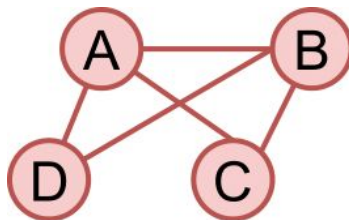


Revealing integrated and segregated structures using a graph neural network

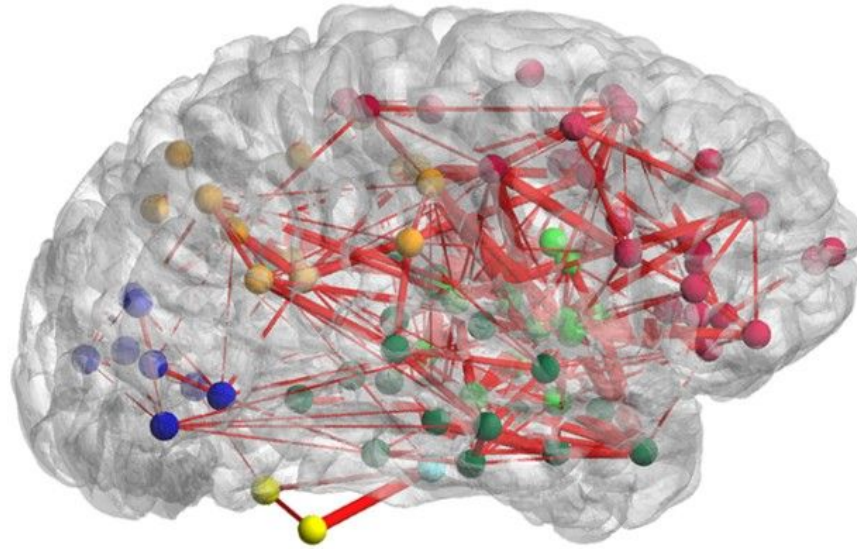
Anna Boronina

Structure

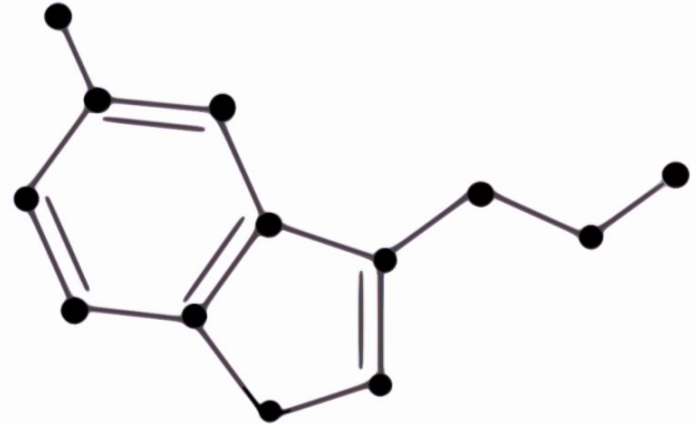
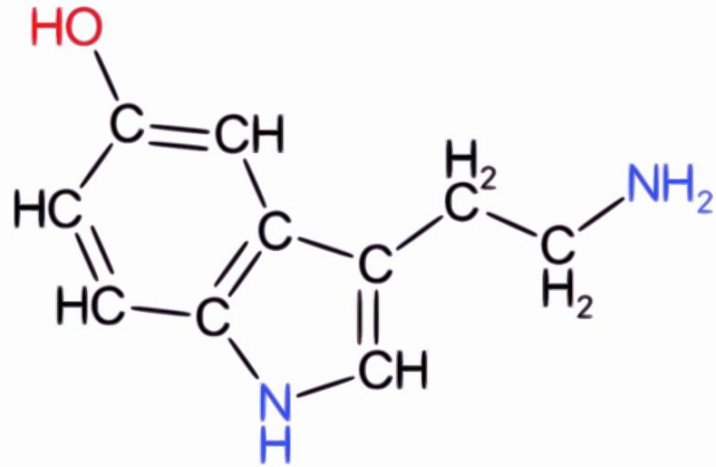
- What are graphs and Graph Neural Networks
- Research gap
- Datasets creation
- GNN architecture
- Results



