

Machine learning for graphs and with graphs

Graph neural networks

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October 18, 2023



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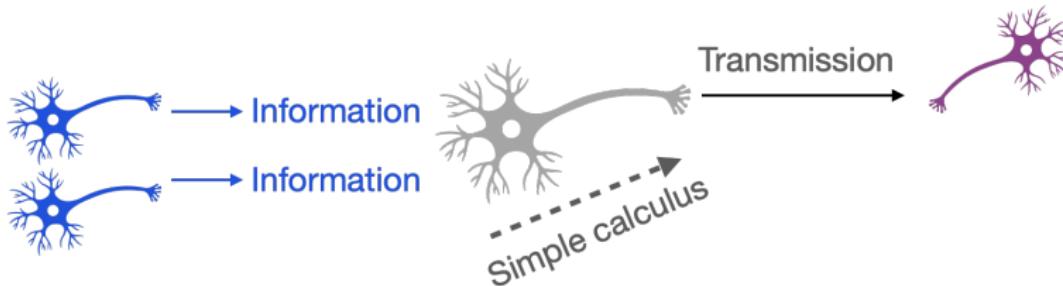
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What is a neural network ?

Neural network is a certain family of functions **parametrized by weights**.

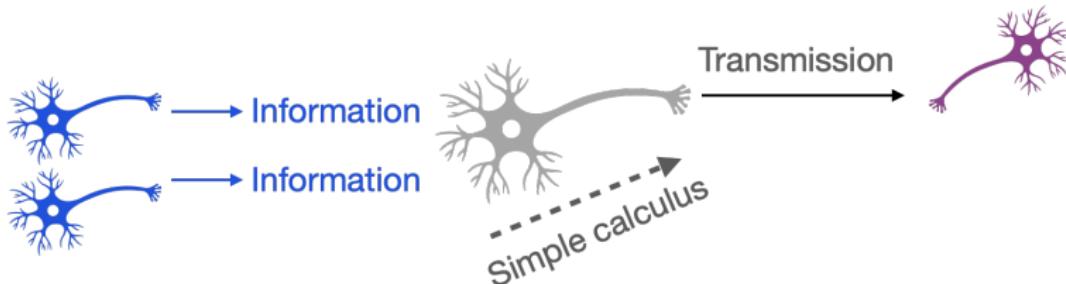
Built upon a biological analogy Rosenblatt 1958



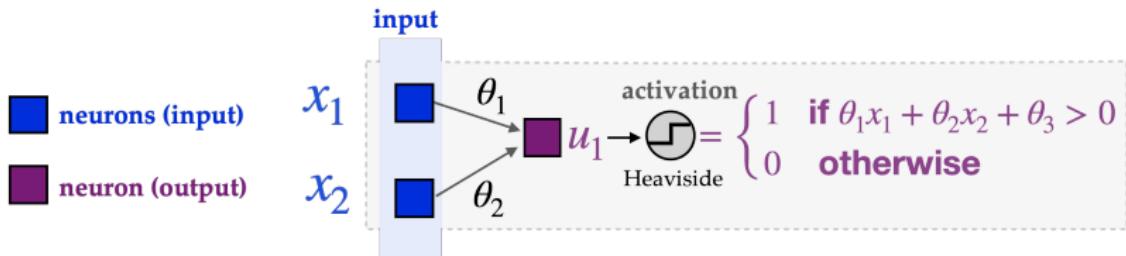
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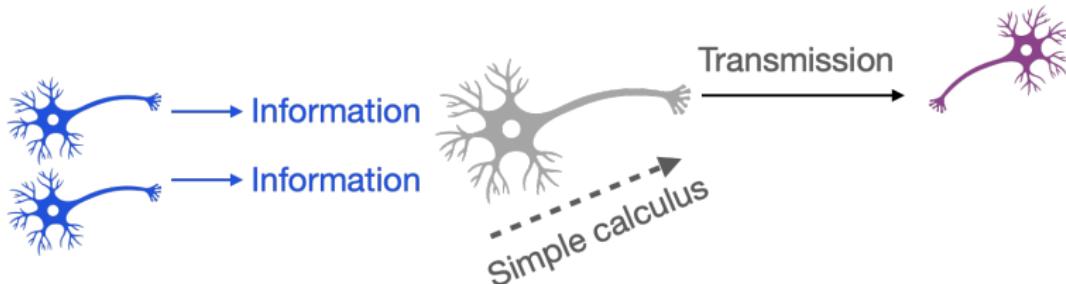
- ▶ First example $f(\mathbf{x} = (x_1, x_2)) = \text{activation}(\theta_1 x_1 + \theta_2 x_2 + \theta_3)$:



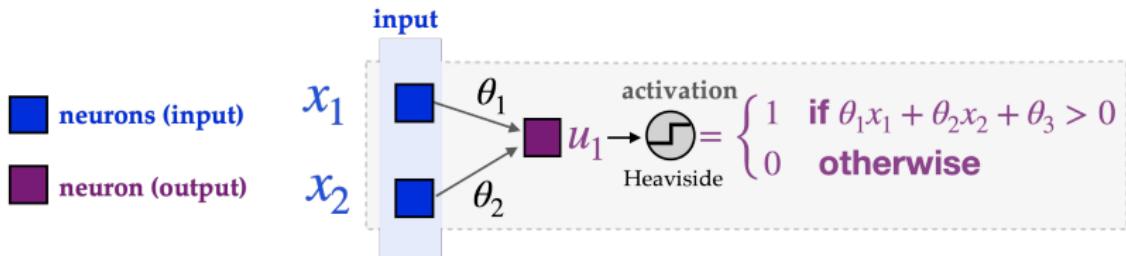
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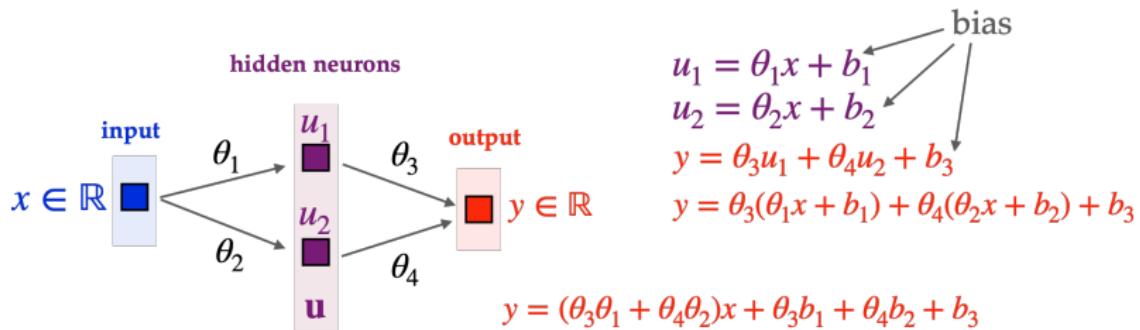
- ▶ Second example $f(\mathbf{x} = (x_1, x_2)) = \text{activation}(\theta_1 x_1 + \theta_2 x_2 + \theta_3)$:



What is a neural network ?

Feed-forward neural networks

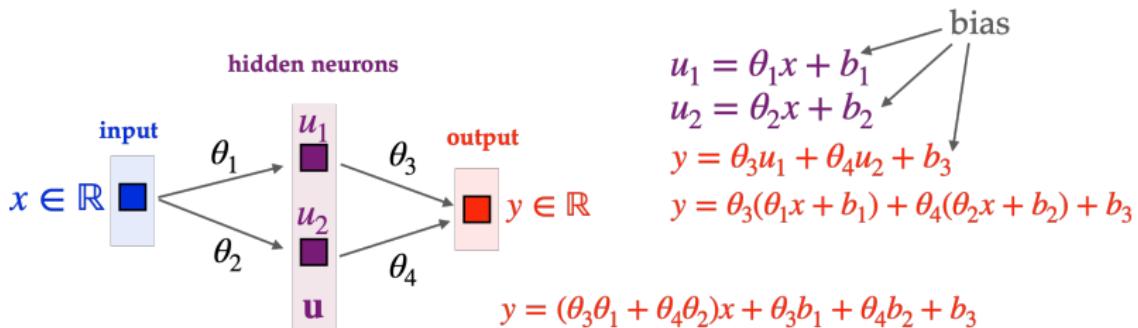
- ▶ Linear neural network:



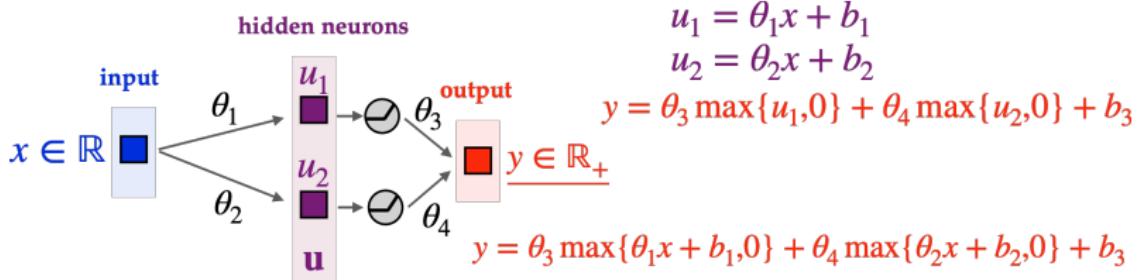
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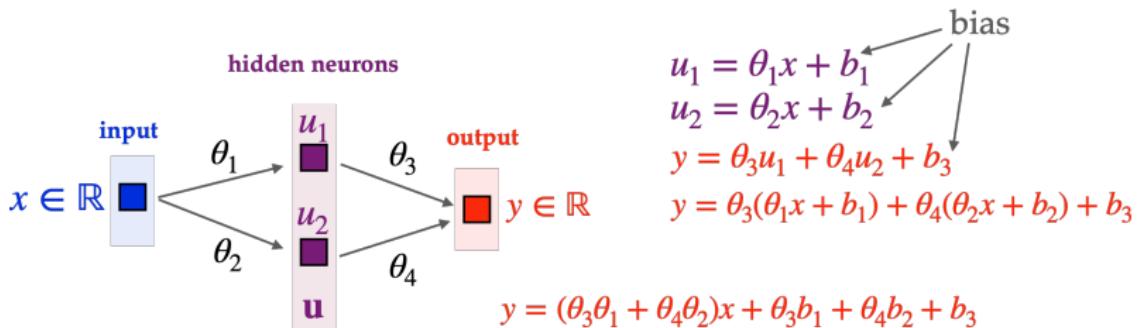
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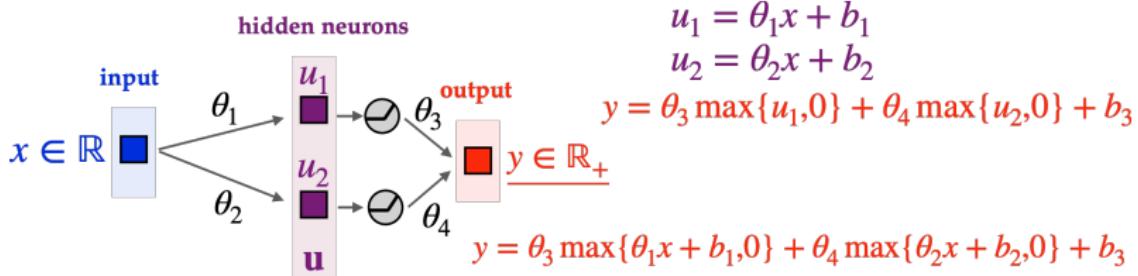
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- ▶ Linear neural network:



- ▶ Non-linearity:

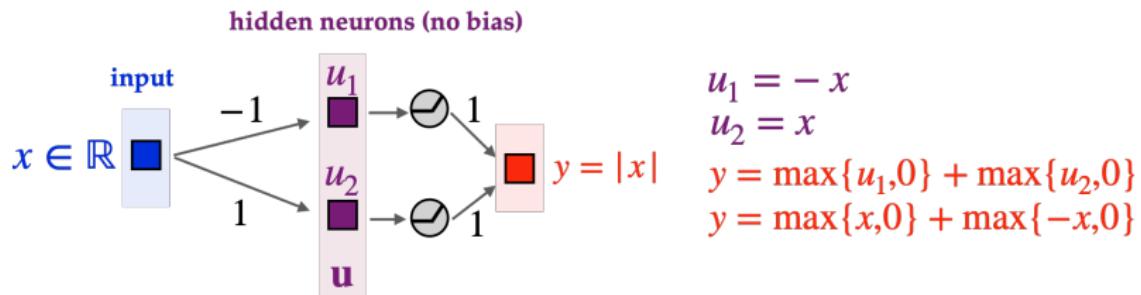


- ▶ Find a neural network that implements the function $f(x) = |x|$.

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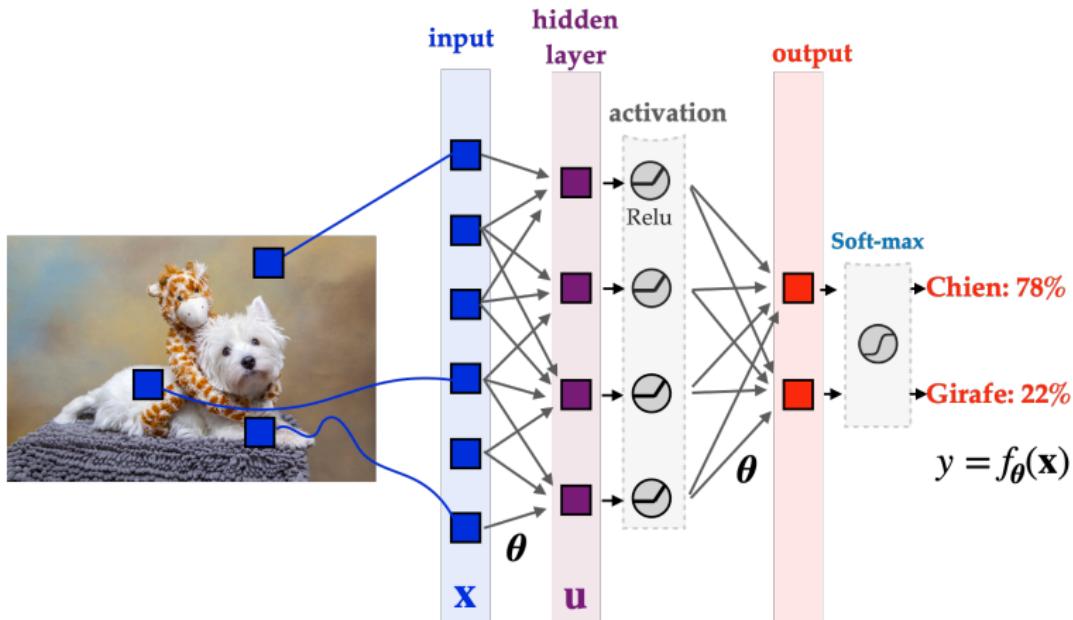
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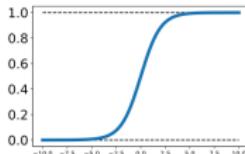
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Feed-forward neural networks



Soft-max:

$$\text{softmax}[u]_i = \frac{\exp(u_i)}{\sum_j \exp(u_j)}$$



What is a neural network ?

Feed-forward neural networks

- ▶ Feed-forward NN are function of the form

$$f(\mathbf{x}) = T_K \circ \sigma_{K-1} \circ \cdots \circ \sigma_1 \circ T_1(\mathbf{x})$$

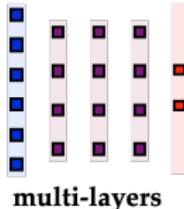
$$\text{where } T_k(\mathbf{z}) = \mathbf{W}^{(k)}\mathbf{z} + \mathbf{b}^{(k)}$$

and σ_k pointwise activation function.

