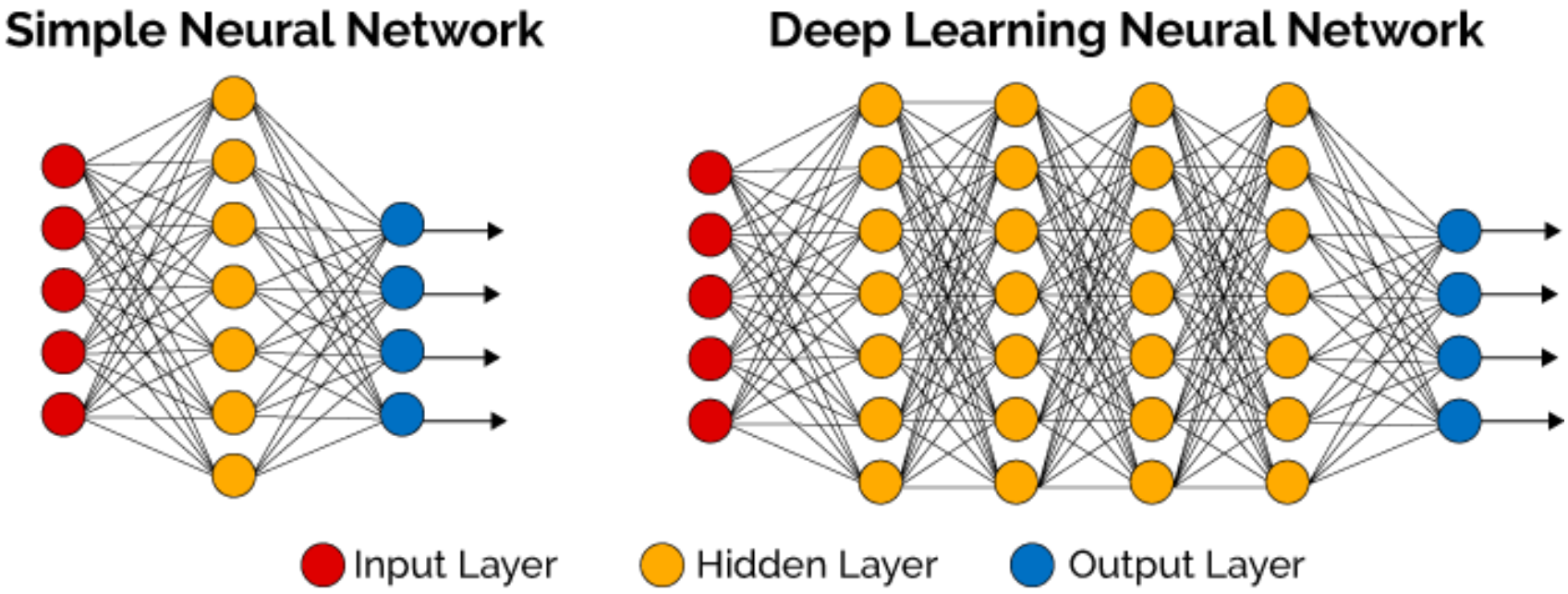


Neural Networks

Architectures



Deep Neural Networks



Width = Number of nodes in a hidden layer
Depth = Number of hidden layers
Deep = depth ≥ 8 (for historical reasons)

Neural Networks

Formal Definition

- Let $\mathbf{x}^l \in \mathbb{R}^{d(l)}$ be all outputs from neurons in layer l, where $d(l)$ is the *width* of layer l.
- Let $y \in V$ be the output.
- Let $\mathbf{x} =: \mathbf{x}^0$ be the input.
- Then

$$\mathbf{x}^l = \mathbf{a}^l(\mathbf{W}^{(l)}\mathbf{x}^{l-1} + \mathbf{b}^l)$$

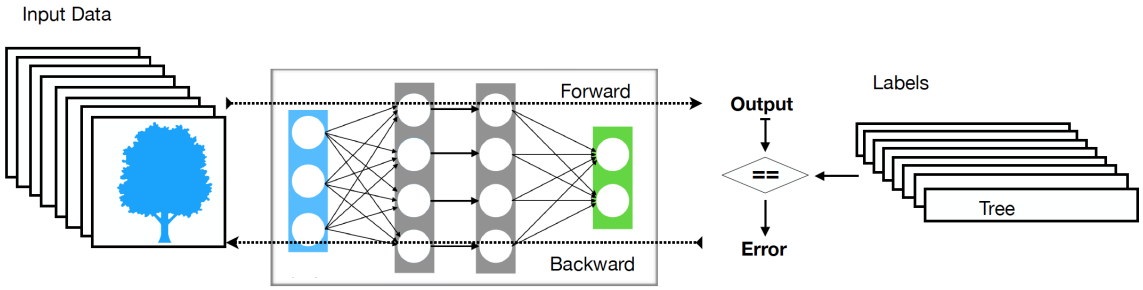
  where $\mathbf{a}^l(.) = (a_1^l(.), ..., a_{d(l)}^l(.))$, $\mathbf{W}^{(l)} \in \mathbb{R}^{d(l)\times d(l-1)}$, $\mathbf{b}^l \in \mathbb{R}^{d(l)}$

- The function f representing a neural network with L layers (with depth L) can be written

$$y = f(\mathbf{x}^0) = f^{(L)}(f^{(L-1)}(...(f^{(1)}(\mathbf{x}^{(0)}))...))$$

  where $\mathbf{x}^l = f^{(l)}(\mathbf{x}^{l-1}) = \mathbf{a}^{\mathbf{l}}(\mathbf{W}^{(\mathbf{l})}\mathbf{x}^{l-1} + \mathbf{b}^{\mathbf{l}})$

Training: Backpropagation



- *E.g.* let X be a set of images, labels 1 and 0: tree or not
- Let

$$f_{(\mathbf{w},\mathbf{b})} : X \to \{0,1\} \quad \text{and} \quad \hat{f} : X \to \{0,1\}$$

  network function ($f_{\mathbf{w},\mathbf{b}}$) and true function ($\hat{f}$)
- $L(f_{(\mathbf{w},\mathbf{b})}, \hat{f})$ loss function, differentiable in network parameters $\mathbf{w}, \mathbf{b}$
- *Back Propagation*: Minimize $L(f, \hat{f})$ through gradient descent
  - ☞ Heavily parallelizable!
- Decisive: Ratio number of parameters and training data

Why Neural Networks?