Graphs in real life



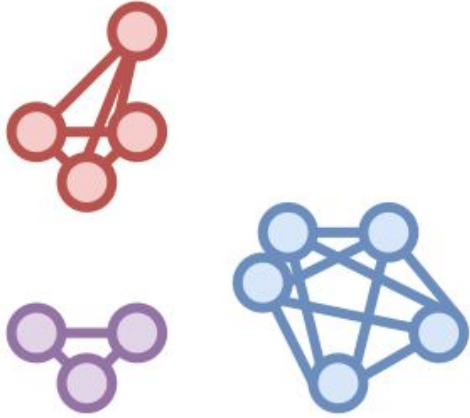
Graphs in real life



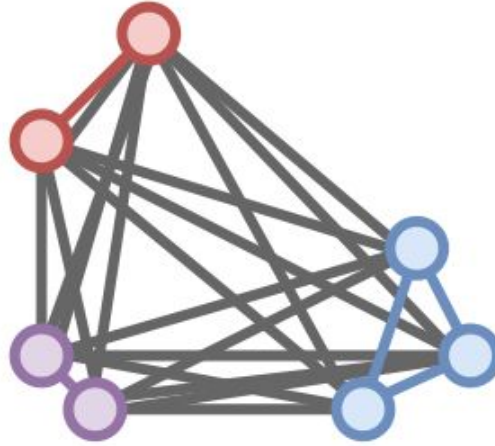
Graphs in real life



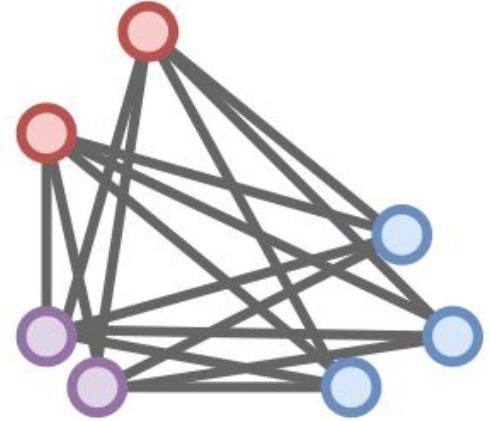
Segregation and integration



Fully segregated



Neutral



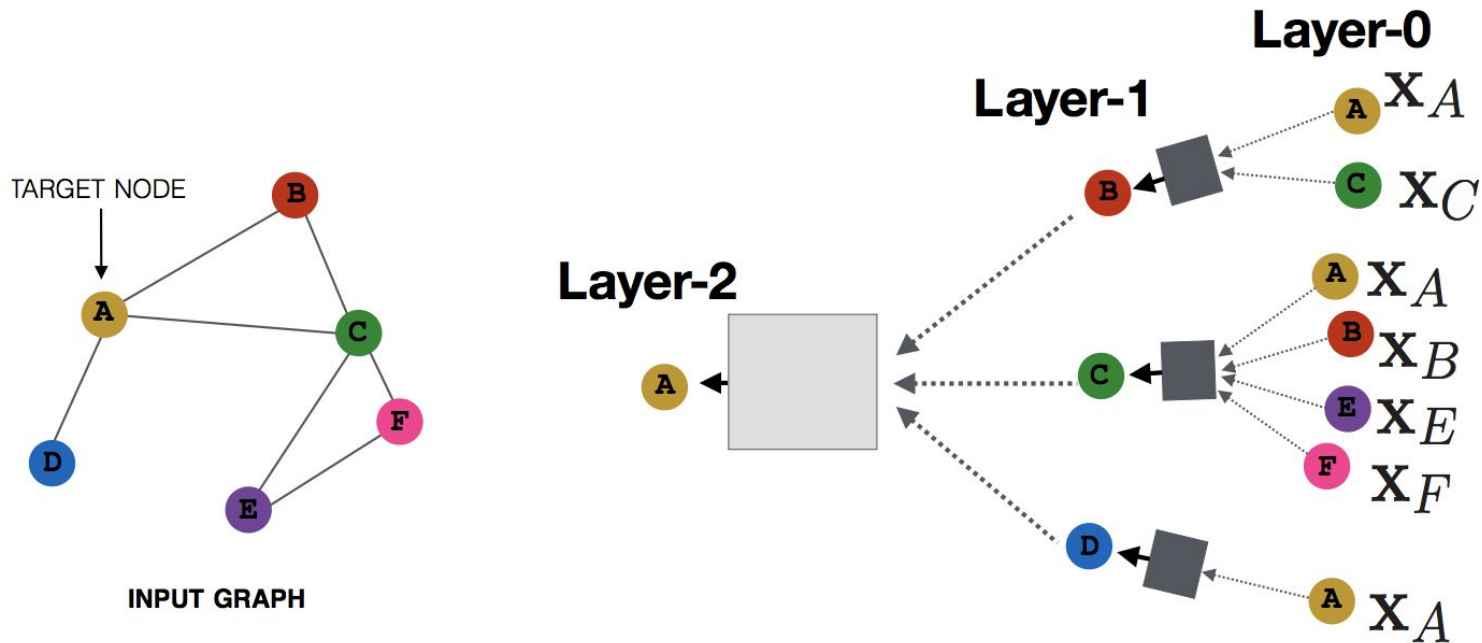
Fully integrated

The balance is important

- **segregation** affects **motor ability** distant brain regions
- **segregation** is important for a **security network**

- **stronger integration** in a brain network implies **better cognitive ability**
- **integration** is important for **city transport system**

Graph Neural Networks



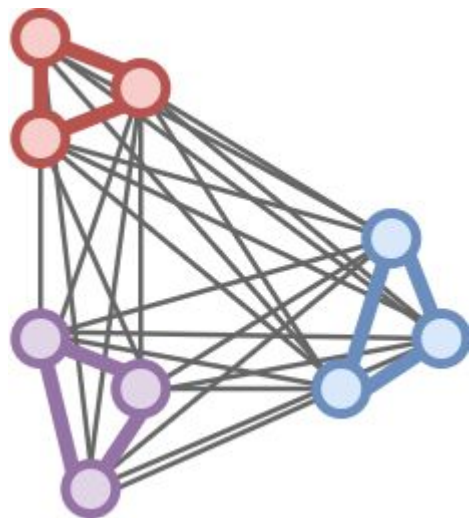
<http://snap.stanford.edu/proj/embeddings-www/>

Research Gap

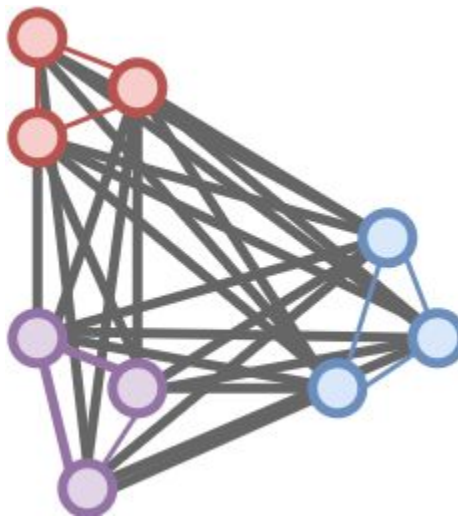
GNNs are mostly applied to real data and rarely interpreted

