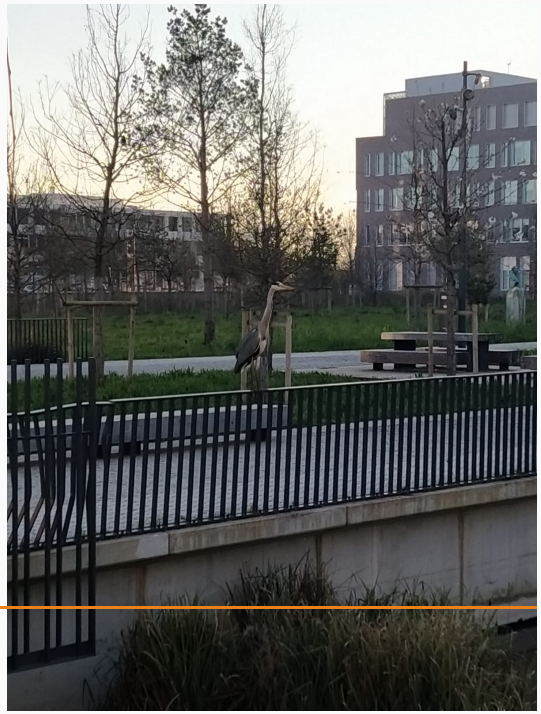
Graph Neural Network: some stuff



Pierre BARBILLON (with a little help from Emre Anakök)

Rochebrune Top, Spring 2024

Outline

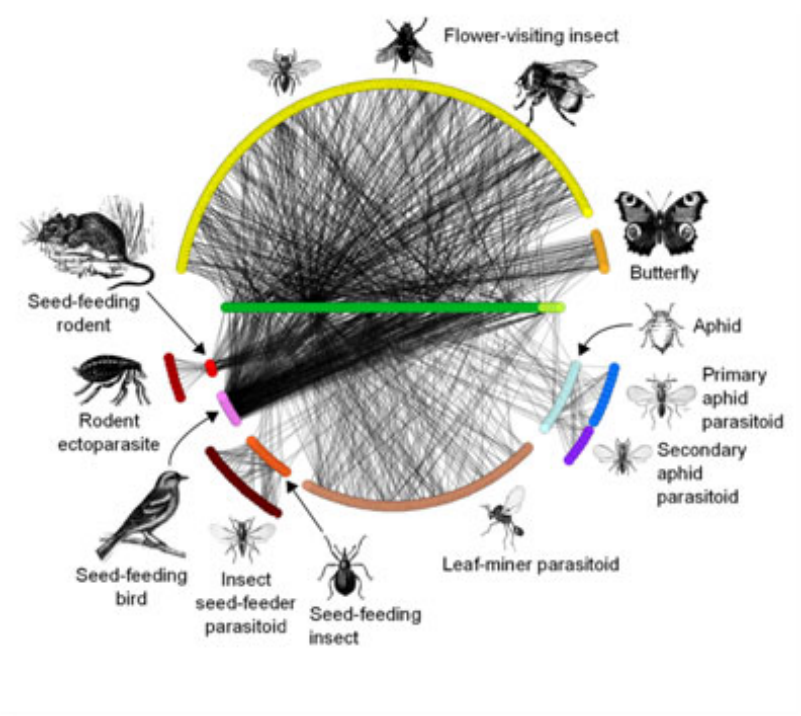
Outline

Sociology

- **Nodes**: individuals or organizations
- **Edges**: advice, competition, ...
- **Examples of objectives**: characterizing the role of individuals in the network, link their role to covariates

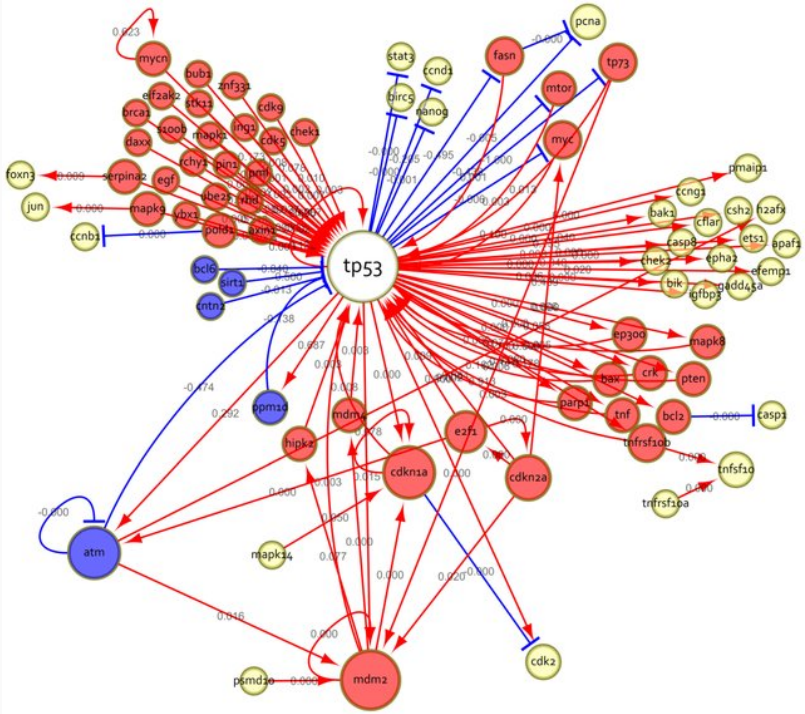
Ecology

- **Nodes:** species (plants or animals)
- **Edges:** predation, pollination, competition...
- **Examples of objectives** : characterizing the structure of the network because it conditions their robustness to the disappearance of species.



Biology

- **Nodes:** genes, metabolites, proteines,
- **Edges:** Regulation, co-expression, reactions,
- **Examples of objectives:** Determine groups of genes co-expressed together under some stresses.



Networks

Graph $G = (V, E, W)$ with

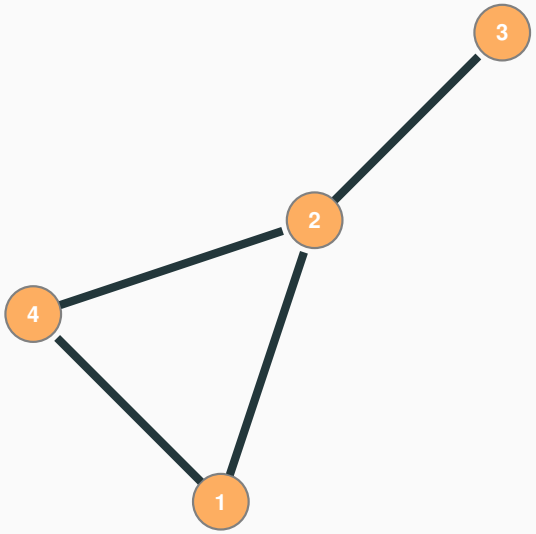
- a set of nodes $V = \{1, \ldots, N\}$,
- a set of edges $E \subset V^2$, particular cases: (un)directed, with(out) loop,...
- additional information on edges, $w \in W$ containing weights (number of interactions, positive or negative interaction,...)

