Machine learning for graphs and with graphs

Graph neural networks

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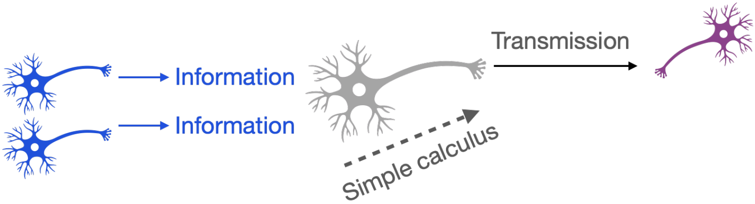
What is a neural network ?

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

Built upon a biological analogy Rosenblatt 1958



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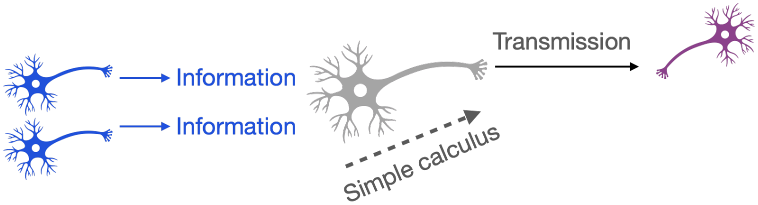
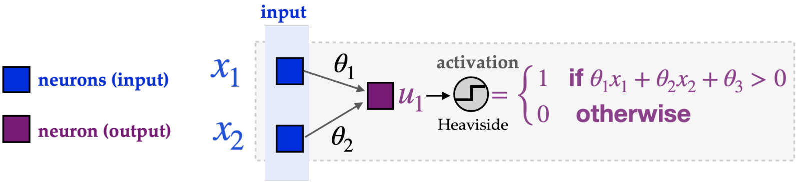


- First example $f(\mathbf{x} = (x_1, x_2)) = \text{activation}(\theta_1 x_1 + \theta_2 x_2 + \theta_3)$:



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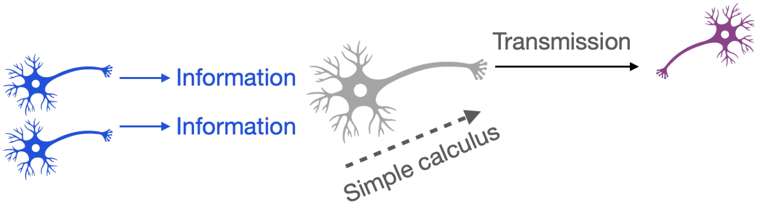

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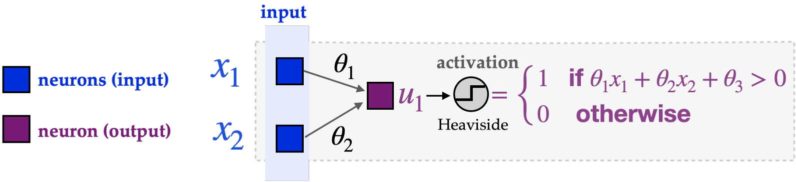
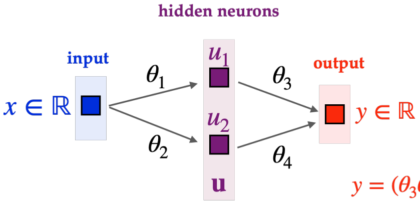


What is a neural network ?

Feed-forward neural networks

- Linear neural network:



bias

$$u_1 = \theta_1 x + b_1$$
$$u_2 = \theta_2 x + b_2$$
$$y = \theta_3 u_1 + \theta_4 u_2 + b_3$$
$$y = \theta_3(\theta_1 x + b_1) + \theta_4(\theta_2 x + b_2) + b_3$$

$$y = (\theta_3\theta_1 + \theta_4\theta_2)x + \theta_3 b_1 + \theta_4 b_2 + b_3$$

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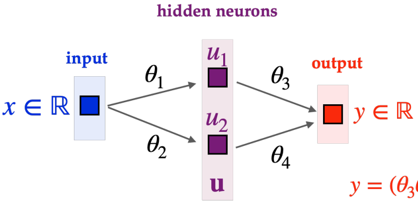

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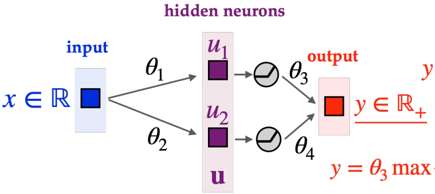

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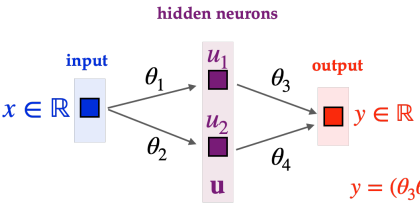

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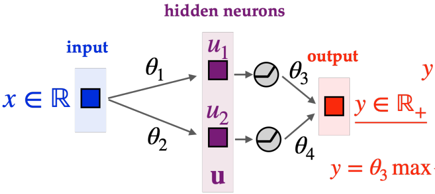

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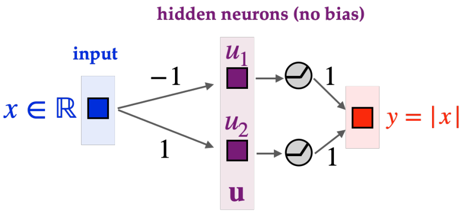
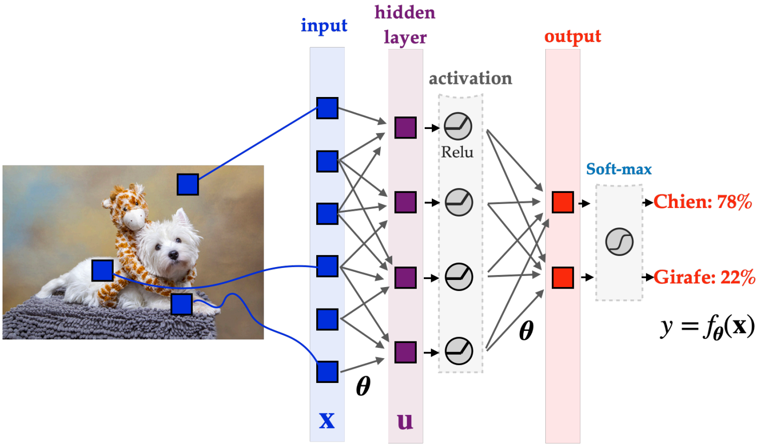


$u_1 = -x$
$u_2 = x$
$y = \max\{u_1, 0\} + \max\{u_2, 0\}$
$y = \max\{x, 0\} + \max\{-x, 0\}$

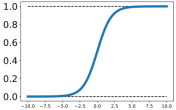
What is a neural network ?

Feed-forward neural networks



Soft-max:

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



What is a neural network ?

Feed-forward neural networks

- Feed-forward NN are function of the form

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

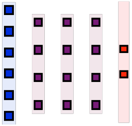
where $T_k(\mathbf{z}) = \mathbf{W}^{(k)}\mathbf{z} + \mathbf{b}^{(k)}$

and σ_k pointwise activation function.

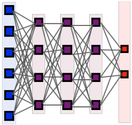
- All the weights: $\boldsymbol{\theta} = (\mathbf{W}^{(1)}, \cdots, \mathbf{W}^{(K)}, \mathbf{b}^{(1)}, \cdots \mathbf{b}^{(K)})$.
- Depending on the task the output of a NN is also transformed $g(\mathbf{x}) = \text{norm}(f(\mathbf{x}))$.
- E.g. $f : \mathbb{R}^d \to \mathbb{R}$ and $g : \mathbb{R}^d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

What is a neural network ?