Data modeling allows to control the input and see what parameters play what role

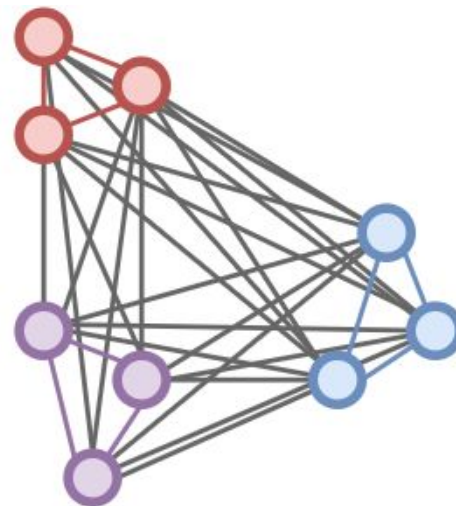
Segregation



Integration



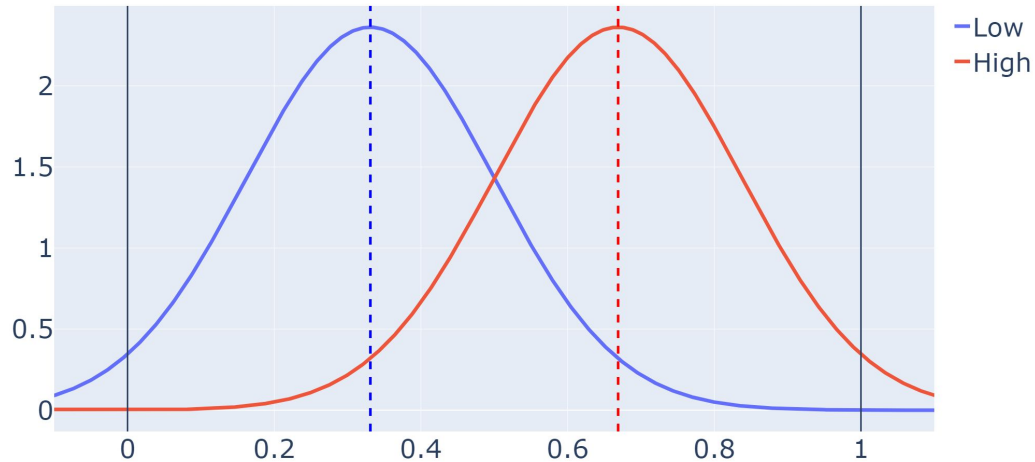
Neutral



OK, so...

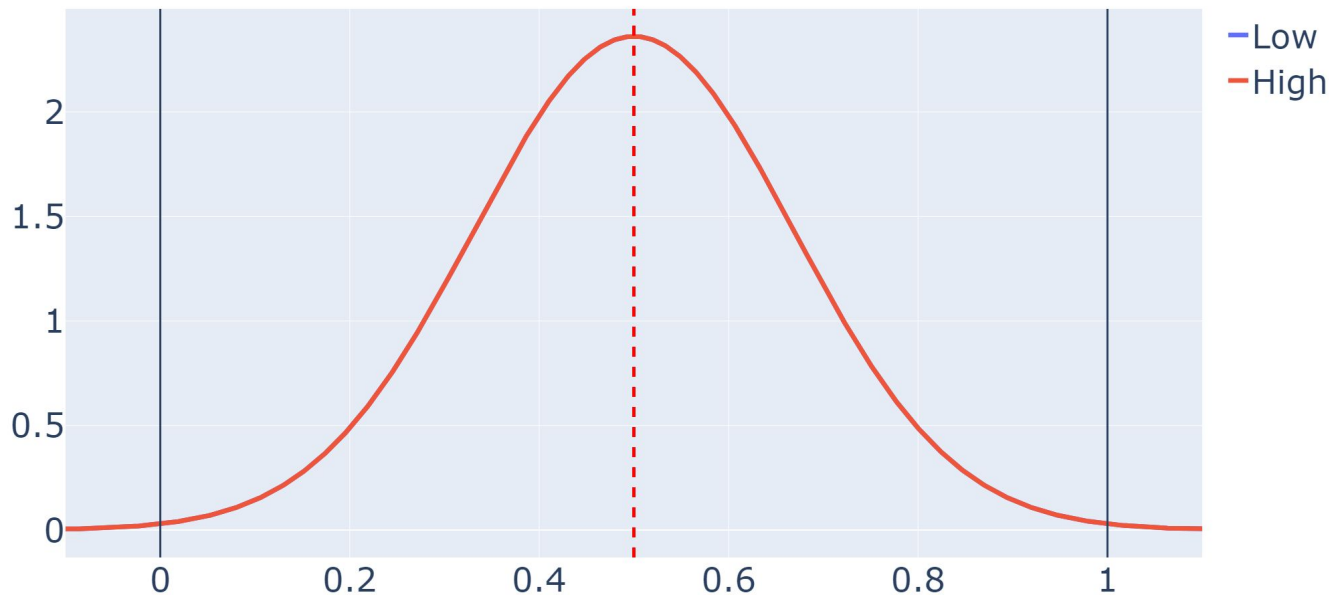
There are two types of connections: **weak** | **strong**

How do we create these connections?



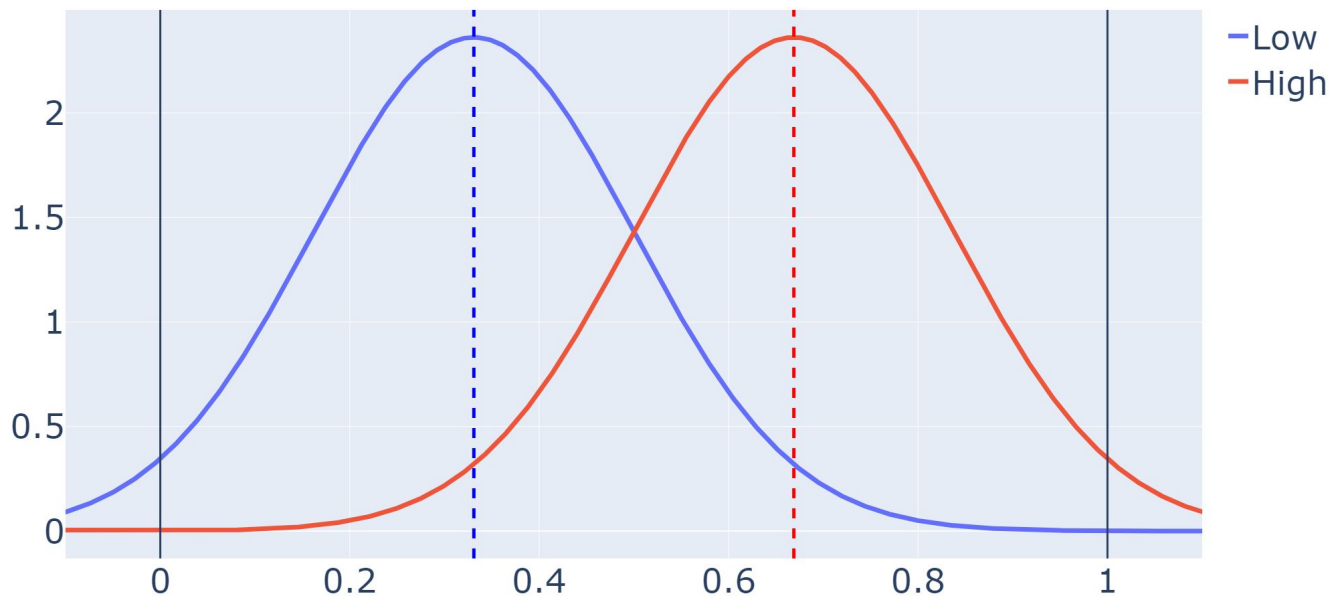
How far L and H distributions should be?