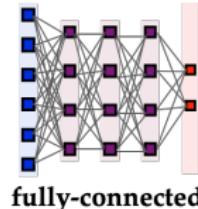
- ▶ All the weights: $\theta = (\mathbf{W}^{(1)}, \dots, \mathbf{W}^{(K)}, \mathbf{b}^{(1)}, \dots, \mathbf{b}^{(K)})$.
- ▶ Depending on the task the output of a NN is also transformed $g(\mathbf{x}) = \text{norm}(f(\mathbf{x}))$.
- ▶ E.g. $f : \mathbb{R}^d \rightarrow \mathbb{R}$ and $g : \mathbb{R}^d \rightarrow (0, 1)$ for binary classification with $\text{norm}(u) = 1/(1 + \exp(-u))$ (logistic/sigmoid function).

What is a neural network ?

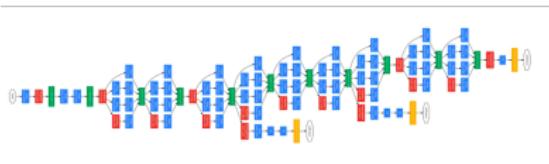
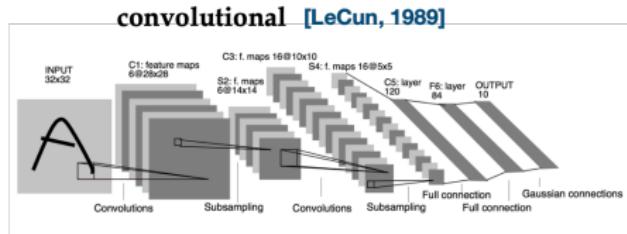
A zoo of architectures



multi-layers



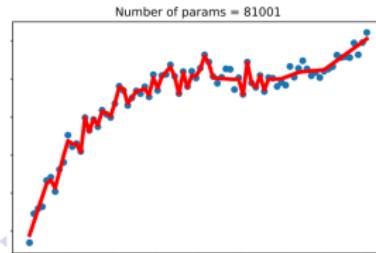
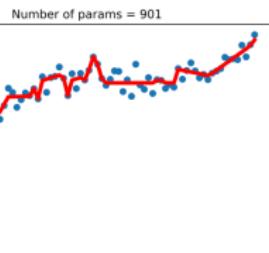
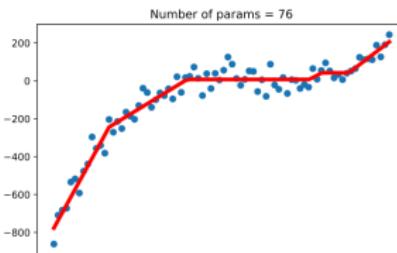
fully-connected



deep-learning

also: generative, recurrent, transformers, attention layer transformers...

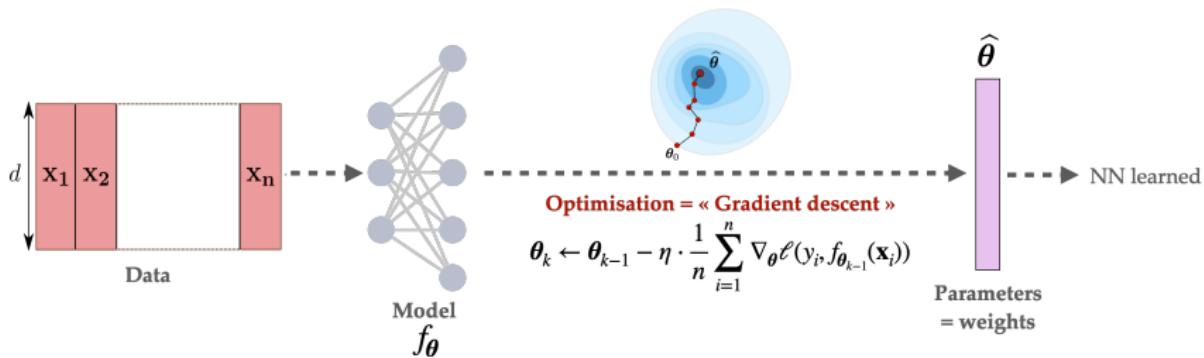
Richness of neural network



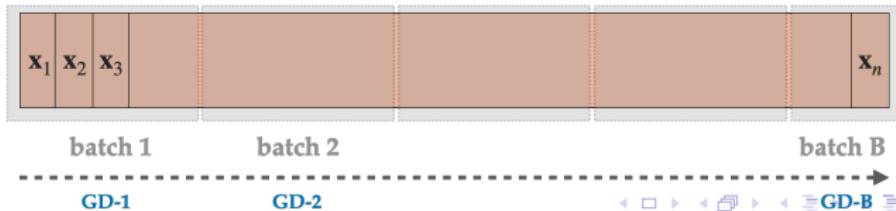
Neural network in practice

The (very) big picture

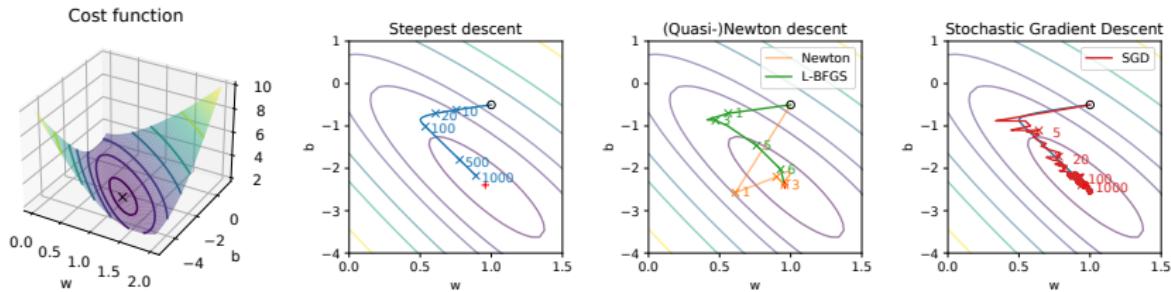
Find the weights that minimizes the empirical minimization loss.



- ▶ In practice gradient descent very slow.
- ▶ We use stochastic gradient descents (and variations) on batches of the data.



(almost) All optimization in one slide



Principle

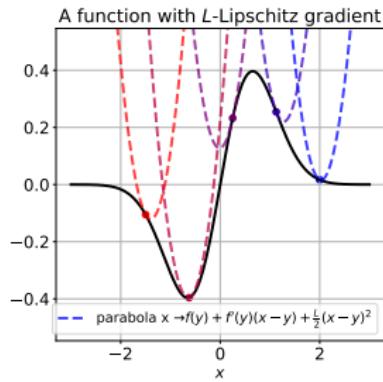
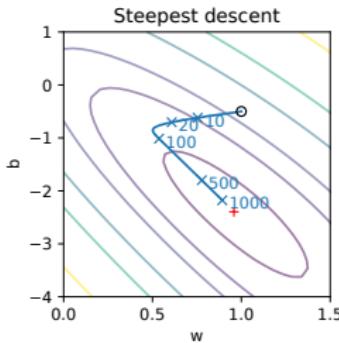
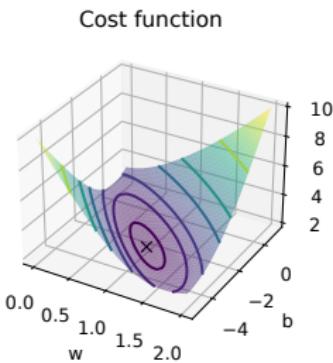
- ▶ Minimize a smooth function $J(\theta)$ using its gradient (or \approx).
- ▶ Initialize a vector $\theta^{(0)}$ and update it at each iteration k as:

$$\theta^{(k+1)} = \theta^{(k)} + \mu_k \mathbf{d}_k$$

where μ_k is a step and \mathbf{d}_k is a descent direction $\mathbf{d}_k^\top \nabla J(\theta^{(k)}) < 0$.

- ▶ Classical descent directions are :
 - ▶ **Steepest descent:** $\mathbf{d}_k = -\nabla J(\theta^{(k)})$ (a.k.a. Gradient descent).
 - ▶ **(Quasi) Newton:** $\mathbf{d}_k = -(\nabla^2 J(\theta^{(k)}))^{-1} \nabla J(\theta^{(k)})$, $\nabla^2 J$ is the Hessian.
 - ▶ **Stochastic Gradient Descent :** $\mathbf{d}_k = -\tilde{\nabla} J(\theta^{(k)})$ with approx. gradient.
- ▶ For NN: gradient computed with **automatic differentiation** (TD).

(almost) All optimization in two slides...



Why is this a good idea ? (on the board)

Let $J : \mathbb{R}^D \rightarrow \mathbb{R}$ with L -Lipschitz gradient¹ and $J^* := \min_{\theta} J(\theta) > -\infty$. Then, provided that $0 < \mu_k < \frac{2}{L}$, the iterations $\theta^{(k+1)} = \theta^{(k)} - \mu_k \nabla J(\theta^{(k)})$ satisfy

$J(\theta^{(k+1)}) < J(\theta^{(k)})$ (decrease the objective function)

$\lim_{k \rightarrow +\infty} \nabla J(\theta^{(k)}) = \mathbf{0}$ (critical point)

¹it means that $\forall \theta_1, \theta_2 \in \mathbb{R}^d$, $\|\nabla J(\theta_1) - \nabla J(\theta_2)\|_2 \leq L\|\theta_1 - \theta_2\|_2$.

(almost) All optimization in three slides...

Be aware of local minima

- ▶ When the functions are not convex, GD and its variants can fall into bad local minima.
- ▶ **Neural networks are not convex w.r.t. the optimized parameters !**

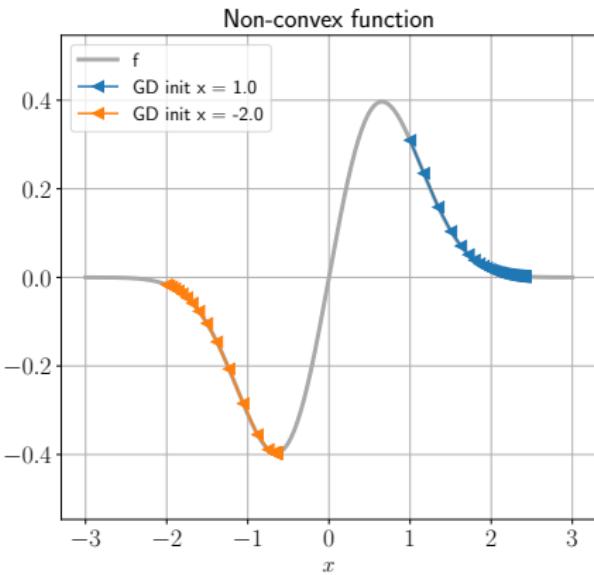
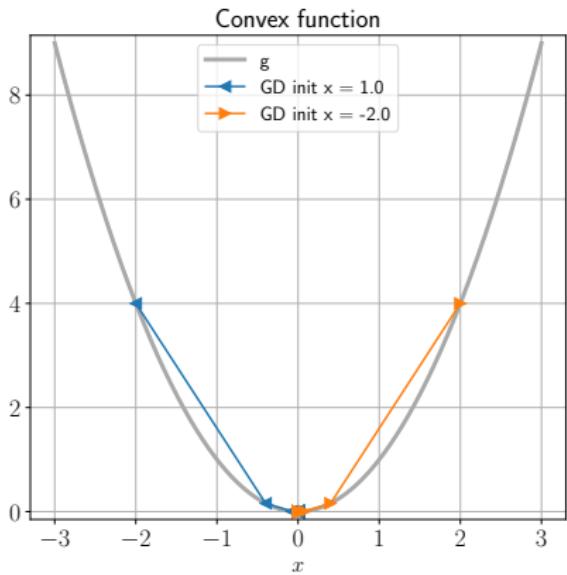


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First simple neural network: logistic regression

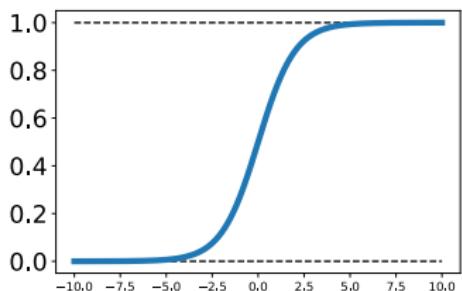
- ▶ It is a **classification method**: input $(\mathbf{x}_i)_i \in \mathbb{R}^d$ and $(y_i)_i \in \{+1, -1\}$.
- ▶ **Probabilistic model**: find a model h_θ s.t. $\mathbb{P}(y = +1|\mathbf{x}) \approx h_\theta(\mathbf{x})$.
- ▶ Bayes decision: $f(\mathbf{x}) = \text{sign}(\mathbb{P}(y = +1|\mathbf{x}) - \mathbb{P}(y = -1|\mathbf{x})) \in \{-1, +1\}$.

First simple neural network: logistic regression

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The sigmoid function

$$\sigma(z) = 1/(1 + \exp(-z)).$$



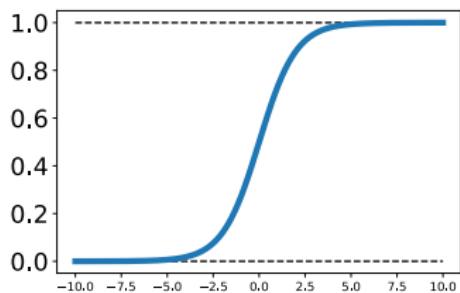
- ▶ Usually used to model probabilities.

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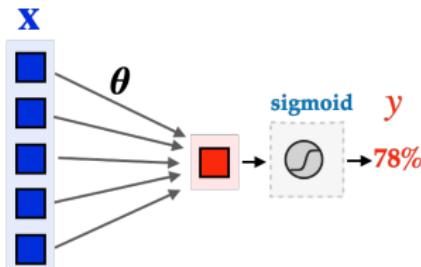


- ▶ Usually used to model probabilities.

The logistic regression model

The model is $\mathbb{P}(y = +1|\mathbf{x}) = \sigma(\boldsymbol{\theta}^\top \mathbf{x} + b)$.

- ▶ $\boldsymbol{\theta} \in \mathbb{R}^d$ are weights, $b \in \mathbb{R}$ is a bias that are to be optimized.
- ▶ It is a **generalized linear model**.
- ▶ Is also a one layer neural-network (no hidden layer).



First simple neural network: logistic regression

One property

$$\mathbb{P}(y = -1 | \mathbf{x}) = 1 - \mathbb{P}(y = 1 | \mathbf{x}) = 1 - \sigma(\boldsymbol{\theta}^\top \mathbf{x} + b) = \sigma(-(\boldsymbol{\theta}^\top \mathbf{x} + b))$$

First simple neural network: logistic regression

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Maximum likelihood estimation

Find $\boldsymbol{\theta} \in \mathbb{R}^d, b \in \mathbb{R}$ that maximize the (conditional) log-likelihood (**board**)

$$\begin{aligned} & \sum_{i:y_i=1} \log \mathbb{P}(y_i = 1 | \mathbf{x}_i) + \sum_{i:y_i=-1} \log \mathbb{P}(y_i = -1 | \mathbf{x}_i) \\ &= \sum_{i:y_i=1} \log \sigma(\boldsymbol{\theta}^\top \mathbf{x}_i + b) + \sum_{i:y_i=-1} \log \sigma(-(\boldsymbol{\theta}^\top \mathbf{x}_i + b)) \\ &= \sum_{i=1}^n \log \sigma(y_i(\boldsymbol{\theta}^\top \mathbf{x}_i + b)). \end{aligned}$$

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Minimizing the logistic loss

$$\min_{\boldsymbol{\theta}, b} \sum_{i=1}^n \log \left[1 + \exp \left(-y_i(\boldsymbol{\theta}^\top \mathbf{x}_i + b) \right) \right].$$

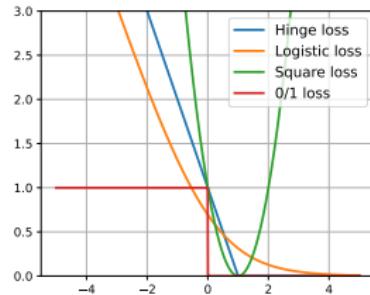
- Convex problem, can be solved with (Quasi) Newton's method.