Attributes of:

- **nodes**, for any $i \in V$, X_i attributes of a node (taxon, gender, age, social group,...), or information derived from the edges: degree of i,
- **edges**, for any $e = (i, j) \in E$, the edges may have an attribute coming from the two nodes (difference of ages, same gender...,) or particular attribute (date of interaction,...)
- **network**, global attribute derived from the edges mean connectivity, diameter, or an associated variable.

Network encoding/representation

Simple network



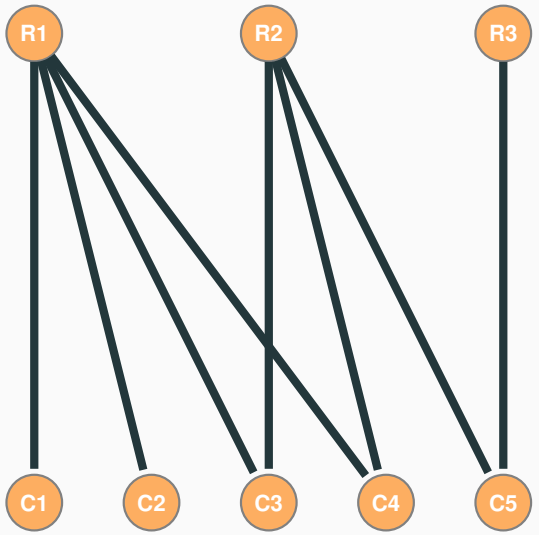
Adjacency matrix:

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

edge list:

E={(1,2),(2,3),(1,4),(2,4)}

Bipartite network



Incidence matrix:

$$B = \begin{pmatrix} 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

edge list:

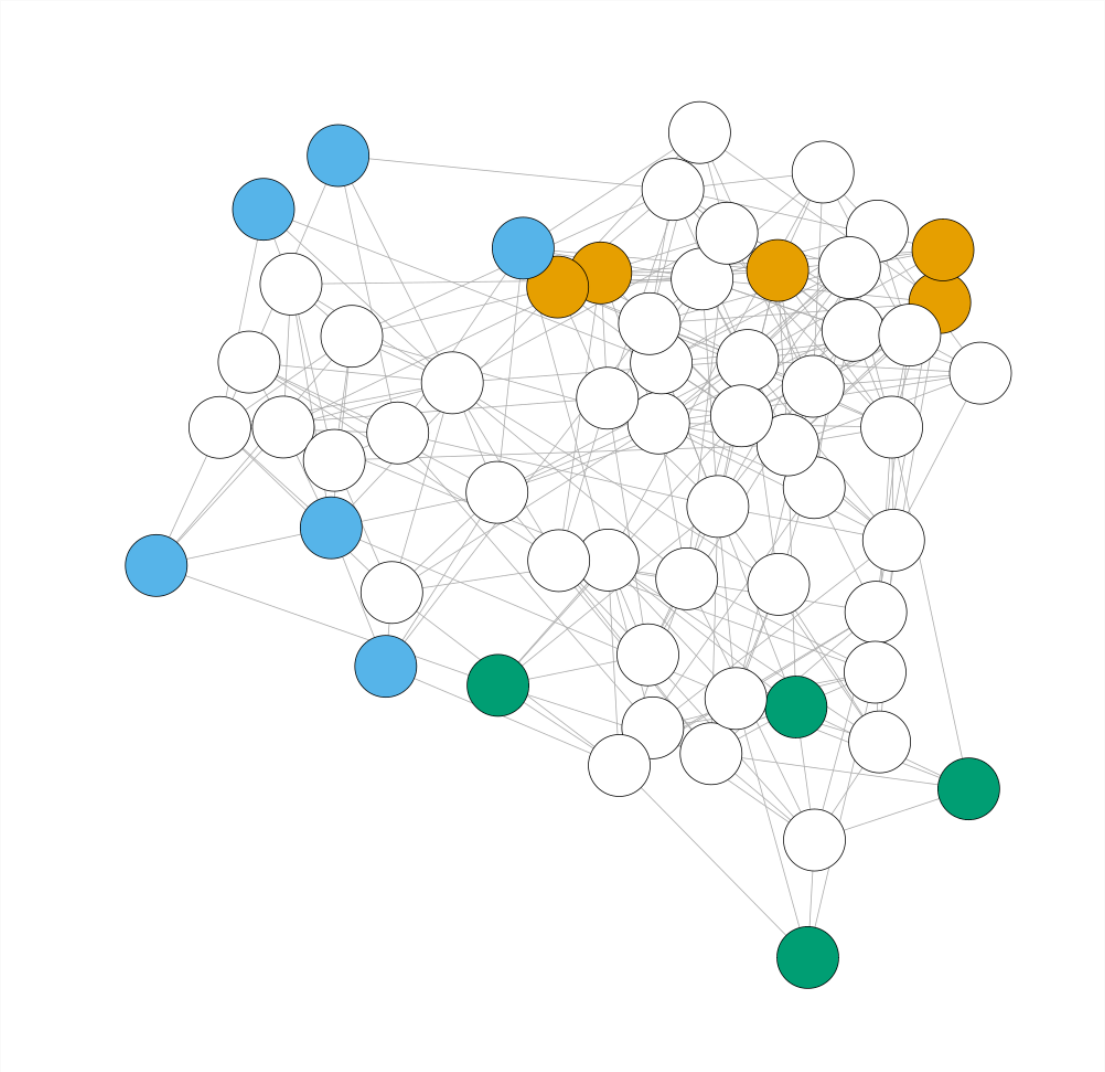
$E = \{(R1, C1), (R1, C2), (R1, C3)...\}$

Outline

Semi-supervised learning on nodes

Data: $G = (V, E)$ and labels in $\{1, \ldots, K\}$ for a subset of V,

- learn $f : i \in V \mapsto \{1, \ldots, K\}$,
- leverage the network structure E.



Clustering of nodes in a graph / Embedding

Data: a graph $G = (V, E)$.

Goal:

- Partition on V.
- Embedding: latent representation of nodes in $\mathbb{R}^d$: $f : i \in V \mapsto \mathbb{R}^d$.