Maybe the same?

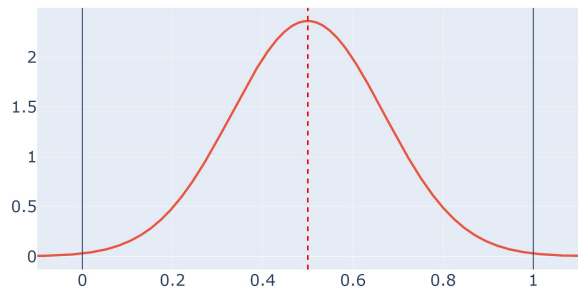


How far L and H distributions should be?

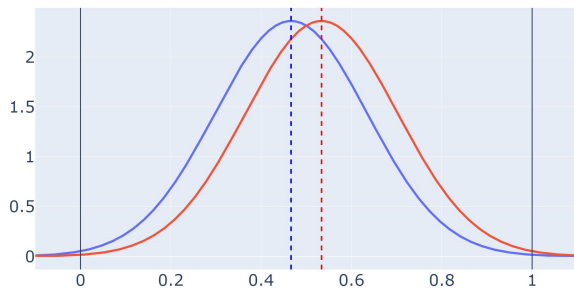
Maybe far away?



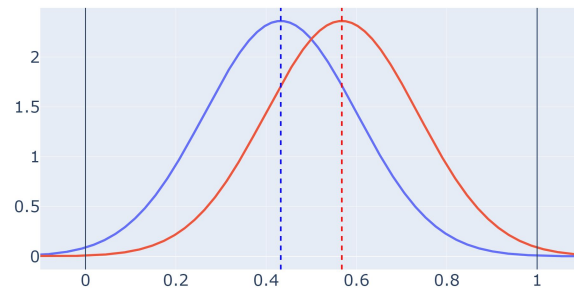
Let's make it a parameter!



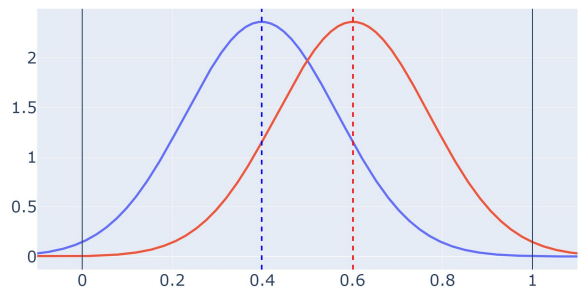
$n = 0$



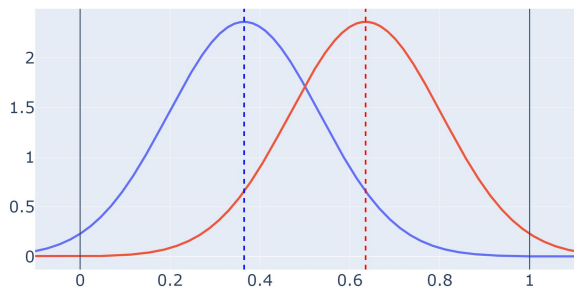
$n = 1$



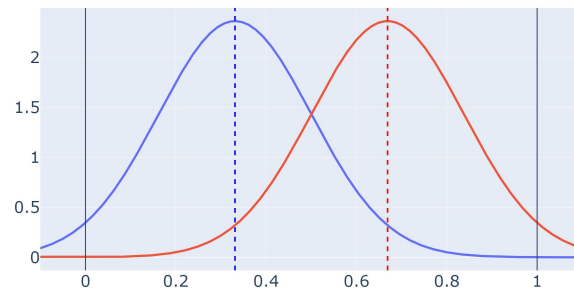
$n = 2$



$n = 3$

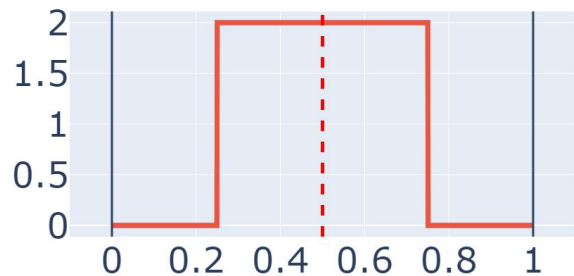


$n = 4$

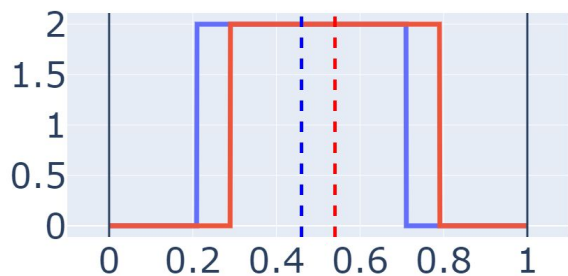


$n = 5$

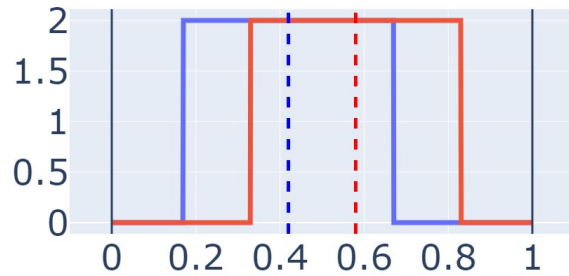
What if we try another distribution?



