Machine learning for graphs and with graphs

Graph neural networks

Titouan Vayer & Pierre Borgnat
email: titouan.vayer@inria.fr, pierre.borgnat@ens-lyon.fr

October 16, 2024

ENS DE LYON

Table of contents

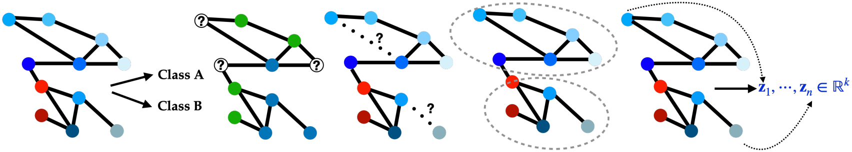
Frameworks considered here

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

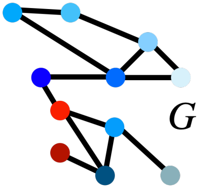
- Approx. 100 GNN papers a month on arXiv.
- Despite 1000s of papers, same ideas coming round: be critical, learn to spot incremental changes!
- We will only see the most well-known architectures (according to me).
- Be aware that it might already be out-of-date.
- Some surveys Wu et al. 2021; Zhang,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

Table of contents

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

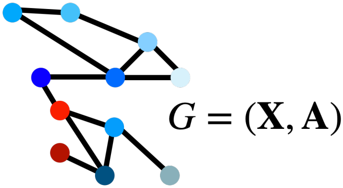


$$G = (\mathbf{X}, \mathbf{A})$$

What is a graph neural network ?

Framework

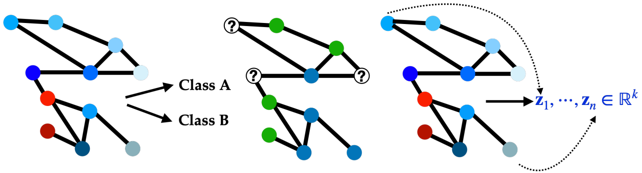
- Graphs considered here:
- $G = (V, E)$ with $|V| = n$, features on the nodes.
- Adjacency matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$.
- Feature matrix $\mathbf{X} \in \mathbb{R}^{n\times d}$, feature $\mathbf{x}_i \in \mathbb{R}^d$.



What is a GNN ?

A **specific parametrized function** that takes a input a graph $G = (\mathbf{X}, \mathbf{A})$

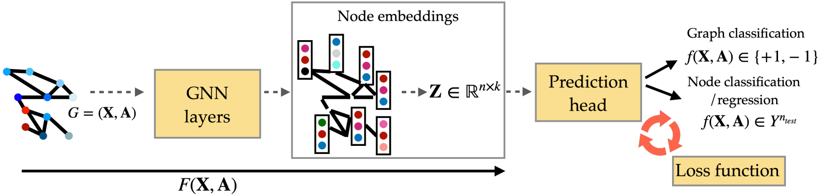
- It is made of a **combination of different layers**.
- Graph classification, node classification/regression, node embedding



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

What properties to ensure ?

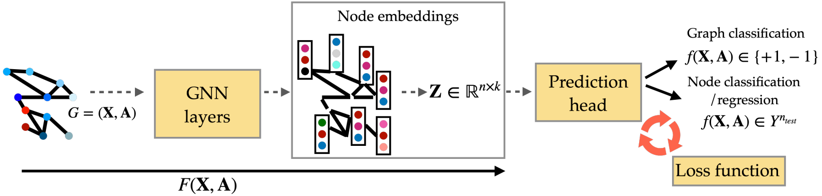
The training pipeline



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

What properties to ensure ?

The training pipeline



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

Properties to ensure

- Prediction on the graph level: the output $f(\mathbf{X}, \mathbf{A})$ must be **invariant to permutations of the graph**.
- Prediction on the node level: permutation of the graph should produce a different result but **be predictable**.
- It will be formalized with the notion of invariance/equivariance.