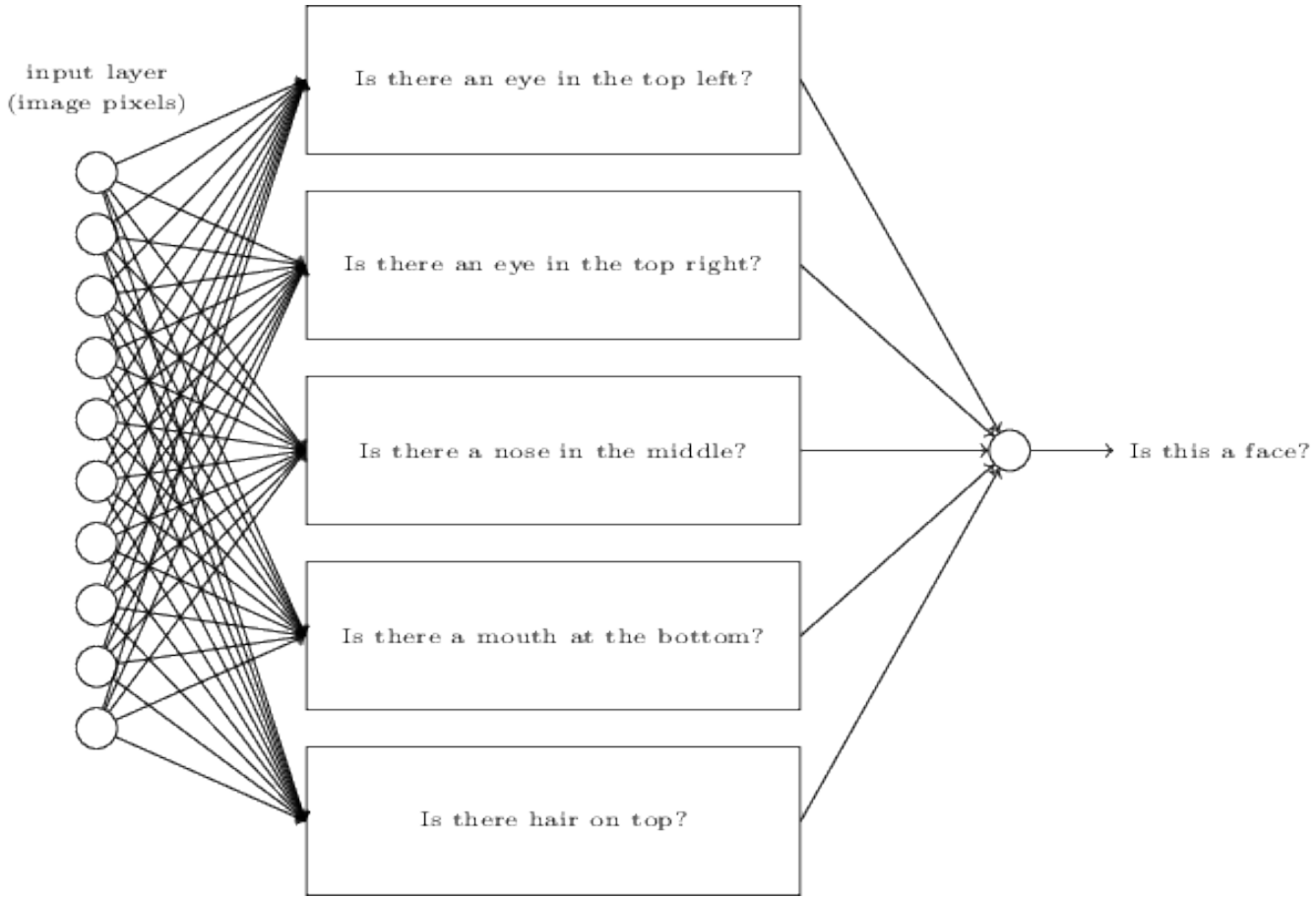
Why Neural Networks?

Given an (unknown) functional relationship $f : \mathbb{R}^d \to V$, why should we learn f by approximating it with a neural network?

Practical, Intuitive Consideration

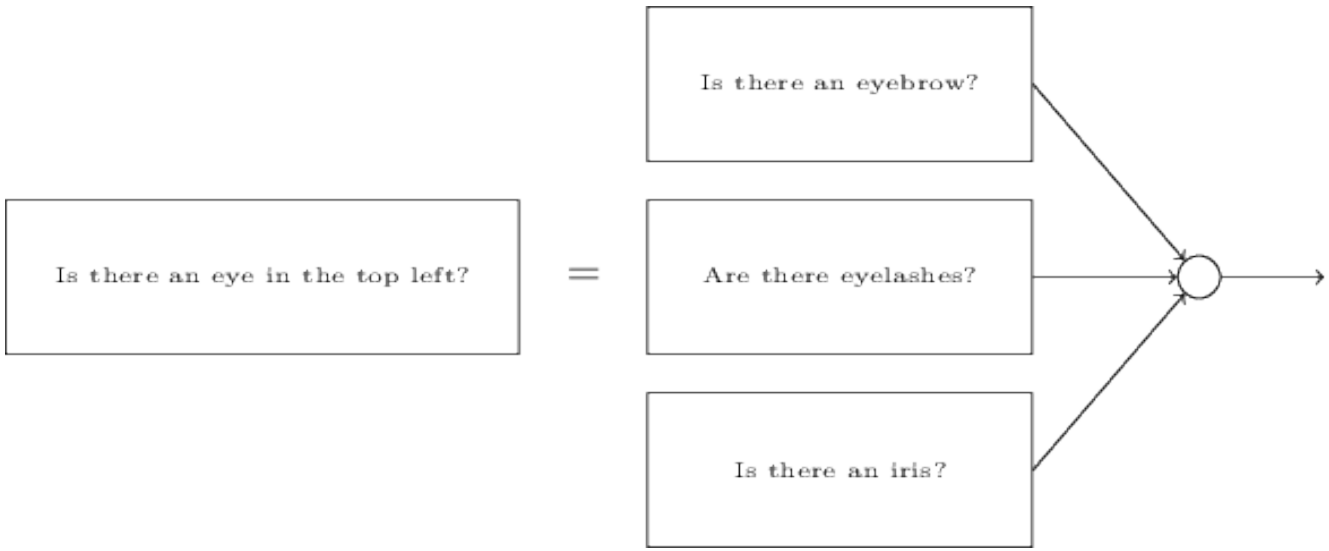
Deep Learning

Intuitive Explanation



- *Face recognition*: decompose classification task into subtasks

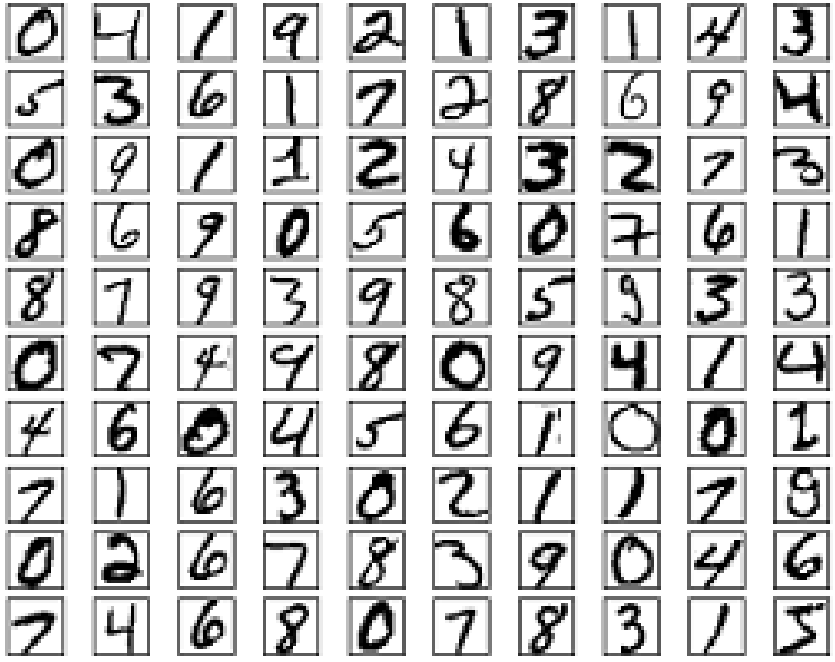
Deep Learning is Intuitive



- *Face recognition*: decompose subtask (eye recognition) into sub-subtasks
- Subtasks are composed into overall task "layer by layer"