A zoo of architectures

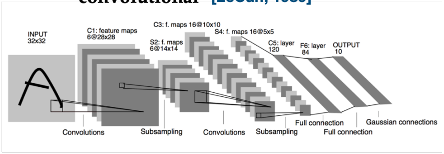


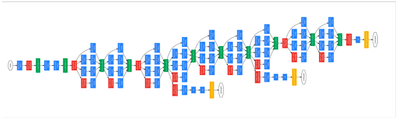
multi-layers



fully-connected

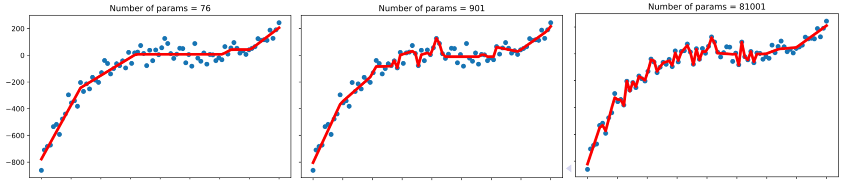
convolutional [LeCun, 1989]





deep-learning **also: generative, recurrent, transformers, attention layer transformers...**

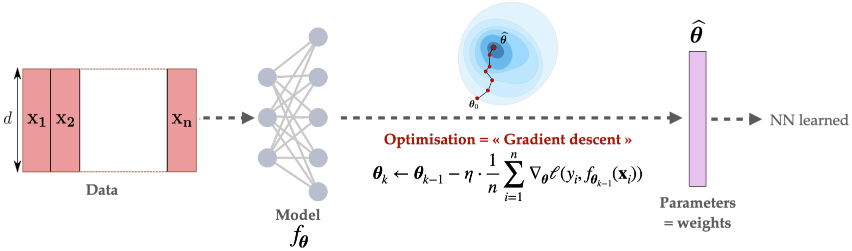
Richness of neural network



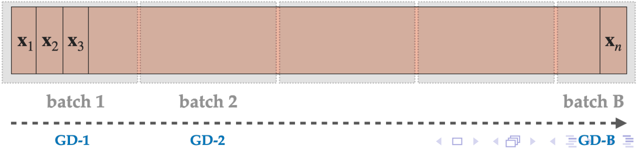
Neural network in practice

The (very) big picture

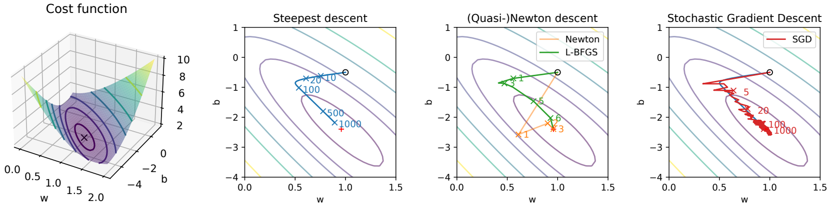
Find the weights that minimizes the empirical minimization loss.



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



(almost) All optimization in one slide



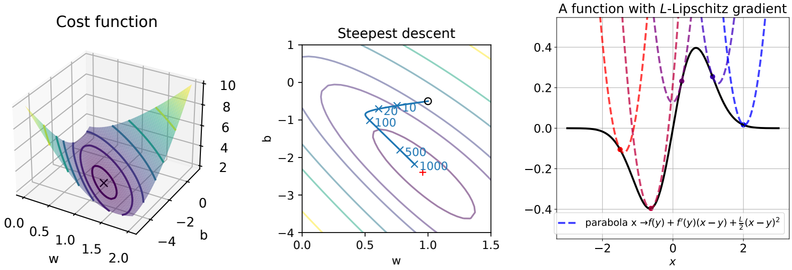
Principle

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

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

  where μ_k is a step and $\mathbf{d}_k$ is a descent direction $\mathbf{d}_k^\top \nabla J(\boldsymbol{\theta}^{(k)}) < 0$.
- Classical descent directions are :
  - **Steepest descent**: $\mathbf{d}_k = -\nabla J(\boldsymbol{\theta}^{(k)})$ (a.k.a. Gradient descent).
  - (Quasi) **Newton**: $\mathbf{d}_k = -(\nabla^2 J(\boldsymbol{\theta}^{(k)}))^{-1} \nabla J(\boldsymbol{\theta}^{(k)})$, $\nabla^2 J$ is the Hessian.
  - **Stochastic Gradient Descent** : $\mathbf{d}_k = -\tilde{\nabla} J(\boldsymbol{\theta}^{(k)})$ 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 $J : \mathbb{R}^D \to \mathbb{R}$ with L-Lipschitz gradient[1] and $J^\star := \min_{\boldsymbol{\theta}} \ J(\boldsymbol{\theta}) > -\infty$. Then, provided that $0 < \mu_k < \frac{2}{L}$, the iterations $\boldsymbol{\theta}^{(k+1)} = \boldsymbol{\theta}^{(k)} - \mu_k \nabla J(\boldsymbol{\theta}^{(k)})$ satisfy

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

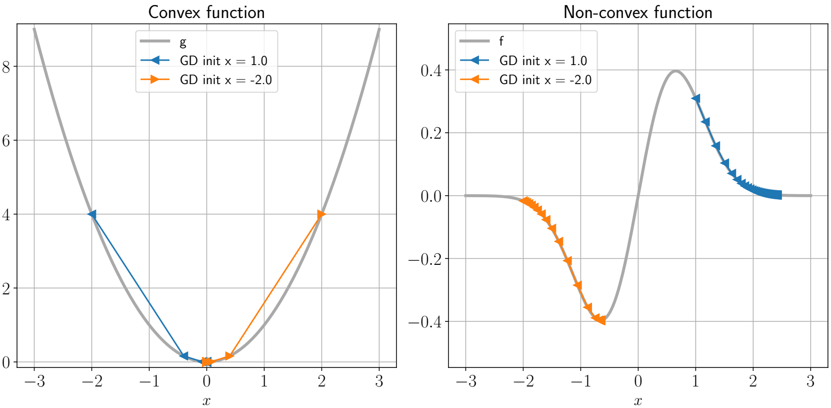
$$\lim_{k \to +\infty} \nabla J(\boldsymbol{\theta}^{(k)}) = \mathbf{0} \text{ (critical point)}$$

[1] it means that $\forall \boldsymbol{\theta}_1, \boldsymbol{\theta}_2 \in \mathbb{R}^d, \ \|\nabla J(\boldsymbol{\theta}_1) - \nabla J(\boldsymbol{\theta}_2)\|_2 \leq L \|\boldsymbol{\theta}_1 - \boldsymbol{\theta}_2\|_2$.

(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 $h_{\boldsymbol{\theta}}$ s.t. $\mathbb{P}(y = +1|\mathbf{x}) \approx h_{\boldsymbol{\theta}}(\mathbf{x})$.
- Bayes decision: $f(\mathbf{x}) = \text{sign}(\mathbb{P}(y = +1|\mathbf{x}) - \mathbb{P}(y = -1|\mathbf{x})) \in \{-1, +1\}$.

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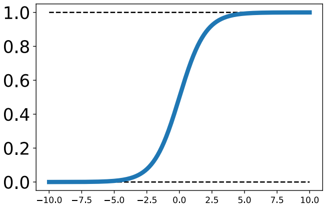
The sigmoid function

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



- Usually used to model probabilities.

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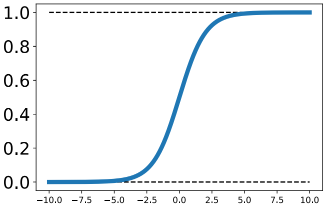
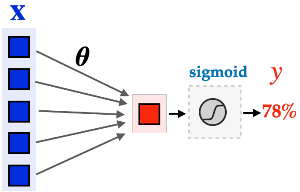


- Usually used to model probabilities.

