Graph clustering of ecological networks

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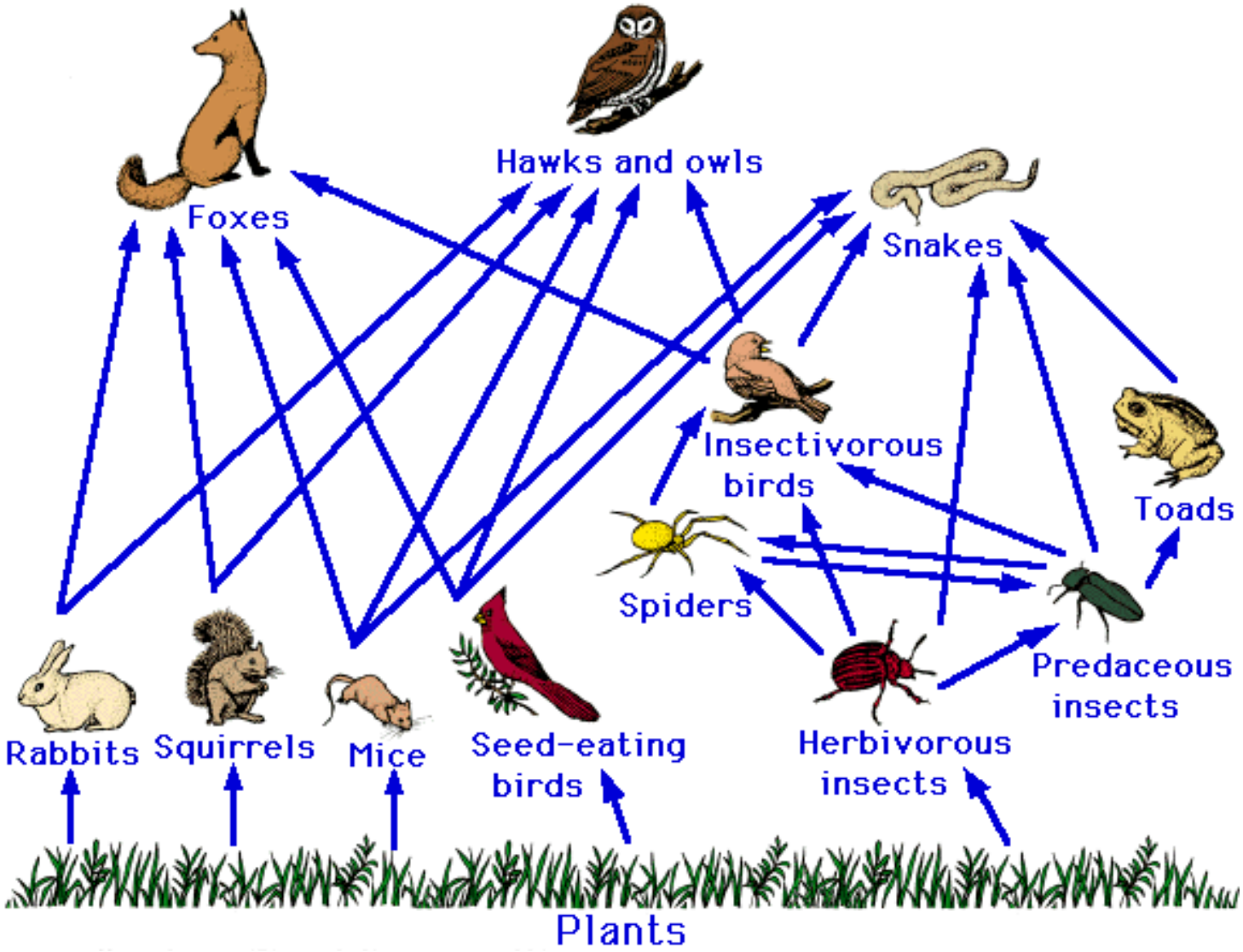
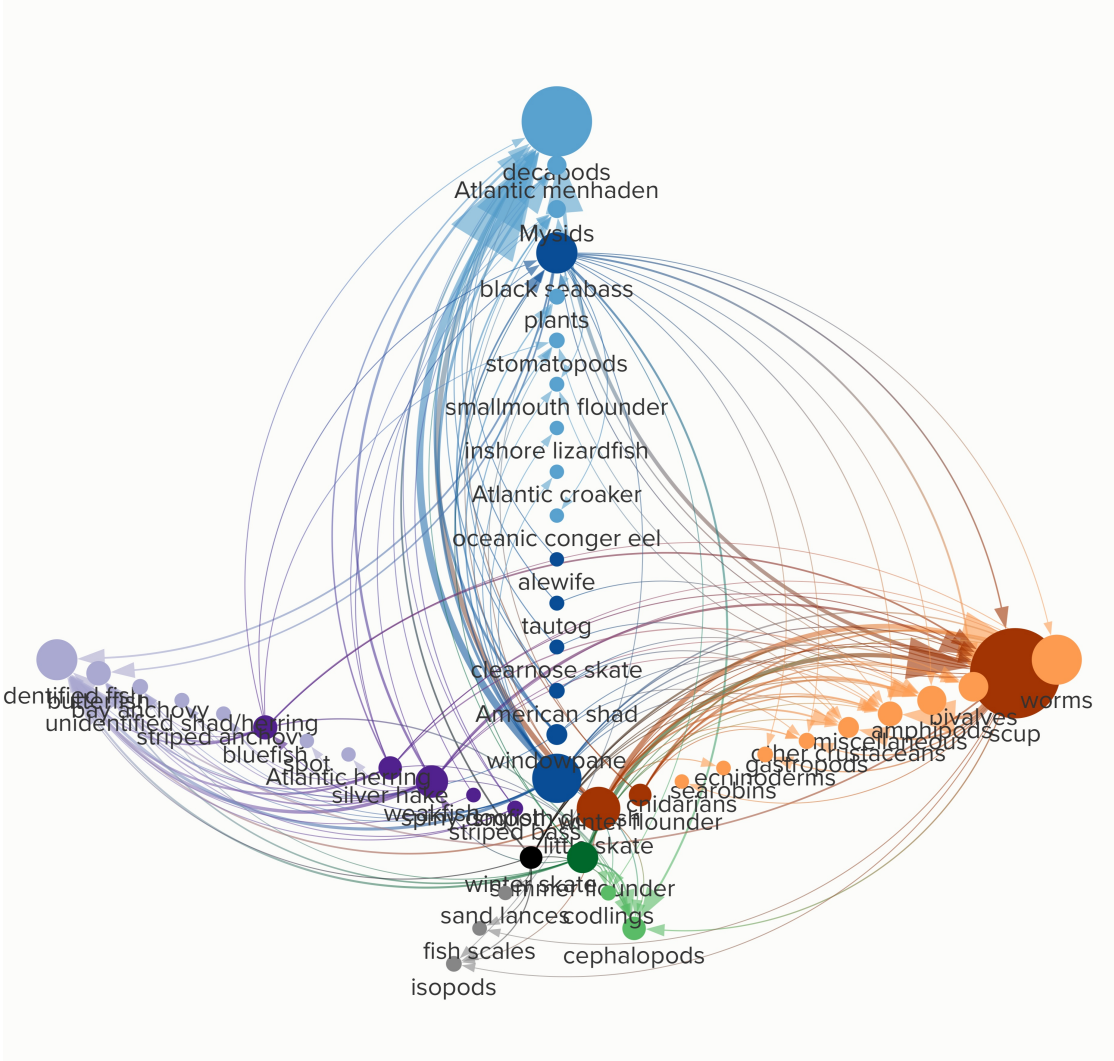
Foodwebs I