Running Example: MNIST Classification

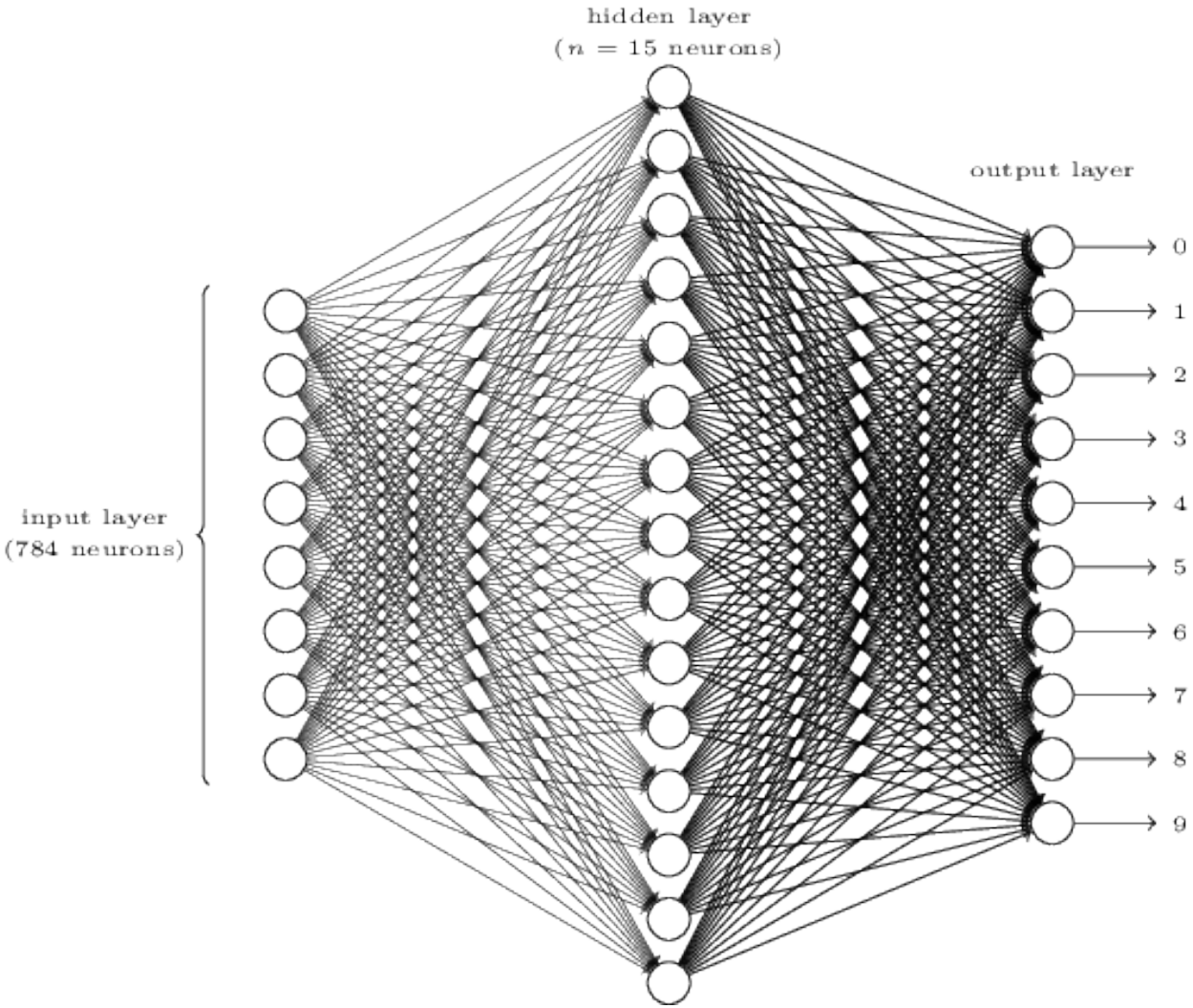
Data, Function



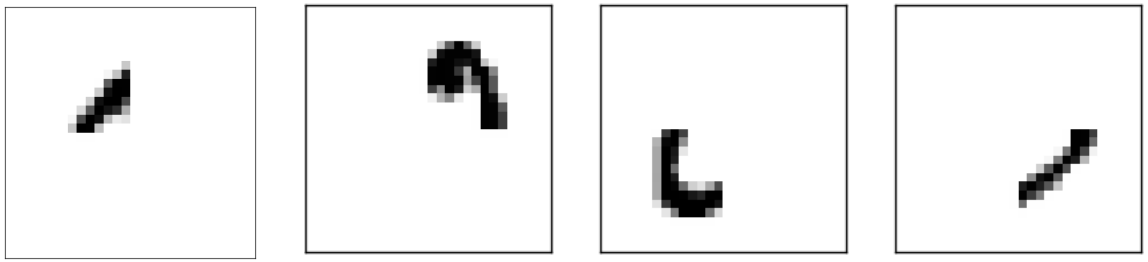
$$f : \mathbb{R}^{28\times 28=784} \longrightarrow \{0, 1, ..., 9\} \tag{1}$$

Running Example

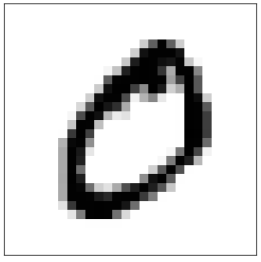
Model Class: NN with 1 hidden layer



Running Example



together makes



Neurons of hidden layer recognize characterizing parts of digit

Theoretical Consideration

The Universal Approximation Theorem

Theorem

A feedforward network with a single hidden layer containing a finite number of neurons can approximate any nonconstant, bounded and continuous function with arbitrary closeness, as long as there are enough hidden nodes.

Step function with n steps as neural network

- requires n hidden nodes
- hence $O(n)$ training data

Why Deep Learning?

The Universal Approximation Theorem

Theorem
A feedforward network with a single hidden layer containing a finite number of neurons can approximate any nonconstant, bounded and continuous function with arbitrary closeness, as long as there are enough hidden nodes.

Example: Step function with n steps as neural network

- requires n hidden nodes
- hence $O(n)$ training data

Rule of Thumb

One needs approximately

as many training data
as there are parameters

in the class of models

More Layers

Motivation

- We have 2 parameters per hidden neuron, amounting to requiring approximately $2n$ data points
- Can we save on neurons/parameters, while increasing number of steps, by increasing depth?