First simple neural network: logistic regression

Remember your losses

With $f : \mathbb{R}^d \rightarrow \mathbb{R}$, many losses can be written as $\ell(y_i, f(\mathbf{x}_i)) = \Phi(y_i f(\mathbf{x}_i))$ with $\Phi \downarrow$.

- ▶ $\ell(y_i, f(\mathbf{x}_i)) = \mathbf{1}_{y_i f(\mathbf{x}_i) \leq 0}$.
- ▶ $\ell(y_i, f(\mathbf{x}_i)) = \max\{0, 1 - y_i f(\mathbf{x}_i)\}$.
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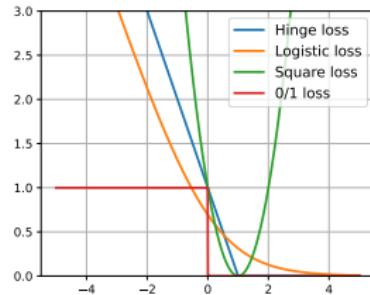


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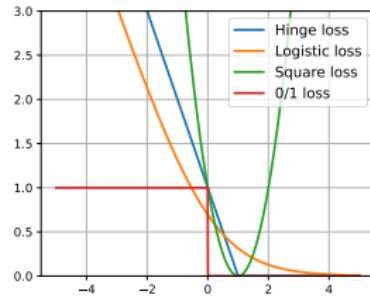
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- ▶ The decision/prediction of the label is $\text{sign}(f(\mathbf{x}))$.
- ▶ So it is a **linear decision boundary** (linear classification).

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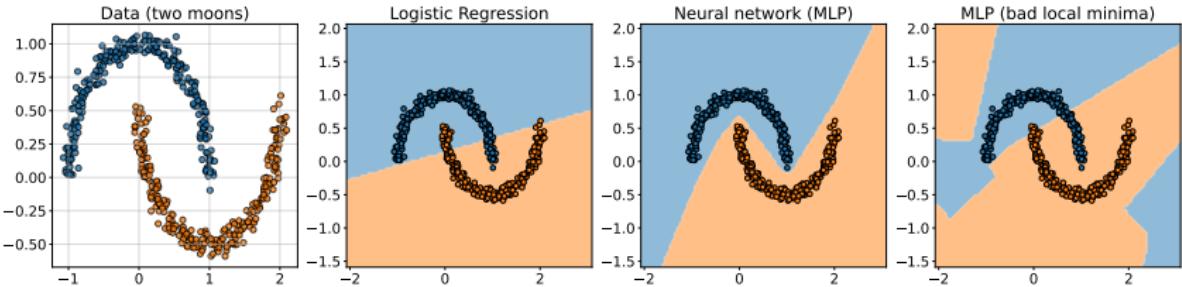


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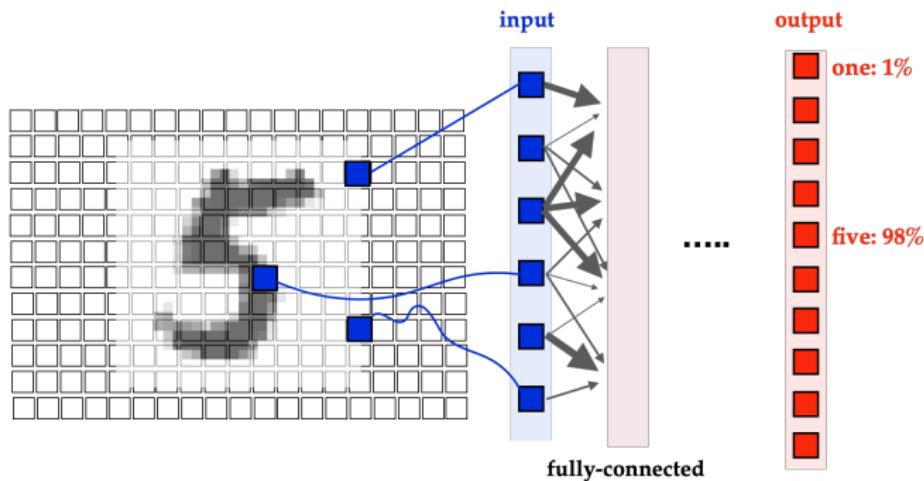
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Convolutional neural networks

- ▶ The core block for deep learning on images.
- ▶ Induces an **implicit bias** on the architecture.

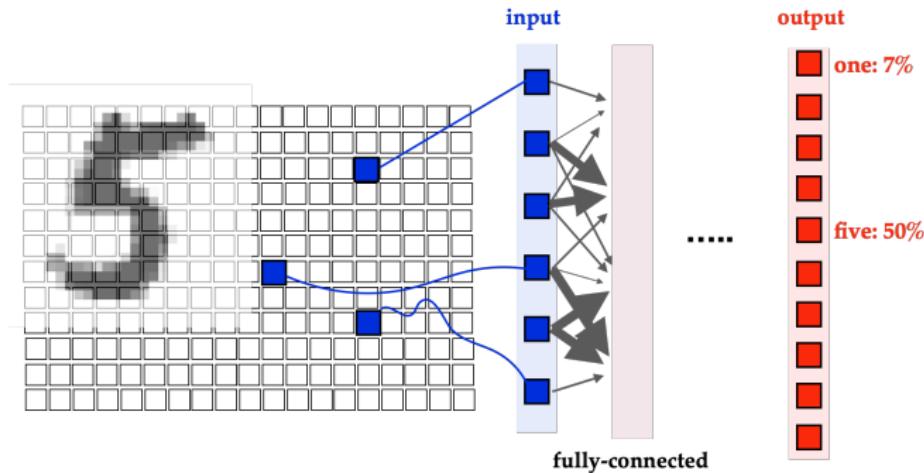
What could happen with a fully-connected architecture?



Convolutional neural networks

- ▶ The core block for deep learning on images.
- ▶ Induces an **implicit bias** on the architecture.

What could happen with a fully-connected architecture?



- ▶ We want a function that doesn't change if we only translate the image.
We want a **translation invariant function**.
- ▶ Convolution: particular structure on the weights that induce
translation equivariance.

Convolutional neural networks

Convolution/correlation of functions

Let $f, h \in L_2(\mathbb{R})$. The convolution $f * h \in L_2(\mathbb{R})$ is defined as

$$f * h(x) = \int_{-\infty}^{+\infty} f(t)h(x-t)dt \text{ and } f \star h(x) = \int_{-\infty}^{+\infty} f(t)h(t+x)dt$$

- ▶ **Translate a filter h** and then take the inner product with² f :

$$f \star h(x) = \langle \tau_{-x}h, f \rangle_{L_2(\mathbb{R})}.$$

- ▶ It weights the local contributions of f by a filter.

² $\tau_x f = t \rightarrow f(t-x)$

Convolutional neural networks

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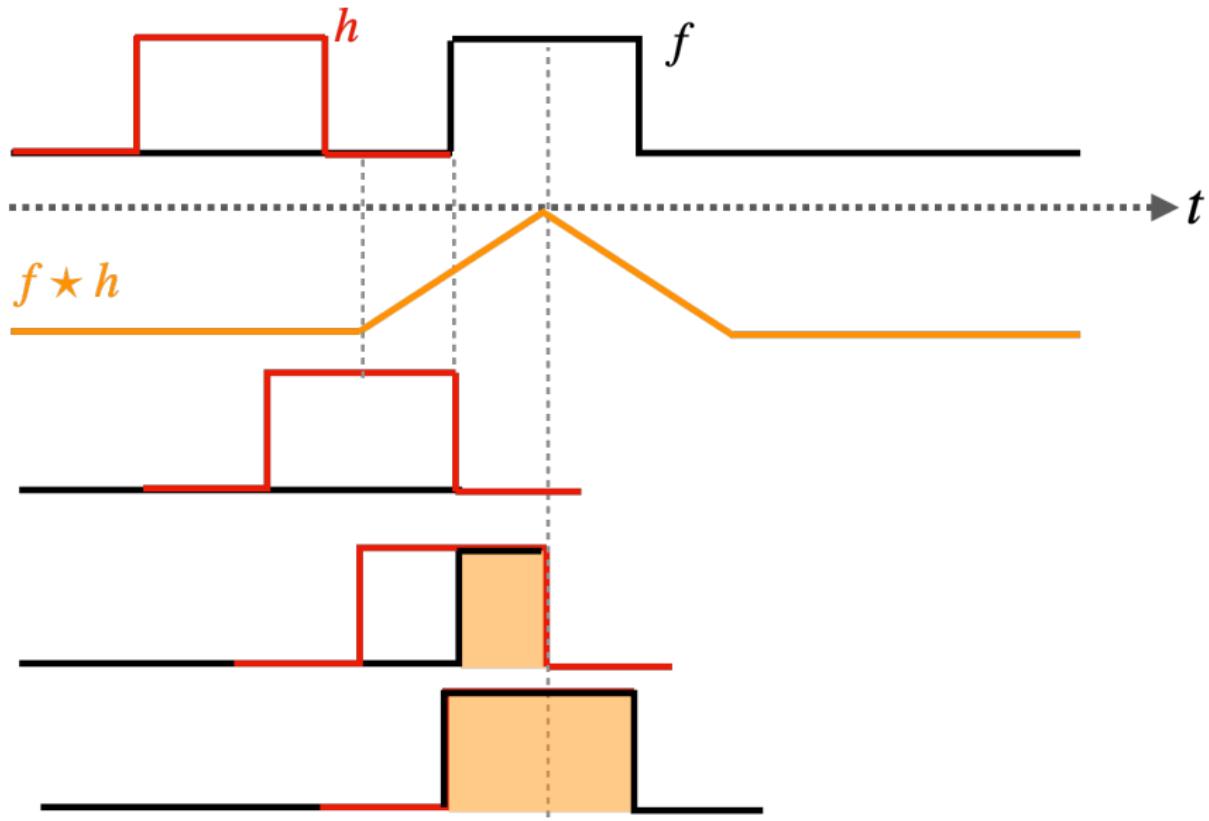
- ▶ It weights the local contributions of f by a filter.
- ▶ It is **translation equivariant**.

$$(\tau_x f) * h = \tau_x(f * h)$$

- ▶ If we translate the input, the output will be equally translated.

² $\tau_x f = t \rightarrow f(t-x)$

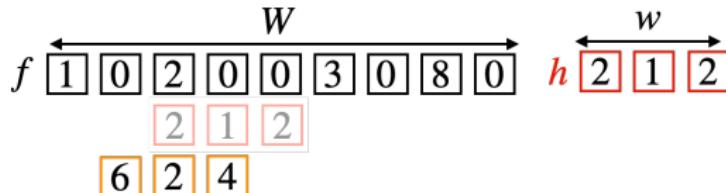
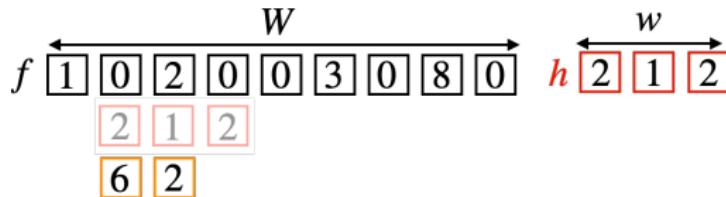
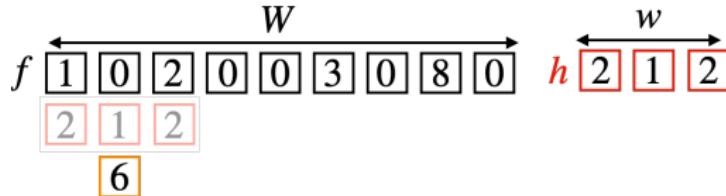
Convolutional neural networks



Convolutional neural networks

In practice convolutions are applied on discrete signals.

Discrete convolutions in 1D

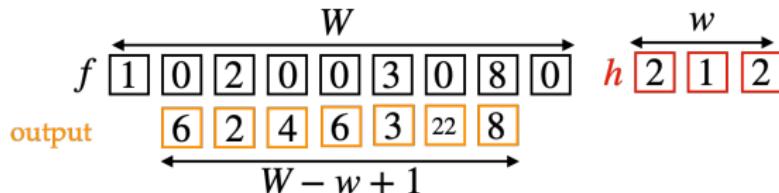


Question: size of the output ?

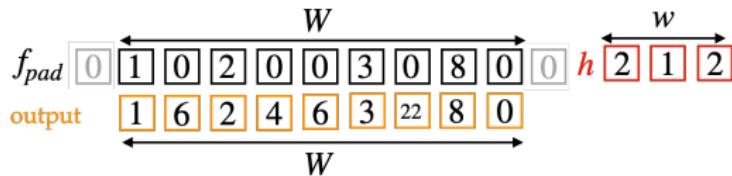
Convolutional neural networks

In practice convolutions are applied on discrete signals.

Discrete convolutions in 1D



- ▶ Padding strategies can be used to have output of the same size.



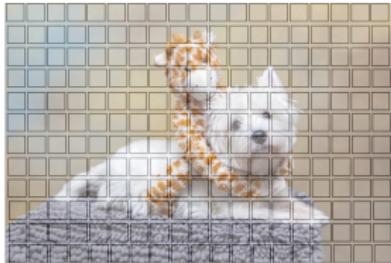
- ▶ Also stride can be used to move the filter from more than one pixel.

Convolutional neural networks

Discrete convolutions **not** in 1D

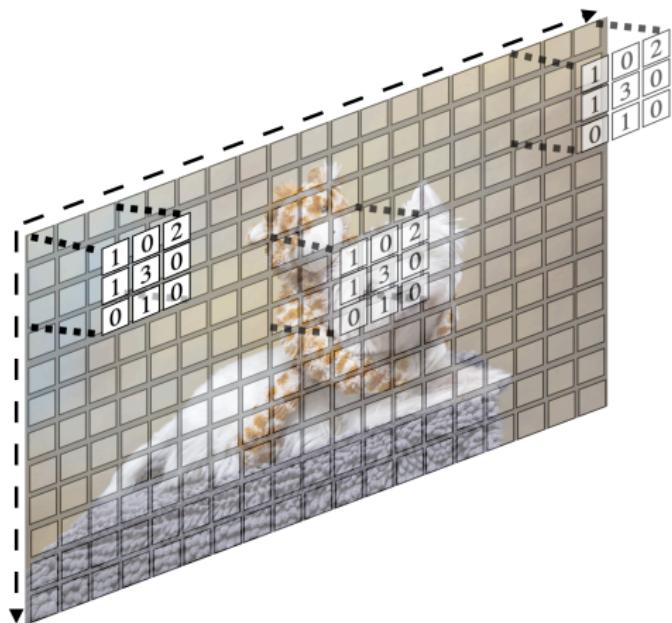
See also https://github.com/vdumoulin/conv_arithmetic.