Table of contents

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

symmetric: $f(-x) = f(x)$ antisymmetric: $f(-x) = -f(x)$

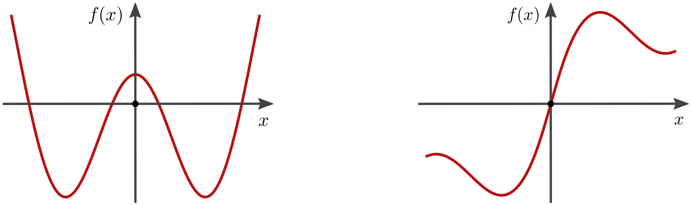


Figure: From Weiler et al. 2023

- 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

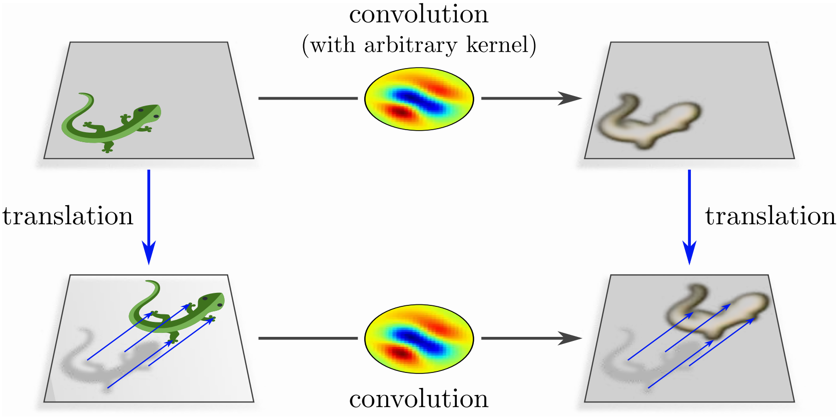


Figure: From Weiler et al. 2023

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 ($\mathfrak{g} \circ \mathfrak{h} \neq \mathfrak{h} \circ \mathfrak{g}$).

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 ($\mathfrak{g} \circ \mathfrak{h} \neq \mathfrak{h} \circ \mathfrak{g}$).

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**.

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**

$$\mathfrak{G} \times \Omega \to \Omega$$
$$(\mathfrak{g}, x) \to \mathfrak{g}x$$

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

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

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**.

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

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**.

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

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

$$\mathfrak{G} \times \Omega \to \Omega$$
$$(\mathfrak{g}, x) \to \mathfrak{g}x$$

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**.

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

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.

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

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

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

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

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.

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

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.

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 $F : \mathbb{R}^{n\times d} \to \mathbb{R}$.

- 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 $\psi : \mathbb{R}^d \to Z, \phi : Z \to Y$.
- $F(\mathbf{X}) = \mathrm{rank}(\mathbf{X})$.

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

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

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

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

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.

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 $h : \Omega_1 \to \Omega_2$ 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.

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

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.

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

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

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

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

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

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

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**.

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.

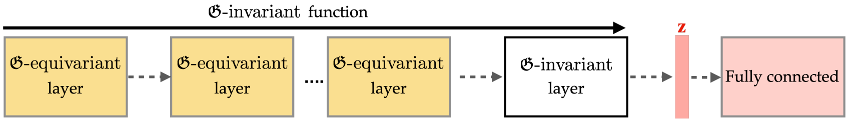
Then $h = g \circ f$ is $\mathfrak{G}$-**invariant**.

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

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

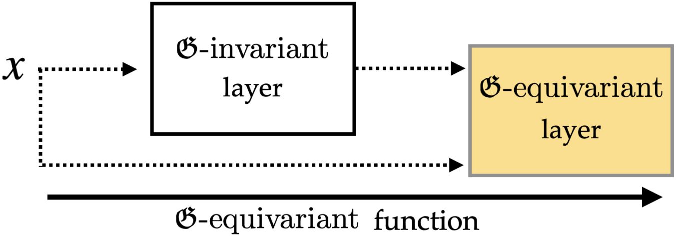


Table of contents

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 $\sigma\mathbf{A} = (A_{\sigma^{-1}(i)\sigma^{-1}(j)})_{ij} = \mathbf{P}_\sigma^\top \mathbf{A}\mathbf{P}_\sigma$.
- An action of S_n on $\mathbb{R}^{n\times d} \times \mathbb{R}^{n\times n}$

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

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 $\sigma\mathbf{A} = (A_{\sigma^{-1}(i)\sigma^{-1}(j)})_{ij} = \mathbf{P}_\sigma^\top \mathbf{A}\mathbf{P}_\sigma$.
- An action of S_n on $\mathbb{R}^{n\times d} \times \mathbb{R}^{n\times n}$

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

Interpretation

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

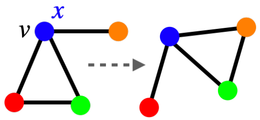


Figure: Is it a valid action of σ ?