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 is also a one layer neural-network (no hidden layer).



First simple neural network: logistic regression

One property

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

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

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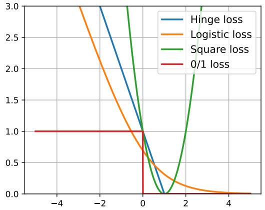

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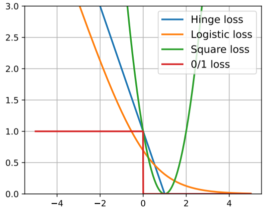

And so ?

- Logistic regression = fitting $f(\mathbf{x}) = \boldsymbol{\theta}^\top \mathbf{x} + b$ with the logistic loss.
- The decision/prediction of the label is $\mathrm{sign}(f(\mathbf{x}))$.
- So it is a **linear decision boundary** (linear classification).

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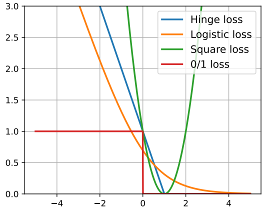

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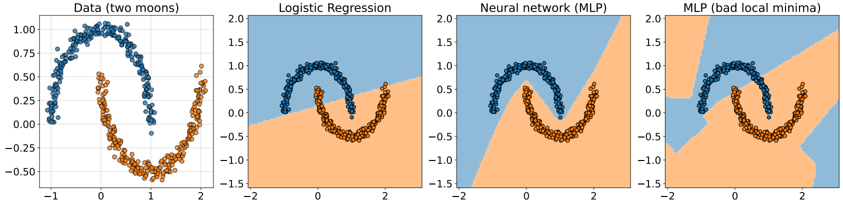

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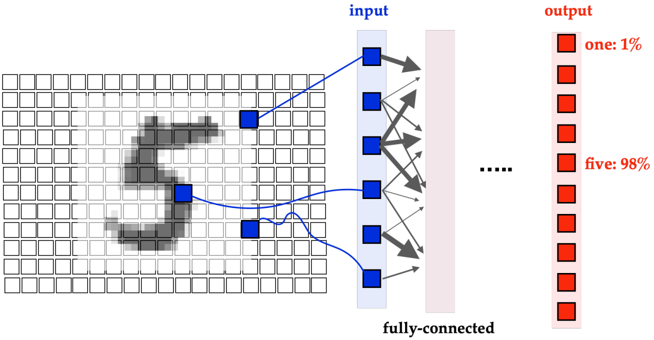
Convolutional neural networks

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

What could happen with a fully-connected architecture?



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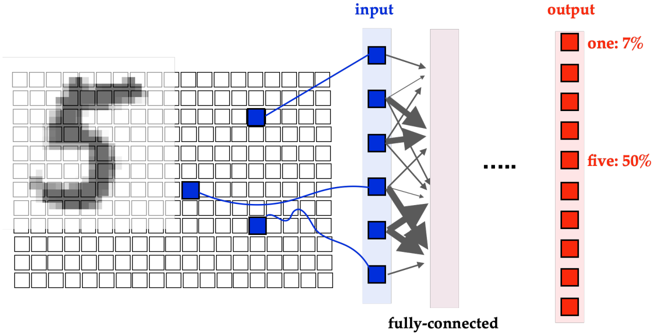

- We want a function that doesn't change if we only translate the image. We want a **translation invariant function**.
- Convolution: particular structure on the weights that induce **translation equivariance**.

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

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

- **Translate a filter** h and then take the inner product with[2] 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] $\tau_x f = t \to f(t-x)$

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Convolution/correlation of functions

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

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

- **Translate a filter** h and then take the inner product with[2] 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.
- It is **translation equivariant**.

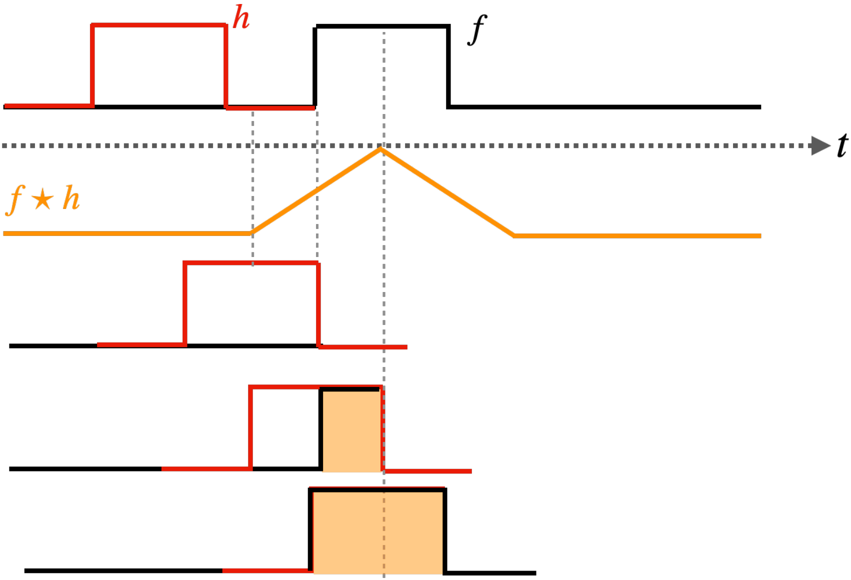
$$(\tau_x f) * h = \tau_x (f * h)$$

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

---

[2] $\tau_x f = t \to f(t-x)$

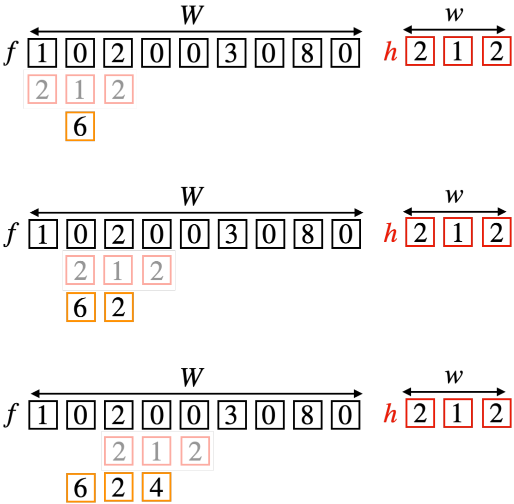
Convolutional neural networks



Convolutional neural networks

In practice convolutions are applied on discrete signals.

Discrete convolutions in 1D



Question: size of the output ?

Convolutional neural networks

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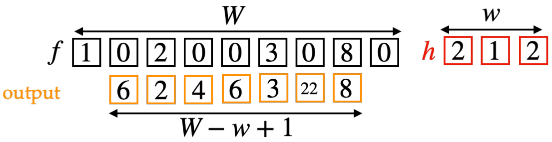
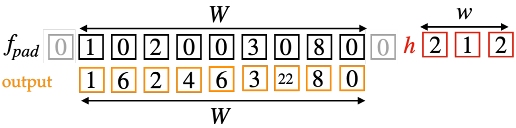


- Padding strategies can be used to have output of the same size.