Image



Filter

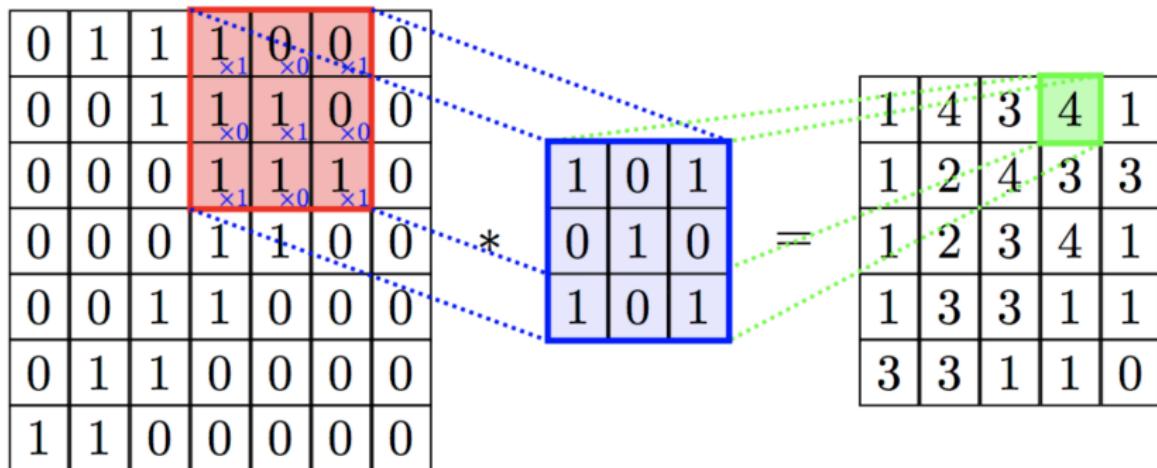
1	0	2
1	3	0
0	1	0



Convolutional neural networks

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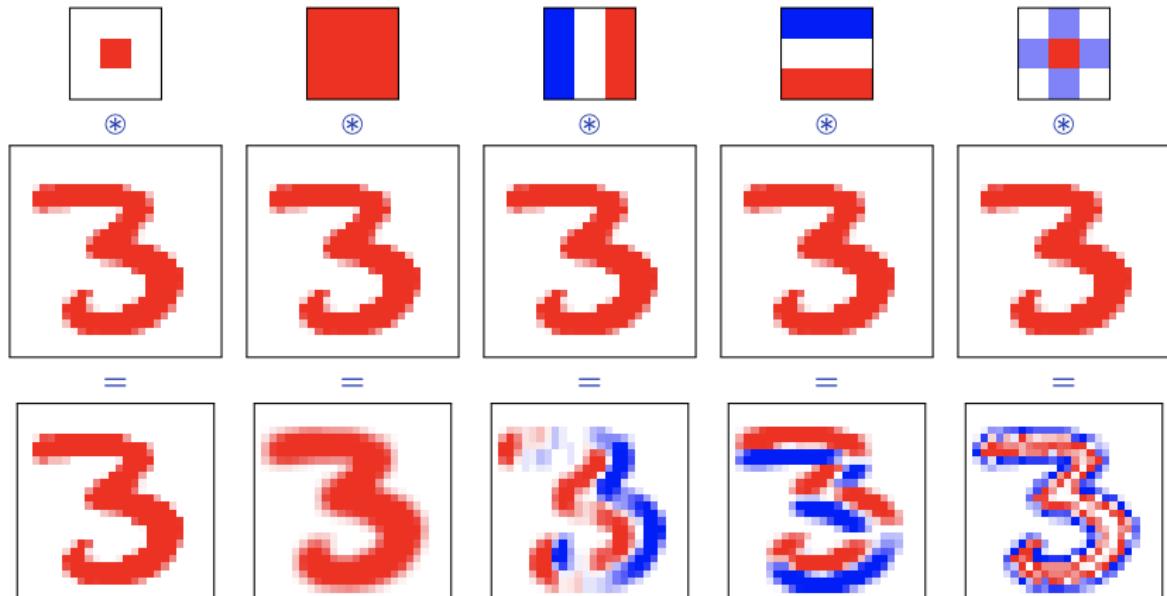


Figure: From Francois Fleuret <https://fleuret.org/dlc/>

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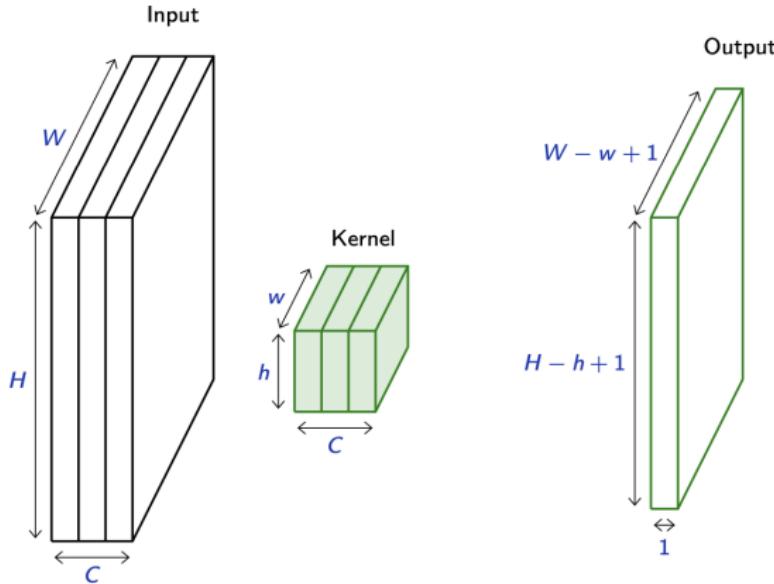


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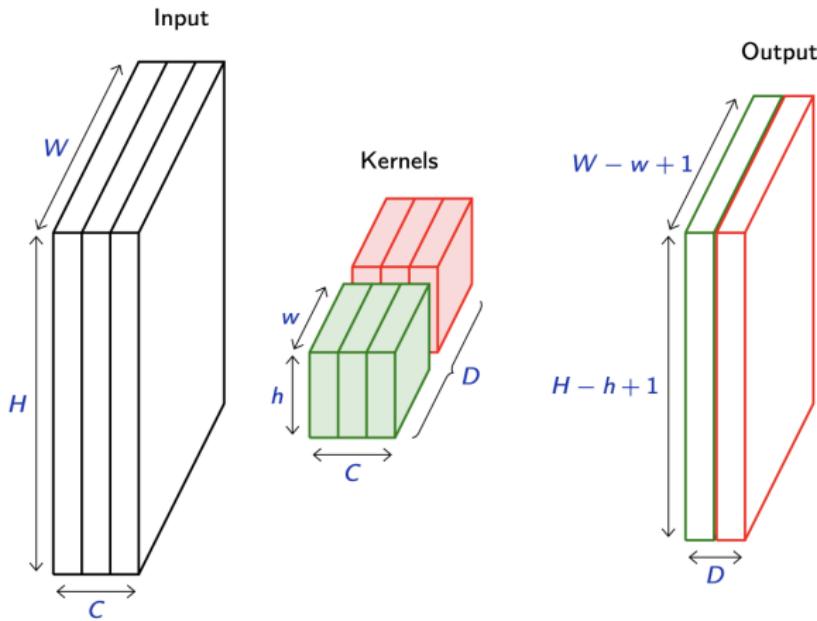


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Convolutional neural networks

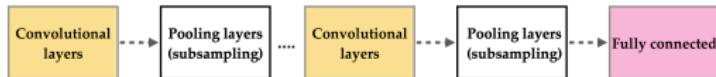
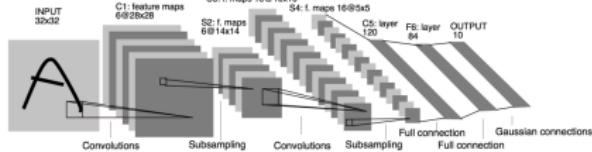


Figure: Schematic view

Figure: LeNet from LeCun et al. 1998

Principle and intuition (Zeiler and Fergus 2014)

- ▶ Define multiple convolutions, **learn the corresponding filter weights**.
- ▶ Recognize local patterns in images.
- ▶ Find intermediate features that are “general” and “adaptive” due to the translation equivariance bias
<https://fabianfuchsml.github.io/equivariance1of2/>.
- ▶ Revealing local features that are shared across the data domain.

Conclusion

- ▶ Deep learning: in almost everything when there are images.
- ▶ Very versatile: learn complex functions.
- ▶ Prior also helps ! (translation equivariance).
- ▶ Side note: still struggles on tabular data ([Grinsztajn, Oyallon, and Varoquaux 2022](#)).

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Graph neural networks ?

- ▶ How do we extend neural networks to graphs?
- ▶ Careful to node ordering: must be invariant to relabelling of the nodes (graph isomorphism).

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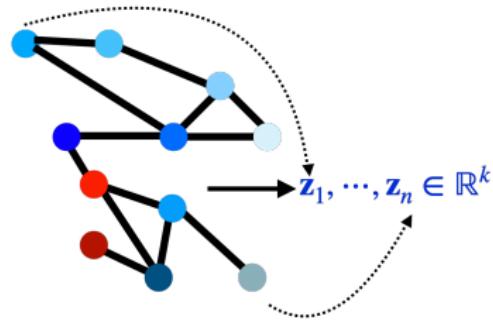
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Objective

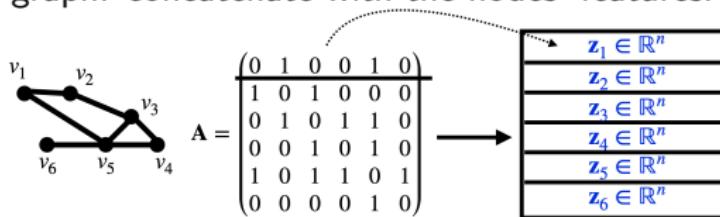
A chronological start

- ▶ Idea: to learn on a graph: nodes → vector → standard ML pipeline.
- ▶ The embedding **must take into account the structure** of the graph.
- ▶ Also useful for visualization.



One naive approach

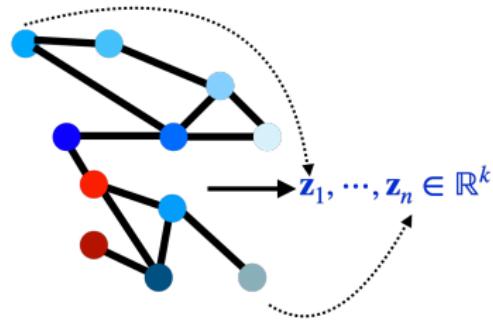
- ▶ Consider each row of the adjacency matrix as an embedding vector.
- ▶ If labelled graph: concatenate with the nodes' features.



Objective

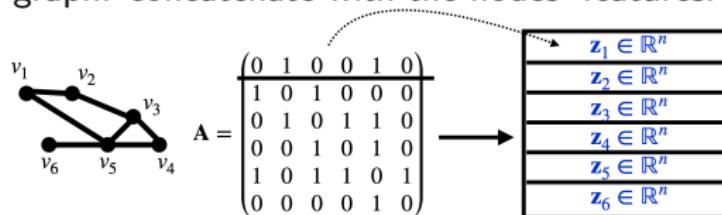
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One naive approach

- ▶ Consider each row of the adjacency matrix as an embedding vector.
- ▶ If labelled graph: concatenate with the nodes' features.



- ▶ Sensitive to the node ordering ! Also, expensive $O(|V|)$!
- ▶ Not applicable to graph with different sizes !

An encoder-decoder perspective

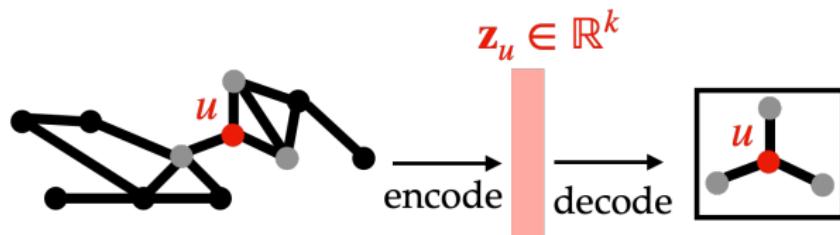
Notations

- ▶ We suppose we have one graph $G = (V, E)$, without features (so far).
- ▶ For each $u \in V$ we look for an embedding $\mathbf{z}_u \in \mathbb{R}^k$.

Principle

We look for a “good” encoder $E : V \rightarrow \mathbb{R}^k$ such that $E(u) = \mathbf{z}_u$.

- ▶ Ideally the embedding \mathbf{z}_u contains the neighbourhood informations of u .

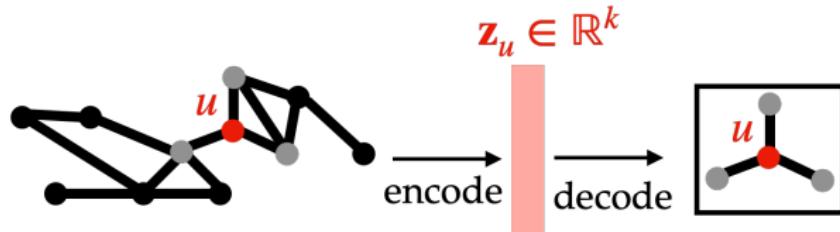


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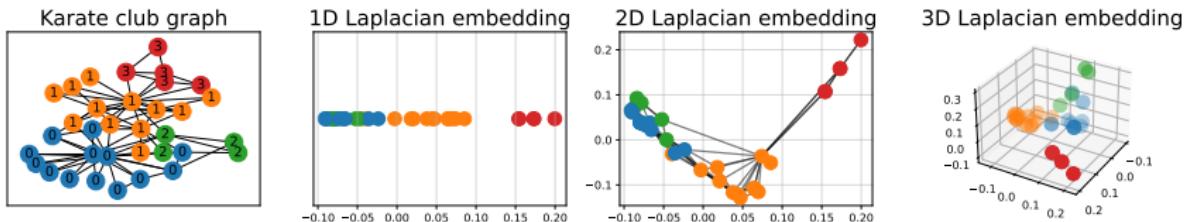
Encoding/decoding scheme

A lot of methods attempt to minimize

$$\mathcal{L} = \sum_{(u,v) \in \mathcal{D}} \ell(\text{similarity}(\mathbf{z}_u, \mathbf{z}_v), S[u, v])$$

- ▶ $\text{similarity}(\mathbf{z}_u, \mathbf{z}_v)$ how close are the embeddings.
- ▶ $S[u, v]$ how close are the nodes in the graph.
- ▶ $\ell : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ is a loss: how similar are the similarities.

Unsupervised node embeddings techniques



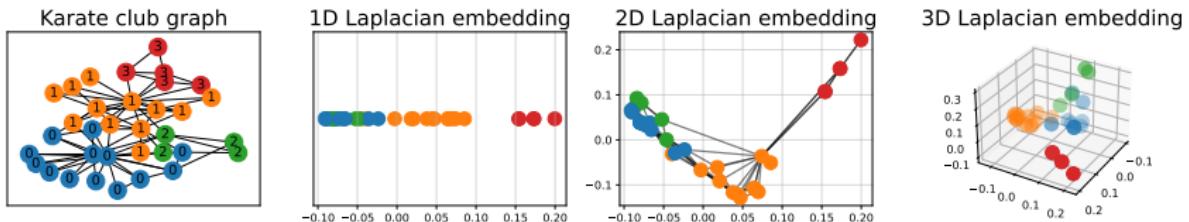
Inspiration from Laplacian eigenmaps Belkin and Niyogi 2003

- ▶ In the embedding space similarity($\mathbf{z}_u, \mathbf{z}_v$) = $\frac{1}{2} \|\mathbf{z}_u - \mathbf{z}_v\|_2^2$.
- ▶ When similiary is $\mathbf{S}[u_i, v_j] = A_{ij} / \sqrt{\text{degree}(u_i)} \sqrt{\text{degree}(u_j)}$, loss to minimize:

$$\frac{1}{2} \sum_{ij} \|\mathbf{z}_i - \mathbf{z}_j\|_2^2 \frac{A_{ij}}{\sqrt{\text{degree}(u_i)} \sqrt{\text{degree}(u_j)}} = \text{tr}(\mathbf{Z}^\top \tilde{\mathbf{L}} \mathbf{Z}).$$

- ▶ Normalized Laplacian $\tilde{\mathbf{L}} = \mathbf{D}^{-1/2} \mathbf{L} \mathbf{D}^{-1/2}$.
- ▶ Interpretation + permutation equivariance of the cost (on the board).