  Example: Symmetric step function with $2n$ steps modeled by NN with 2 hidden layers one with n and one with 2 neurons

Why Deep Learning

- We need only $O(n+1)$ (and not $O(2n)$) many parameters to model a constellation with $2n$ steps and one symmetry axis
- Hence, we only need $O(n+1)$ many training data, and not $O(2n)$ (like SVM's or Nearest Neighbor)
- In general $O(n^l)$ (symmetric) steps need only $O(nl)$ training data
- This illustrates why deeper NN's can deal with symmetry invariance in images

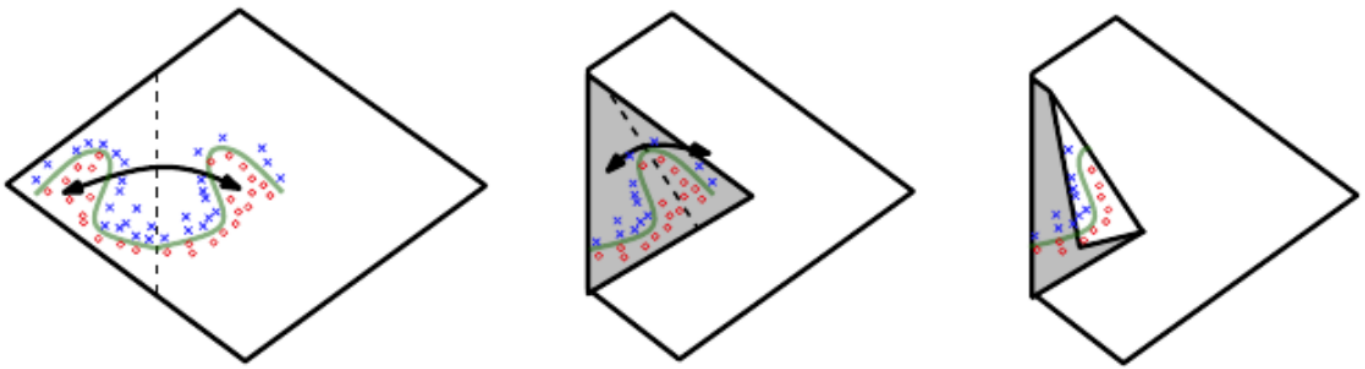
Why Deep Learning

Theorem (Universal Approximation; Montufar (2014))

Let f be an NN with d inputs, l hidden layers (depth l) of width n each. Then the number of differently labeled regions is

$$O\left(\binom{n}{d}^{d(l-1)} n^d\right) \tag{2}$$

That is, the number of regions that can receive different labels is exponential in the depth (the number of hidden layers) l.



[Montufar 2014]: Every neuron can fold space along an axis

Deep Learning

Assumptions

- Model classes make certain assumptions about properties of the functions they aim to approximate
- Many model classes (such as Nearest Neighbors and SVM's) require *local consistency* and *smoothness*: nearby points are likely to receive the same label
- Deep neural networks make further assumptions such as invariance to shifts, rotations and mirroring

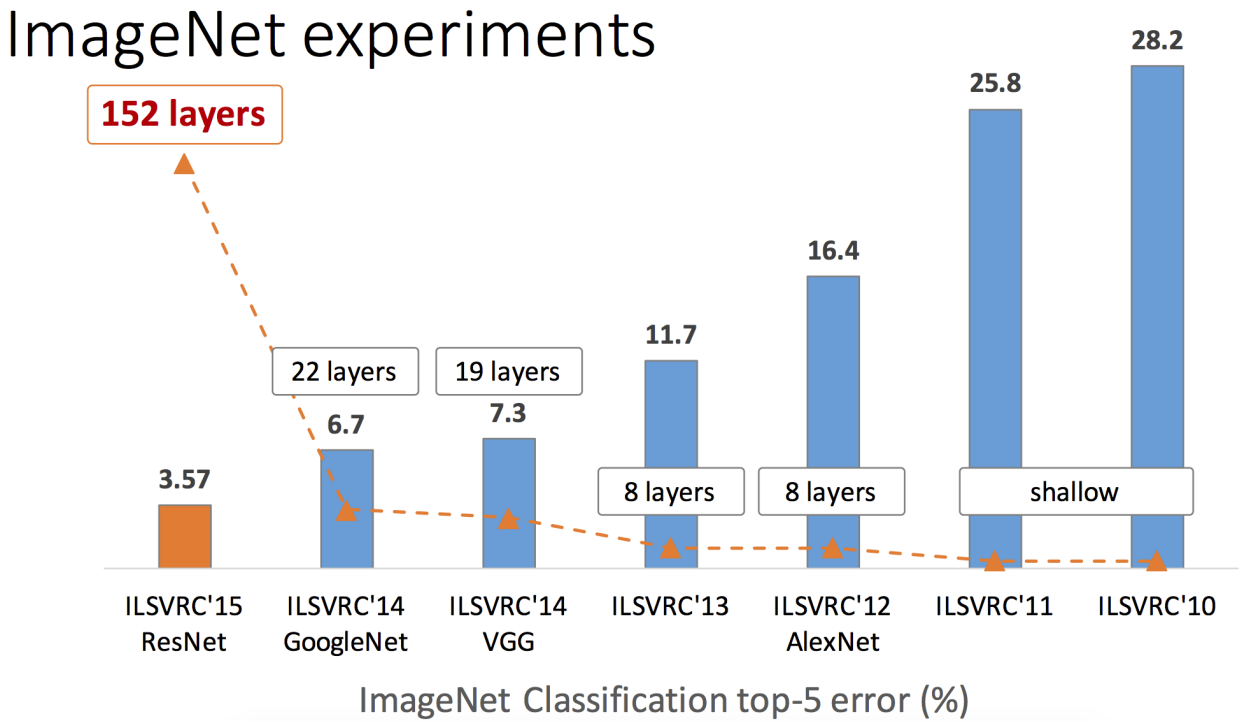
ImageNet and ILSVRC

Dataset and First Results

ImageNet examples: “beading plane”, “brown root rot fungus”, “scalded milk”, “common roundworm”

- *ImageNet dataset*: 16 million full color images; 20 000 categories
- *Starting point*: Le, Ranzato, Monga, Devin, Chen, Corrado, Dean & Ng: “Building high-level features using large scale unsupervised learning”, 2012, `https://ai.google/research/pubs/pub38115` achieved 15.3 % test accuracy
- *ILSVRC*: Image-Net Large-Scale Visual Recognition Challenge
  - *2012*: 1000 categories; Training 1.2 million images; Validation 50 000 images; Test 150 000 images

Going Deeper

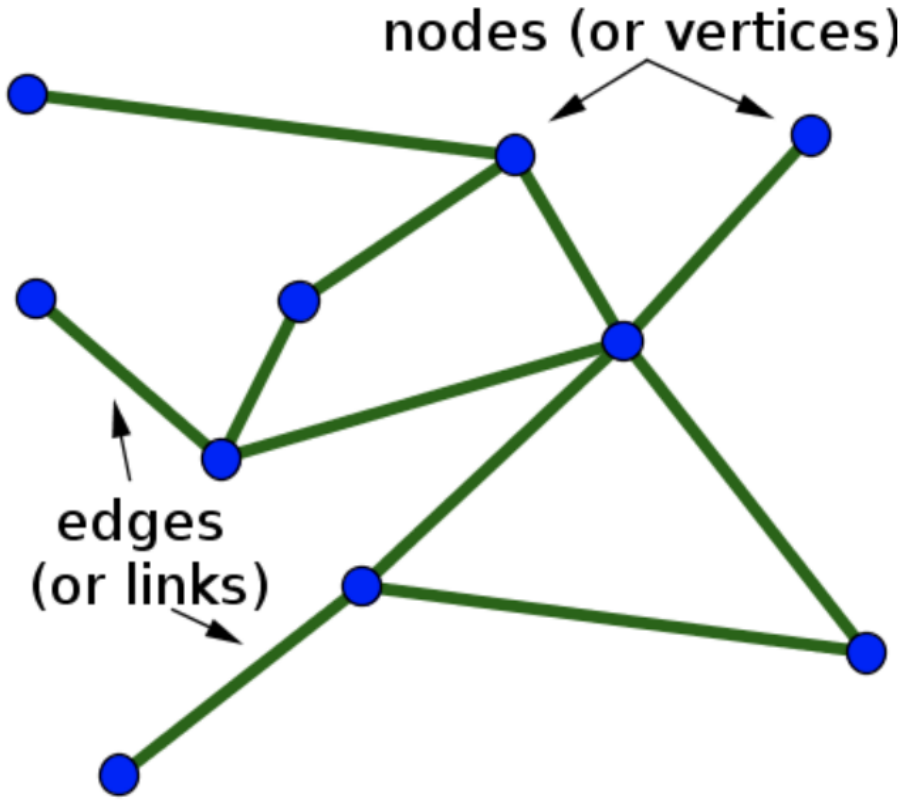


https://icml.cc/2016/tutorials/icml2016_tutorial_deep_residual_networks_kaiminghe.pdf; Note: correct error rate for AlexNet is 15.4%