Source: www.pw.live/chapter-our-environment/food-web

Foodwebs II



Fall 2021 NEAMAP Food Webs – Mid-Atlantic Coastal Food Web

Source: Virginia Institute of Marine Science

Foodwebs III

Mangal database

- collection of foodwebs on a planetary scale
- 1.300 networks, 120.000 interactions across 7.000 taxa
- contains further information on
  - type (predation, mutualism, parasitism)
  - geographic location
  - climate conditions
- Poisot et al. (2016) + R package `rmangal`

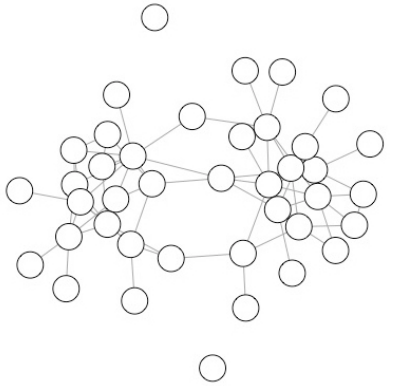
Foodwebs IV

Questions

- analyze and compare many networks
- identify networks with similar structure/organization
- detect outliers/changes...

$\hookrightarrow$ do it in an **automatic** way
$\hookrightarrow$ use an **objective criterion** for comparison

Graph clustering task



From a **mathematical point of view**.

- consider a **collection of networks** or graphs
- goal: graph **clustering**
- many other fields of application : social sciences, transport, biology and medicine (e.g. metabolic networks)

Clustering in machine learning literature

Classical clustering approaches

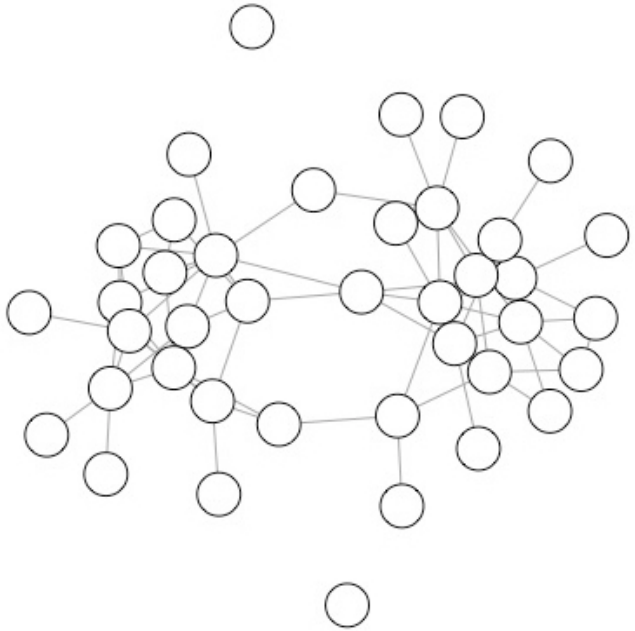
- clustering of **vectors**: kmeans, DBSCAN, GMM
- straightforward solution for networks:
  - compute a **graph embedding** (based on hand-designed statistics or deep learning)
  - apply classical ML clustering method

New network clustering approach

Our approach

- is a statistical one
- introduce a **statistical model** for each graph
- perform **model-based clustering** (like a classical mixture model)
- hierarchical **agglomerative cluster algorithm**
- interpretable output