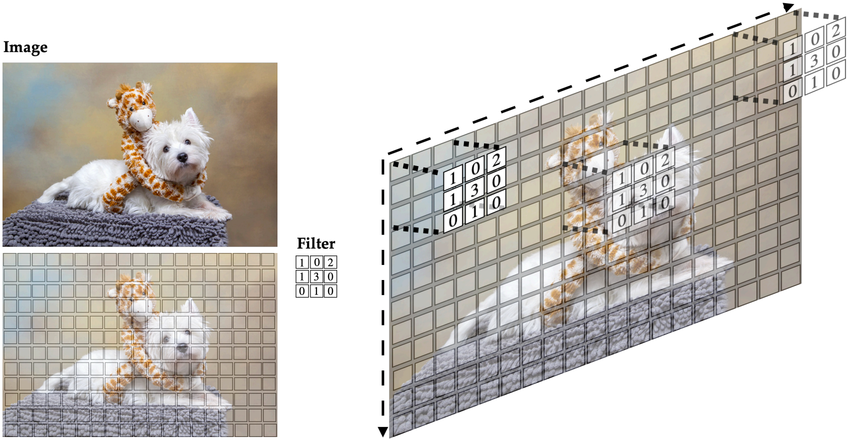


- Also stride can be used to move the filter from more than one pixel.

Convolutional neural networks

Discrete convolutions **not** in 1D

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



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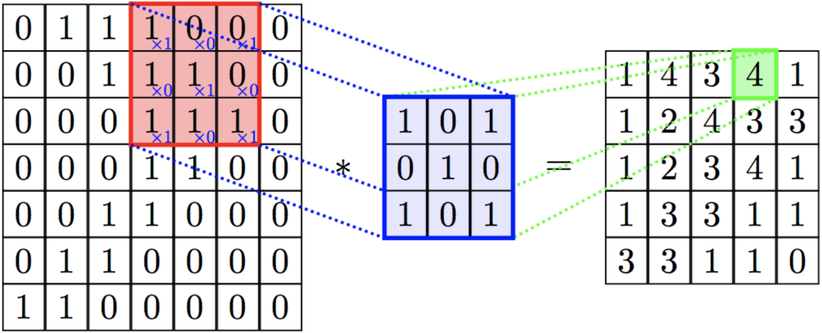

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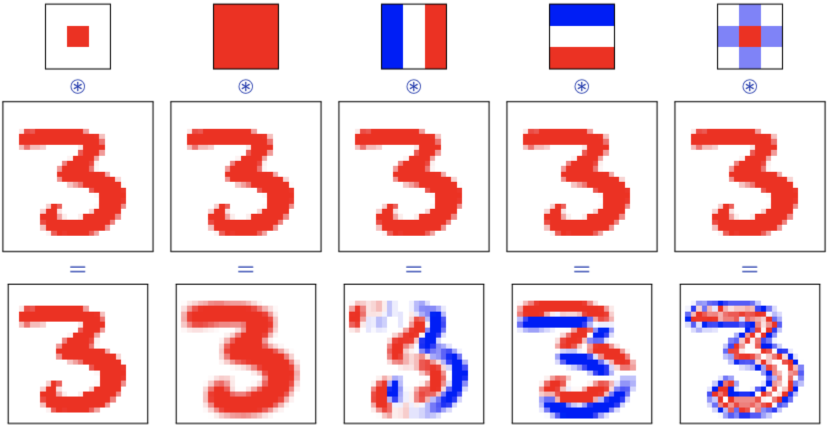

Figure: From Franccois Fleuret `https://fleuret.org/dlc/`

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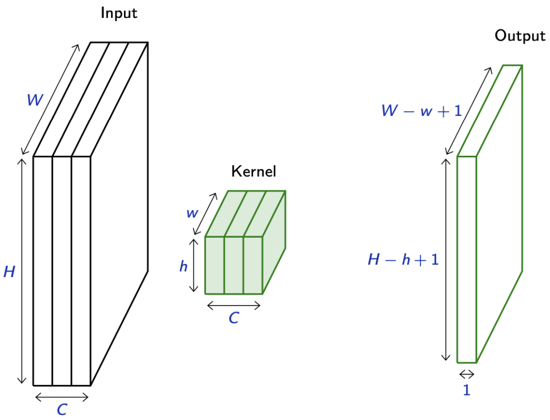

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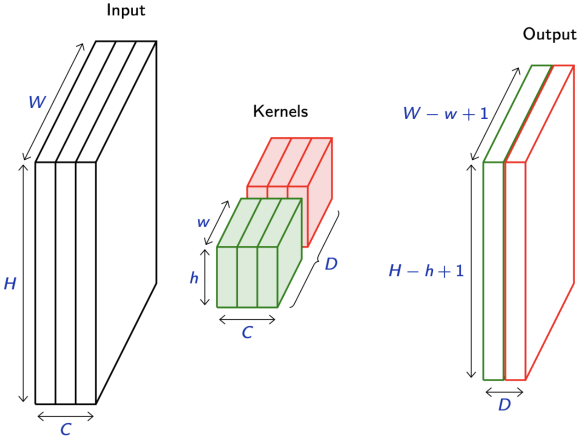

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Convolutional neural networks

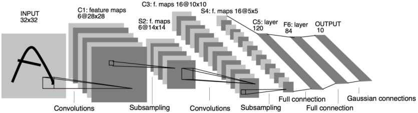

Figure: LeNet from LeCun et al. 1998

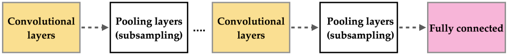

Figure: Schematic view

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).

Conclusion

- Deep learning: in almost everything when there are images.
- Very versatile: learn complex functions.
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- Side note: still struggles on tabular data (Grinsztajn, Oyallon, and Varoquaux 2022).

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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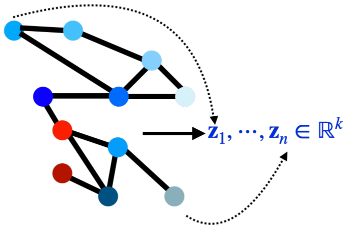
Objective

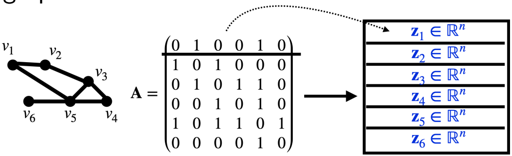
A chronological start

- Idea: to learn on a graph: nodes $\rightarrow$ vector $\rightarrow$ 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.



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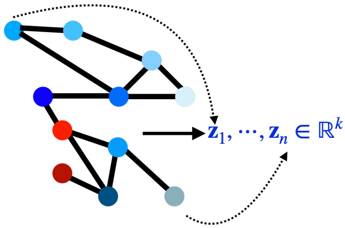

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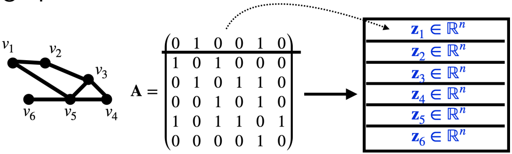


- Sensitive to the node ordering ! Also, expensive $O(|V|)$!
- Not applicable to graph with different sizes !

An encoder-decoder perspective

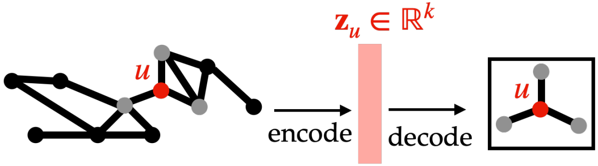
Notations

- 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 $E : V \to \mathbb{R}^k$ such that $E(u) = \mathbf{z}_u$.