Graph Neural Networks: Introduction

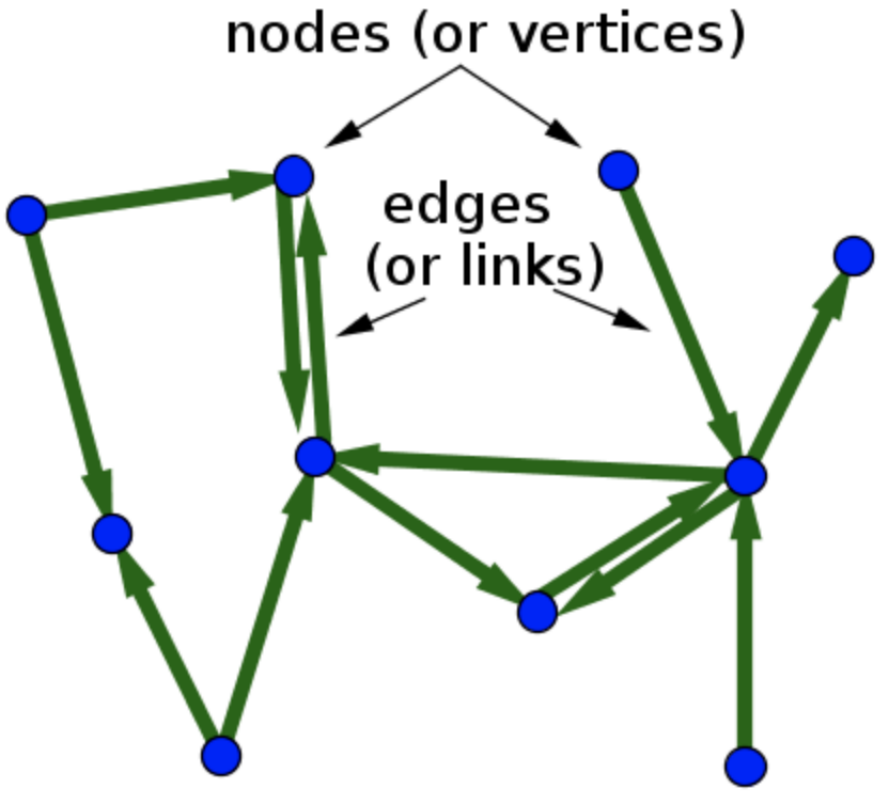
Graphs

Graphs: Introduction



From `https://mathinsight.org/network_introduction`

Directed Graph



From `https://mathinsight.org/network_introduction`

Graphs, Adjacency Matrix: Definition

Definition [Graph]:
A graph $G = (V, E)$ has vertices V and edges $E \subset V \times V$. If G is *directed*, the order $(i, j) := (v_i, v_j) \in E$ matters (and edges are often referred to as *arcs*). If G is undirected, (i, j) can be considered unordered, so $(i, j) = (j, i)$.

Definition [Adjacency Matrix]:
Let $G = (V, E)$ be a graph with vertices V and (directed) edges E. The *adjacency matrix* $A = (a_{ij})_{1 \leq i,j \leq |V|}$ is defined by

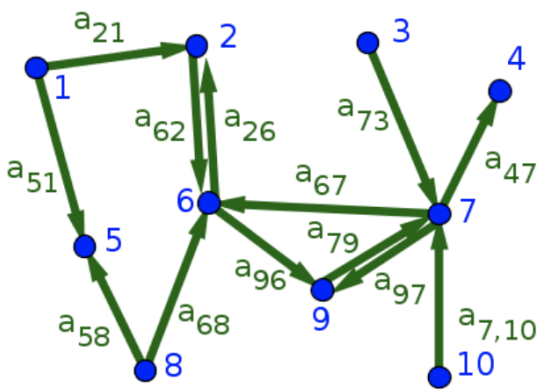
$$a_{ij} = \begin{cases} 1 & \text{if } (i, j) \in E \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

Remark: If G is undirected, $a_{ij} = 1$ implies $a_{ji} = 1$. Hence A is symmetric.

Adjacency Matrix: Example

Definition [Adjacency Matrix]:
Let $G = (V, E)$ be a graph with vertices V and (directed) edges E. The *adjacency matrix* $A = (a_{ij})_{1 \le i,j \le |V|}$ is defined by

$$a_{ij} = \begin{cases} 1 & \text{if } (i,j) \in E \\ 0 & \text{otherwise} \end{cases} \tag{4}$$



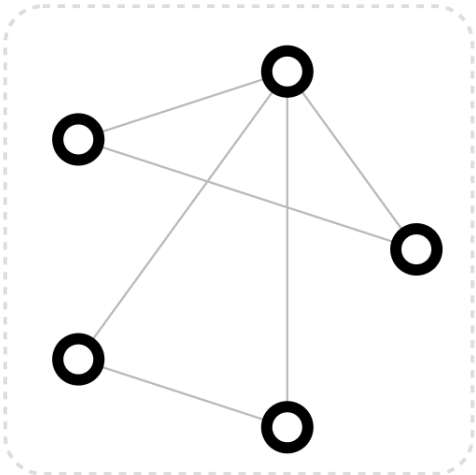
$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

From `https://mathinsight.org/network_introduction`

Graphs: Storing Information

Graphs: Storing Information I

Graphs can store information in various ways



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

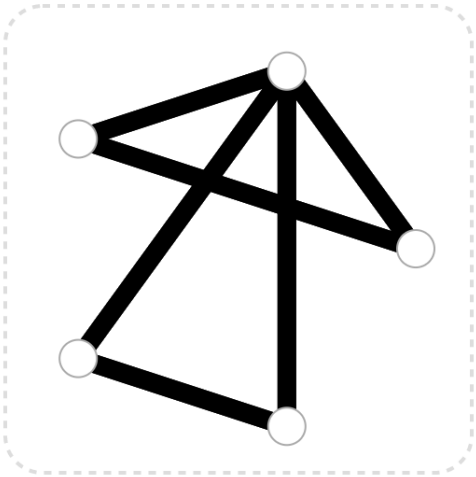
U Global (or master node) attributes
e.g., number of nodes, longest path