Focus on permutation invariance/equivariance

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 $\mathbb{R}^{n\times d} \times \mathbb{R}^{n\times n}$

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

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 $F : G = (\mathbf{X}, \mathbf{A}) \to \mathbf{Z} \in \mathbb{R}^{n\times k}$

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 $\sigma \mathbf{A} = (A_{\sigma^{-1}(i)\sigma^{-1}(j)})_{ij} = \mathbf{P}_\sigma^\top \mathbf{A} \mathbf{P}_\sigma$.
- An action of S_n on $\mathbb{R}^{n \times d} \times \mathbb{R}^{n \times n}$

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

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 $F : G = (\mathbf{X}, \mathbf{A}) \to \mathbf{Z} \in \mathbb{R}^{n \times k}$

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

Focus on permutation invariance/equivariance

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

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**.

Focus on permutation invariance/equivariance

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

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**.

Focus on permutation invariance/equivariance

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

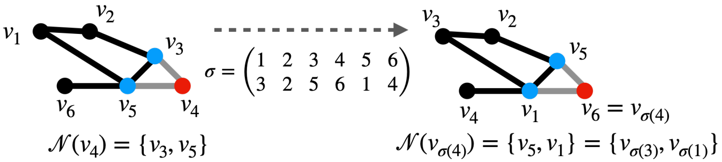
Examples: equivariance (1/2)

- 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)

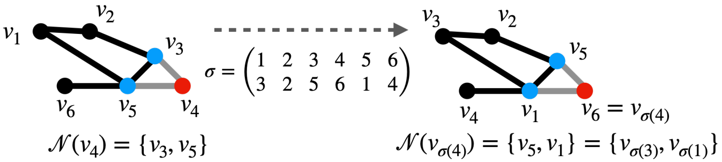
- Take $\mathbf{X} = \begin{pmatrix} \mathbf{x}_1^\top \\ \vdots \\ \mathbf{x}_n^\top \end{pmatrix}$ and define the multiset $X_i := \{\{\mathbf{x}_j : j \in \mathcal{N}(i)\}\}$.
- Then $X_{\sigma(i)} = \{\{\mathbf{x}_{\sigma(j)} : j \in \mathcal{N}(i)\}\}$:



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 $X_{\sigma(i)} = \{\{\mathbf{x}_{\sigma(j)} : j \in \mathcal{N}(i)\}\}$:



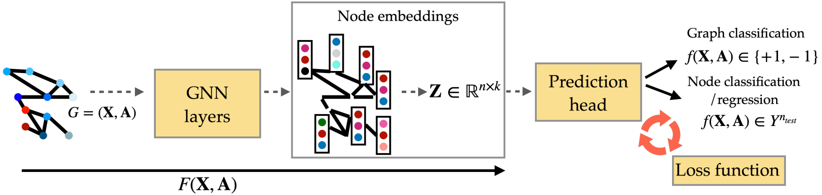
- A function AGGREGATE operating on **multisets of vectors**.
- Then the following function is permutation equivariant.

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

Table of contents

Remember

The training pipeline

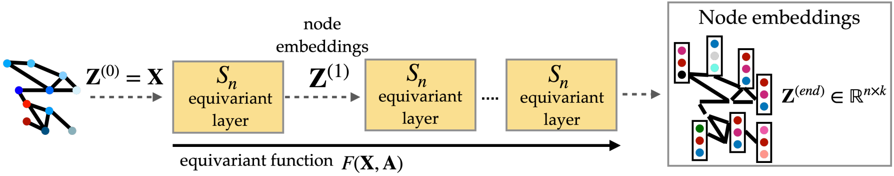


- Find an embedding of the nodes $F(\mathbf{X}, \mathbf{A}) \in \mathbb{R}^{n \times k}$ and then do stuff.