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



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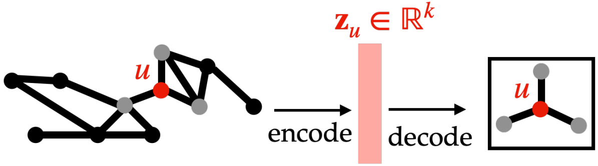


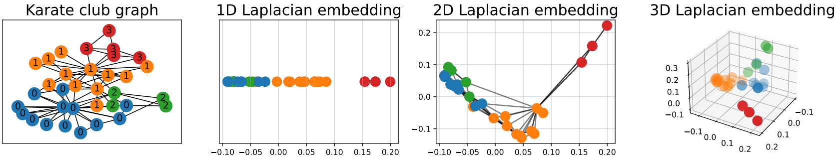
Encoding/decoding scheme

A lot of methods attempt to minimize

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

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

Unsupervised node embeddings techniques



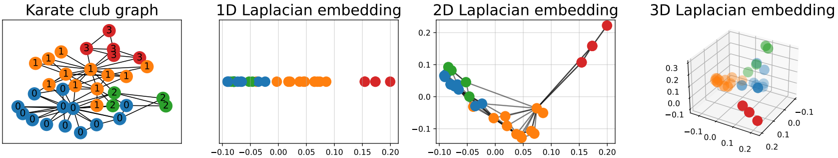
Inspiration from Laplacian eigenmaps Belkin and Niyogi 2003

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

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

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

Unsupervised node embeddings techniques



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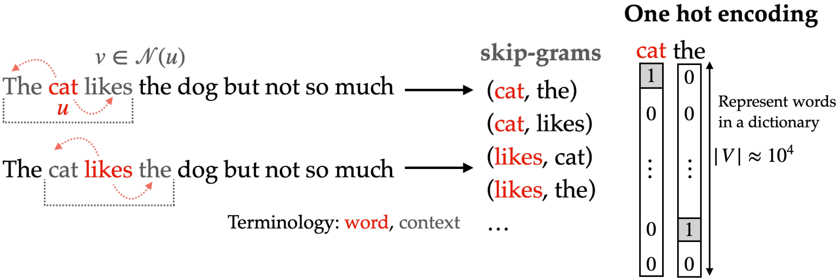
- Normalized Laplacian $\widetilde{\mathbf{L}} = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2}$.
- Interpretation + permutation equivariance of the cost (on the board).
- With the constraint $\mathbf{Z}^\top\mathbf{Z} = \mathbf{I}_d$ it recovers Laplacian eigenmaps.
- Sol. is the d eigenvectors associated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

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 $\mathbb{P}(\text{context}|\text{input word})$.



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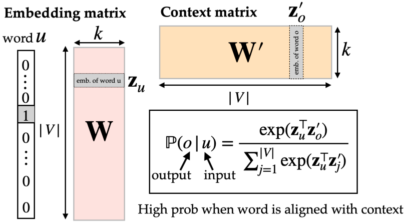

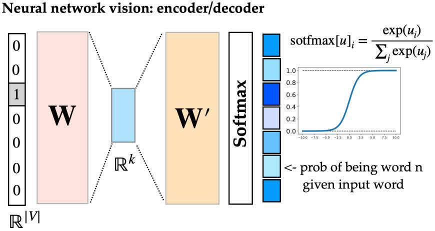

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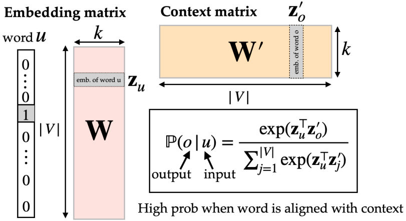
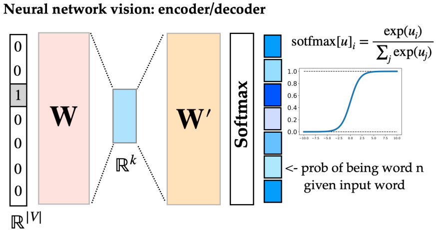




- Dataset $\mathcal{D}$ of input/output words (surrounding). Loss to minimize is:

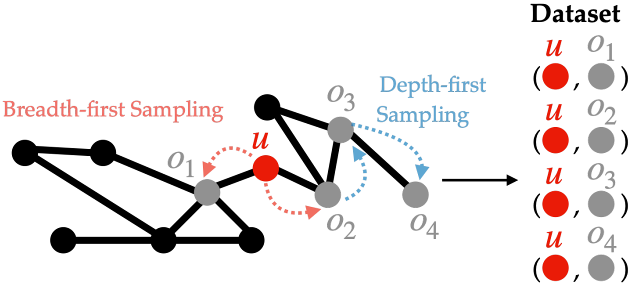
$$- \sum_{(u,o)\in\mathcal{D}} \log \mathbb{P}(o|u)\,.$$

- 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:

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

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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 draws 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 $\sigma(x) = \dfrac{1}{1 + \exp(-x)}$.

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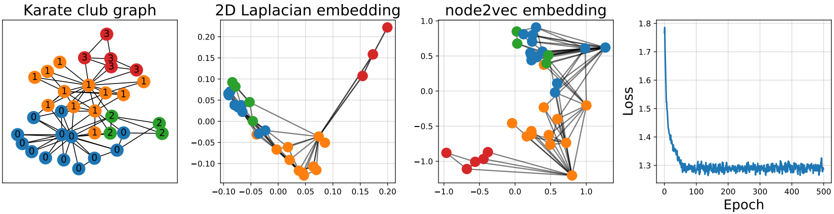

Unsupervised node embeddings techniques

Limitations of previous embeddings techniques

- The previous embeddings are called **shallow**: encoder function $E : V \to \mathbb{R}^k$ 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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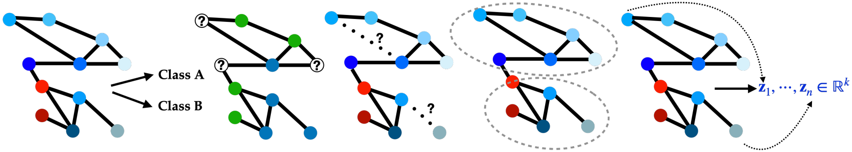
Frameworks considered here

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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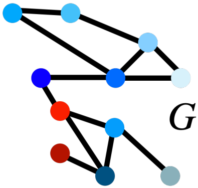
What is a graph neural network ?

Framework

- 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 $\mathbf{x}_i \in \mathbb{R}^d$.



$G = (\mathbf{X}, \mathbf{A})$

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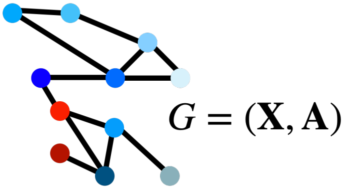
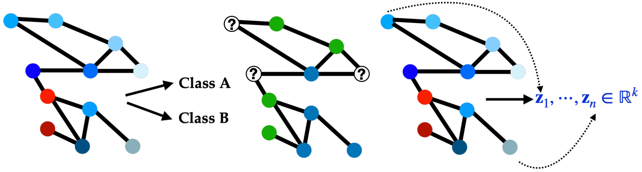


GNN general definition

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).