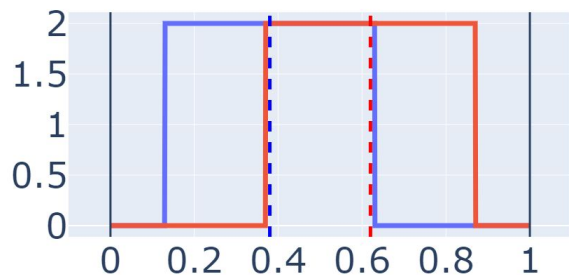
$n = 0$



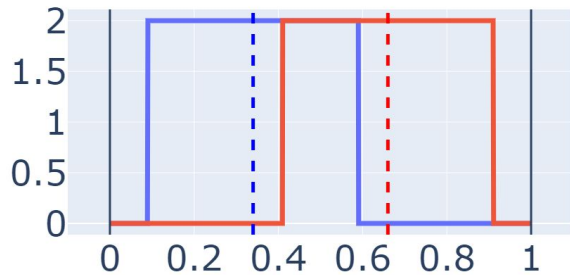
$n = 1$



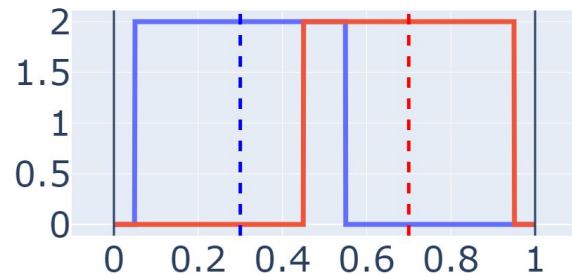
$n = 2$



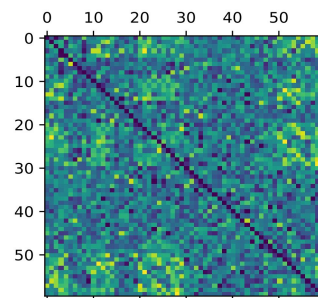
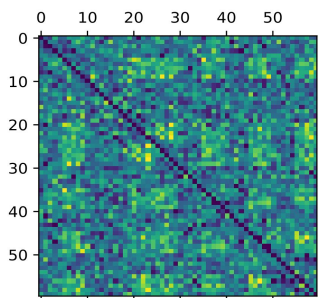
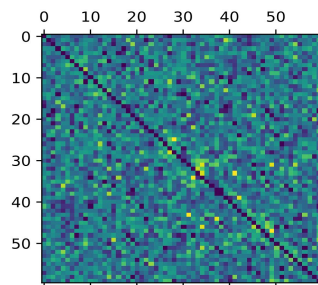
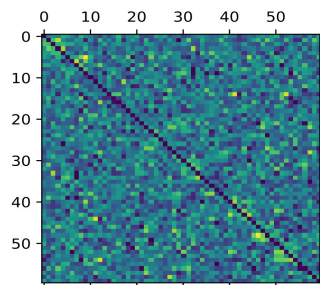
$n = 3$



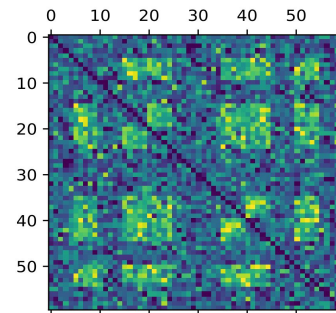
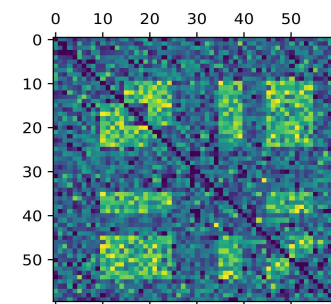
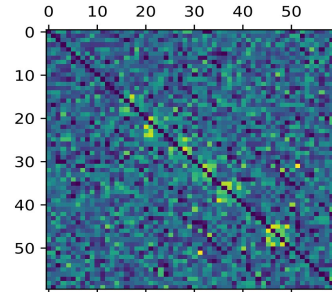
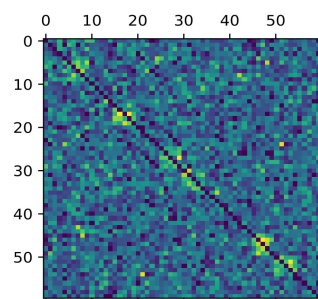
$n = 4$



$n = 5$



$n = 3$



$n = 5$

OK, so...

Two types of connections: **weak** | **strong**

Distributions for connections: **Normal** | **Uniform**

Three types of graphs: **segregated** | **integrated** | **neutral**

Before finally modeling the graphs

How to choose...

- **number of regions?**
- **number of nodes per region?**

Modularity and Participation

These metrics **reflect degree of segregation and integration** considering **regional information**

$$Q_i = \frac{1}{I} \sum_{i,j \in \mathbb{N}} \left[w_{ij} - \frac{k_i k_j}{I} \right] \delta_{r_i, r_j}$$