Modelling I

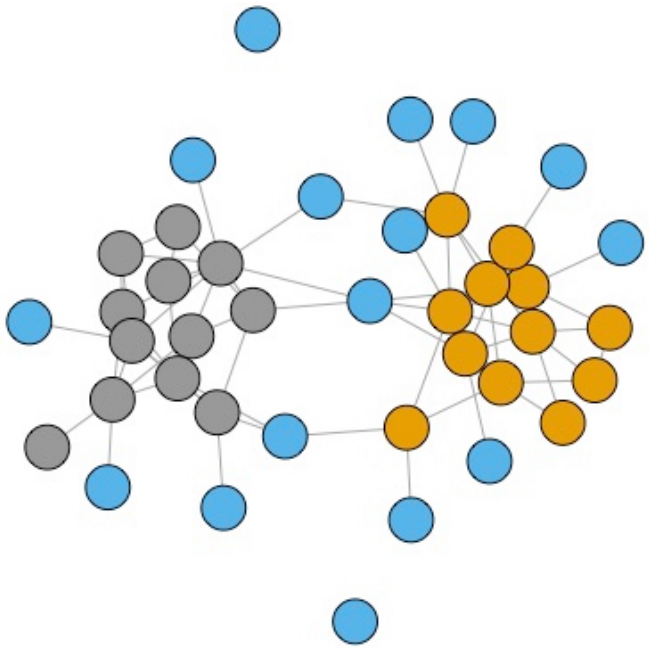


$\Longleftrightarrow$

```
> adjMatrix
      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10] [,11] [,12] [,13]
 [1,]    0    0    0    0    0    0    0    0    0     0     1     0     1
 [2,]    0    0    0    0    0    0    0    0    0     0     0     0     0
 [3,]    0    0    0    0    0    0    0    0    0     0     0     0     0
 [4,]    0    0    0    0    0    0    0    0    1     0     0     0     0
 [5,]    0    0    0    0    0    0    0    0    0     0     0     0     0
 [6,]    0    0    0    0    0    0    0    0    0     0     0     0     0
 [7,]    0    0    0    0    0    0    0    0    0     0     0     0     0
 [8,]    0    0    0    0    0    0    0    0    0     1     0     0     0
 [9,]    0    0    0    1    0    0    0    0    0     0     0     0     0
[10,]    0    0    0    0    0    0    0    1    0     0     1     0     0
[11,]    1    0    0    0    0    0    0    0    0     1     0     0     0
[12,]    0    0    0    0    0    0    0    0    0     0     0     0     0
[13,]    1    0    0    0    0    0    0    0    0     0     0     0     0
```

Adjacency matrix

Modelling II



Stochastic block model (SBM)

- **Block memberships** For node i, $Z_i \in \{1, \ldots, K\}$ is drawn independently with probabilities

$$\mathbb{P}(Z_i = \bullet) = \pi_\bullet$$

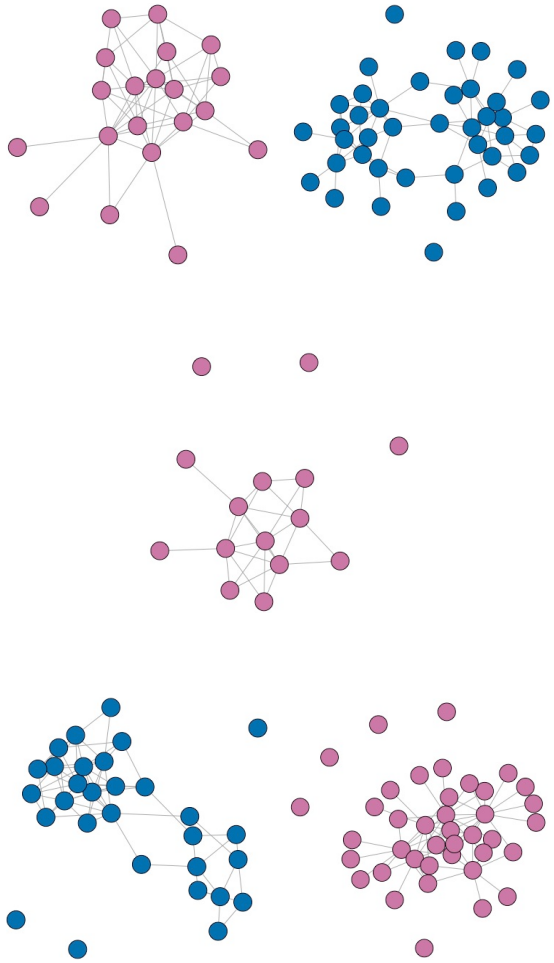
- **Edges** Conditionally on $Z_1, \ldots, Z_n$, $A_{i,j}$ are drawn independently

$$A_{i,j} | (Z_i = \bullet, Z_j = \bullet) \sim \text{Bernoulli}(\gamma_{\bullet\bullet})$$

- **Model parameters** of the SBM:

$$\theta^{\text{SBM}} = ((\pi_k)_{1 \leq k \leq K}, (\gamma_{k,l})_{1 \leq k,l \leq K})$$

Modelling III



Mixture model of SBMs

- C different SBM parameters $\theta_c^{\mathrm{SBM}}, c = 1, \ldots, C$
- **Cluster membership** For network m, $U_m \in \{1, \ldots, C\}$ is drawn independently with probabilities

$$\mathbb{P}(U_m = c) = p_c$$

- Conditionally on $U_1, \ldots, U_M$, the adjacency matrix $A^{(m)}$ is drawn from a SBM:

$$A^{(m)} | (U_m = c) \sim \mathrm{SBM}(\theta_c^{\mathrm{SBM}})$$

Estimation I

- Observed collection of networks: $\mathcal{A} = \{A^{(m)}, m = 1, \ldots, M\}$
- Latent variables: $\mathcal{U} = (U_1, \ldots, U_M)$, $\mathcal{Z} = \{Z^{(m)}, m = 1, \ldots, M\}$
- Model parameters of the mixture:
  $\theta = \left((p_1, \ldots, p_C), (\boldsymbol{\pi}^{(c)}, \boldsymbol{\gamma}^{(c)})_{c=1,\ldots,C}\right)$