Classification of graphs or regression on graphs

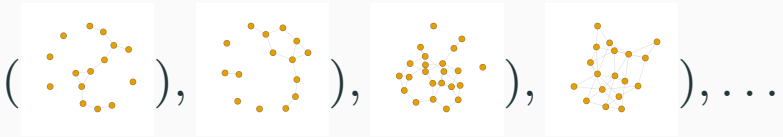
Data:

$$(\ \text{  }\ , y_1),\ \text{  }\ , y_2),\ \text{  }\ , y_3),\ \text{  }\ , y_4), \ldots$$

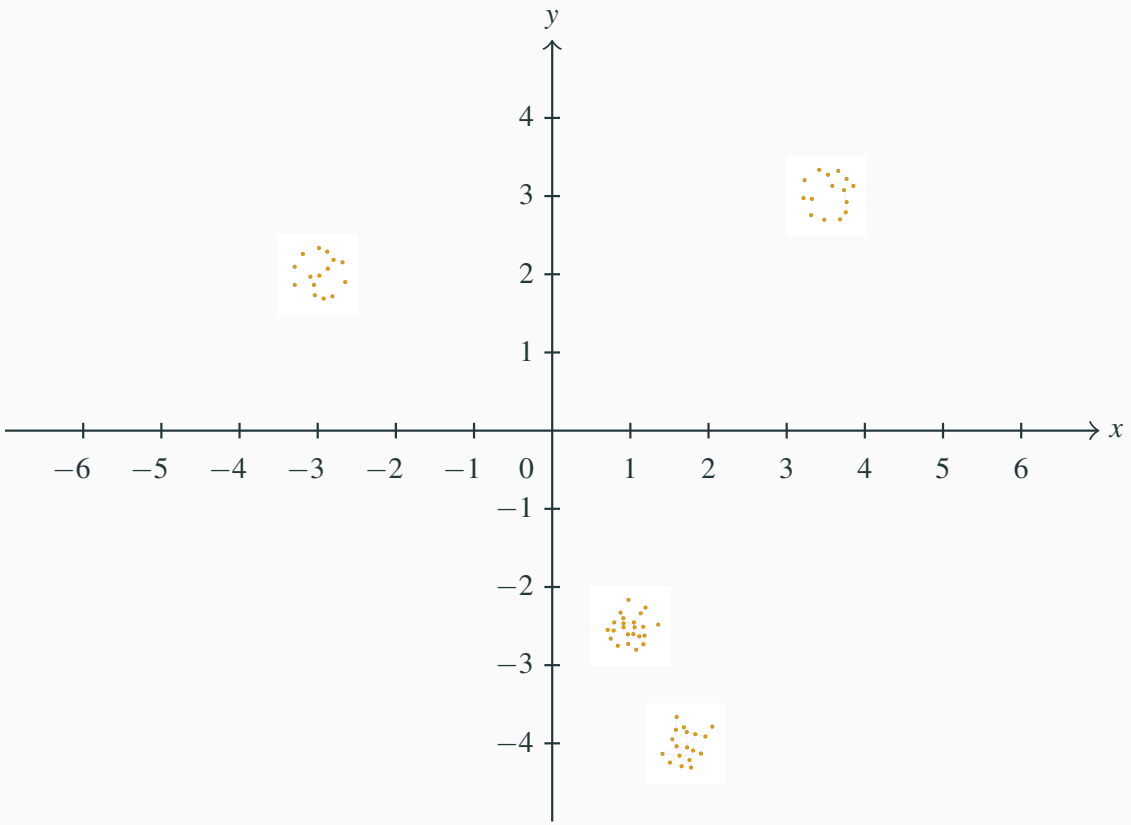
Goal: learn $f : G = (V, E) \mapsto y \in \{1, \ldots, K\}$ or $f : G = (V, E) \mapsto y \in \mathbb{R}$.

Clustering of graphs / Embeddings

Data:



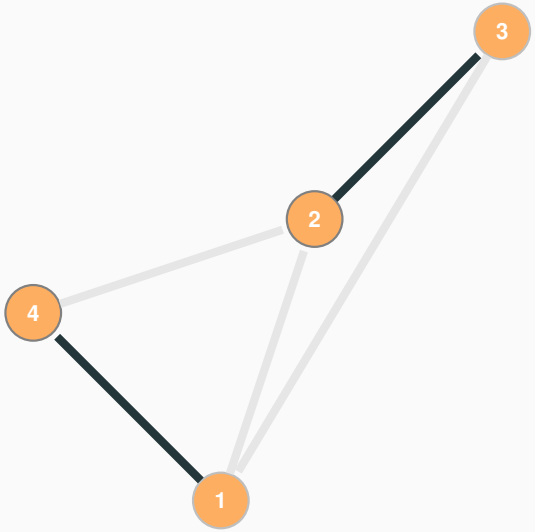
Goal: learn a partition of graphs , learn an embedding:



Predict of dyads, missing links

Data: a graph G with missing or incomplete data.

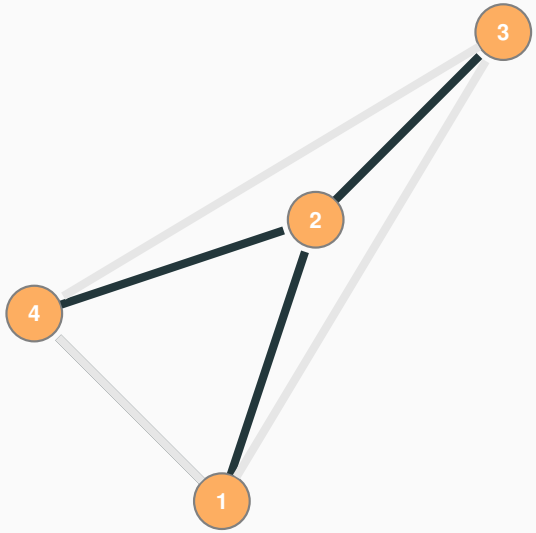
missing data



Adjacency matrix:

$$A = \begin{pmatrix} 0 & \texttt{NA} & \texttt{NA} & 1 \\ \texttt{NA} & 0 & 1 & \texttt{NA} \\ \texttt{NA} & 1 & 0 & 0 \\ 1 & \texttt{NA} & 0 & 0 \end{pmatrix}$$

incomplete data



Adjacency matrix:

$$A = \begin{pmatrix} 0 & 1 & \texttt{NA} & \texttt{NA} \\ 1 & 0 & 1 & 1 \\ \texttt{NA} & 1 & 0 & \texttt{NA} \\ \texttt{NA} & 1 & \texttt{NA} & 0 \end{pmatrix}$$

Goal: Predict NA to $\{0, 1\}$ or predict most likely existing links.