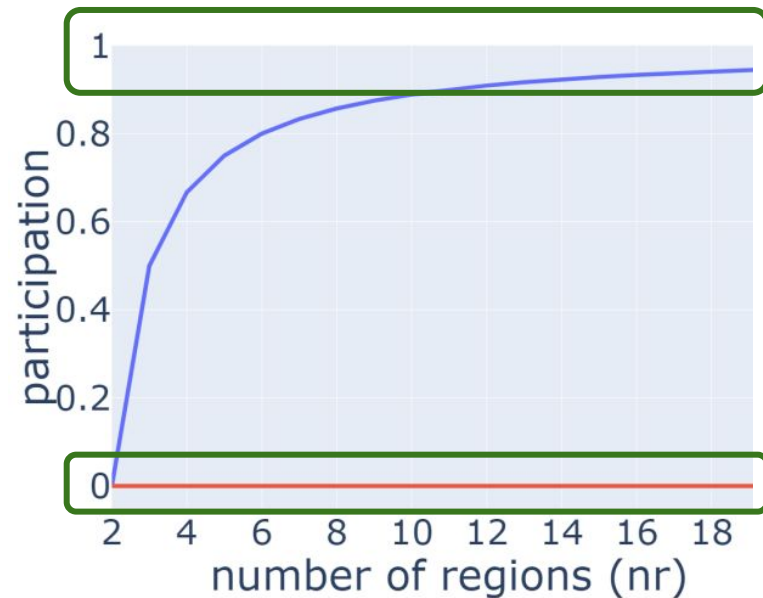
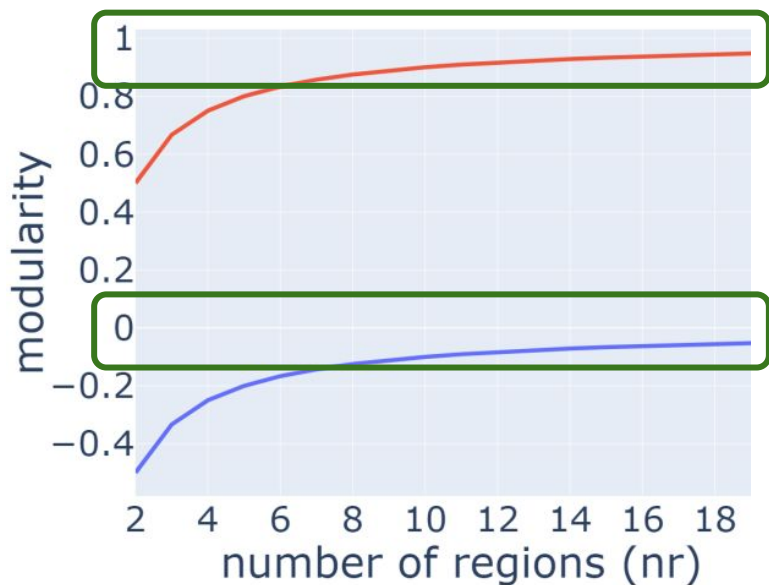
$$\delta_{r_i, r_j} = \begin{cases} 1, & \text{if nodes } i \text{ and } j \text{ are in the same region} \\ 0, & \text{otherwise} \end{cases}$$

$$PC_i = 1 - \sum_{r=1}^R \left(\frac{k_i(r)^2}{k_i} \right)$$

$k_i(r)$ - connectivity strength of node i within region r
 R - region number

Modularity and Participation

— integration
— segregation



The final choice

Number of regions: 12

Number of nodes per region: 5

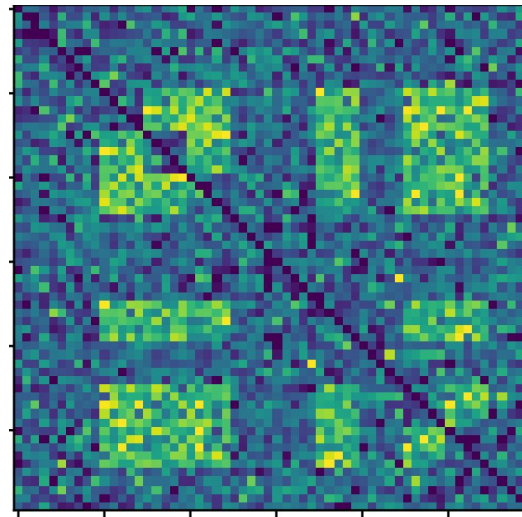
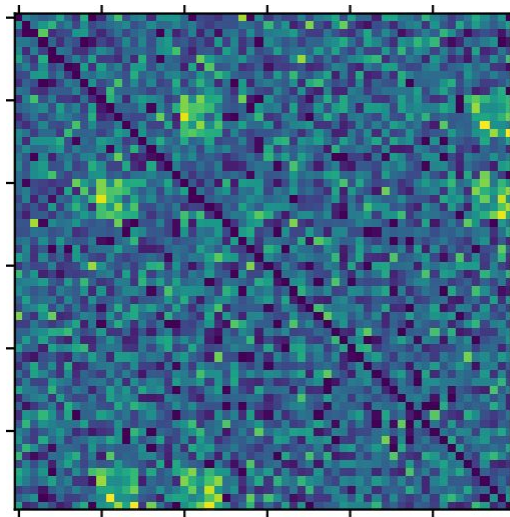
The final choice