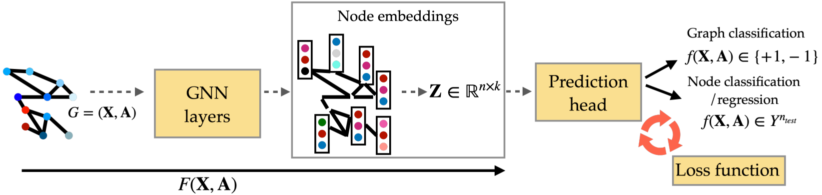
- It is made of a **combination of different layers**.
- Graph classification, node classification/regression, node embedding



- 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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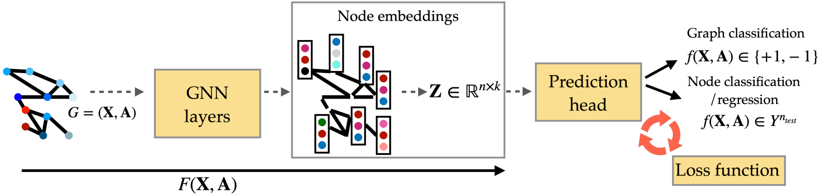

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Properties to ensure

- 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

The right symmetries can facilitate learning

- Fit a polynomial $\hat{f}(x) = \sum_{n=0}^{N} \theta_n x^n$ on

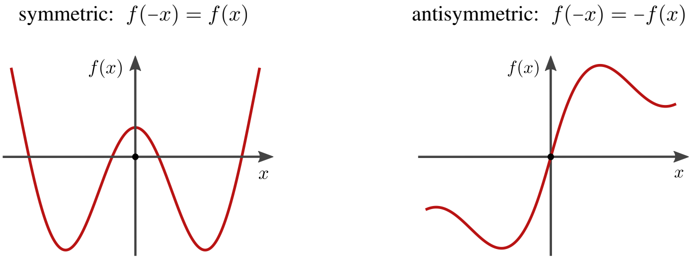

Figure: From Weiler et al. 2023

- Ignore prior knowledge about the function.
- Better: fit $\sum_{n \text{ even}}^{N} \theta_n x^n$ (invariant) or $\sum_{n \text{ odd}}^{N} \theta_n x^n$ (equivariant).
- Need half of the parameters + generalize well.

On invariance and equivariance

On the previous episodes

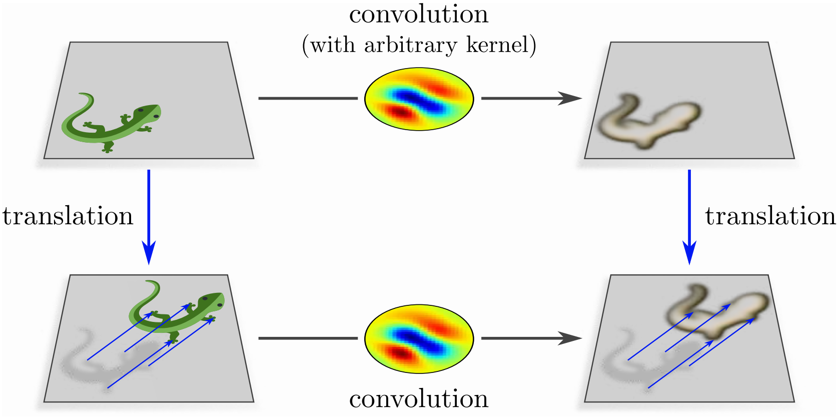

Figure: From Weiler et al. 2023

On invariance and equivariance

A little bit of group theory

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

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

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

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A little bit of group theory

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

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

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

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 $S_n = \{\sigma : [\![n]\!] \to [\![n]\!], \sigma \text{ is a bijection}\}$ 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**

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

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**.

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- It acts on the element of the sets via the group.
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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

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

On invariance and equivariance

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Permutation of vectors

- Group of permutations S_n with composition $\circ$. Identity element id.
- For $\mathbf{x} \in \mathbb{R}^n$ a group action is $\sigma\mathbf{x} = (x_{\sigma(1)}, x_{\sigma(2)}, \cdots, x_{\sigma(n)})$.
- Is it a left group action ?

On invariance and equivariance

Group action

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- **A set endowed with an action of $\mathfrak{G}$ on it is called a $\mathfrak{G}$-set**.

Permutation of vectors

- For $\mathbf{x} \in \mathbb{R}^n$ a group action is $\sigma\mathbf{x} = (x_{\sigma(1)}, x_{\sigma(2)}, \cdots, x_{\sigma(n)})$.
- Def $(\sigma_1\mathbf{x})_i = x_{\sigma_1(i)}$. So $(\sigma_2(\sigma_1\mathbf{x}))_i = (\sigma_1\mathbf{x})_{\sigma_2(i)} = x_{\sigma_1(\sigma_2(i))} = x_{\sigma_1\circ\sigma_2(i)}$.
- Thus $\sigma_2(\sigma_1\mathbf{x}) = (\sigma_1 \circ \sigma_2)\mathbf{x} \neq (\sigma_2 \circ \sigma_1)\mathbf{x}$.

On invariance and equivariance

Group action

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Permutation of vectors

- For $\mathbf{x} \in \mathbb{R}^n$ a **left** group action is $\sigma\mathbf{x} = (x_{\sigma^{-1}(1)}, x_{\sigma^{-1}(2)}, \cdots, x_{\sigma^{-1}(n)})$.
- Def $(\sigma_1\mathbf{x})_i = x_{\sigma_1^{-1}(i)}$. So $(\sigma_2(\sigma_1\mathbf{x}))_i = (\sigma_1\mathbf{x})_{\sigma_2^{-1}(i)} = x_{\sigma_1^{-1}(\sigma_2^{-1}(i))} = x_{(\sigma_2\circ\sigma_1)^{-1}(i)}$.
- Thus $\sigma_2(\sigma_1\mathbf{x}) = (\sigma_2 \circ \sigma_1)\mathbf{x}$.

Table of contents

A formal definition of invariance

Invariance

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

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

- 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 $f, g, h : \mathbb{R}^n \to \mathbb{R}$ that are S_n-invariant.

A formal definition of invariance

Invariance

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

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

Permutation invariant functions

- $f(\mathbf{x}) = \sum_{i=1}^{n} x_i, g(\mathbf{x}) = \max_{i \in [\![n]\!]} x_i, h(\mathbf{x}) = \mathrm{sort}(\mathbf{x})$ (to $\mathbb{R}^n$).
- Characterization of all linear permutation invariant functions $L : \mathbb{R}^{n^k} \to \mathbb{R}$ (Maron et al. 2018).

A formal definition of invariance

Invariance

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Permutation invariant functions

Let $\mathbf{X} \in \mathbb{R}^{n\times d}$. The action of σ on $\mathbf{X}$ is $\sigma\mathbf{X} = (X_{\sigma^{-1}(i)j})_{ij}$. Find a permutation invariant function $F : \mathbb{R}^{n\times d} \to \mathbb{R}$.

A formal definition of invariance

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Let $\mathbf{X} \in \mathbb{R}^{n\times d}$. The action of σ on $\mathbf{X}$ is $\sigma\mathbf{X} = (X_{\sigma^{-1}(i)j})_{ij}$. Find a permutation invariant function $F : \mathbb{R}^{n\times d} \to \mathbb{R}$.

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

A formal definition of invariance

Function operating on sets/multisets

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

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

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

A formal definition of invariance

Function operating on sets/multisets

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

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

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

- 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 $h : \Omega_1 \to \Omega_2$ is $\mathfrak{G}$-**equivariant** if

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

- 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

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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 $H : \Omega = L_2(\mathbb{R}) \to L_2(\mathbb{R})$ 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

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

Permutation equivariant functions

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

A formal definition of equivariance

Equivariance

Let Ω_1, Ω_2 be two $\mathfrak{G}$-sets (of the same group). A function $h : \Omega_1 \to \Omega_2$ 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 $F(\mathbf{X}) = \mathbf{X}\mathbf{W}$.
- Let $\mathbf{X} = \begin{pmatrix} \mathbf{x}_1^\top \\ \vdots \\ \mathbf{x}_n^\top \end{pmatrix}$ previous example $F(\mathbf{X}) = \begin{pmatrix} (\mathbf{W}^\top \mathbf{x}_1)^\top \\ \vdots \\ (\mathbf{W}^\top \mathbf{x}_n)^\top \end{pmatrix}$.
- More generally $F(\mathbf{X}) = \begin{pmatrix} \psi(\mathbf{x}_1)^\top \\ \vdots \\ \psi(\mathbf{x}_n)^\top \end{pmatrix}$ where $\psi : \mathbb{R}^{d_1} \to \mathbb{R}^{d_2}$.