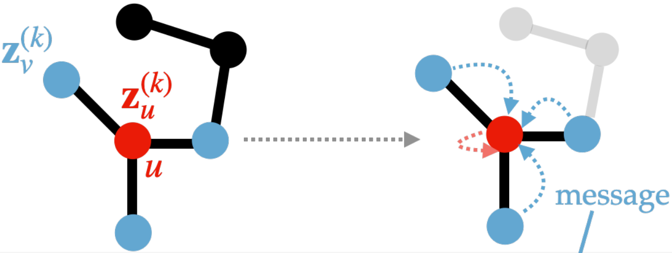
Message-passing for node embeddings

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



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

One of the most used GNN framework in practice

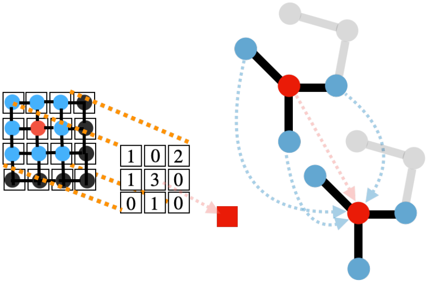
- At each iteration, **every node aggregates information from its local neighborhood**.
- A zoo of methods for different COMBINE, AGGREGATE functions.
- Why is this defining a permutation equivariant layer ?

The message passing framework

Similarities with CNN

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

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

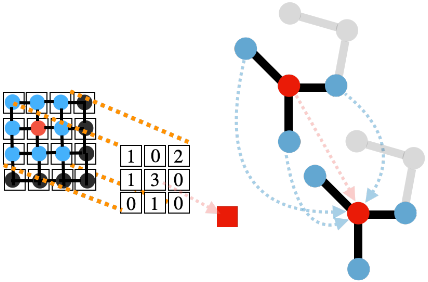


The message passing framework

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.

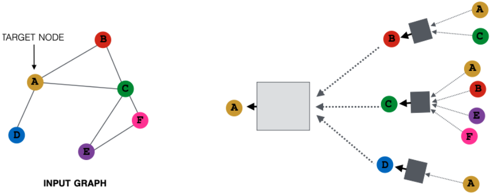


Figure: From Jure Leskovec course *Machine Learning with Graphs*.

Table of contents

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.

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.

Answers

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

A first GNN with message passing

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.

Answers

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

Graph convolutional neural networks

Most popular baseline model

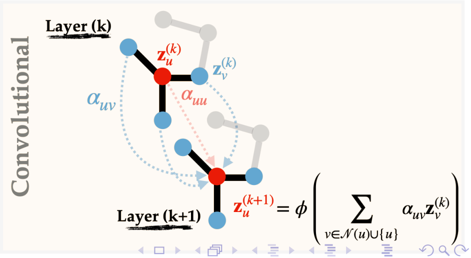
Introduced by Kipf and Welling 2016 for semi-supervised node classification.

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

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

In matrix form

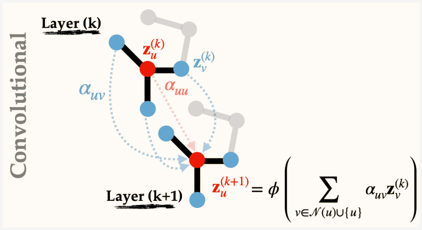
- With $\mathbf{W}_{\text{self}} = \mathbf{W}_{\text{neigh}}$, $\mathbf{Z}^{(k+1)} = \mathrm{Relu}\left((\mathbf{I} + \mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}})\mathbf{Z}^{(k)}\mathbf{W}^{(k)\top}\right)$.
- First-order approximation of localized spectral filters on graphs.



Graph Attention Networks

Motivations

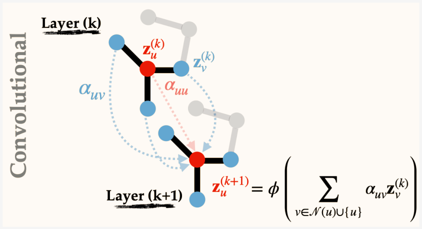
- In many MP-GNN layers weights of the convolutions **are fixed**.
- What if we also learn them ?
- Learn the importance of the neighbours contributions.