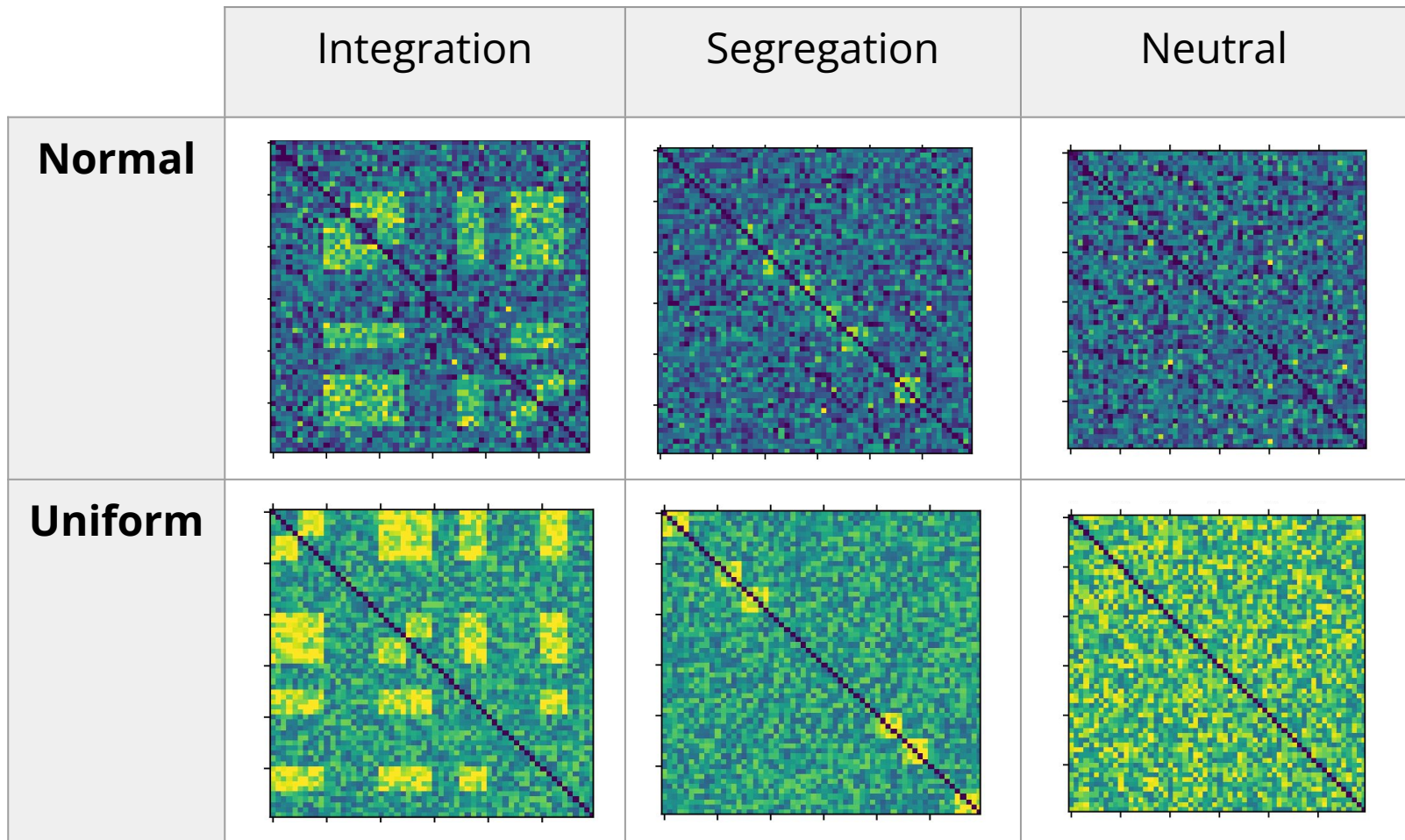
Number of regions: 12

How many are **active**?

3 | 6 | 9 | **all**

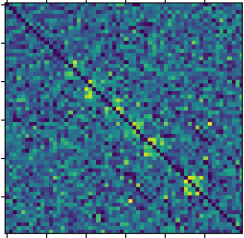
Number of nodes per region: 5





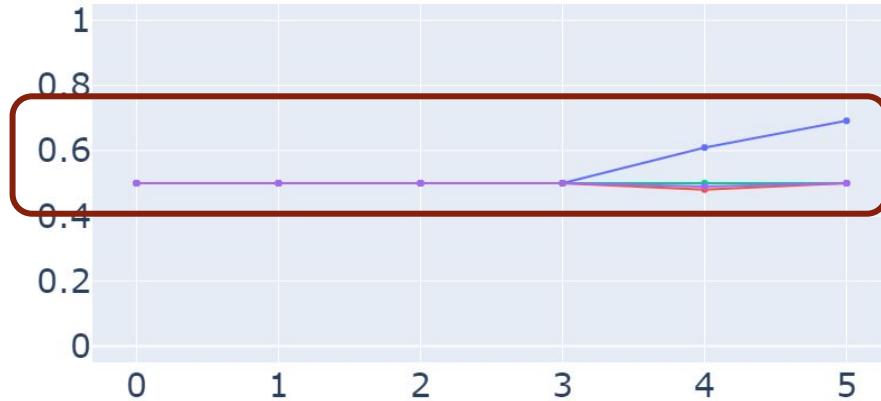
? Research Questions

- Will a GNN show **better results** for either segregation or integration?
- Is there any difference depending on the **difference between weak and strong connections** in a graph?
- Does a **type of distribution** play a role?