Estimation II

Integrated classification likelihood (ICL)

- Bayesian approach: put a prior $p(\theta)$ on the parameters θ
- Likelihood criterion:

$$\mathrm{ICL}(\mathcal{U}, \mathcal{Z}; \mathcal{A}) = \log(p(\mathcal{U}, \mathcal{Z}, \mathcal{A})) = \log\left(\int p(\mathcal{U}, \mathcal{Z}, \mathcal{A}|\theta)p(\theta)\mathrm{d}\theta\right)$$

- Estimates of $\mathcal{U}$ and $\mathcal{Z}$:

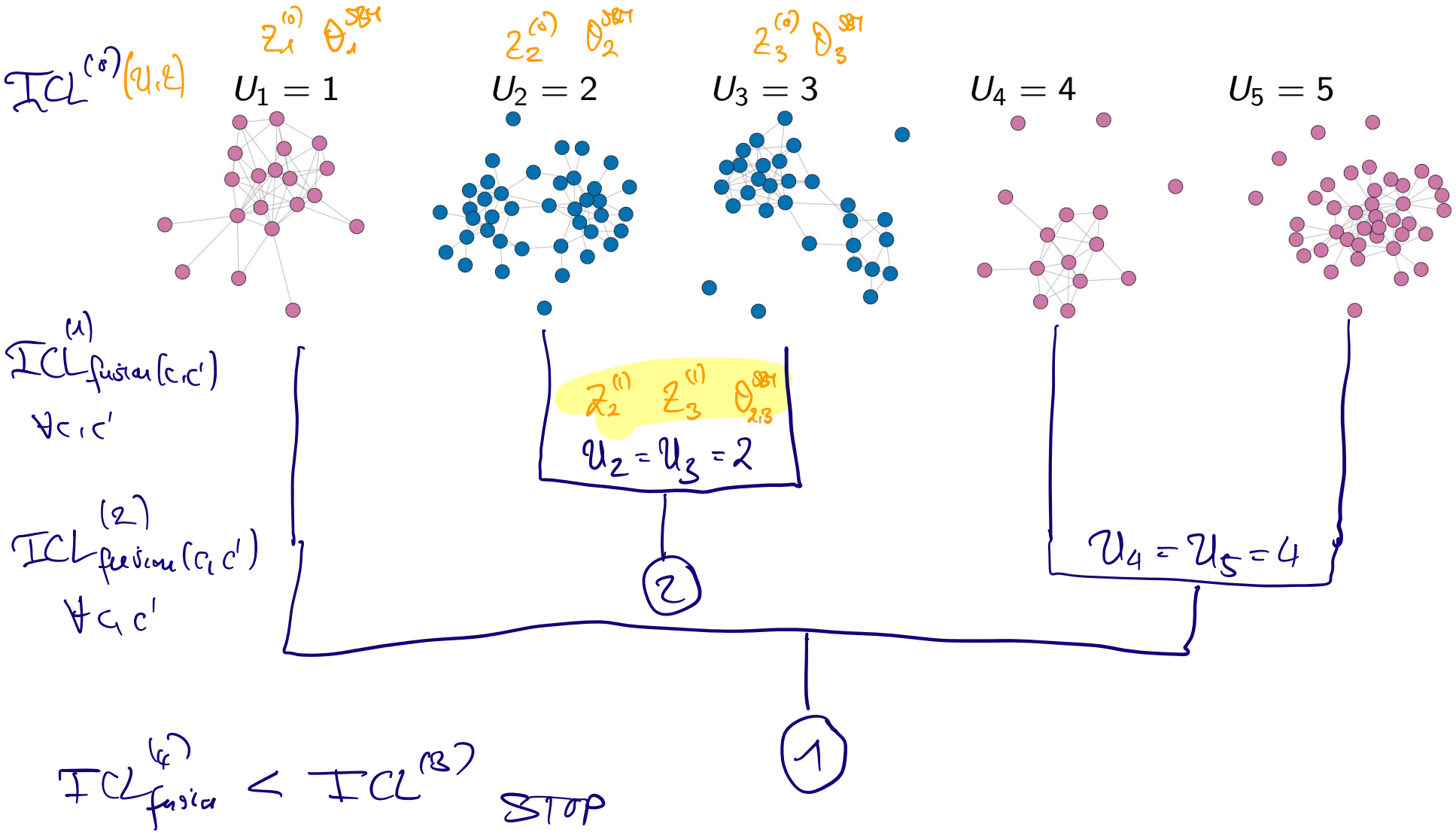
$$(\hat{\mathcal{U}}, \hat{\mathcal{Z}}) = \arg\max_{\mathcal{U},\mathcal{Z}} \mathrm{ICL}(\mathcal{U}, \mathcal{Z}; \mathcal{A})$$

(Côme and Latouche, 2015)