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 (Velivcković et al. 2017)

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

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

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

- 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.

Spectral GNN

Learning filters

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

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

- $\mathcal{L}(\mathbf{A}) = \mathrm{diag}(\mathbf{A1}) - \mathbf{A}$ 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.

Limitations

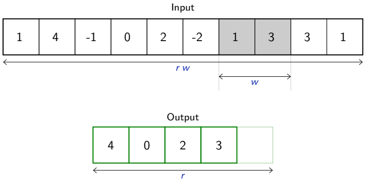
- Niave complexity in $O(|V|^3)$ (eigen-decomposition).
- Any perturbation to a graph results in a change of eigenbasis $\mathbf{U}$.
- Learned filters are domain dependent.
- Alternative ChebNet Defferrard, Bresson, and Vandergheynst 2017 relies on Chebyshev polynomials with $O(|E|M)$ complexity.

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.

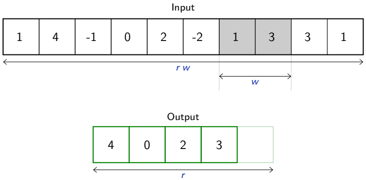


Graph pooling

Pooling layers in neural networks

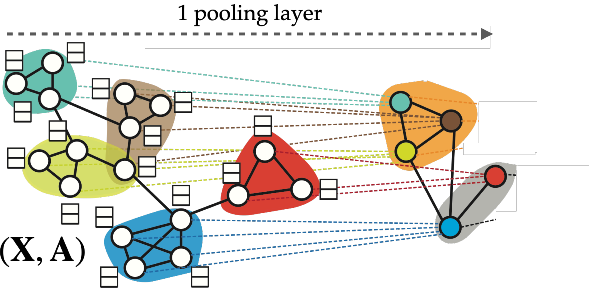
At the core of many NN architectures.

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



Pooling in GNN

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



$$\mathbf{Z} = F(\mathbf{X}, \mathbf{A})$$

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

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

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

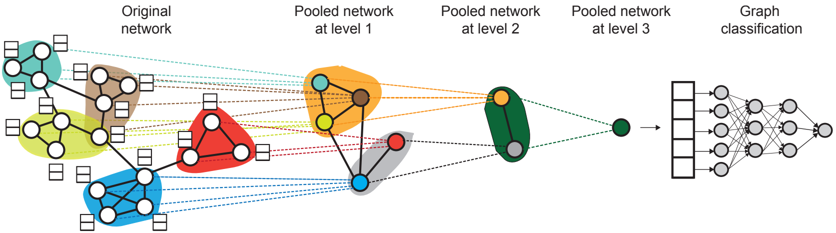
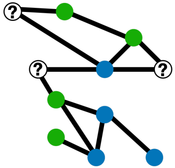


Table of contents

Applications

Node classification

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



Train GNNs in a fully-supervised manner by minimizing

$$\mathcal{L} = \mathrm{CE} = \sum_{u \in V_{train}} \sum_{k \in [\![K]\!]} -[\mathbf{y}_u]_k \log([\mathrm{softmax}(\mathbf{z}_u)]_k)$$

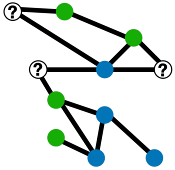
Applications

Node classification

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

Train GNNs in a fully-supervised manner by minimizing

$$\mathcal{L} = \mathrm{CE} = \sum_{u \in V_{train}} \sum_{k \in [\![K]\!]} -[\mathbf{y}_u]_k \log([\mathrm{softmax}(\mathbf{z}_u)]_k)$$



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

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

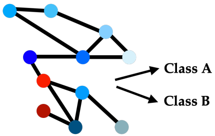


Table of contents

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.