Unsupervised node embeddings techniques



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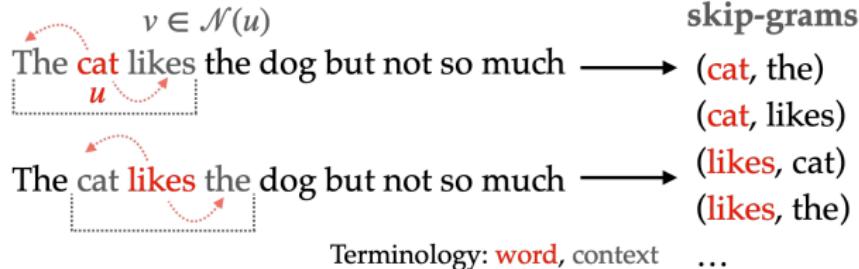
- ▶ Normalized Laplacian $\tilde{\mathbf{L}} = \mathbf{D}^{-1/2} \mathbf{L} \mathbf{D}^{-1/2}$.
- ▶ Interpretation + permutation equivariance of the cost (on the board).
- ▶ With the constraint $\mathbf{Z}^\top \mathbf{Z} = \mathbf{I}_d$ it recovers Laplacian eigenmaps.
- ▶ Sol. is the d eigenvectors associated to the d smallest eigenvalues of $\tilde{\mathbf{L}}$.

Unsupervised node embeddings techniques

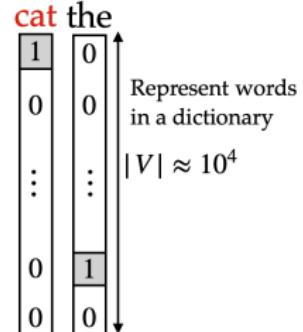
Skip-Gram and the Word2vec model (Mikolov et al. 2013)

The meaning of a word is its use in language (Wittgenstein).

- ▶ Objective: “similar” words are embedded into “similar” vectors.
- ▶ Goal: predict context words from each **input word**.
- ▶ We want to maximize $\mathbb{P}(\text{context}|\text{input word})$.



One hot encoding

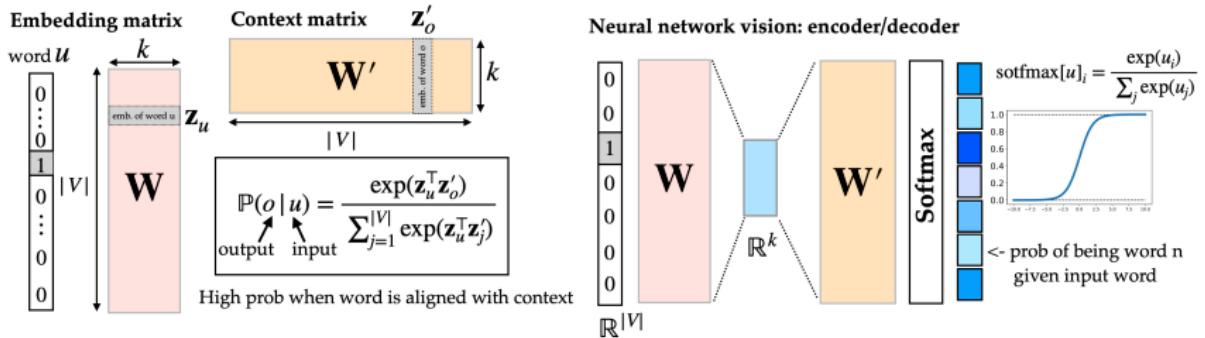


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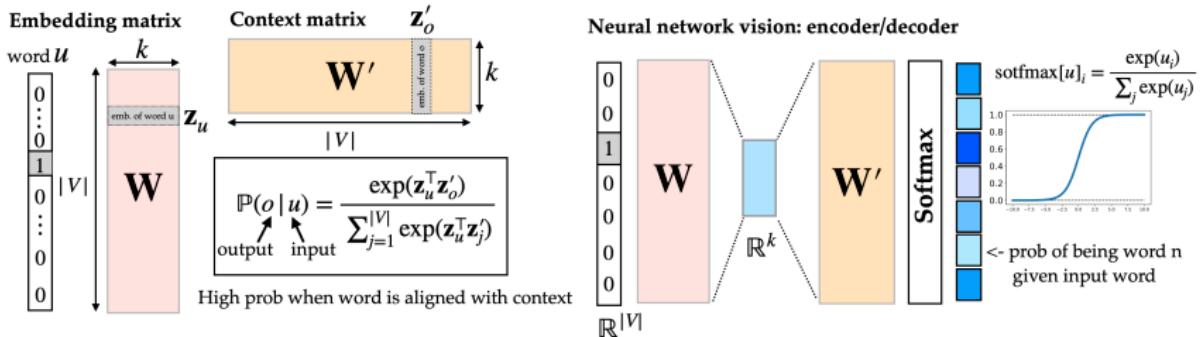


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- ▶ Dataset \mathcal{D} of input/output words (surrounding). Loss to minimize is:

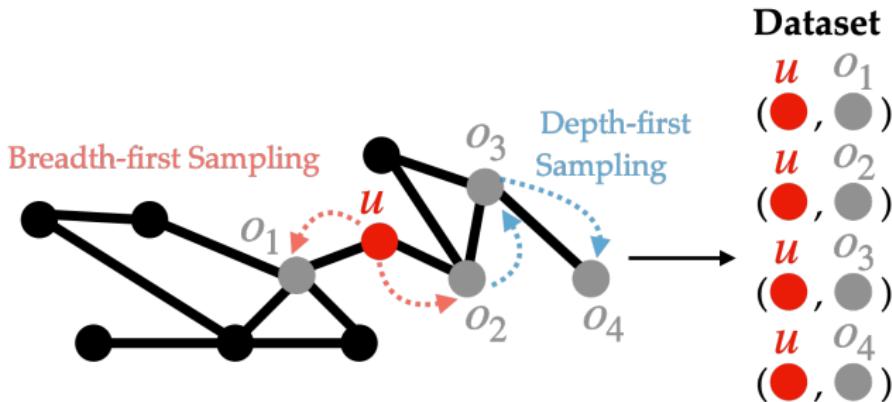
$$-\sum_{(u,o) \in \mathcal{D}} \log \mathbb{P}(o|u).$$

- ▶ But computing it in $\mathcal{O}(|V| \times |\{\text{words to embed}\}|)$: negative sampling.

Unsupervised node embeddings techniques

The node2vec model (Grover and Leskovec 2016)

- ▶ Similar as before: each node $u \in V$ is embedded as $\mathbf{z}_u \in \mathbb{R}^k$.
- ▶ Goal of the embedding: reflect the neighboring nodes of u .
- ▶ Sampling strategies based on random walks (BFS/DFS).



- ▶ With a dataset \mathcal{D} of input/output nodes. Loss to minimize:

$$\mathcal{L} = - \sum_{(u,o) \in \mathcal{D}} \log \frac{\exp(\mathbf{z}_u^\top \mathbf{z}_o)}{\sum_{w \in V} \exp(\mathbf{z}_u^\top \mathbf{z}_w)}$$

Unsupervised node embeddings techniques

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Negative sampling (NS)

- ▶ Loss is too expensive to compute $\mathcal{O}(|V|^2)$.
- ▶ NS: introduce negative data samples.
- ▶ Goal: distinguish between neighboring points of a target node u and random nodes drawn from a noise distribution using logistic regression.
- ▶ New loss (explanations on the board) (Goldberg and Levy 2014):

$$\mathcal{L} = - \left(\sum_{(u_+, o_+) \in \mathcal{D}_+} \log \sigma(\mathbf{z}_u^\top \mathbf{z}_o) + \sum_{(u_-, o_-) \in \mathcal{D}_-} \log \sigma(-\mathbf{z}_u^\top \mathbf{z}_o) \right)$$

with sigmoid function $\sigma(x) = \frac{1}{1 + \exp(-x)}$.

Unsupervised node embeddings techniques

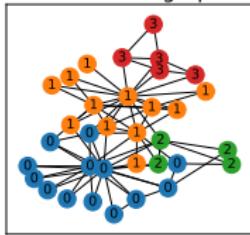
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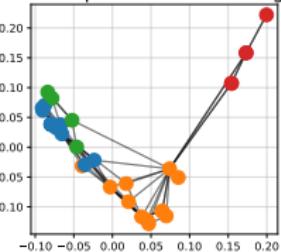
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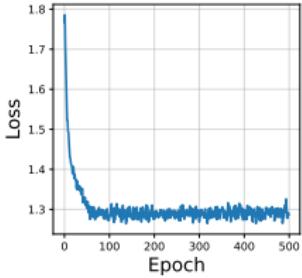
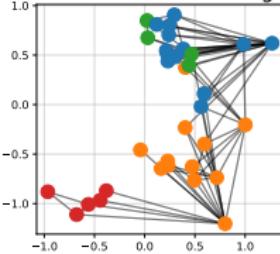
Karate club graph



2D Laplacian embedding



node2vec embedding



Unsupervised node embeddings techniques

Limitations of previous embeddings techniques

- ▶ The previous embeddings are called **shallow**: encoder function $E : V \rightarrow \mathbb{R}^k$ is simply an embedding lookup based on the node ID.

$$E(u) = \mathbf{Z}[:, u] = \mathbf{z}_u .$$

Unsupervised node embeddings techniques

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$$E(u) = \mathbf{Z}[:, u] = \mathbf{z}_u .$$

- ▶ Lack of parameter sharing between nodes in the encoder.
- ▶ Do not leverage node features !
- ▶ Inherently **transductive**: these methods can only generate embeddings for nodes that were present during the training phase.
- ▶ **If new nodes must retrain everything.**

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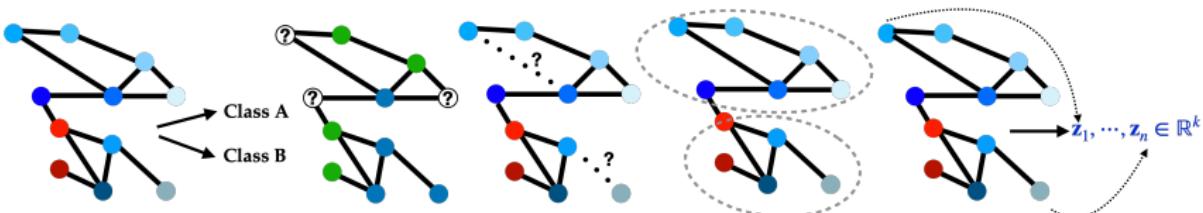
Frameworks considered here

Supervised:

- ▶ Graph classification: labelled graphs → label new graph (molecule classification, drug efficiency prediction).
- ▶ Node (or edge) classification: labelled nodes → label other nodes (advertisement, protein interface prediction).

Unsupervised (semi-supervised):

- ▶ Community detection: one graph → group nodes (social network analysis).
- ▶ Link prediction: one graph → potential new edge.
- ▶ Unsupervised node embeddings.



Some limitations

Tip of the iceberg

- ▶ Approx. 100 GNN papers a month on arXiv.
- ▶ Despite 1000s of papers, same ideas coming round: be critical, learn to spot incremental changes!
- ▶ We will only see the most well-known architectures (according to me).
- ▶ Be aware that it might already be out-of-date.
- ▶ Some surveys [Wu et al. 2021](#); [Zhang, Cui, and Zhu 2020](#); [William L Hamilton 2020](#).
- ▶ See also <https://github.com/houchengbin/awesome-GNN-papers>.

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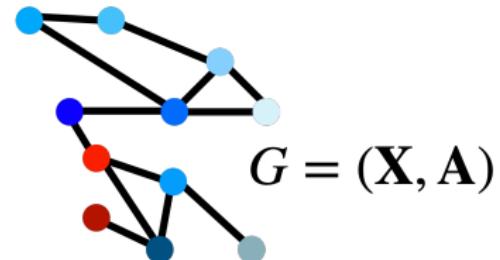
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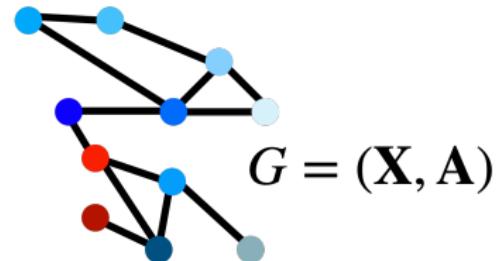
- ▶ Graphs considered here:
- ▶ $G = (V, E)$ with $|V| = n$, features on the nodes.
- ▶ Adjacency matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$.
- ▶ Feature matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$, feature $\mathbf{x}_i \in \mathbb{R}^d$.



What is a graph neural network ?

Framework

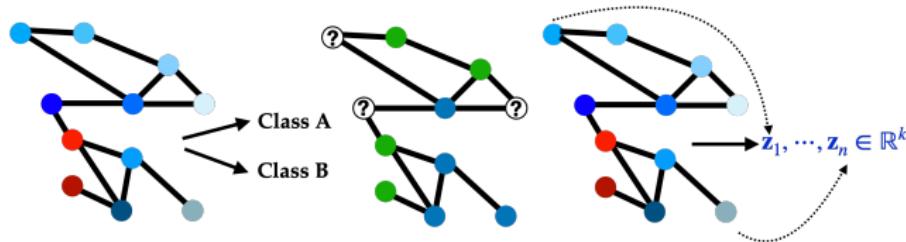
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GNN general definition

A GNN is a **specific parametrized function** that takes a input a graph $G = (\mathbf{X}, \mathbf{A})$ and outputs “something” (depends on the application).

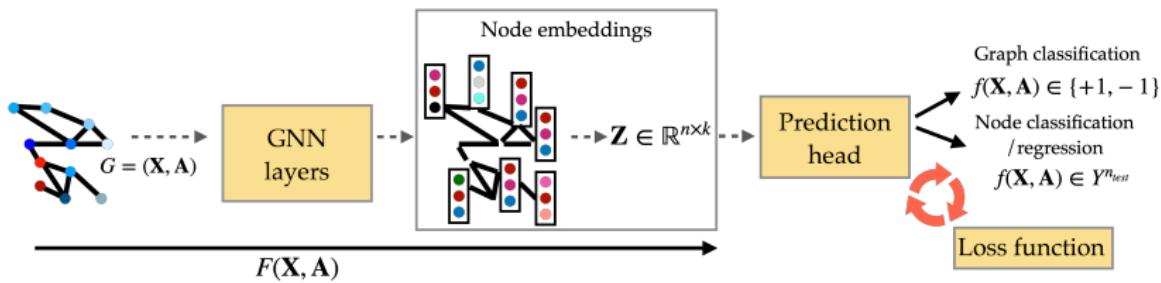
- ▶ It is made of a **combination of different layers**.
- ▶ Graph classification, node classification/regression, node embedding



- ▶ Notations: vector output $f(\mathbf{X}, \mathbf{A})$, matrix output $F(\mathbf{X}, \mathbf{A})$.

What properties to ensure ?

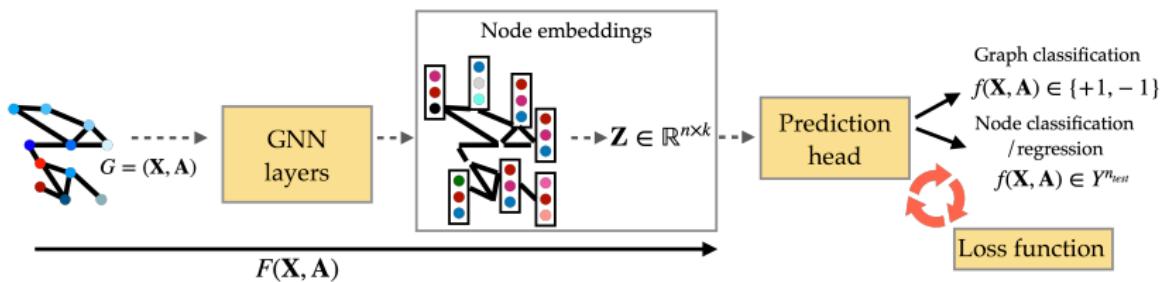
The training pipeline



- ▶ Overall the same procedure: find an embedding of the nodes $F(\mathbf{X}, \mathbf{A}) \in \mathbb{R}^{n \times k}$ (supervised or unsupervised) and then do stuff.

