ENS Lyon
2023/2024 **Titouan Vayer**

Homework 2 : A bit of GNN theory

You have three weeks to do this homework: it must be return by Monday, November 4.

- You can do it by group of 2.
- Send the homework to titouan.vayer@inria.fr with the header "Homework 1 Name 1 Name 2".
- For the maths send a scan by mail or give it by hand on 4th november.

- Exercise 1: Invariance and equivariance on graphs ($\approx$ 2H). -

For this exercise you need first too look at the slides of the course, specifically the part "A bit of group theory" and "Invariance and equivariance". For $n \in [\![N]\!]$ we note $S_n = \{\sigma : [\![n]\!] \to [\![n]\!] : \sigma \text{ is a bijection}\}$ the permutation group of $[\![n]\!]$.

Let $\Omega_1 = \mathbb{R}^{n\times d}$ and consider the action of S_n on Ω_1 as $\sigma \cdot \mathbf{X} = (X_{\sigma^{-1}(i),j})_{(i,j)\in[\![n]\!]\times[\![d]\!]}$ for $\sigma \in S_n, \mathbf{X} \in \Omega_1$. The action is simply permuting the rows of $\mathbf{X}$, that we denote by $\mathbf{x}_1, \cdots, \mathbf{x}_n$, i.e. $\mathbf{X} = (\mathbf{x}_1, \cdots, \mathbf{x}_n)^\top$. Let $\mathbf{W} \in \mathbb{R}^{d\times p}$ be fixed, and $\phi : \mathbb{R}^d \to \mathbb{R}^p$. We define the functions $F : \mathbf{X} \to \mathbf{XW}$ and $f : \mathbf{X} \to \sum_{i=1}^n \phi(\mathbf{x}_i)$.

(i) Show that $\sigma \cdot \mathbf{X}$ defines a left group action on Ω_1.

(ii) Show that F is S_n-equivariant, and f is S_n-invariant.

Now consider $\Omega_2 = \mathbb{R}^{n\times n}$ and the action of S_n on Ω_2 defined by $\sigma \cdot \mathbf{A} = (A_{\sigma^{-1}(i),\sigma^{-1}(j)})_{(i,j)\in[\![n]\!]^2}$. We consider the Laplacian function defined by $\mathcal{L} : \mathbf{A} \to \text{diag}(\mathbf{A1}) - \mathbf{A}$ where for a vector $\mathbf{x} = (x_1, \cdots, x_n)^\top$, $\text{diag}(\mathbf{x})$ is the diagonal matrix with elements $x_1, \cdots, x_n$ and $\mathbf{1} = (1, \cdots, 1)^\top$.

(iii) Show that $\mathcal{L}$ is S_n-equivariant.

(iv) What about the normalized graph Laplacian $\mathcal{L}_N : \mathbf{A} \to \mathbf{I} - \text{diag}(\mathbf{A1})^{-\frac{1}{2}}\mathbf{A}\text{diag}(\mathbf{A1})^{-\frac{1}{2}}$?

(v) Let $P[\mathcal{L}] = \sum_m c_m \mathcal{L}^m$ be a polynomial of $\mathcal{L}$, where $\mathcal{L}^m$ is understood with respect to the composition of functions i.e. $\mathcal{L}^m = \overbrace{\mathcal{L} \circ \cdots \circ \mathcal{L}}^{m \text{ times}}$. Show that $P[\mathcal{L}]$ is S_n-equivariant.

Finally, consider $\Omega_3 = \mathbb{R}^{n\times d} \times \mathbb{R}^{n\times n}$ with the group action $\sigma \cdot (\mathbf{X}, \mathbf{A}) = \big((X_{\sigma^{-1}(i),j})_{ij}, (A_{\sigma^{-1}(i),\sigma^{-1}(j)})_{ij}\big)$. Consider $\Psi : \mathbb{R}^{n\times p} \to \mathbb{R}^{n\times p}$ a function that applies *independently on each row of the input matrix.*

(vi) Show that $F : (\mathbf{X}, \mathbf{A}) \to \Psi(P[\mathcal{L}](\mathbf{A})\mathbf{XW})$ is S_n-equivariant.

(vii) What about $F : (\mathbf{X}, \mathbf{A}) \to \Psi(P[\mathcal{L}_N](\mathbf{A})\mathbf{XW})$? In this case when the degree of the polynomial is equal to one, which GGN does it correspond to ?