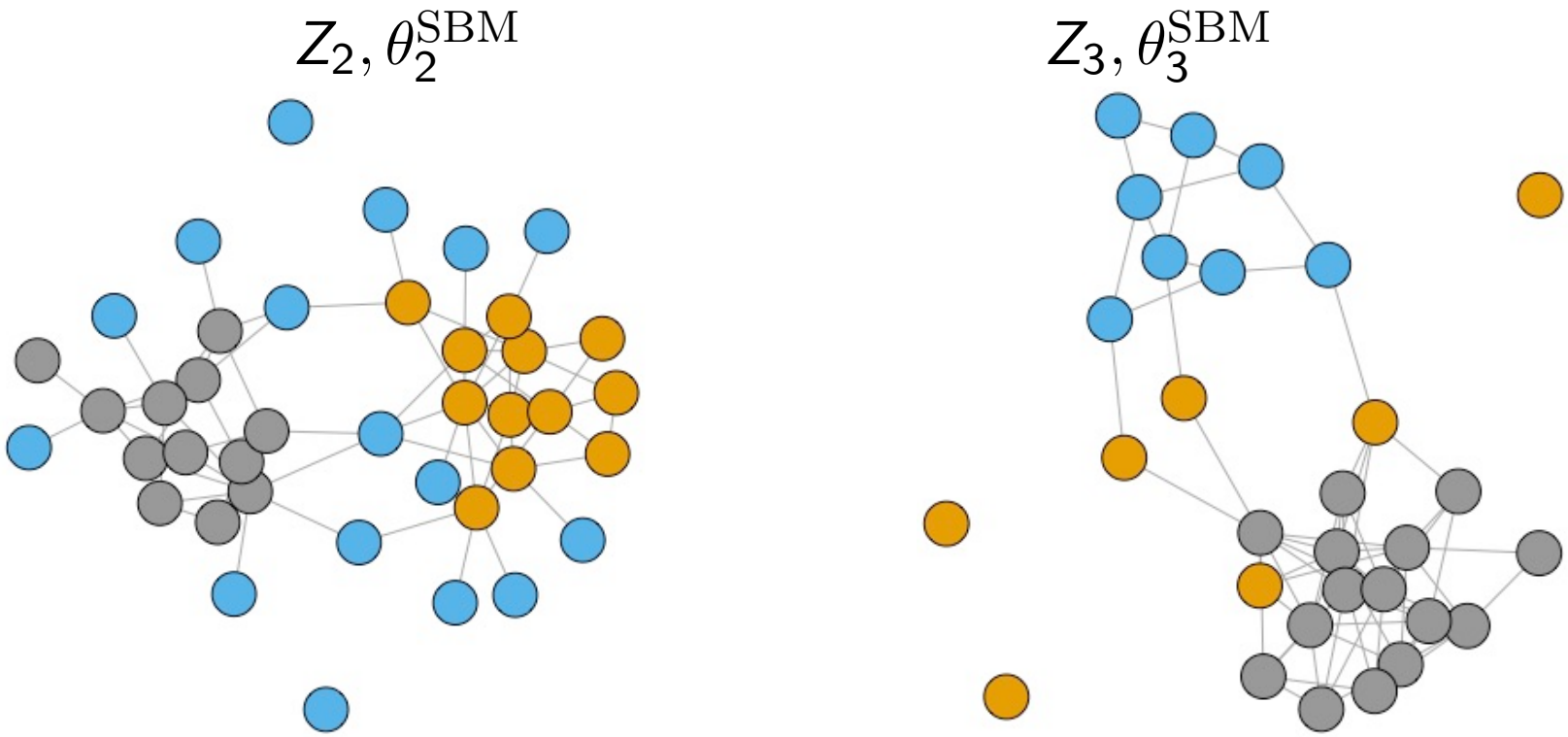
- With an appropriate prior $p(\theta)$, the ICL has closed-form expression
- Discrete optimization

Estimation III

Agglomerative algorithm



Fusion of two clusters I

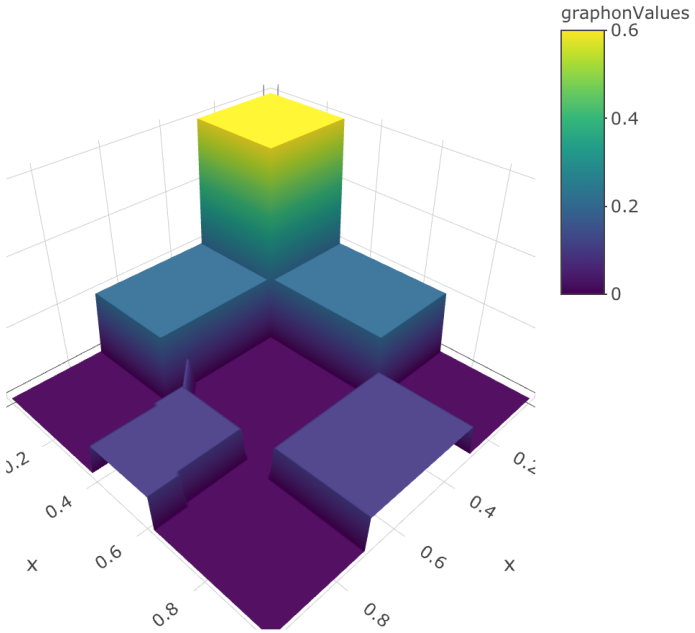


Label-switching problem in the SBM

Fusion of two clusters II

$$\boldsymbol{\pi} = (0.3, 0.4, 0.3)$$

$$\gamma = \begin{pmatrix} 0.6 & 0.2 & 0 \\ 0.2 & 0 & 0.1 \\ 0 & 0.1 & 0 \end{pmatrix}$$



Graphon of a SBM

- $g(u, v) = \gamma_{k,l}$ for all $u \in I_k$, $v \in I_l$
- intervals $I_k = \left(\sum_{s=1}^{k-1} \pi_s, \sum_{s=1}^{k} \pi_s\right]$
- piecewise constant function
- Graphon g depends on the block labelling!