A formal definition of equivariance

Equivariance

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

Laplacian matrix

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

$$\sigma\mathbf{A} = (A_{\sigma^{-1}(i),\sigma^{-1}(j)})_{ij}$$

- $\mathcal{L} : \mathrm{sym}_n(\mathbb{R}) \to \mathrm{sym}_n(\mathbb{R})$ which takes a symmetric matrix $\mathbf{A}$ and outputs the Laplacian matrix $\mathcal{L}(\mathbf{A}) = \mathrm{diag}(\mathbf{A1}) - \mathbf{A}$
- **Show that $\mathcal{L}$ is S_n-permutation equivariant**.

Combining them together

Composition of invariant/equivariant functions

Let Ω_1, Ω_2 be $\mathfrak{G}$-sets.

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

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

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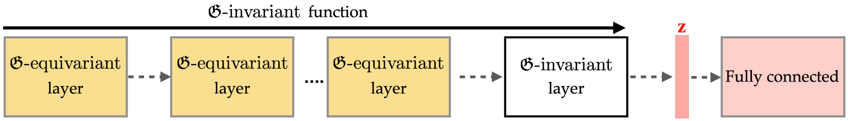
Then $h = g \circ f$ is $\mathfrak{G}$-**invariant**.

Proof

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

$$h(\mathfrak{g}x) = g(f(\mathfrak{g}x)) = g(\mathfrak{g}f(x)) = g(f(x)) = (g \circ f)(x) = h(x) \,.$$

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



Combining them together

Composition of invariant/equivariant functions

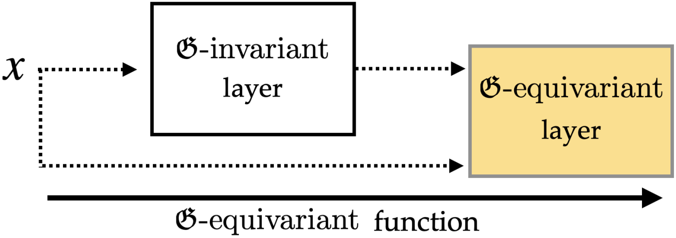
Let Ω_1, Ω_2 be $\mathfrak{G}$-sets.

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

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

Proof

$h(\mathfrak{g}x) = f(\mathfrak{g}x, g(\mathfrak{g}x)) = f(\mathfrak{g}x, g(x)) = \mathfrak{g}f(x, g(x)) = \mathfrak{g}h(x)$.



Focus on permutation invariance/equivariance

Permutations as matrices

- $\sigma \in S_n$ can be described as $\mathbf{P}_\sigma = \begin{pmatrix} \mathbf{e}_{\sigma(1)}^\top \\ \vdots \\ \mathbf{e}_{\sigma(n)}^\top \end{pmatrix} \in \{0,1\}^{n\times n}$. $\mathbf{P}_{\sigma^{-1}} = \mathbf{P}_\sigma^\top$.
- For $\mathbf{A} \in \mathbb{R}^{n\times n}$, the previous action is $\sigma\mathbf{A} = \left(A_{\sigma^{-1}(i)\sigma^{-1}(j)}\right)_{ij} = \mathbf{P}_\sigma^\top \mathbf{A} \mathbf{P}_\sigma$.
- An action of S_n on $\mathbb{R}^{n\times d} \times \mathbb{R}^{n\times n}$

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

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

Interpretation

- $\sigma\ (\mathbf{X}, \mathbf{A})$ permutes the nodes of the graph **and** the features **in the same manner**.

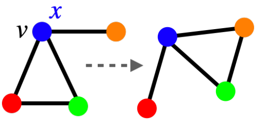

Figure: Is it a valid action of σ ?

Focus on permutation invariance/equivariance

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Back to the GNN context

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

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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**.

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

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

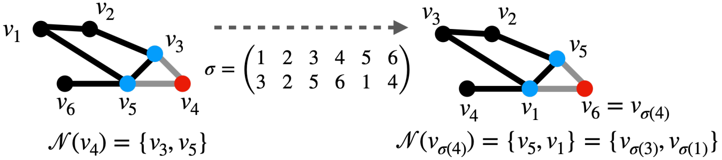
Examples: equivariance (1/2)

- 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.
- $F(\mathbf{X}, \mathbf{A}) = \Psi(\mathbf{AXW})$ is S_n-**equivariant**.
- In particular when Ψ is **element-wise**.
- But also $F(\mathbf{X}, \mathbf{A}) = \Psi(G(\mathbf{A})\mathbf{XW})$ where G is S_n-**equivariant**.
- E.g. $F(\mathbf{X}, \mathbf{A}) = \Psi(\mathcal{L}(\mathbf{A})\mathbf{XW})$ where $\mathcal{L}$ computes the Laplacian.
- E.g. $F(\mathbf{X}, \mathbf{A}) = \Psi(P[\mathcal{L}](\mathbf{A})\mathbf{XW})$ 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 $X_{\sigma(i)} = \{\{\mathbf{x}_{\sigma(j)} : j \in \mathcal{N}(i)\}\}$:



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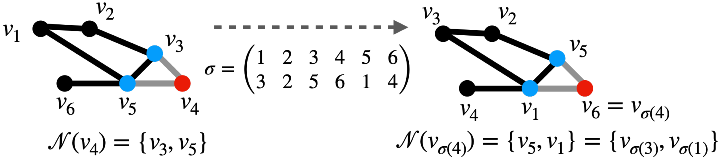

- A function AGGREGATE operating on **multisets of vectors**.
- Then the following function is permutation equivariant.

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

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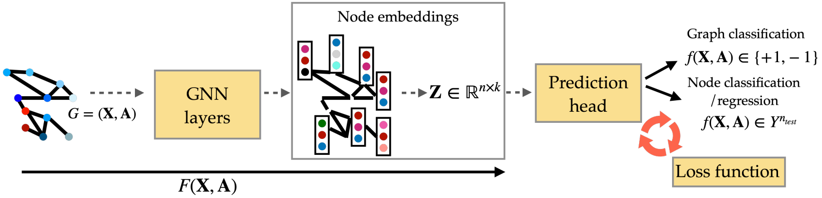
Remember

The training pipeline

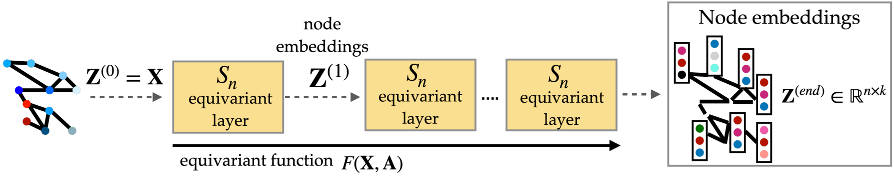


- Overall the same procedure: find an embedding of the nodes $F(\mathbf{X}, \mathbf{A}) \in \mathbb{R}^{n \times k}$ (supervised or unsupervised) and then do stuff.