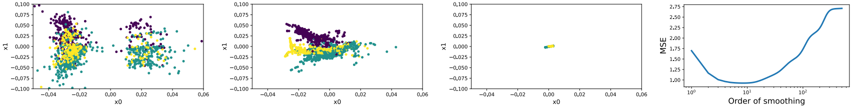


Figure: From Keriven 2022

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

Table of contents

Conclusion

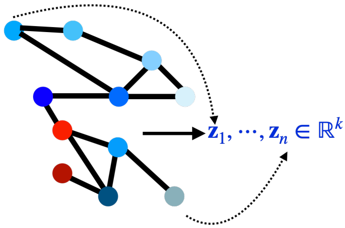
- Flexible: graph/node/edge classification, semi-supervised learning, link prediction...
- Generally state-of-the-art, but...
- ... sometimes do not work "that well" (compared to other DL)
- Simple methods may perform better but might be "forgotten" in benchmarks
- Room for improvement (many interesting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

Table of contents

Objective

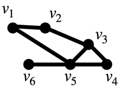
A chronological start

- 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.



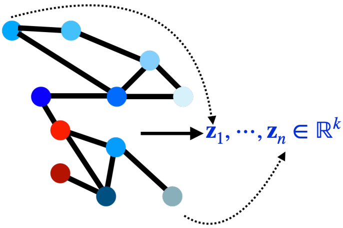
$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \longrightarrow$$

$\mathbf{z}_1 \in \mathbb{R}^n$
$\mathbf{z}_2 \in \mathbb{R}^n$
$\mathbf{z}_3 \in \mathbb{R}^n$
$\mathbf{z}_4 \in \mathbb{R}^n$
$\mathbf{z}_5 \in \mathbb{R}^n$
$\mathbf{z}_6 \in \mathbb{R}^n$

Objective

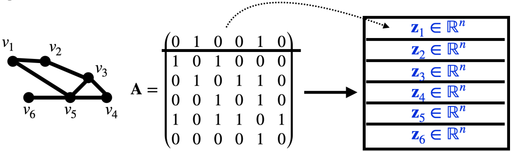
A chronological start

- 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.



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

An encoder-decoder perspective

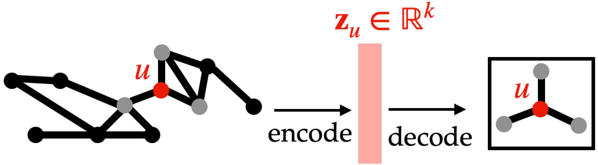
Notations

- 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.

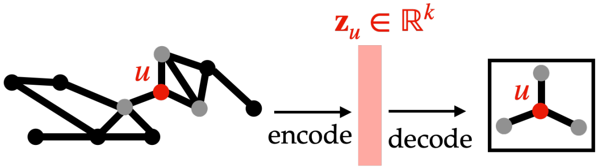


An encoder-decoder perspective

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.



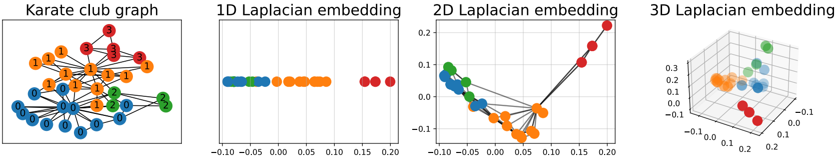
Encoding/decoding scheme

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



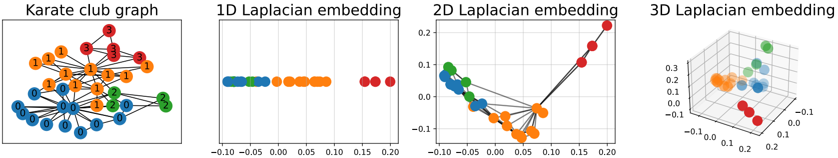
Inspiration from Laplacian eigenmaps Belkin and Niyogi 2003

- 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



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:

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

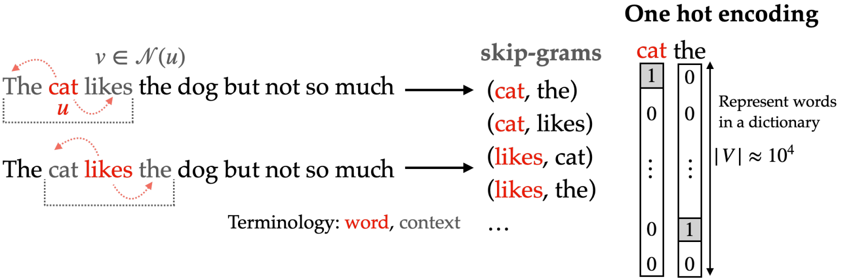
- Normalized Laplacian $\widetilde{\mathbf{L}} = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2}$.
- Interpretation + permutation equivariance of the cost (on the board).
- With the constraint $\mathbf{Z}^\top\mathbf{Z} = \mathbf{I}_d$ it recovers Laplacian eigenmaps.
- Sol. is the d eigenvectors associated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

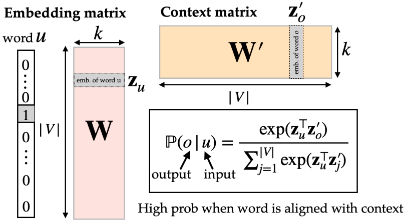


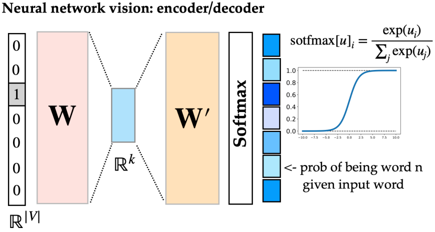
Unsupervised node embeddings techniques

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



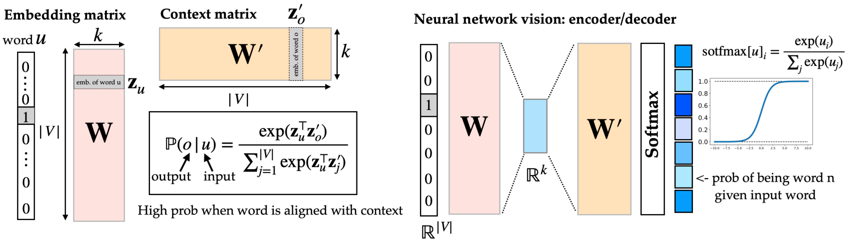


Unsupervised node embeddings techniques

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



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

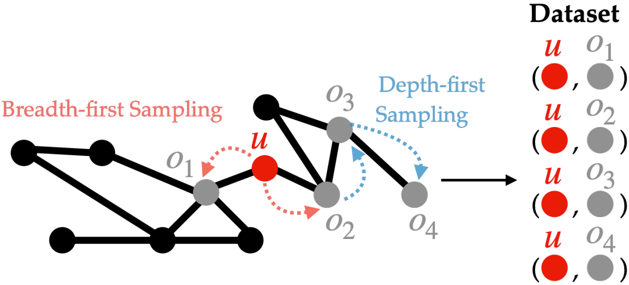
$$- \sum_{(u,o) \in \mathcal{D}} \log \mathbb{P}(o|u)\,.$$

- 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

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).

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

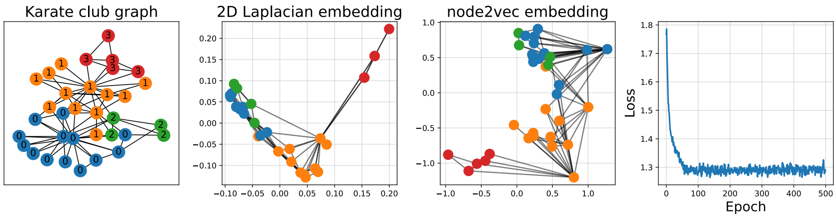
Unsupervised node embeddings techniques

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).

Negative sampling (NS)

- Goal: distinguish between neighboring points of a target node u and random draws from a noise distribution using logistic regression.



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

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.

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

- 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**.

References I

Belkin, Mikhail and Partha Niyogi (2003). "Laplacian eigenmaps for dimensionality reduction and data representation". In: *Neural computation* 15.6, pp. 1373–1396.

Bruna, Joan et al. (2013). "Spectral networks and locally connected networks on graphs". In: *arXiv preprint arXiv:1312.6203*.