(Lovász, 2012)

Fusion of two clusters III

- Consider L^2-distance of two graphons:

$$\|g_{\theta_1} - g_{\theta_2}\|_2 = \left(\int_{[0,1]^2} (g_{\theta_1}(u,v) - g_{\theta_2}(u,v))^2 \mathrm{d}(u,v) \right)^{\frac{1}{2}}$$

Matching blocks of two SBMs

Search the best permutations of block labels by

$$(\hat{\sigma}_1, \hat{\sigma}_2) \in \arg \min_{\sigma_1 \in \mathfrak{S}_{K_1}, \sigma_2 \in \mathfrak{S}_{K_2}} \|g_{\sigma_1(\theta_1)} - g_{\sigma_2(\theta_2)}\|_2,$$

where $\mathfrak{S}_K$ denotes the set of all permutations of $\{1, \ldots, K\}$ and $\sigma(\theta) = \left((\pi_{\sigma(1)}, \ldots, \pi_{\sigma(K)}), (\gamma_{\sigma(k),\sigma(l)})_{k,l} \right)$.

- does not depend on the clusterings, the data, the number of networks or the number nodes
- works also for $K_1 \neq K_2$

Mangal Foodwebs I

Data

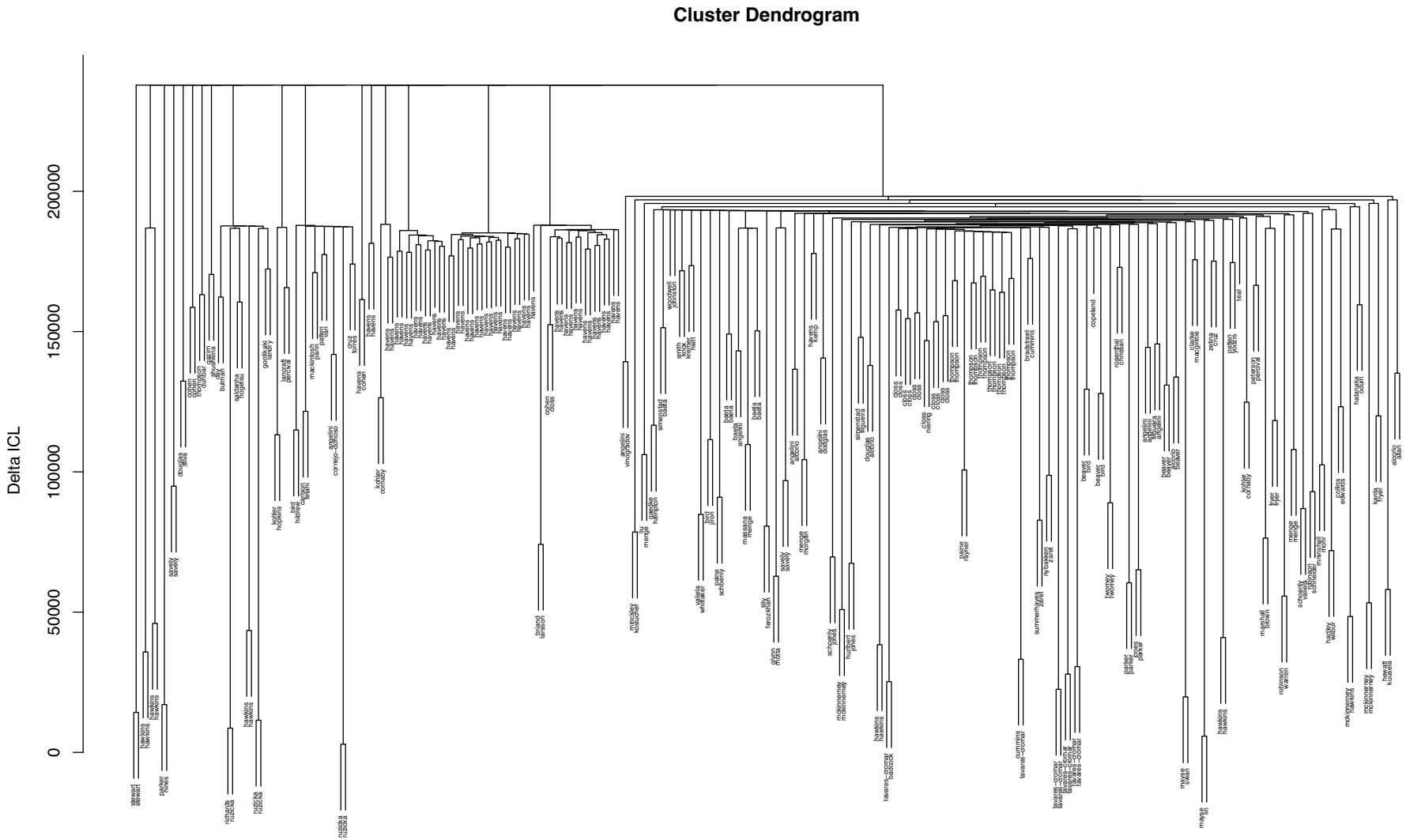
- 270 predator foodwebs
- mean number of species: 33 (min=5, max=317)
- mean number of edges: 120 (min=5, max=1.086)
- mean density: 0,12 (min=0,01, max=0,41)