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Properties to ensure

- ▶ If graph classification then $f(\mathbf{X}, \mathbf{A}) \in \pm 1$: the function must be **invariant to permutations of the graph**.
- ▶ Prediction on the node level: we want to let the permutation of the graph produce a different result but while **making this phenomena predictable**.
- ▶ It will be formalized with the notion of invariance/equivariance.

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On invariance and equivariance

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A group \mathfrak{G} is a set along with a binary operation $\circ : \mathfrak{G} \times \mathfrak{G} \rightarrow \mathfrak{G}$ satisfying

- ▶ *Associativity*: $\forall g, h, i \in \mathfrak{G}, (g \circ h) \circ i = g \circ (h \circ i)$.
- ▶ *Identity*: there exists $e \in \mathfrak{G}$ such that $\forall g \in \mathfrak{G}, g \circ e = e \circ g = g$.
- ▶ *Inverse*: For each $g \in \mathfrak{G}$ there exists $g^{-1} \in \mathfrak{G}$ such that
 $g \circ g^{-1} = g^{-1} \circ g = e$.
- ▶ *Closure*: $\forall g, h \in \mathfrak{G}, g \circ h \in \mathfrak{G}$.

Commutativity is not part of this definition ($g \circ h \neq h \circ g$).

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Some examples

- ▶ Translation group on \mathbb{Z}^2 is an Abelian group:

$$(m, n) \circ (p, q) = (n + p, m + q).$$

- ▶ Translation + rotations, mirror reflections.
- ▶ Permutation group $S_n = \{\sigma : \llbracket n \rrbracket \rightarrow \llbracket n \rrbracket, \sigma \text{ is a bijection}\}$ with the composition of functions.

On invariance and equivariance

Group action

Given a set Ω and a group \mathfrak{G} , a (left) **group action** of \mathfrak{G} on Ω is a function

$$\begin{aligned}\mathfrak{G} \times \Omega &\rightarrow \Omega \\ (\mathfrak{g}, x) &\rightarrow \mathfrak{g}x\end{aligned}$$

satisfying

- ▶ $\forall x \in \Omega, \mathfrak{e}x = x$
- ▶ *Compatibility:* $\forall \mathfrak{g}, \mathfrak{h} \in \mathfrak{G}, \forall x \in \Omega, \mathfrak{g}(\mathfrak{h}x) = (\mathfrak{g} \circ \mathfrak{h})x.$
- ▶ It acts on the element of the sets via the group.
- ▶ **A set endowed with an action of \mathfrak{G} on it is called a \mathfrak{G} -set.**

On invariance and equivariance

Group action

Given a set Ω and a group \mathfrak{G} , a (left) **group action** of \mathfrak{G} on Ω is a function

$$\begin{aligned}\mathfrak{G} \times \Omega &\rightarrow \Omega \\ (\mathfrak{g}, x) &\mapsto \mathfrak{g}x\end{aligned}$$

satisfying

- ▶ $\forall x \in \Omega, \mathfrak{e}x = x$
- ▶ *Compatibility:* $\forall \mathfrak{g}, \mathfrak{h} \in \mathfrak{G}, \forall x \in \Omega, \mathfrak{g}(\mathfrak{h}x) = (\mathfrak{g} \circ \mathfrak{h})x.$
- ▶ It acts on the element of the sets via the group.
- ▶ **A set endowed with an action of \mathfrak{G} on it is called a \mathfrak{G} -set.**

Translation of functions

- ▶ Group of translations $\mathfrak{G} = \{\tau_x, x \in \mathbb{R}\}$ with $\tau_x \circ \tau_y = \tau_{x+y}$. Identity element τ_0 .
- ▶ For a function f and τ_x the group action

$$\tau_x f := t \rightarrow f(t - x).$$

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A formal definition of invariance

Invariance

Let Ω be a \mathfrak{G} -set. A function $f : \Omega \rightarrow Y$ is **\mathfrak{G} -invariant** if

$$\forall x \in \Omega, \forall g \in \mathfrak{G}, f(gx) = f(x).$$

- ▶ f is \mathfrak{G} -invariant if its output is unaffected by the group action.

A formal definition of invariance

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Permutation invariant functions

Find three functions $f, g, h : \mathbb{R}^n \rightarrow \mathbb{R}$ that are S_n -invariant.

A formal definition of invariance

Invariance

Let Ω be a \mathfrak{G} -set. A function $f : \Omega \rightarrow Y$ is **\mathfrak{G} -invariant** if

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Permutation invariant functions

$$f(\mathbf{x}) = \sum_{i=1}^n x_i, g(\mathbf{x}) = \max_{i \in [\mathfrak{n}]} x_i, h(\mathbf{x}) = \text{sort}(\mathbf{x}).$$

- ▶ The action of group $\sigma\mathbf{x} = (x_{\sigma(i)})_{i \in [\mathfrak{n}]} \in \mathbb{R}^n$.
- ▶ It is compatible $\sigma_1(\sigma_2\mathbf{x}) = (\sigma_1 \circ \sigma_2)\mathbf{x}$.
- ▶ Then f, g, h are S_n -invariant.
- ▶ Characterization of all permutation invariant functions $L : \mathbb{R}^{n^k} \rightarrow \mathbb{R}$ (Maron et al. 2018).

A formal definition of invariance

Invariance

Let Ω be a \mathfrak{G} -set. A function $f : \Omega \rightarrow Y$ is **\mathfrak{G} -invariant** if

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Permutation invariant functions

Let $\mathbf{X} \in \mathbb{R}^{n \times d}$. The action of σ on \mathbf{X} is $\sigma\mathbf{X} = (X_{\sigma(i)j})_{ij}$. Find a permutation invariant function $F : \mathbb{R}^{n \times d} \rightarrow \mathbb{R}$.

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Permutation invariant functions

Let $\mathbf{X} \in \mathbb{R}^{n \times d}$. The action of σ on \mathbf{X} is $\sigma\mathbf{X} = (X_{\sigma(i)j})_{ij}$. Find a permutation invariant function $F : \mathbb{R}^{n \times d} \rightarrow \mathbb{R}$.

- ▶ With $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)^\top$ and $F(\mathbf{X}) = \phi(\sum_{i=1}^n \psi(\mathbf{x}_i))$ with any $\psi : \mathbb{R}^d \rightarrow Z, \phi : Z \rightarrow Y$.

A formal definition of invariance

Function operating on sets/multisets

Let \mathcal{X} be a **countable set**. By construction, any function acting on sets $f : 2^{\mathcal{X}} \rightarrow Y$ for some Y is **permutation invariant**. That is

$$\forall \{x_1, \dots, x_n\} \in 2^{\mathcal{X}}, \forall \sigma \in S_n, f(\{x_1, \dots, x_n\}) = f(\{x_{\sigma(1)}, \dots, x_{\sigma(n)}\}).$$

Simply because $\{x_1, \dots, x_n\} = \{x_{\sigma(1)}, \dots, x_{\sigma(n)}\}$.

A formal definition of invariance

Function operating on sets/multisets

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Simply because $\{x_1, \dots, x_n\} = \{x_{\sigma(1)}, \dots, x_{\sigma(n)}\}$.

- ▶ Any function $f : 2^{\mathcal{X}} \rightarrow \mathbb{R}$ has the form ([Zaheer et al. 2018](#))

$$f(X) = \phi\left(\sum_{x \in X} \psi(x)\right) \text{ for some } \psi : \mathcal{X} \rightarrow \mathbb{R}, \phi : \mathbb{R} \rightarrow \mathbb{R}.$$

- ▶ See prev. course: a multiset is a “set” where element can be repeated several times e.g. $\{\{a, a, b\}\}$.
- ▶ Same representation result holds for functions on multisets ([Wagstaff et al. 2019](#)).

A formal definition of equivariance

Equivariance

Let Ω_1, Ω_2 be two \mathfrak{G} -sets (of the same group). A function $h : \Omega_1 \rightarrow \Omega_2$ is **\mathfrak{G} -equivariant** if

$$\forall x \in \Omega_1, \forall g \in \mathfrak{G}, h(gx) = gh(x).$$

- ▶ Pay attention to the input/output spaces and the compatibility.
- ▶ Transform the input + apply $h =$ apply h and transform the result.

A formal definition of equivariance

Equivariance

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- ▶ Transform the input + apply h = apply h and transform the result.

Convolutions

Prove that the convolution with a filter $h \in L_2(\mathbb{R})$ is translation equivariant.

A formal definition of equivariance

Equivariance

Let Ω_1, Ω_2 be two \mathfrak{G} -sets (of the same group). A function $h : \Omega_1 \rightarrow \Omega_2$ is **\mathfrak{G} -equivariant** if

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- ▶ Pay attention to the input/output spaces and the compatibility.
- ▶ Transform the input + apply h = apply h and transform the result.

Convolutions

Consider a filter $h \in L_2(\mathbb{R})$.

- ▶ The convolution with a filter is $H : \Omega = L_2(\mathbb{R}) \rightarrow L_2(\mathbb{R})$ such that $H(g) := g * h = h * g$.
- ▶ For any translation τ_x

$$\forall g \in L_2(\mathbb{R}), H(\tau_x g) = (\tau_x g) * h = \tau_x(g * h) = \tau_x H(g).$$

- ▶ Translate then convolve = convolve then translate.

A formal definition of equivariance

Equivariance

Let Ω_1, Ω_2 be two \mathfrak{G} -sets (of the same group). A function $h : \Omega_1 \rightarrow \Omega_2$ is **\mathfrak{G} -equivariant** if

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- ▶ Pay attention to the input/output spaces and the compatibility.
- ▶ Transform the input + apply h = apply h and transform the result.

Permutation equivariant functions

- ▶ Action of S_n on $\Omega_1 = \mathbb{R}^{n \times d_1}, \Omega_2 = \mathbb{R}^{n \times d_2}$ defined as

$$\sigma \mathbf{X} = (X_{\sigma(i),j})_{ij}$$

for $\sigma \in S_n, \mathbf{X} \in \mathbb{R}^{n \times d_1} \cup \mathbb{R}^{n \times d_2}$.

- ▶ Find two permutation equivariant functions $F : \mathbb{R}^{n \times d_1} \rightarrow \mathbb{R}^{n \times d_2}$.

A formal definition of equivariance

Equivariance

Let Ω_1, Ω_2 be two \mathfrak{G} -sets (of the same group). A function $h : \Omega_1 \rightarrow \Omega_2$ is **\mathfrak{G} -equivariant** if

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- ▶ Pay attention to the input/output spaces and the compatibility.
- ▶ Transform the input + apply h = apply h and transform the result.

Permutation equivariant functions

- ▶ Let $\mathbf{W} \in \mathbb{R}^{d_1 \times d_2}$ and $F(\mathbf{X}) = \mathbf{XW}$.

$$\text{▶ Let } \mathbf{X} = \begin{pmatrix} \mathbf{x}_1^\top \\ \vdots \\ \mathbf{x}_n^\top \end{pmatrix} \text{ previous example } F(\mathbf{X}) = \begin{pmatrix} (\mathbf{W}^\top \mathbf{x}_1)^\top \\ \vdots \\ (\mathbf{W}^\top \mathbf{x}_n)^\top \end{pmatrix}.$$

$$\text{▶ More generally } \Psi(\mathbf{X}) = \begin{pmatrix} \psi(\mathbf{x}_1)^\top \\ \vdots \\ \psi(\mathbf{x}_n)^\top \end{pmatrix} \text{ where } \psi : \mathbb{R}^{d_1} \rightarrow \mathbb{R}^{d_2}.$$

A formal definition of equivariance

Equivariance

Let Ω_1, Ω_2 be two \mathfrak{G} -sets (of the same group). A function $h : \Omega_1 \rightarrow \Omega_2$ is **\mathfrak{G} -equivariant** if

$$\forall x \in \Omega_1, \forall g \in \mathfrak{G}, h(gx) = gh(x).$$

- ▶ Pay attention to the input/output spaces and the compatibility.
- ▶ Transform the input + apply h = apply h and transform the result.

Laplacian matrix

- ▶ The action of S_n on $\mathbb{R}^{n \times n}$ defined as

$$\sigma \mathbf{A} = (A_{\sigma(i), \sigma(j)})_{ij}$$

- ▶ $\mathcal{L} : S_n(\mathbb{R}) \rightarrow S_n(\mathbb{R})$ which takes a symmetric matrix $\mathbf{A} \in S_n(\mathbb{R})$ and outputs the Laplacian matrix $\mathcal{L}(\mathbf{A}) = \text{diag}(\mathbf{A}\mathbf{1}) - \mathbf{A}$
- ▶ **Show that \mathcal{L} is permutation equivariant.**

Combining them together

Composition of invariant/equivariant functions

Let Ω_1, Ω_2 be \mathfrak{G} -sets.

- ▶ Let $f : \Omega_1 \rightarrow \Omega_2$ be a **\mathfrak{G} -equivariant** function.
- ▶ Let $g : \Omega_2 \rightarrow Y$ be a **\mathfrak{G} -invariant** function.

Then $h = g \circ f$ is **\mathfrak{G} -invariant**.

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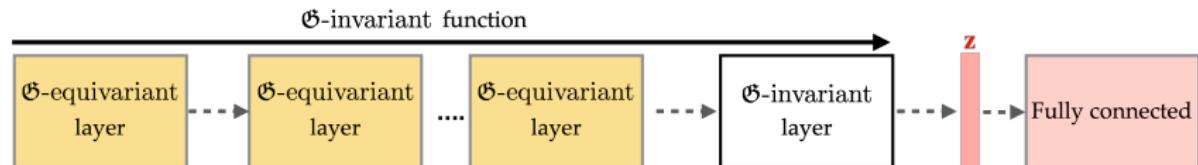
Then $h = g \circ f$ is **\mathfrak{G} -invariant**.

Proof

Indeed with $x \in \Omega_1, g \in \mathfrak{G}$

$$h(gx) = g(f(gx)) = g(gf(x)) = g(f(x)) = (g \circ f)(x) = h(x).$$

Simple but powerful: one of the reason CNNs work so well



Combining them together

Composition of invariant/equivariant functions

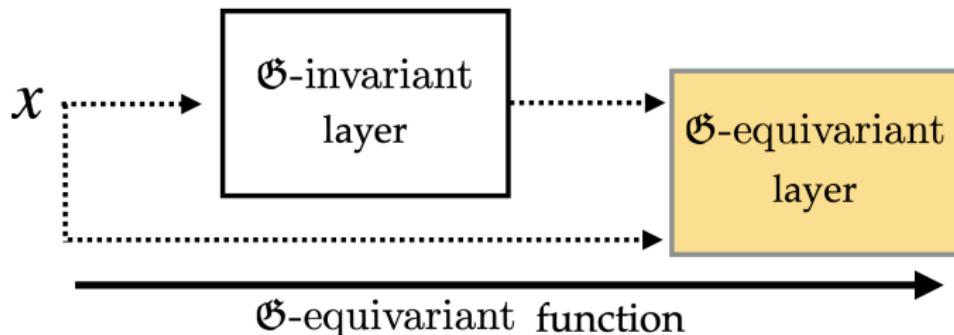
Let Ω_1, Ω_2 be \mathfrak{G} -sets.

- ▶ Let $f : \Omega_1 \times Y \rightarrow \Omega_2$ be a **\mathfrak{G} -equivariant** function **with respect to its first variable** i.e. $\forall y \in \Omega_1, \forall g \in \mathfrak{G}, \forall y \in Y, f(gx, y) = gf(gx, y)$.
- ▶ Let $g : \Omega_1 \rightarrow Y$ be a **\mathfrak{G} -invariant** function.

Then the function h defined by $h(x) = f(x, g(x))$ is **\mathfrak{G} -equivariant**.