Outline

Models with latent variables

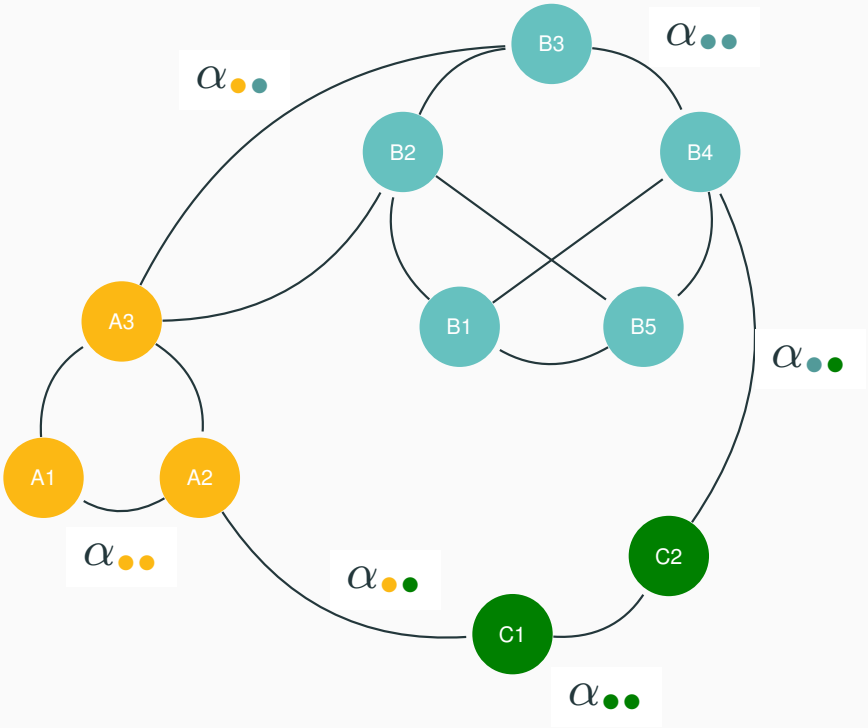
Review: [Matias and Robin, 2014]

- $\boldsymbol{Z} = (Z_1, \ldots, Z_N)$ independent latent variables in $\{1, \ldots, K\}$ or in $\mathbb{R}^d$,
- $Y_{ij}|Z_i, Z_j \overset{ind}{\sim} \mathcal{F}(\alpha_{Z_i,Z_j})$ for all dyads (i, j).
- can include covariates: $Y_{ij}|Z_i, Z_j \overset{ind}{\sim} \mathcal{F}(\alpha_{Z_i,Z_j}, x_{i,j})$.
- e.g. $Y_{ij}|Z_i, Z_j \overset{ind}{\sim} b\Big(1/\big(1 + \exp(-\alpha_{Z_i,Z_j} + \beta^\top x_{i,j})\big)\Big)$.

Two classical families:

- if Zs are categorical $\rightarrow$ Stochastic Block Models [Nowicki and Snijders, 2001],
- if Zs are in a continuous space $\rightarrow$ Latent space models [Peter D Hoff and Handcock, 2002]

Stochastic Block Model : illustration



Parameters

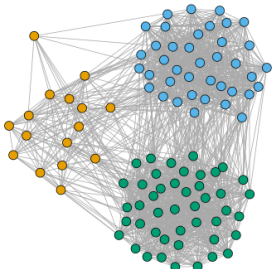
Let N nodes divided into 3 clusters

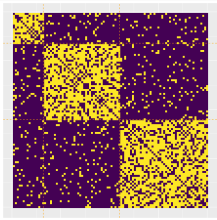
- $\{\bullet, \bullet, \bullet\}$ clusters
- $\pi_\bullet = \mathbb{P}(i \in \bullet),\ i = 1, \ldots, N$
- $\alpha_{\bullet\bullet} = \mathbb{P}(i \leftrightarrow j | i \in \bullet, j \in \bullet)$

$$\mathbf{Y} \sim \mathrm{SBM}_N(Q, \boldsymbol{\pi}, \boldsymbol{\alpha})\,.$$

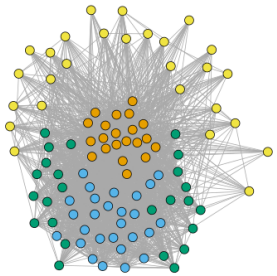
Simulations under the SBM

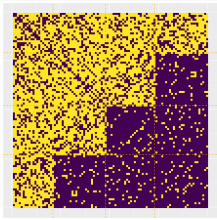
$$\alpha = \begin{pmatrix} 0.70 & 0.09 & 0.09 \\ 0.09 & 0.70 & 0.09 \\ 0.09 & 0.09 & 0.70 \end{pmatrix}$$



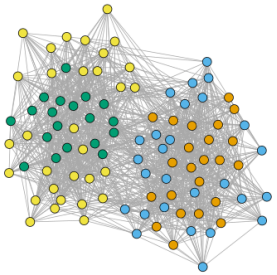


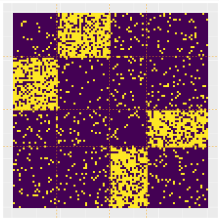
$$\alpha = \begin{pmatrix} 0.70 & 0.70 & 0.70 & 0.70 \\ 0.70 & 0.70 & 0.70 & 0.09 \\ 0.70 & 0.70 & 0.09 & 0.09 \\ 0.70 & 0.09 & 0.09 & 0.09 \end{pmatrix}$$





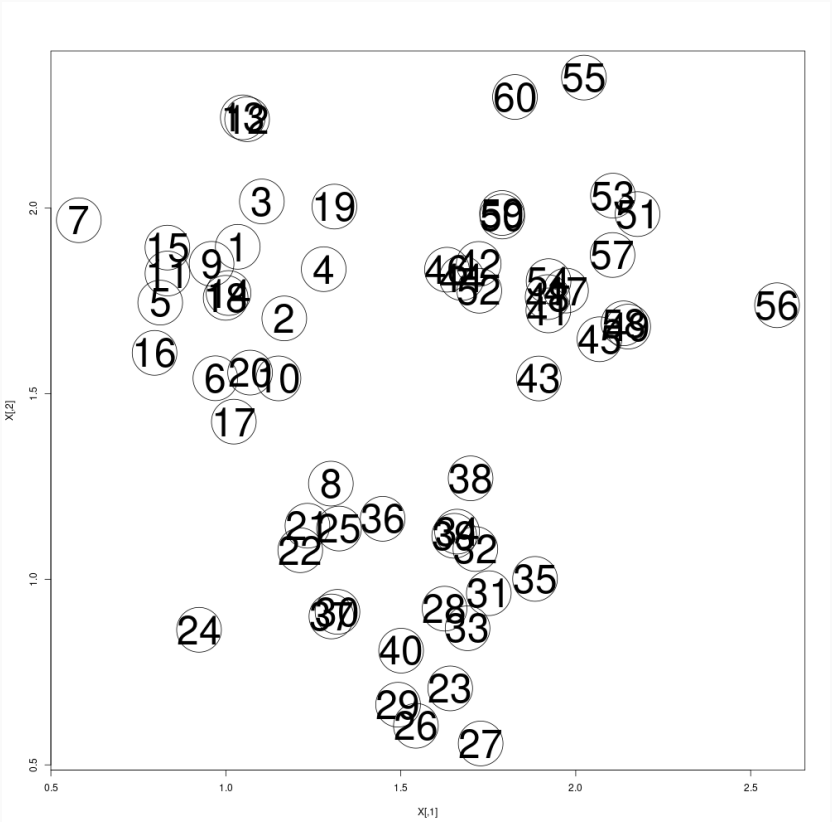
$$\alpha = \begin{pmatrix} 0.09 & 0.70 & 0.09 & 0.09 \\ 0.70 & 0.09 & 0.09 & 0.09 \\ 0.09 & 0.09 & 0.09 & 0.70 \\ 0.09 & 0.09 & 0.70 & 0.09 \end{pmatrix}$$