Clustering results

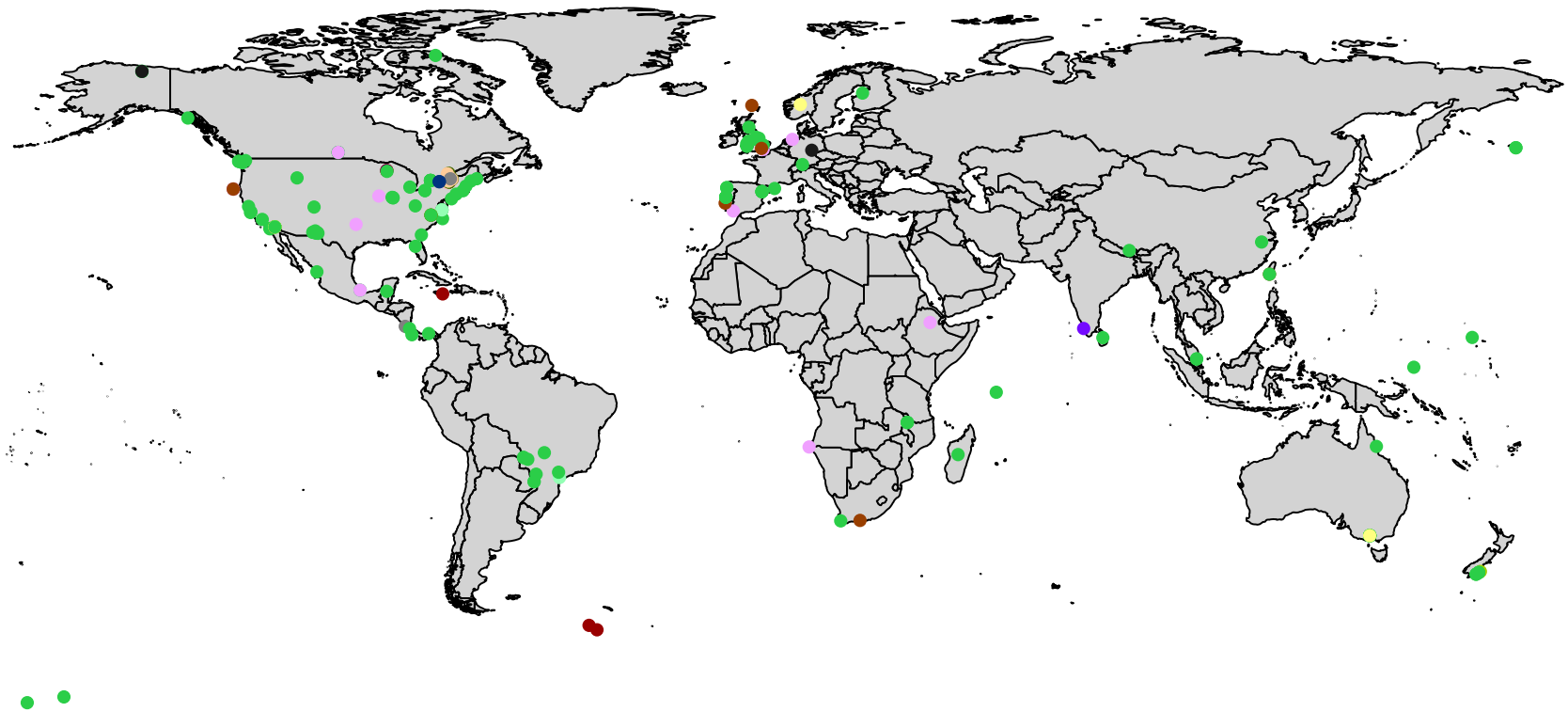
- partition into 18 clusters
- cluster sizes:

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
166	19	18	11	4	2	2	14	4	12	2	2	2	2	2	2	4	2