Proof

$$h(gx) = f(gx, g(gx)) = f(gx, g(x)) = gf(x, g(x)) = gh(x).$$



Focus on permutation invariance/equivariance

Permutations as matrices

- ▶ Each permutation $\sigma \in S_n$ can be uniquely described as $\mathbf{P}_\sigma \in \{0, 1\}^{n \times n}$.
- ▶ For $\mathbf{A} \in \mathbb{R}^{n \times n}$, the action is $\sigma \mathbf{A} = \mathbf{P}_\sigma \mathbf{A} \mathbf{P}_\sigma^\top$.
- ▶ We define the action of S_n on $\mathbb{R}^{n \times d} \times \mathbb{R}^{n \times n}$ as

$$\sigma(\mathbf{X}, \mathbf{A}) = (\mathbf{P}_\sigma \mathbf{X}, \mathbf{P}_\sigma^\top \mathbf{A} \mathbf{P}_\sigma)$$

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Interpretation

- ▶ A_{ij} = adjacency between nodes described by the i th and j th rows of \mathbf{X} .
- ▶ $\sigma(\mathbf{X}, \mathbf{A})$ permutes the nodes of the graph **and** the features **in the same manner**, indeed:
- ▶ $A_{\sigma(i)\sigma(j)}$ = adjacency between the nodes described by the $\sigma(i)$ th and $\sigma(j)$ th rows of \mathbf{X} .

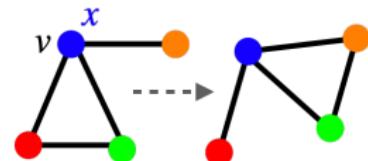


Figure: Is it a valid action of σ ?

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Back to the GNN context

- ▶ In classification/regression $f : G = (\mathbf{X}, \mathbf{A}) \rightarrow y \in Y$ such as $Y = \{+1, -1\}$.
- ▶ For node embeddings $F : G = (\mathbf{X}, \mathbf{A}) \rightarrow \mathbf{Z} \in \mathbb{R}^{n \times k}$

Focus on permutation invariance/equivariance

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Ensuring invariance/equivariance is key when learning on graphs

Find f that are S_n -**invariant**, F that are S_n -**equivariant**.

- ▶ $f(\mathbf{P}_\sigma \mathbf{X}, \mathbf{P}_\sigma^\top \mathbf{A} \mathbf{P}_\sigma) = f(\mathbf{X}, \mathbf{A})$ and $F(\mathbf{P}_\sigma \mathbf{X}, \mathbf{P}_\sigma^\top \mathbf{A} \mathbf{P}_\sigma) = \mathbf{P}_\sigma F(\mathbf{X}, \mathbf{A})$.

Focus on permutation invariance/equivariance

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Examples: equivariance (1/2)

- ▶ Take $\mathbf{X} \in \mathbb{R}^{n \times d_1}$, $\mathbf{W} \in \mathbb{R}^{d_1 \times d_2}$ and a function Ψ that applies **independently on each row** of a matrix.
- ▶ $F(\mathbf{X}, \mathbf{A}) = \Psi(\mathbf{A}\mathbf{X}\mathbf{W})$ is S_n -**equivariant**.

Focus on permutation invariance/equivariance

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- ▶ In particular when Ψ is **element-wise**.

Focus on permutation invariance/equivariance

Ensuring invariance/equivariance is key when learning on graphs

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- ▶ $f(\mathbf{P}_\sigma \mathbf{X}, \mathbf{P}_\sigma^\top \mathbf{A} \mathbf{P}_\sigma) = f(\mathbf{X}, \mathbf{A})$ and $F(\mathbf{P}_\sigma \mathbf{X}, \mathbf{P}_\sigma^\top \mathbf{A} \mathbf{P}_\sigma) = \mathbf{P}_\sigma F(\mathbf{X}, \mathbf{A})$.

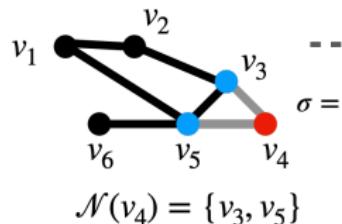
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- ▶ $F(\mathbf{X}, \mathbf{A}) = \Psi(\mathbf{A}\mathbf{X}\mathbf{W})$ is S_n -**equivariant**.
- ▶ In particular when Ψ is **element-wise**.
- ▶ But also $F(\mathbf{X}, \mathbf{A}) = \Psi(G(\mathbf{A})\mathbf{X}\mathbf{W})$ where G is S_n -**equivariant**.
- ▶ E.g. $F(\mathbf{X}, \mathbf{A}) = \Psi(\mathcal{L}(\mathbf{A})\mathbf{X}\mathbf{W})$ where \mathcal{L} computes the Laplacian.
- ▶ E.g. $F(\mathbf{X}, \mathbf{A}) = \Psi(P[\mathcal{L}](\mathbf{A})\mathbf{X}\mathbf{W})$ where P is a polynomial $P[\mathcal{L}] = \sum_m c_m \mathcal{L}^m$.

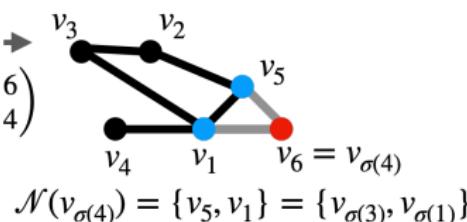
Focus on permutation invariance/equivariance

Examples: equivariance (2/2)

- Take $\mathbf{X} = \begin{pmatrix} \mathbf{x}_1^\top \\ \vdots \\ \mathbf{x}_n^\top \end{pmatrix}$ and define the multiset $X_i := \{\{\mathbf{x}_j : j \in \mathcal{N}(i)\}\}$.
- Then $X_{\sigma(i)} = \{\{\mathbf{x}_{\sigma(j)} : j \in \mathcal{N}(i)\}\}$:



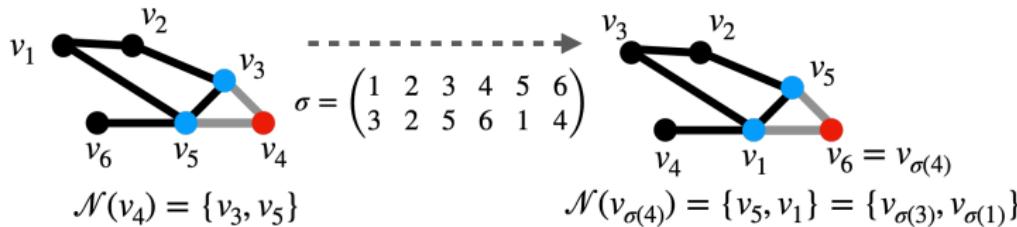
$$\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 3 & 2 & 5 & 6 & 1 & 4 \end{pmatrix}$$



Focus on permutation invariance/equivariance

Examples: equivariance (2/2)

- Take $\mathbf{X} = \begin{pmatrix} \mathbf{x}_1^\top \\ \vdots \\ \mathbf{x}_n^\top \end{pmatrix}$ and define the multiset $X_i := \{\{\mathbf{x}_j : j \in \mathcal{N}(i)\}\}$.
- Then $X_{\sigma(i)} = \{\{\mathbf{x}_{\sigma(j)} : j \in \mathcal{N}(i)\}\}$:



- A function AGGREGATE operating on **multisets of vectors**.
- Then the following function is permutation equivariant.

$$F(\mathbf{X}, \mathbf{A}) = \begin{pmatrix} \psi(\mathbf{x}_1, \text{AGGREGATE}(X_1)) \\ \vdots \\ \psi(\mathbf{x}_n, \text{AGGREGATE}(X_n)) \end{pmatrix}$$

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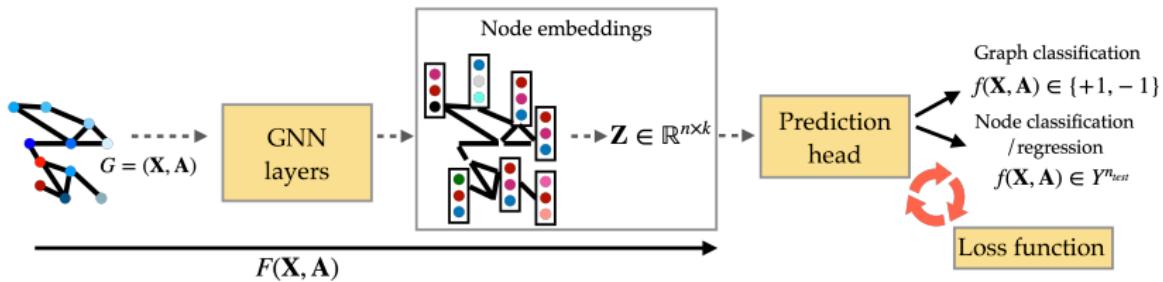
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The training pipeline

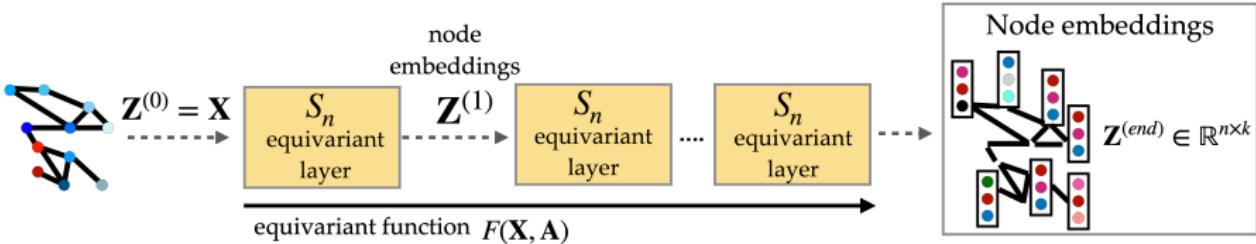


- ▶ Overall the same procedure: find an embedding of the nodes $F(\mathbf{X}, \mathbf{A}) \in \mathbb{R}^{n \times k}$ (supervised or unsupervised) and then do stuff.

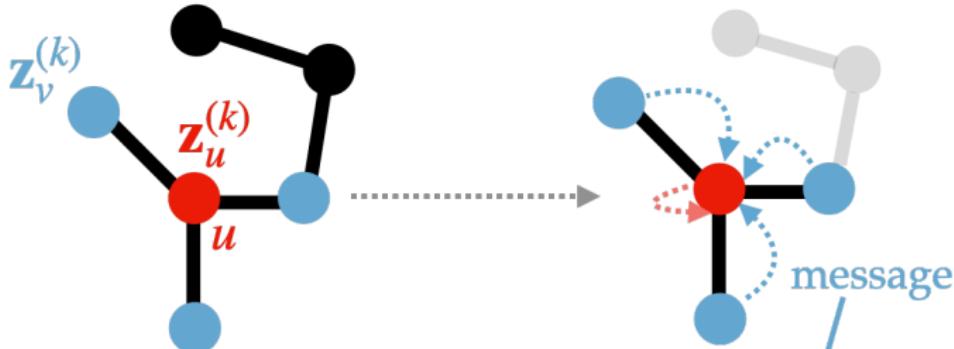
Message-passing for node embeddings

Goal of the message passing framework

- ▶ Defines specific S_n -equivariant layers/functions.
- ▶ Can be used for node embeddings.
- ▶ Usually $\mathbf{Z}^{(0)} = \mathbf{X}$ but when no node features are available several options (e.g. node statistics).
- ▶ Notation: $\mathbf{z}_u^{(k)}$ is the embedding of the node $u \in V$ at the k -layer.



The message passing framework



$$\mathbf{z}_u^{(k+1)} = \text{COMBINE}^{(k)} \left(\mathbf{z}_u^{(k)}, \text{AGGREGATE}^{(k)} \left(\{\{\mathbf{z}_v^{(k)} : v \in \mathcal{N}(u)\}\} \right) \right)$$

One of the most used GNN framework in practice

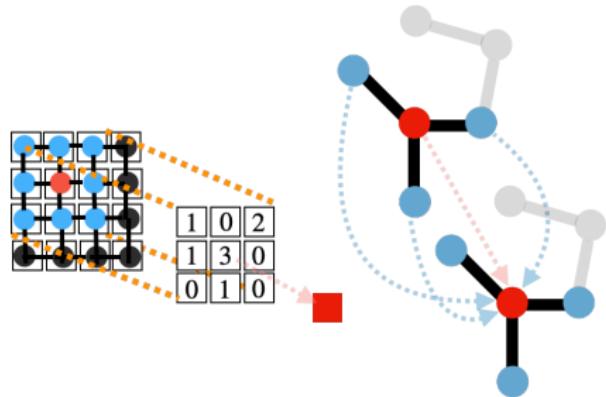
- ▶ At each iteration, **every node aggregates information from its local neighborhood.**
- ▶ A zoo of methods for different COMBINE, AGGREGATE functions.
- ▶ Why is this defining a permutation equivariant layer ?

The message passing framework

Similarities with CNN

- ▶ One layer of message-passing GNN shares similarities to convolutional layers.
- ▶ Usually it takes the form

$$\mathbf{z}_u^{(k+1)} = \phi \left(\sum_{v \in \mathcal{N}(u) \cup \{u\}} \alpha_{uv} \mathbf{z}_v^{(k)} \right).$$

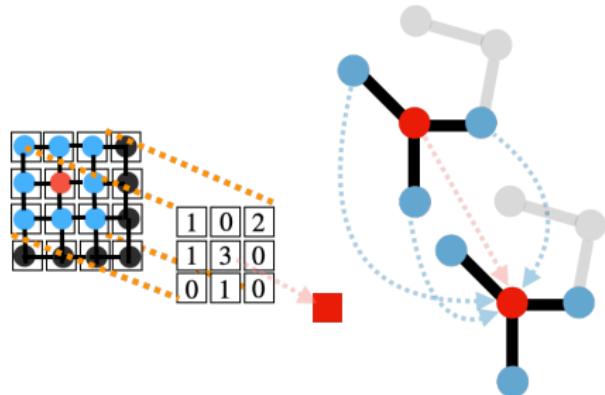


The message passing framework

Similarities with CNN

- ▶ One layer of message-passing GNN shares similarities to convolutional layers.
- ▶ Usually it takes the form

$$\mathbf{z}_u^{(k+1)} = \phi \left(\sum_{v \in \mathcal{N}(u) \cup \{u\}} \alpha_{uv} \mathbf{z}_v^{(k)} \right).$$



k-hop neighbourhood

After k -steps each node has received the informations from its k -hop neighbourhood.

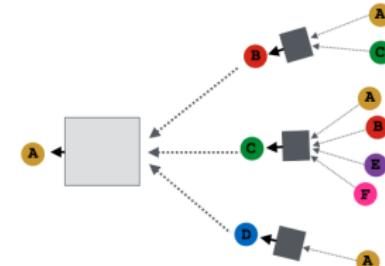
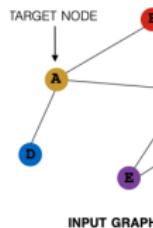


Figure: From Jure Leskovec course *Machine Learning with Graphs*.

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A first GNN with message passing

Sum/mean aggregation (Scarselli et al. 2008)

A first idea would be

$$\mathbf{z}_u^{(k+1)} = \phi(\mathbf{W}_{\text{self}}^{(k)} \mathbf{z}_u^{(k)} + \mathbf{W}_{\text{neigh}}^{(k)} \sum_{v \in \mathcal{N}(u)} \mathbf{z}_v^{(k)} + \mathbf{b}^{(k)})$$

- ▶ $\mathbf{W}_{\text{self}}^{(k)}, \mathbf{W}_{\text{neigh}}^{(k)} \in \mathbb{R}^{d_{k+1} \times d_k}$ are matrices of **learnable parameters**.
- ▶ Do not depend on the number of nodes ! .
- ▶ Complexity of computing it for all nodes is $O(|E|)$.
- ▶ $\mathbf{b}^{(k)} \in \mathbb{R}^{d_{k+1}}$ is a bias term (often omitted to simplify notations).
- ▶ ϕ is a pointwise non-linearity such as ReLu.

Questions

- ▶ What is COMBINE, AGGREGATE ?
- ▶ Write this in matrix form.