Defferrard, Michaël, Xavier Bresson, and Pierre Vandergheynst (2017). *Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering*. arXiv: `1606.09375 [cs.LG]`.

Goldberg, Yoav and Omer Levy (2014). "word2vec Explained: deriving Mikolov et al.'s negative-sampling word-embedding method". In: *arXiv preprint arXiv:1402.3722*.

Grinsztajn, Léo, Edouard Oyallon, and Gaël Varoquaux (2022). "Why do tree-based models still outperform deep learning on typical tabular data?" In: *Advances in Neural Information Processing Systems* 35, pp. 507–520.

Grover, Aditya and Jure Leskovec (2016). "node2vec: Scalable feature learning for networks". In: *Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining*, pp. 855–864.

References II

Hamilton, William L (2020). *Graph representation learning*. Morgan & Claypool Publishers.

Hamilton, William L., Rex Ying, and Jure Leskovec (2018). *Inductive Representation Learning on Large Graphs*. arXiv: 1706.02216 [cs.SI].

Keriven, Nicolas (2022). "Not too little, not too much: a theoretical analysis of graph (over) smoothing". In: *Advances in Neural Information Processing Systems* 35, pp. 2268–2281.

Kipf, Thomas N and Max Welling (2016). "Semi-supervised classification with graph convolutional networks". In: *arXiv preprint arXiv:1609.02907*.

LeCun, Yann et al. (1998). "Gradient-based learning applied to document recognition". In: *Proceedings of the IEEE* 86.11, pp. 2278–2324.

Luan, Sitao et al. (2022). "Revisiting heterophily for graph neural networks". In: *Advances in neural information processing systems* 35, pp. 1362–1375.

Maron, Haggai et al. (2018). "Invariant and equivariant graph networks". In: *arXiv preprint arXiv:1812.09902*.

Mikolov, Tomas et al. (2013). "Distributed representations of words and phrases and their compositionality". In: *Advances in neural information processing systems* 26.

References III

Rosenblatt, Frank (1958). "The perceptron: a probabilistic model for information storage and organization in the brain.". In: *Psychological review* 65.6, p. 386.

Scarselli, Franco et al. (2008). "The graph neural network model". In: *IEEE transactions on neural networks* 20.1, pp. 61–80.

Vaswani, Ashish et al. (2023). *Attention Is All You Need*. arXiv: 1706.03762 [cs.CL].

Velivcković, Petar et al. (2017). "Graph attention networks". In: *arXiv preprint arXiv:1710.10903*.

Wagstaff, Edward et al. (2019). "On the limitations of representing functions on sets". In: *International Conference on Machine Learning*. PMLR, pp. 6487–6494.

Weiler, Maurice et al. (2023). *Equivariant and Coordinate Independent Convolutional Networks. A Gauge Field Theory of Neural Networks*. URL: https://maurice-weiler.gitlab.io/cnn_book/EquivariantAndCoordinateIndependentCNNs.pdf.

References IV

Wu, Zonghan et al. (Jan. 2021). "A Comprehensive Survey on Graph Neural Networks". In: *IEEE Transactions on Neural Networks and Learning Systems* 32.1, pp. 4–24. DOI: 10.1109/tnnls.2020.2978386. URL: https://doi.org/10.1109%2Ftnnls.2020.2978386.

Xu, Keyulu et al. (2019). *How Powerful are Graph Neural Networks?* arXiv: 1810.00826 [cs.LG].

Ying, Zhitao et al. (2018). "Hierarchical graph representation learning with differentiable pooling". In: *Advances in neural information processing systems* 31.

Zaheer, Manzil et al. (2018). *Deep Sets*. arXiv: 1703.06114 [cs.LG].

Zeiler, Matthew D and Rob Fergus (2014). "Visualizing and understanding convolutional networks". In: *Computer Vision–ECCV 2014: 13th European Conference, Zurich, Switzerland, September 6-12, 2014, Proceedings, Part I 13*. Springer, pp. 818–833.

Zhang, Ziwei, Peng Cui, and Wenwu Zhu (2020). *Deep Learning on Graphs: A Survey*. arXiv: 1812.04202 [cs.LG].