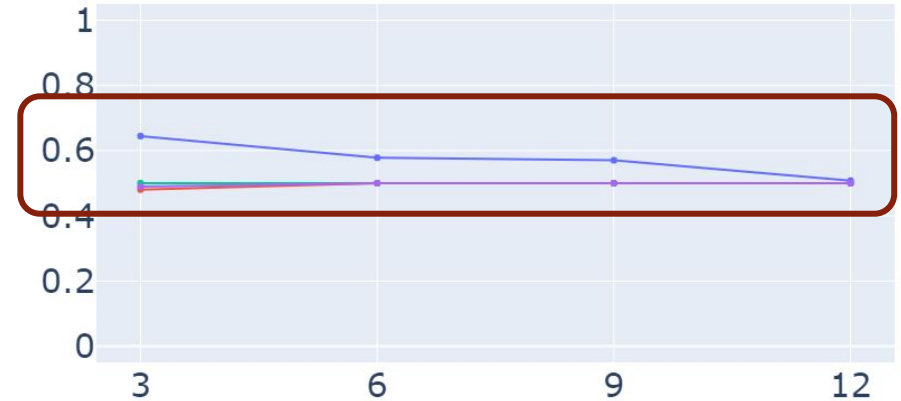


Segregation based on **Normal** distribution

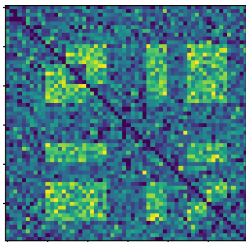
metrics depending on n



metrics depending on nar for $n > 1$



— accuracy
— recall
— precision
— f1

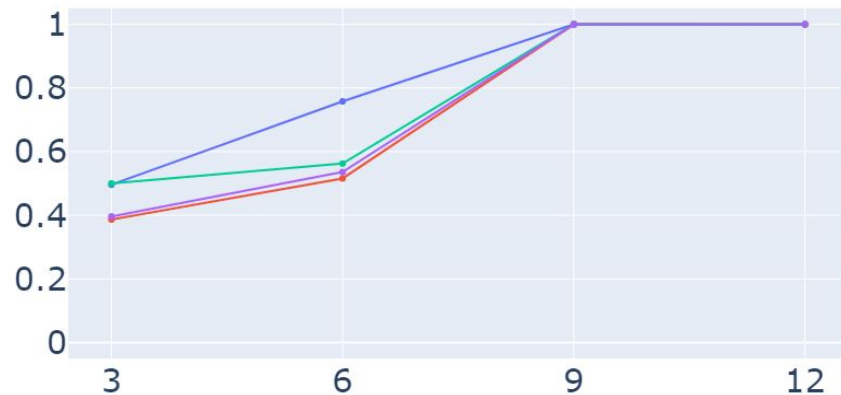


Integration based on **Normal** distribution

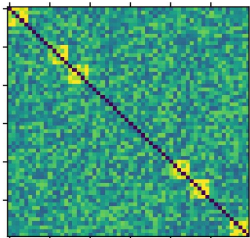
metrics depending on n



metrics depending on nar for $n > 1$



— accuracy
— recall
— precision
— f1

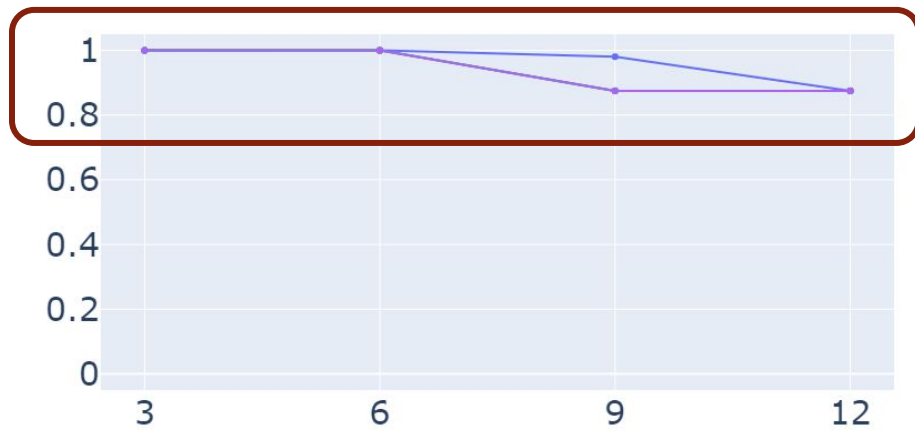


Segregation based on **Uniform** distribution

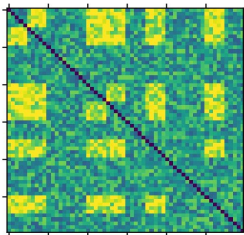
metrics depending on n



metrics depending on nar for $n > 1$

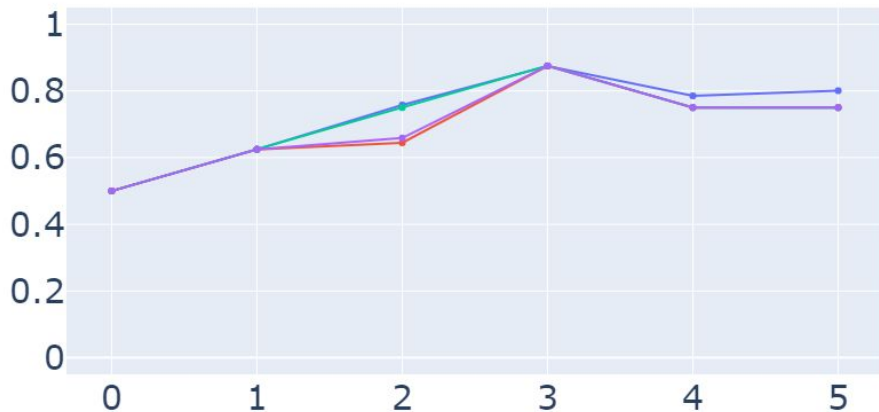


- accuracy
- recall
- precision
- f1

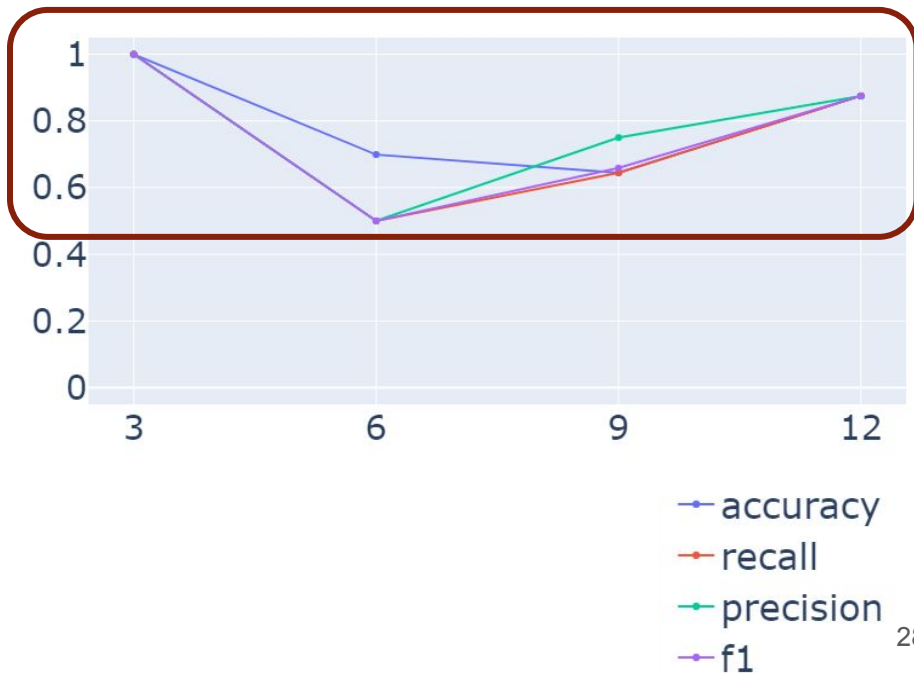


Integration based on **Uniform** distribution

metrics depending on n



metrics depending on nar for $n > 1$





Conclusion

Normal distribution: it is easier to predict integration rather than segregation.

Segregation: It is easier to predict it based on uniform than on normal distribution.

In most cases performance improves as n increases.

Distribution type plays a role in the GNN's performance.



Further work

- Creating not fully connected graphs
- Use an **interpreter**

Acknowledgements

- **Vladimir Maksimenko:** supervision, support, and knowledge sharing
- **Creators of *bctpy* library**