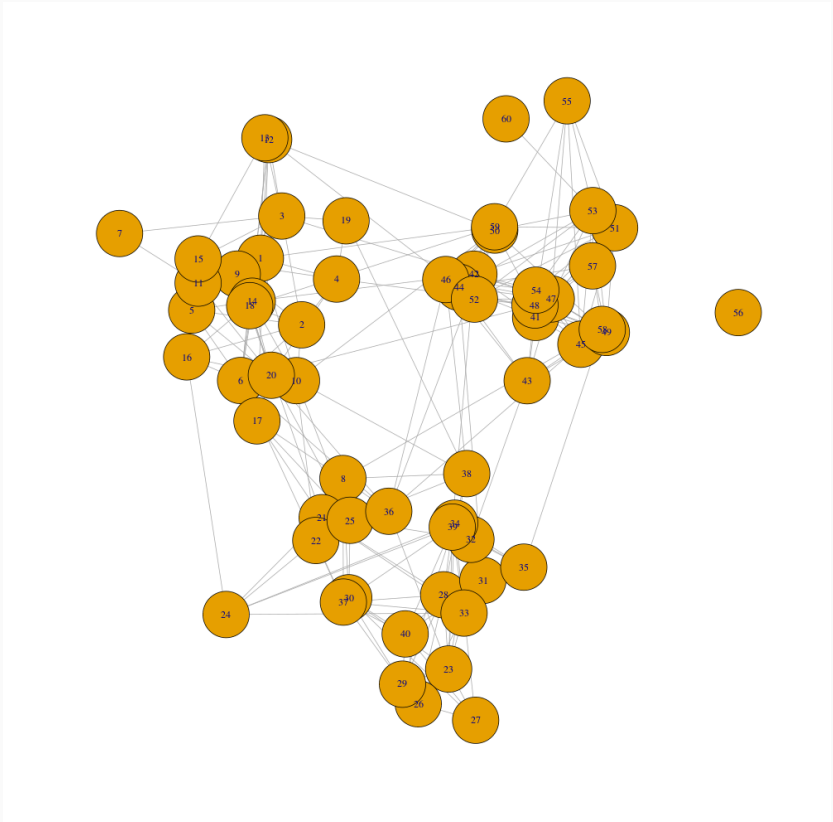




Latent space model

- $\forall i \in \{1, \ldots, N\}$, $Z_i \overset{ind}{\sim}$ Mixture$\mathcal{N}((\mu_k)_k, (\Sigma_k)_k)$,
- $\forall (i,j)$,$Y_{ij}|Z_i, Z_j \overset{ind}{\sim} b(\exp(-\|Z_i - Z_j\|/\sigma^2))$.





(Generalised) random dot product graph

Alternative to the distance between latent positions, the dot product can be used:

$$\forall (i,j),\ Y_{ij} | Z_i, Z_j \overset{ind}{\sim} b(Z_i \cdot Z_j = Z_i^\top Z_j).$$

[Rubin-Delanchy et al., 2022] proposed a generalisation:

$$\forall (i,j),\ Y_{ij} | Z_i, Z_j \overset{ind}{\sim} b(Z_i I_{p,q} Z_j)$$

with

$$I_{p,q} \begin{bmatrix} I_p & 0 \\ 0 & -I_q \end{bmatrix}.$$

Outline

Laplacian of a graph

For $G = (V, E)$ an undirected graph s.t. $V = \{1, \ldots, N\}$ and A the corresponding adjacency matrix.

- Degree of a vertex/node: $d_i = \sum_j A_{ij}$,
- Unnormalized Laplacian: $L = D - A$ with $D = \text{diag}(d_1, \ldots, d_N)$,

Properties:

- for $x \in \mathbb{R}^n$, $x^\top L x = \frac{1}{2} \sum_j^N A_{ij}(x_i - x_j)^2$,
- L is symmetric and positive definite,
- the smallest eigenvalue is 0 and associated with the vector $\mathbb{1}$,
- the order of multiplicity of 0 is the number of connected components.

[Von Luxburg, 2007]

Normalized Laplacians:

$$
\begin{aligned}
L_{sym} &= D^{-1/2} L D^{-1/2} = I_N - D^{-1/2} A D^{-1/2} \\
L_{rw} &= D^{-1} L = I_N - D^{-1} A
\end{aligned}
$$

Properties:

- for $x \in \mathbb{R}^n$, $x^\top L_{sym} x = \frac{1}{2} \sum_j^N A_{ij} (x_i/\sqrt{d_i} - x_j/\sqrt{d_j})^2$,
- L_{sym} and L_{rw} are symmetric and positive definite,
- the smallest eigenvalue is 0,
- the order of multiplicity of 0 is the number of connected components.

Spectral Clustering:

Input: Adjacency Matrix $A \in \mathbb{R}^{N \times N}$, number k of clusters to construct.

- Compute the unnormalized Laplacian L.
- Compute the first k eigenvectors $u_1, \ldots, u_k$ of L.
- Let $U \in \mathbb{R}^{N \times k}$ be the matrix containing the vectors $u_1, \ldots, u_k$ as columns.
- For $i = 1, \ldots, N$, let $z_i \in \mathbb{R}^k$ be the vector corresponding to the i-th row of U.
- Cluster the points $(z_i)_{i=1,\ldots,N}$ in $\mathbb{R}^k$ with the k-means algorithm into clusters $C_1, \ldots, C_k$.

Random walks point of view

Transition from vertex v_i to vertex v_j given by $p_{ij} := \frac{A_{ij}}{d_i}$.

Transition matrix:

$$P = (p_{ij})_{i,j=1,\dots,n}, \quad P = D^{-1}W.$$

Stationary distribution: if G is connected, unique stationary distribution $\pi = (\pi_1, \dots, \pi_n)^T$ with $\pi_i = \frac{d_i}{\mathrm{vol}(V)}$.

Relation with Laplacian: $L_{\mathrm{rw}} = I - P \Rightarrow$ same eigenvectors.

Node2vec: proposes an embedding from random walks on graph [Grover and Leskovec, 2016].