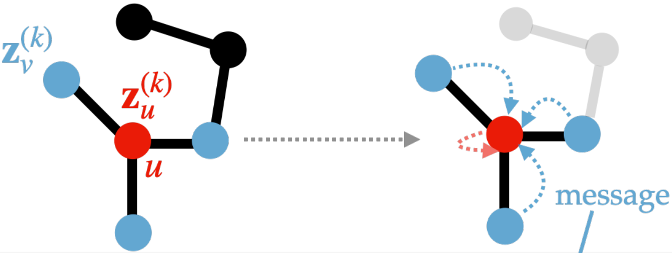
Message-passing for node embeddings

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

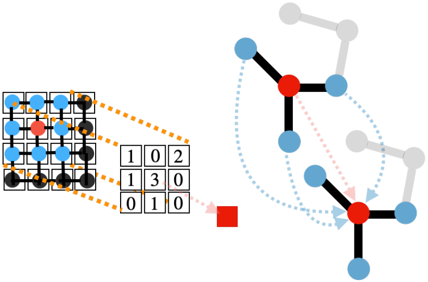
- At each iteration, **every node aggregates information from its local neighborhood**.
- A zoo of methods for different COMBINE, AGGREGATE functions.
- Why is this defining a permutation equivariant layer ?

The message passing framework

Similarities with CNN

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

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



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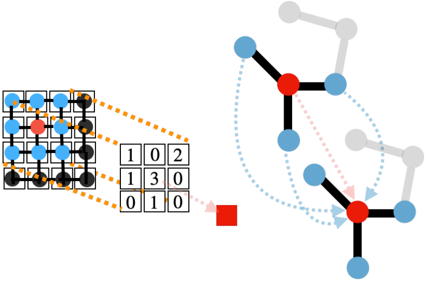

k-hop neighbourhood

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

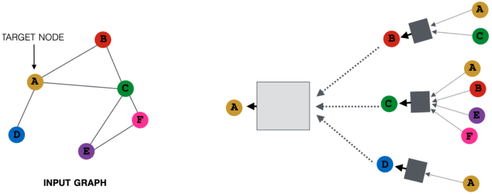

Figure: From Jure Leskovec course *Machine Learning with Graphs*.

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

A first GNN with message passing

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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

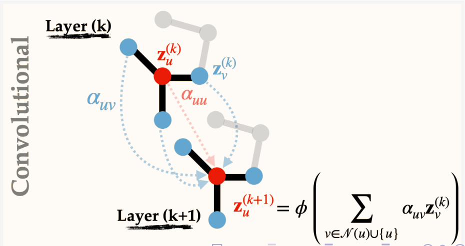
Introduced by Kipf and Welling 2016 for semi-supervised node classification.

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

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

In matrix form

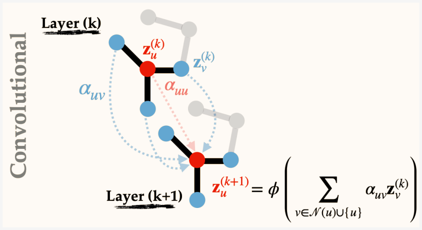
- With $\mathbf{W}_{\text{self}} = \mathbf{W}_{\text{neigh}}$, $\mathbf{Z}^{(k+1)} = \text{Relu}\left((\mathbf{I} + \mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}})\mathbf{Z}^{(k)}\mathbf{W}^{(k)}\right)$.
- First-order approximation of localized spectral filters on graphs.



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.



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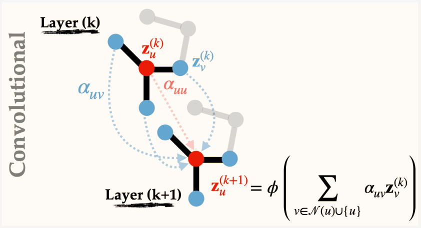

GAT networks (Velivcković et al. 2017)

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

- Here α_{uv} are **learnable weights**.
- $e_{uv} = \text{NN}(\mathbf{\Theta}_1\mathbf{z}_u, \mathbf{\Theta}_2\mathbf{z}_u)$ with learnable matrices $\mathbf{\Theta}_1, \mathbf{\Theta}_2$ 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

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

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

Spectral GNN

Learning filters

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

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

- $\mathcal{L}(\mathbf{A}) = \mathrm{diag}(\mathbf{A}\mathbf{1}) - \mathbf{A}$ 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.
- 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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- Connections with the Fourier transform on graphs: $P[\mathcal{L}]$ acts as a filter.

Limitations

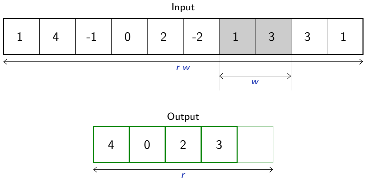
- Niave complexity in $O(|V|^3)$ (eigen-decomposition).
- Any perturbation to a graph results in a change of eigenbasis $\mathbf{U}$.
- Learned filters are domain dependent.
- Alternative ChebNet Defferrard, Bresson, and Vandergheynst 2017 relies on Chebyshev polynomials with $O(|E|M)$ complexity.

Graph pooling

Pooling layers in neural networks

At the core of many NN architectures.

- Most standard type is **max-pooling**.
- $\downarrow$ the number of parameters to learn.
- Improves robustness.



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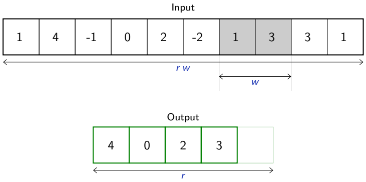
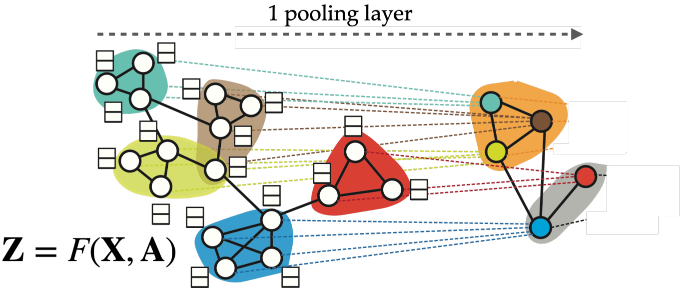


Pooling in GNN

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



Diffpool

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 $\mathbf{z}_G = f(\mathbf{X}, \mathbf{A}) = \frac{1}{|V|} \sum_{u \in V} \mathbf{z}_u \in \mathbb{R}^k$.

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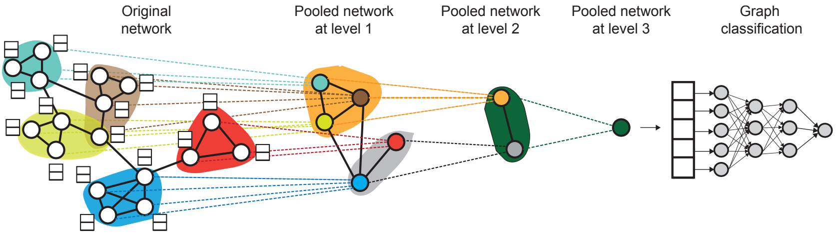
Better idea: hierarchical pooling (Z. Ying et al. 2018)



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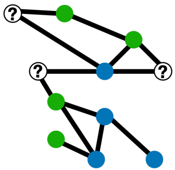
Applications

Node classification

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

Train GNNs in a fully-supervised manner by minimizing

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



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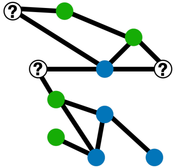
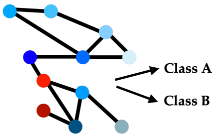


Graph classification

- **Many graphs** $G_1, \cdots, G_n$ 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

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

- 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.

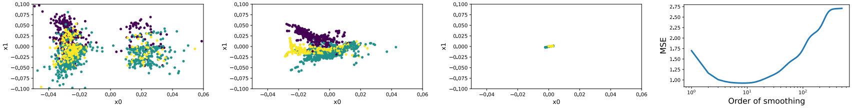

Figure: From Keriven 2022

- **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 -¿ several recent initiatives for bigger datasets and more complex tasks (eg Open Graph Benchmark)

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