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Answers

- ▶ What is COMBINE, AGGREGATE ?
- ▶ $\forall k, \text{AGGREGATE}^{(k)}(\{\{\mathbf{z}_v : v \in \mathcal{N}(u)\}\}) = \sum_{v \in \mathcal{N}(u)} \mathbf{z}_v$.
- ▶ $\text{COMBINE}^{(k)}(\mathbf{z}_1, \mathbf{z}_2) = \mathbf{W}_{\text{self}}^{(k)} \mathbf{z}_1 + \mathbf{W}_{\text{neigh}}^{(k)} \mathbf{z}_2 + \mathbf{b}^{(k)}$.

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Answers

- ▶ Write this in matrix form.

$$\mathbf{Z}^{(k+1)} = \phi \left(\mathbf{A} \mathbf{Z}^{(k)} \mathbf{W}_{\text{neigh}}^{(k)} + \mathbf{Z}^{(k)} \mathbf{W}_{\text{self}}^{(k)} + \begin{pmatrix} \mathbf{b}^{(k)} \\ \vdots \\ \mathbf{b}^{(k)} \end{pmatrix} \right).$$

Graph convolutional neural networks

Most popular baseline model

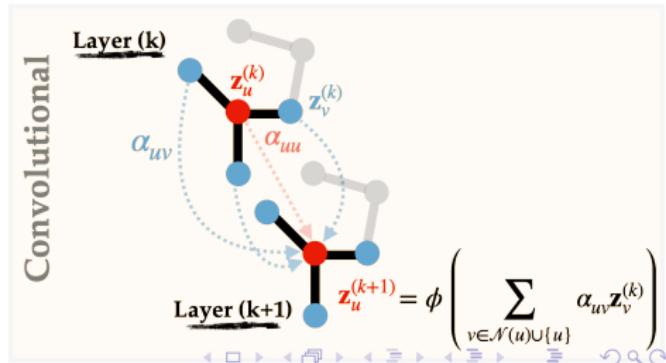
Introduced by Kipf and Welling 2016 for semi-supervised node classification.

$$\mathbf{z}_u^{(k+1)} = \text{Relu}(\mathbf{W}_{\text{self}}^{(k)} \mathbf{z}_u^{(k)} + \mathbf{W}_{\text{neigh}}^{(k)} \frac{1}{\sqrt{|\mathcal{N}(u)|}} \sum_{v \in \mathcal{N}(u)} \frac{\mathbf{z}_v^{(k)}}{\sqrt{|\mathcal{N}(v)|}})$$

- ▶ Also GraphSage framework (William L. Hamilton, R. Ying, and Leskovec 2018).
- ▶ What is COMBINE, AGGREGATE ?

In matrix form

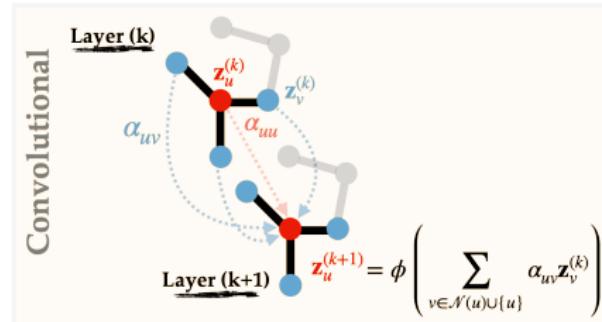
- ▶ With $\mathbf{W}_{\text{self}} = \mathbf{W}_{\text{neigh}}$, $\mathbf{Z}^{(k+1)} = \text{Relu} \left((\mathbf{I} + \mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}}) \mathbf{Z}^{(k)} \mathbf{W}^{(k)} \right)$.
- ▶ First-order approximation of localized spectral filters on graphs.



Graph Attention Networks

Motivations

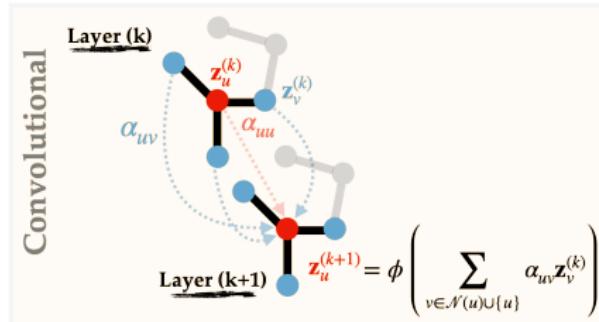
- ▶ In many MP-GNN layers weights of the convolutions **are fixed**.
- ▶ What if we also learn them ?
- ▶ Learn the importance of the neighbours contributions.



Graph Attention Networks

Motivations

- ▶ In many MP-GNN layers weights of the convolutions **are fixed**.
- ▶ What if we also learn them ?
- ▶ Learn the importance of the neighbours contributions.



GAT networks (Veličković et al. 2017)

$$\mathbf{z}_u^{(k+1)} = \text{Relu}(\mathbf{W}^{(k)} \sum_{v \in \mathcal{N}(u) \cup \{u\}} \alpha_{uv} \mathbf{z}_v^{(k)})$$

- ▶ Here α_{uv} are **learnable weights**.
- ▶ $e_{uv} = \text{NN}(\Theta_1 \mathbf{z}_u, \Theta_2 \mathbf{z}_u)$ with learnable matrices Θ_1, Θ_2 and

$$\alpha_{uv} = \text{softmax}_v(e_{uv}) = \frac{\exp(e_{uv})}{\sum_{v' \in \mathcal{N}(u)} e_{uv'}}$$

- ▶ It is based on attention mechanisms (Vaswani et al. 2023).

Graph Isomorphism Networks (GIN)

The problem of injectivity

Xu et al. 2019 provide a detailed discussion of the relative power of GNN.

- ▶ One interesting property is **injectivity** of COMBINE, AGGREGATE.
- ▶ They propose

$$\mathbf{z}_u^{(k+1)} = \text{MLP}^{(k)} \left((1 + \theta^{(k)}) \mathbf{z}_u^{(k)} + \sum_{v \in \mathcal{N}(u)} \mathbf{z}_v^{(k)} \right)$$

- ▶ MLP : $\mathbb{R}^{d_k} \rightarrow \mathbb{R}^{d_{k+1}}$ is a fully connected neural-network.

Spectral GNN

Learning filters

Originally introduced by Bruna et al. 2013. The idea is

$$\mathbf{Z}^{(k+1)} = \text{Relu}(P[\mathcal{L}](\mathbf{A})\mathbf{Z}^{(k)}\mathbf{W}^{(k)})$$

- ▶ $\mathcal{L}(\mathbf{A}) = \text{diag}(\mathbf{A}\mathbf{1}) - \mathbf{A}$ is the Laplacian (or normalized version).
- ▶ $P[\mathcal{L}] = \sum_{m=0}^M c_m \mathcal{L}^m$ is a **learnable** polynomial of the Laplacian operator.
- ▶ As $\mathcal{L}(\mathbf{A}) = \mathbf{U}\Lambda\mathbf{U}^\top$, $P[\mathcal{L}](\mathbf{A}) = \mathbf{U}P[\Lambda]\mathbf{U}^\top$.
- ▶ Connections with the Fourier transform on graphs: $P[\mathcal{L}]$ acts as a filter.

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Limitations

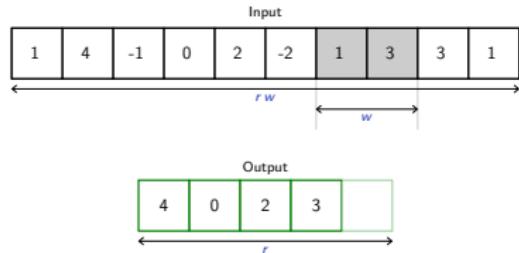
- ▶ Complexity in $O(|V|^3)$ (eigen-decomposition).
- ▶ Any perturbation to a graph results in a change of eigenbasis \mathbf{U} .
- ▶ Learned filters are domain dependent.
- ▶ Alternative ChebNet Defferrard, Bresson, and Vandergheynst 2017 relies on Chebyshev polynomials for computing in $O(|E|M)$.

Graph pooling

Pooling layers in neural networks

At the core of many NN architectures.

- ▶ Most standard type is **max-pooling**.
- ▶ ↓ the number of parameters to learn.
- ▶ Improves robustness.

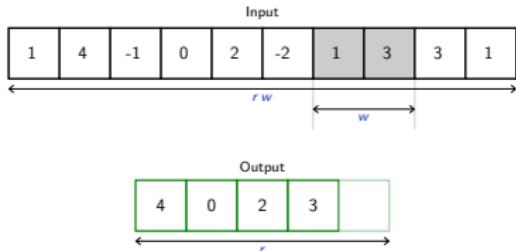


Graph pooling

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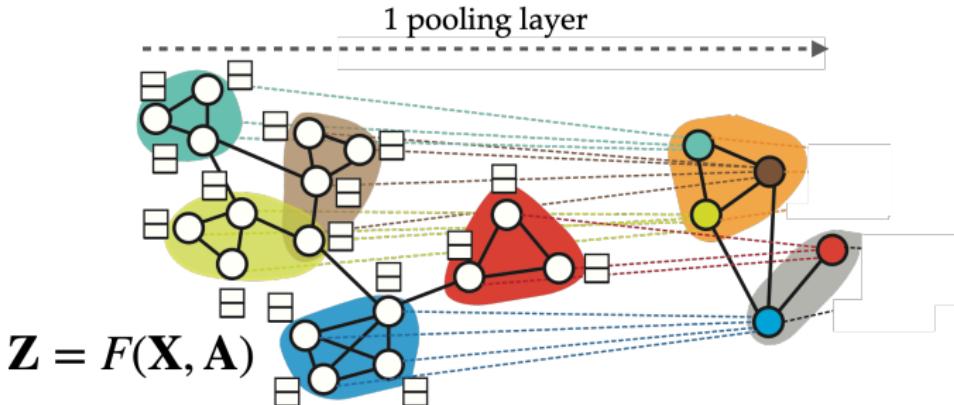
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Pooling in GNN

Equivalent to down-sampling = reducing the number of nodes.



Learning at the graph level

- ▶ The neural message passing approach produces a set of node embeddings $F(\mathbf{X}, \mathbf{A}) = \mathbf{Z} \in \mathbb{R}^{n \times k}$.
- ▶ What about predictions at the graph level ? E.g. in graph classification.
- ▶ **We want one embedding for the entire graph \mathbf{z}_G .**
- ▶ It should be a permutation invariant function $f(\mathbf{X}, \mathbf{A})$.
- ▶ E.g. global average pooling $\mathbf{z}_G = f(\mathbf{X}, \mathbf{A}) = \frac{1}{|V|} \sum_{u \in V} \mathbf{z}_u \in \mathbb{R}^k$.

Diffpool

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Better idea: hierarchical pooling (Z. Ying et al. 2018)

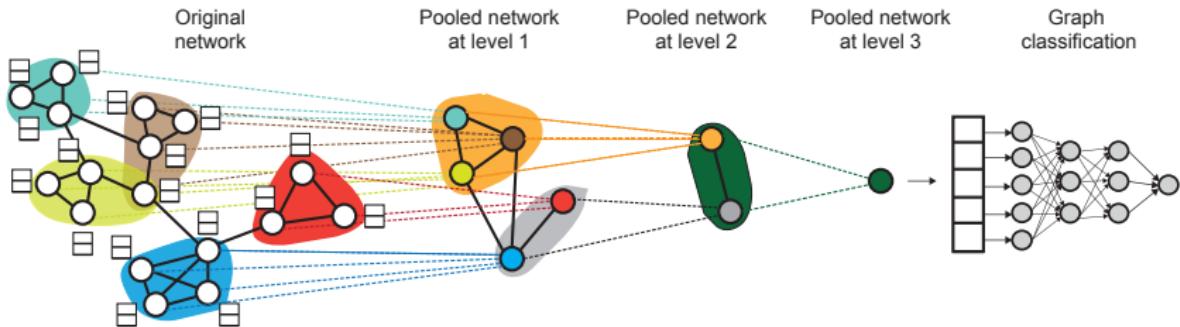


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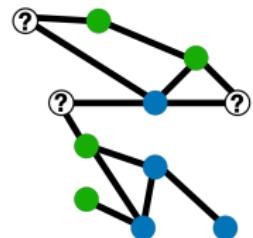
Applications

Node classification

- ▶ **One graph** G where each node has a class.

Train GNNs in a fully-supervised manner by minimizing

$$\mathcal{L} = \sum_{u \in V_{train}} -\log(\text{softmax}(\mathbf{z}_u, \mathbf{y}_u))$$



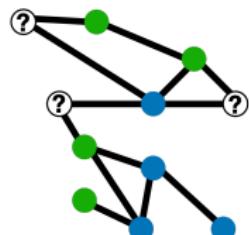
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Graph classification

- **Many graphs** G_1, \dots, G_n associated with classes $(y_{G_i})_i$.

Train GNNs in a fully-supervised manner by minimizing

$$\mathcal{L} = \sum_{G \in T_{train}} \ell(\text{MLP}(\mathbf{z}_G), y_G)$$

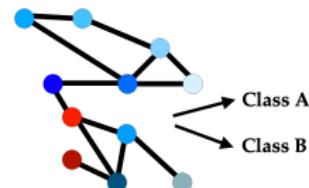


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Connection with the WL test

WL algorithm and MP-GNN

- ▶ WL algorithm and the message passing GNN approach are very similar.
- ▶ Iteratively aggregate information from local node neighborhoods.

Connection with the WL test

WL algorithm and MP-GNN

- ▶ WL algorithm and the message passing GNN approach are very similar.
- ▶ Iteratively aggregate information from local node neighborhoods.

Message passing neural networks are not that powerful ?

- ▶ Consider a MP-GNN with K layers

$$\mathbf{z}_u^{(k+1)} = \text{COMBINE}^{(k)} \left(\mathbf{z}_u^{(k)}, \text{AGGREGATE}^{(k)} \left(\{\{\mathbf{z}_v^{(k)} : v \in \mathcal{N}(u)\}\} \right) \right)$$

- ▶ Suppose that discrete node labels $\mathbf{Z}^{(0)} = \mathbf{X} \in \mathbb{Z}^{n \times d}$.
- ▶ Then Xu et al. 2019 show that

$\mathbf{z}_u^{(K)} \neq \mathbf{z}_v^{(K)} \iff$ labels of u and v are \neq after K iter. of the WL algorithm.

- ▶ If the WL test cannot distinguish between G_1, G_2 , then MP-GNN also incapable of doing it.
- ▶ Ability of solving isomorphism = good measure of “expressivity” ?

Other limitations

- ▶ **The oversmoothing problem:** if too many layers of MP-GNN, the node features tend to converge to a non-informative limit.

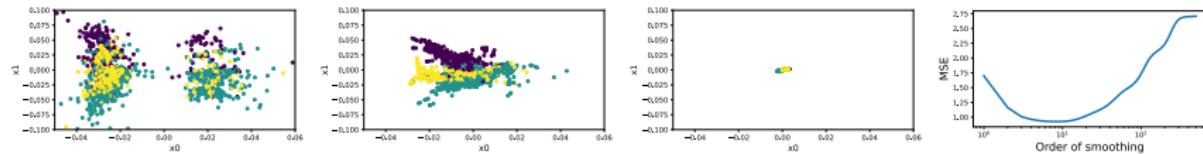


Figure: From Keriven 2022

- ▶ **Heterophily vs homophilie:** neighbours should have similar embeddings ? ([Luan et al. 2022](#)).

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Conclusion

- ▶ Flexible: graph/node/edge classification, semi-supervised learning, link prediction...
- ▶ Generally state-of-the-art, but...
- ▶ ... sometimes do not work “that well” (compared to other DL)
- ▶ Simple methods may perform better but might be “forgotten” in benchmarks
- ▶ Room for improvement (many interesting challenges), but conventional DL wisdom might not hold
- ▶ Arguably, no real “ImageNet moment” yet for GNNs -*i* several recent initiatives for bigger datasets and more complex tasks (eg Open Graph Benchmark)

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