Diffusion point of view

Heat equation on graph:

- S given subset of V with fixed temperature,
- heat exchanges according to (for $i \notin S$):

$$\frac{dT_i}{dt} = \sum_i^n A_{ij}(T_j - T_i) = -(LT)_i \,.$$

- Equilibrium: Laplace equation when $(LT)_i = 0$ or with RW $T_i = (PT)_i$.

[Bonald and De Lara, 2023] relies on this to semi-supervised the graph.

Outline

Convolution on graphs

- particular structure,
- isomorphism of graphs up to relabelling the nodes,
- large graphs but sparse,
- convolution on graph, convolution on images (images can be seen as graph with fixed number of neighbors)

Convolution with neighbors: x features on nodes:

$$h_i = \sum_{j \in \mathcal{N}(i)} x_j$$

$\mathcal{N}(i)$ is the set of neighbors of node i.

Polynomial filters

- Polynomial

$$p_w(L) = w_0 + w_1 L + w_2 L^2 + \ldots + w_d L^d = \sum_{r=0}^{d} w_r L^r.$$

- Convolution of node feature $\mathbf{x}$:

$$h = p_w(L)\mathbf{x}.$$

- if $p_w(L) = 1$, $\mathbf{h} = p_w(L)\mathbf{x} = w_0 I\mathbf{x} = \mathbf{x}$,
- if $p_w(L) = L$, $h_i = (L\mathbf{x})_i = \sum_j (D_{ij} - A_{ij})x_j = D_i x_i - \sum_{j \in \mathcal{N}_i} x_j$,
- $\text{dist}_G(i,j) > r \implies L^r_{vu} = 0$,
- $h_i = (p_w(L)\mathbf{x})_i = (p_w(L))_i\mathbf{x} = \sum_{r=0}^{d} w_r (L^r\mathbf{x})_i = \sum_{r=0}^{d} w_r \sum_j L^r_{ij} x_j = \sum_{r=0}^{d} w_r \sum_{j,\text{dist}_G(j,i) \leq r} L^r_{ij} x_j$.
- independent of the ordering of the node.

[Defferrard et al., 2016]

Convolution with polynomial filters

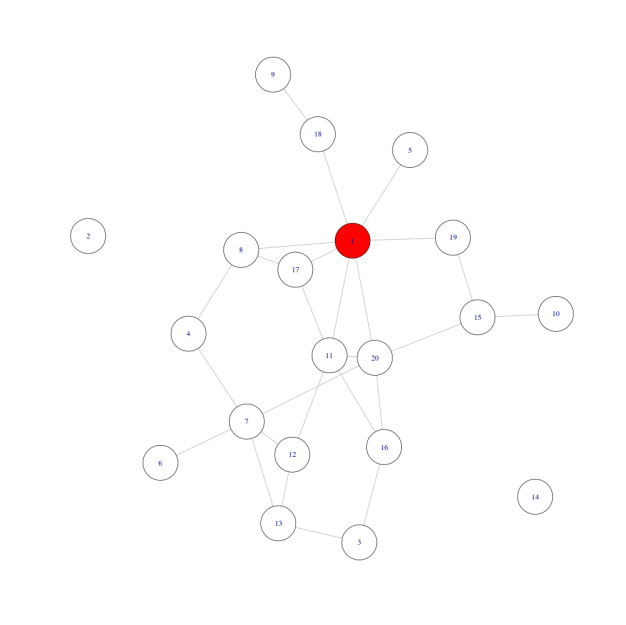
If we have K polynomial filters $p_{w^{(k)}}(L)$ with $w^{(k)}$ trainable parameters.

- $h^{(0)} = x$,
- iterate from $k = 1, \ldots$
  - compute $p^{(k)} = p_{w^{(k)}}(L)$,
  - Matrix computation: $g^{(k)} = p^{(k)} \cdot h^{(k-1)}$,
  - non linear function: $h^{(k)} = \sigma(g^{(k)})$.

If we use $p_{w^{(k)}}(L) = L$:

- $$h_i = (L\mathbf{x})_i = \sum_j (D_{ij} - A_{ij})x_j = D_i x_i - \sum_{j \in \mathcal{N}_i} x_j$$
- we aggregate over immediate neighbors,
- and we combine with the node feature,
- the aggregation is node-order equivariant $\Rightarrow$ overall convolution is node-order equivariant,
- convolutions can be thought of as 'message-passing' between adjacent nodes,
- repeating 1-hop localized convolutions K times makes convolution effective K hops away.

convolutional layer



Graph Convolution Networks

[Kipf and Welling, 2016]

$$h_i^{(\ell+1)} = \sigma\left(\mathbf{W}^{(\ell+1)} \sum_{j \in \mathcal{N}(i) \cup \{i\}} \frac{1}{c_{i,j}} \cdot \mathbf{x}_j^{(\ell)}\right)$$

Importance of normalization $c_{i,j}$.

Matrix form

$$H^{(l+1)} = \sigma\left(\tilde{D}^{-1/2}\tilde{A}\tilde{D}^{-1/2}H^{(l)}W^{(l)}\right)$$

with

- $W^{(l)}$ a matrix of trainable parameters,
- $\tilde{A} = A + I$,
- D the diagonal matrix of degrees of $\tilde{A}$.

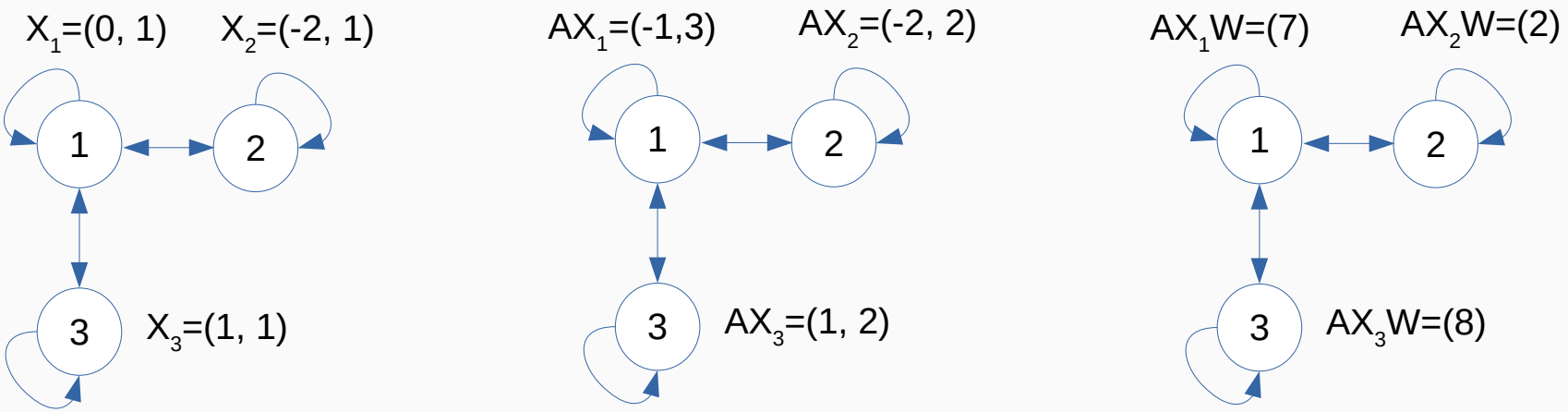
first-order approximation of localized spectral filters proposed in [Defferrard et al., 2016]