Vertex attributes

From `https://distill.pub/2021/gnn-intro/`

Graphs: Storing Information II

Graphs can store information in various ways



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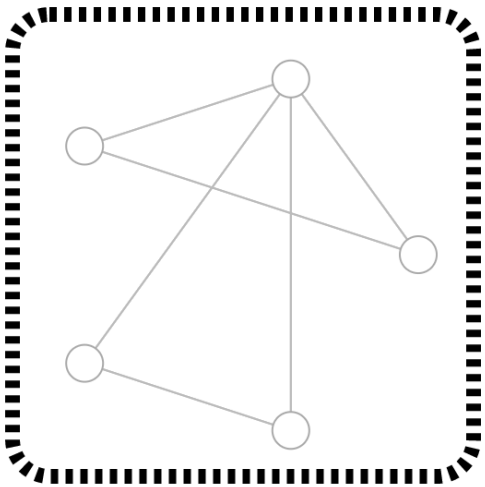
Edge attributes

From `https://distill.pub/2021/gnn-intro/`

Graphs: StoringInformation III

Graphs can store information in various ways



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e.g., node identity, number of neighbors

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

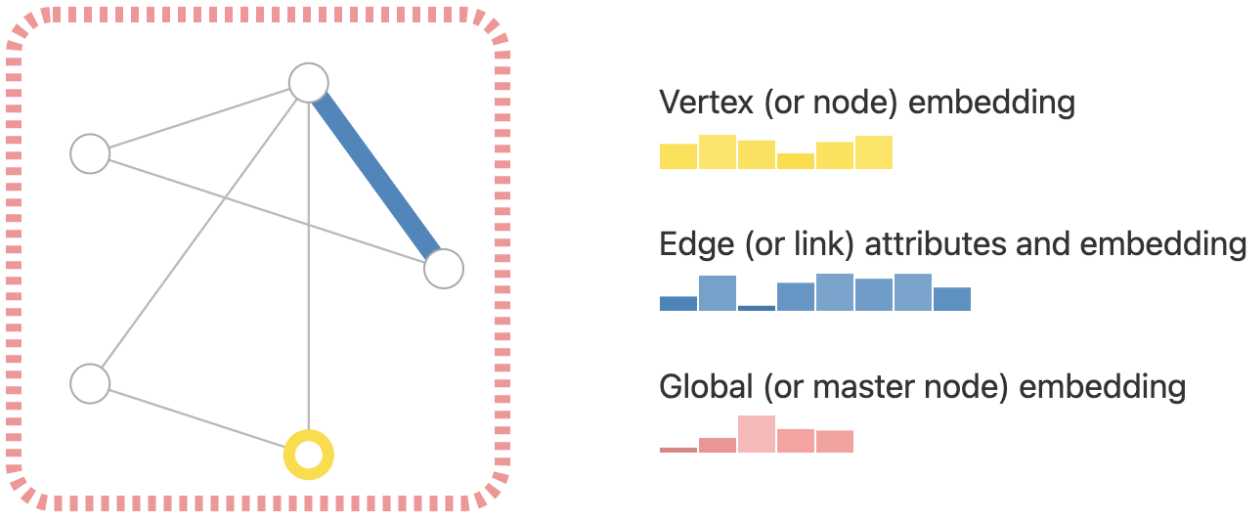
U Global (or master node) attributes
e.g., number of nodes, longest path

Global attributes

From `https://distill.pub/2021/gnn-intro/`

Graphs: StoringInformation IV

Graphs can store information in various ways

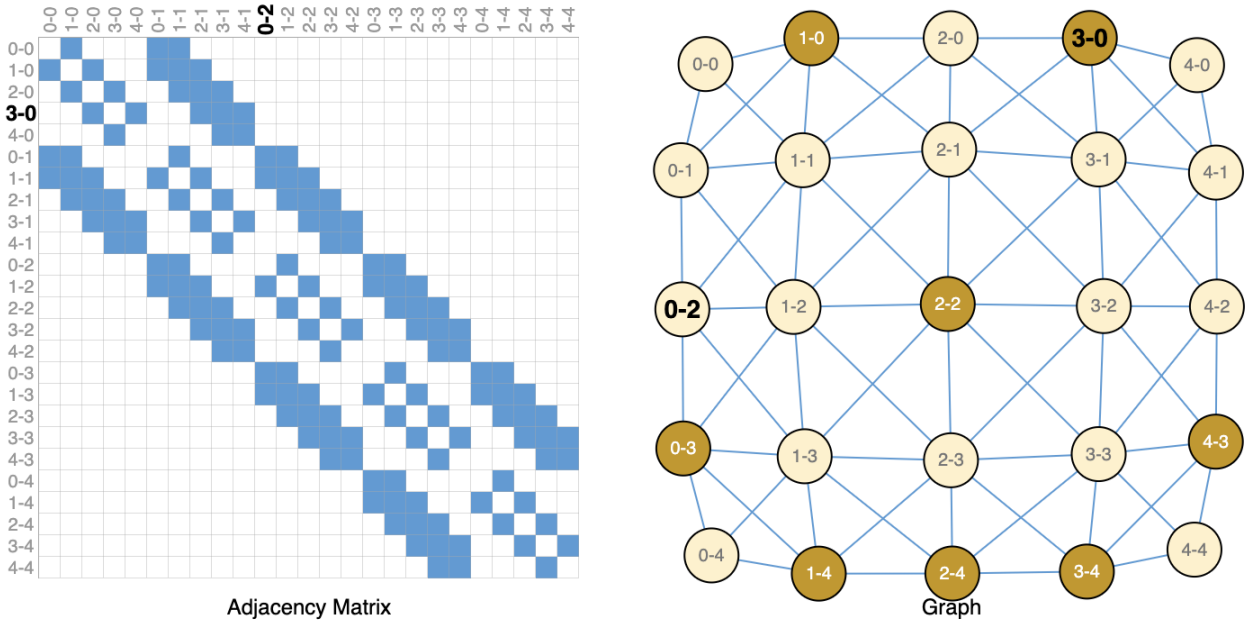


Embeddings: vector-valued information

From `https://distill.pub/2021/gnn-intro/`

Graphs: Examples

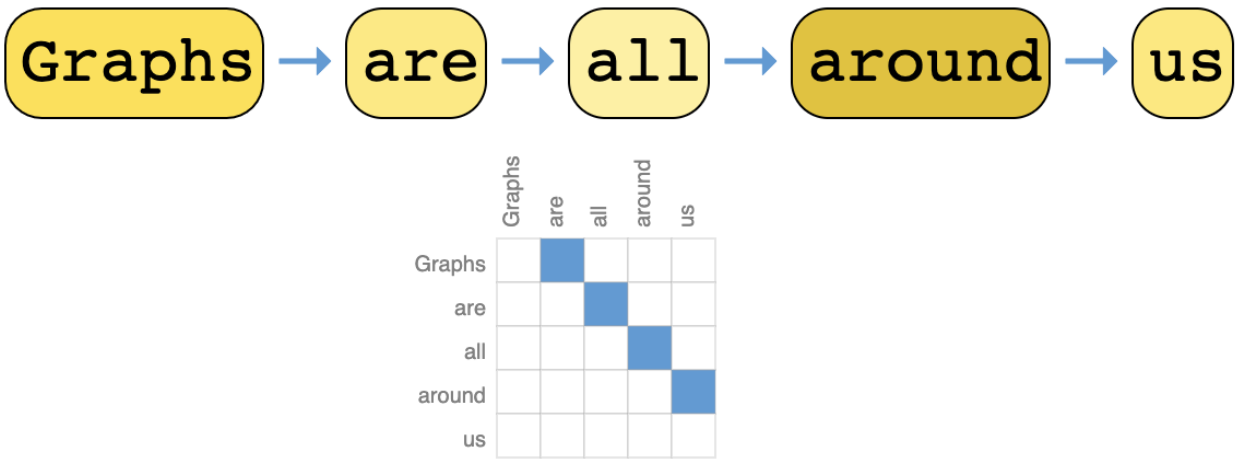
Graphs: Images



Graph and adjacency matrix of an image

From `https://distill.pub/2021/gnn-intro/`

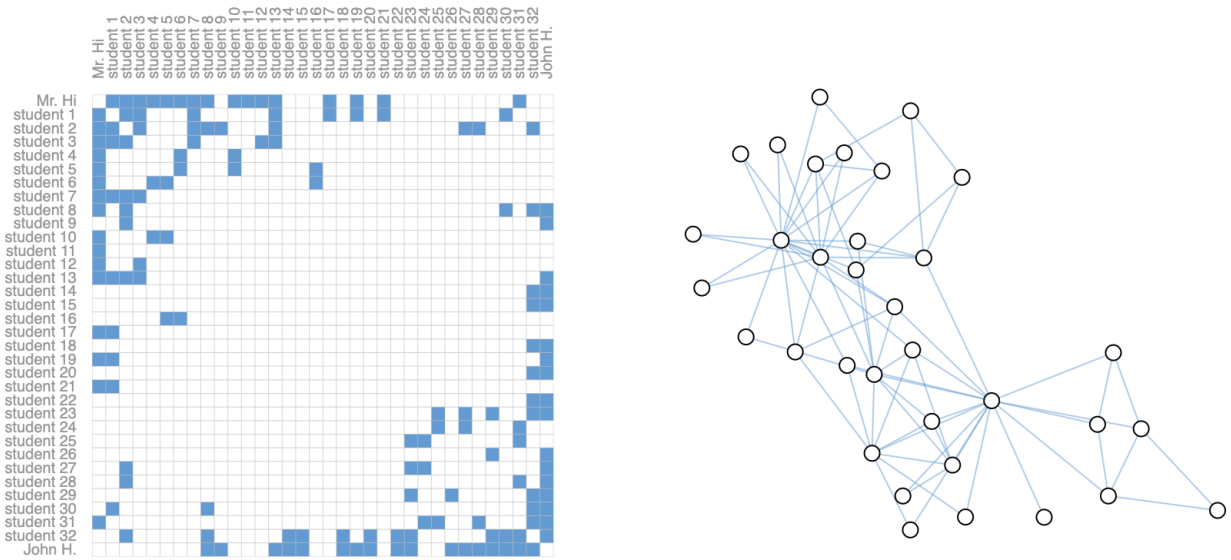
Graphs: Texts



Graph and adjacency matrix of a piece of text

From `https://distill.pub/2021/gnn-intro/`

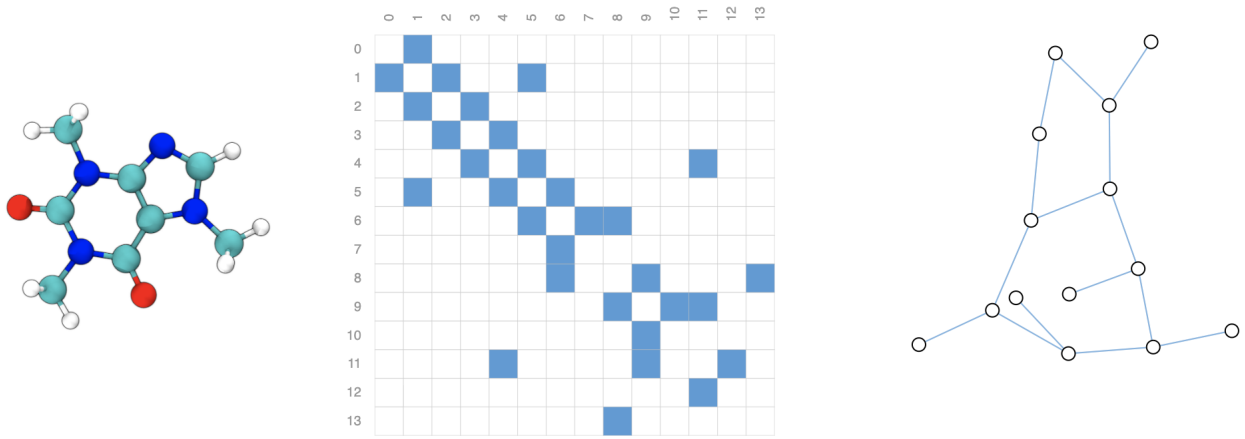
Graphs: Social Networks



Graph and adjacency matrix displaying interactions in karate club

From `https://distill.pub/2021/gnn-intro/`

Graphs: Molecules

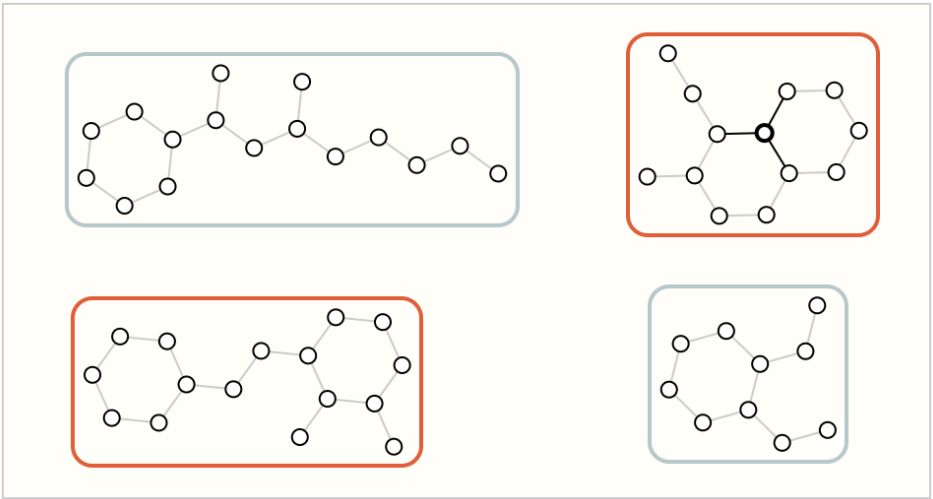


Graph and adjacency matrix displaying interactions in karate club

From `https://distill.pub/2021/gnn-intro/`

Graphs: Learning Tasks

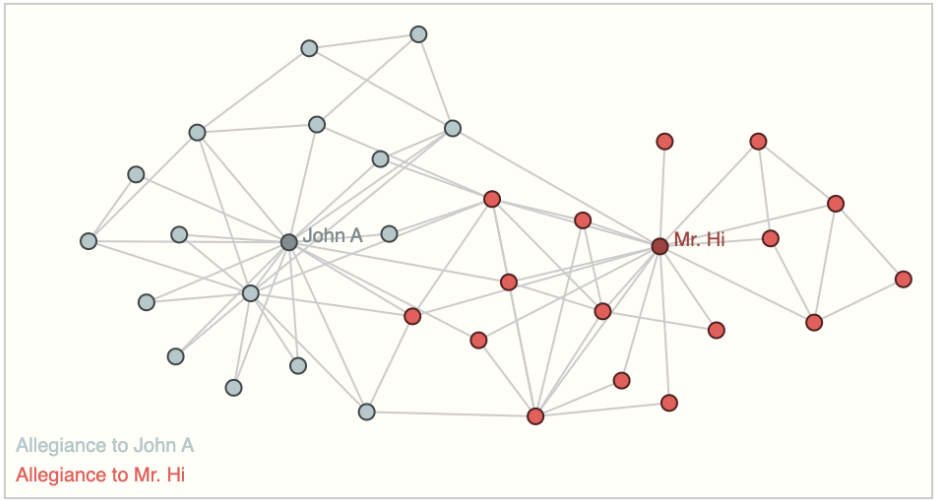
Graph Level Tasks



Structures in molecule graphs. Two rings (red) or not (black).
From `https://distill.pub/2021/gnn-intro/`

- Labels reflect statements about the entire graph.
- If unknown, determine using machine learning.