Importance of normalization

Different choices:

- No normalization $\tilde{A}$
  - $h_i^{l+1} = \sum_{j, j \in \mathcal{N}(i)} A_{ij} h_j^l$,
  - Eigenvalue of $\tilde{A}$ larger than $1 \Rightarrow$ exploding largest eigenvalue when stacking layers,
- row normalization $A_{\text{row}} = D^{-1} A$,
  - $h_i^{l+1} = \sum_{j, j \in \mathcal{N}(i)} A_{ij} \frac{h_j^l}{d_i}$
  - largest eigenvalue is 1 but not taken into account connectivity of neighbors,
- col normalization $A_{\text{col}} = A D^{-1}$
  - $h_i^{l+1} = \sum_{j, j \in \mathcal{N}(i)} A_{ij} \frac{h_j^l}{d_j}$
  - largest eigenvalue is 1 but put too much weight on well connected nodes,
- Naive normalization $A_{\text{naive}} = D^{-1} A D^{-1}$
  - $h_i^{l+1} = \sum_{j, j \in \mathcal{N}(i)} A_{ij} \frac{h_j^l}{d_j d_i}$
  - largest eigenvalue is < 1 and vanishes when stacking layers,
- symmetric normalization $A_{\text{sym}} = D^{-1/2} A D^{-1/2}$
  - $h_i^{l+1} = \sum_{j, j \in \mathcal{N}(i)} A_{ij} \frac{h_j^l}{\sqrt{d_j d_i}}$
  - largest eigenvalue is 1, combine row and col normalization.

Graph Convolutional Network



$$\tilde{A} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}, X = \begin{pmatrix} 0 & 1 \\ -2 & 1 \\ 1 & 1 \end{pmatrix}, W = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$$

Other kinds of GNN

- Graph Convolution Networks as we have seen,
- Graph Attention Networks (GAT) [Casanova et al., 2018],
  - $h_i^l = \sigma\left(\sum_{j \in \mathcal{N}(i)} \alpha^l(i,j) W h_j^{l-1}\right)$,
  - $\alpha^l(i,j)$ is the attention function,
  - $\alpha^l(i,j) = \text{softmax}\left(\sigma'\left(a^\top \cdot (Wh_i, Wh_j)\right)\right)$.
- Graph SAGE (SAmple and agGrEgate) [Hamilton et al., 2017],
  - $h_{\mathcal{N}(i)}^l = AGGREGATE_k(\{h_j^{l-1}, j \in \mathcal{N}(i)\})$,
  - $h_i^l = \sigma(W^l \cdot CONCAT(h_i^{l-1}, h_{\mathcal{N}(i)}^l)$,
  - $h_i^l = h_i^l / \|h_i^l\|$.
- Graph Isomorphism Network (GIN) [Xu et al., 2018].

see https://distill.pub/2021/understanding-gnns/

Outline

Semi-supervised learning on nodes

Data: $G = (V, E)$ a network with N nodes, $m\%$ of nodes with an observed labels in $\{1, \ldots, Q\}$, V set of edges is known, (features on nodes X).

Goal: Classify nodes without labels.

Architecture:

- X can be a vector of the degrees of nodes, a number for each node, or an identity matrix...
- 2 or 3 GCN layers with given numbers of features,
- Last layer is a linear transformation in a K dimension space : for each p point from the dataset $(h^L_{p1}, \ldots, h^L_{pK})$.

Loss: Cross entropy:

$$loss(x, y) = \frac{1}{n_{\text{train}}} \sum_{p=1}^{n_{\text{train}}} \log \left(\frac{\exp(h^L_{p,y_p})}{\sum_{k=1}^{K} \exp(h^L_{p,k})} \right) .$$

Graph clustering

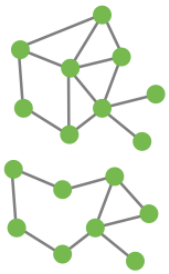
Data: $G_1, \dots G_n$ and labels on graphs.

Goal: Learn the Classification function $f : G \mapsto \{1, \dots, K\}$

Architecture:

$\mathcal{G}_1 = (\mathbf{X}_1, \mathbf{A}_1)$

$\mathcal{G}_2 = (\mathbf{X}_2, \mathbf{A}_2)$



$$\text{GNN}\left(\begin{bmatrix} \mathbf{A}_1 & \\ & \mathbf{A}_2 \end{bmatrix}, \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{bmatrix}\right) = \begin{bmatrix} \mathbf{X}'_1 \\ \mathbf{X}'_2 \end{bmatrix}$$

and batches

Average over nodes in the same graph in order to have a layer at the graph level and use a classifier.

Loss: cross entropy.

Link Prediction

Data: $G = (V, E)$, V is incomplete.
Goal: Find edges that are likely to exist for a given set of non-observed edges...

Architecture: GCN layers with V as the set of edges... Last layer uses a "decoder" for dyads:

$$g(\text{Dist}(h_i^l, h_j^l)) \text{ or } h_i^{l\top} h_j^l$$

Loss: Cross entropy computed on a set of trainable DYADS (usually half of edges and half of non edges).

Remark: Autoencoder directly derived from link prediction task by using h_i^l as the embedding.

GVAE

Data: $G = (V, E)$.

Goal: Find an embedding of nodes in a small dimension (Euclidean) space as a conditional distribution.

Architecture: GCN layers to embed the nodes in the parameters of a Gaussian distribution, simulation under the distribution and a last decoder layer to predict edges.

$$(X_i)_i \to (m_i, s_i)_i \to (Z_i = m_i + s_i \cdot \mathcal{N}(0,1))_i \to (Z_i^\top Z_j)_{ij}$$

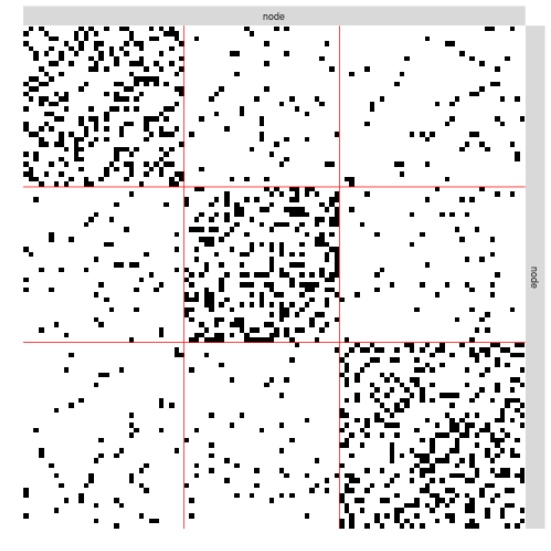
Loss: Cross entropy with a KL on the set of trainable DYADS:

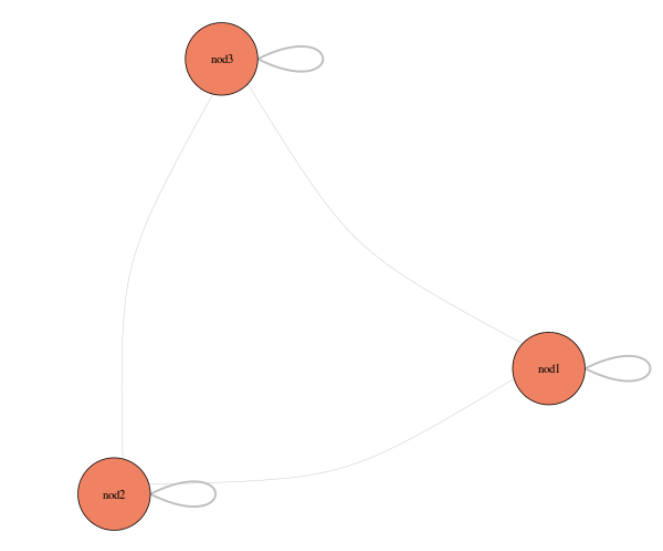
$$\mathbb{E}_{q(Z|X,A)}\big(\log p(A_{\text{train}}|Z)\big) - KL(q(Z|X,A)||p(Z))$$

where $p(Z)$ is a prior distribution chosen as $\mathcal{N}(0,1)$.

Some Examples

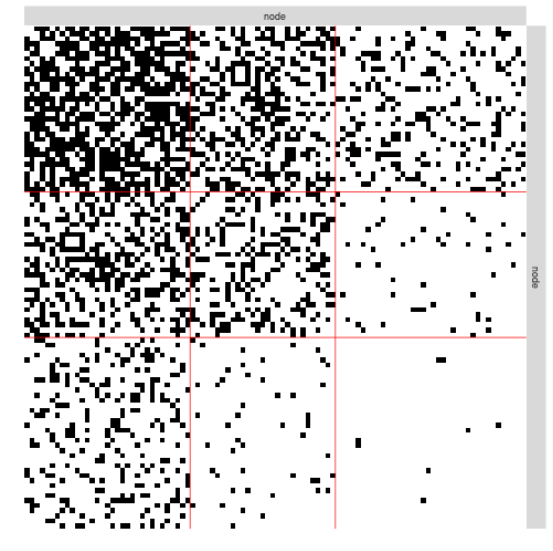
Communities

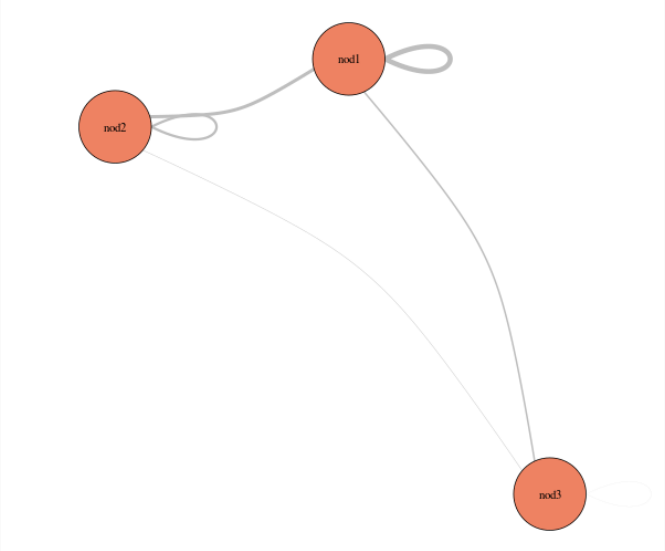




Some Examples

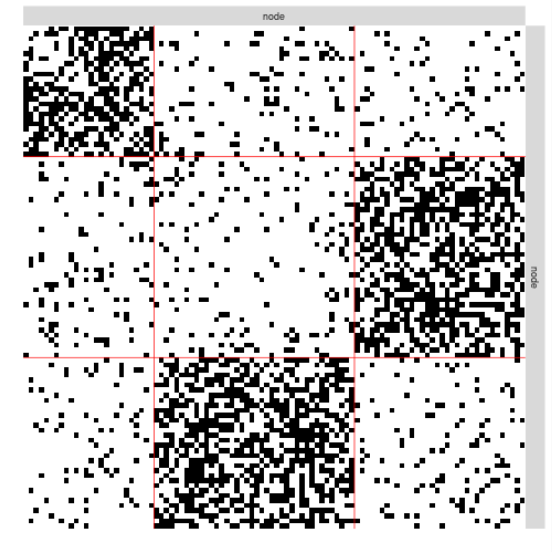
Nestedness

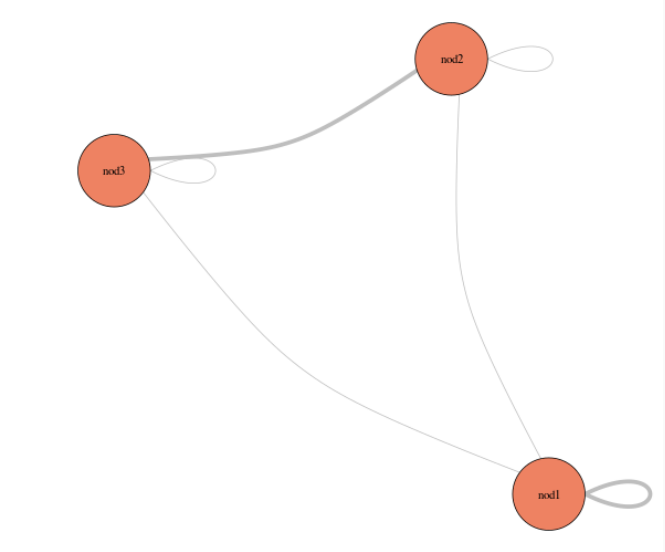




Some Examples

Community and antagonism





Many resources online

- introduction to GNN https://distill.pub/2021/gnn-intro/,
- convolution on graphs https://distill.pub/2021/understanding-gnns/,
- google colabs for pytorch geometric https://pytorch-geometric.readthedocs.io/en/latest/get_started/colabs.html.

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