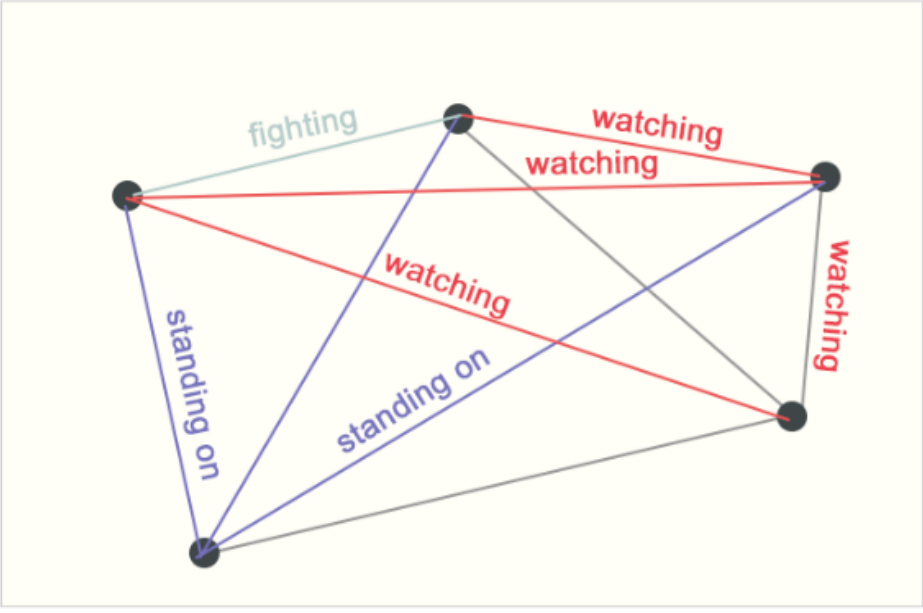
Node Level Tasks



Karate club: Allegiance to either Mr. Hi (red) or John A. (gray)
From `https://distill.pub/2021/gnn-intro/`

- Labels reflect statements about individual nodes.
- Some may be known. Others not: determine using ML.

Edge Level Tasks



Fight scene in image: elements (two fighters, arbiter, audience, mat).
Labels: relationships.
From `https://distill.pub/2021/gnn-intro/`

- Labels reflect statements about edges, so indicate relationships.
- Some relationships known. If not known: determine using ML.

Graphs: Machine Learning Challenges

Neural Networks and Graphs

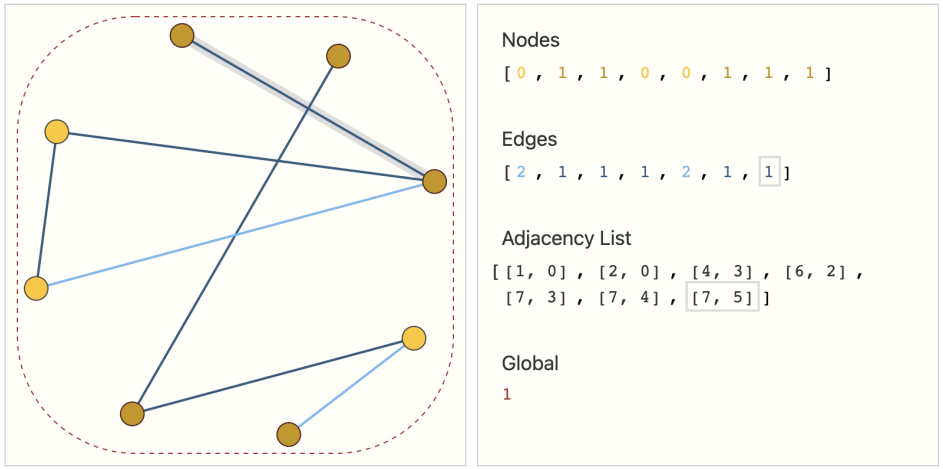
- Techniques for certain graphs available:
  - *Images = Grids:* Convolutional neural networks
  - *Text = Sequences:* Recurrent neural networks, attention networks
- Techniques for arbitrary graphs desirable:
  - *Social networks:* vary (heavily) by application
  - *Molecules:* plenty of different structures
  - *Other applications:* manifold interaction networks
- *Motivation:* Extend existing techniques to general graphs
- *Issue:* Get rid of regularity as a necessary condition

General Graphs: Input

- Neural networks usually expect well-arranged input:
  - Rectangular, grid-like input
  - Sequence type input
  - Arrangement in terms of graph-type evaluation obvious
- Graphs may harbor four types of information:
  - Node information
  - Edge information
  - Global information
  - Connectivity

How to exploit them by appropriately arranging input?

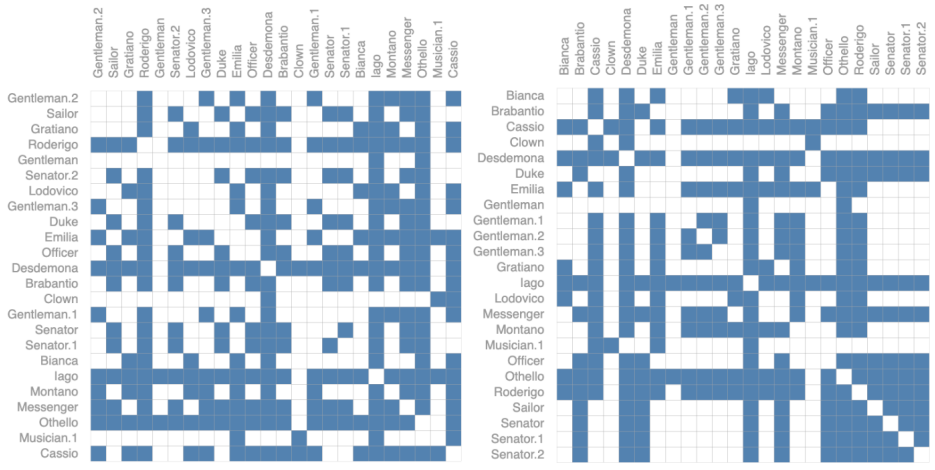
Challenge: Representing Input



Suitable way of storing graph information. Colors: different information.
From `https://distill.pub/2021/gnn-intro/`

- Nodes: node information
- Edges: edge information
- Global: global information
- Adjacency List: connectivity information

Challenge: Permutation Invariance



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From `https://distill.pub/2021/gnn-intro/`

- Graphs are permutation invariant
- *Goal:* Exploit data in permutation invariant way

Thanks for your attention!