Mangal Foodwebs II

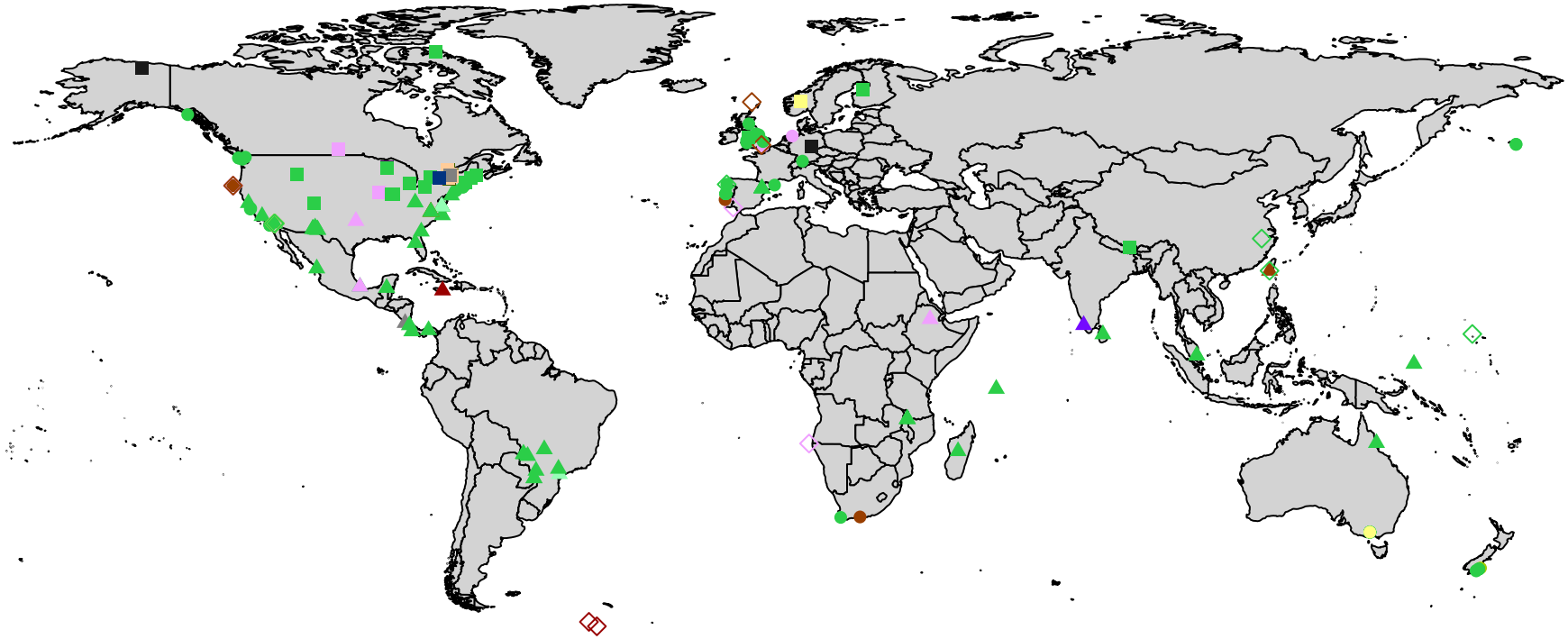


Mangal Foodwebs III



Sampling bias: the planet is not observed uniformly (Poisot et al., 2020)

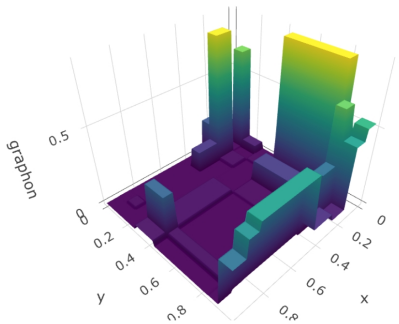
Mangal Foodwebs IV



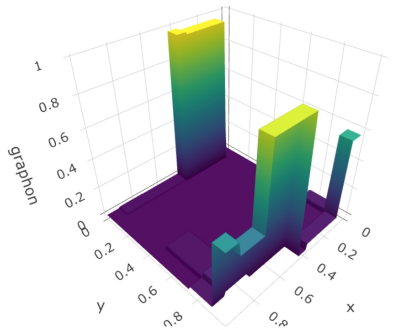
Impact of climat conditions

Mangal Foodwebs V

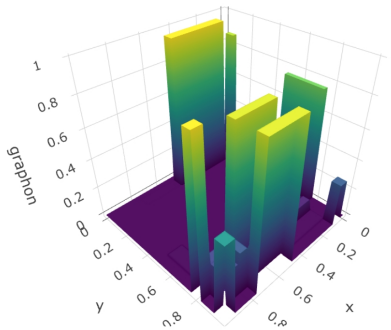
Cluster 1



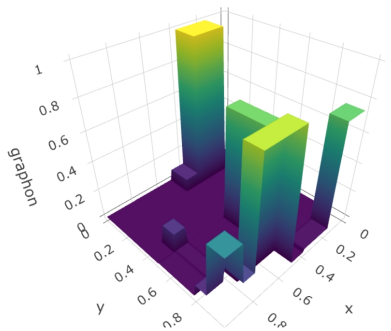
Cluster 2



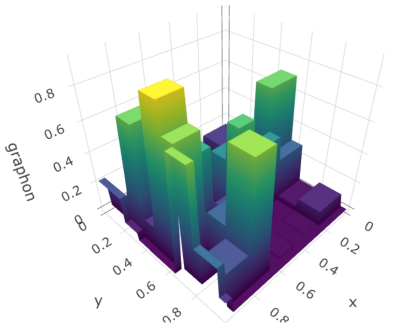
Cluster 3



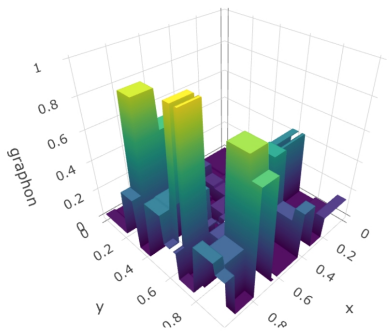
Cluster 4



Cluster 8

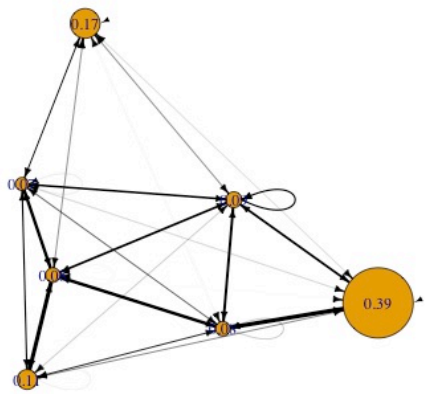


Cluster 10

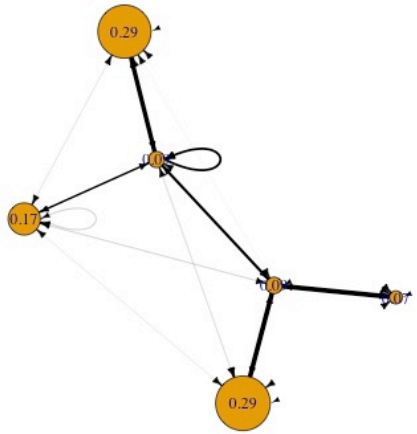


Mangal Foodwebs VI

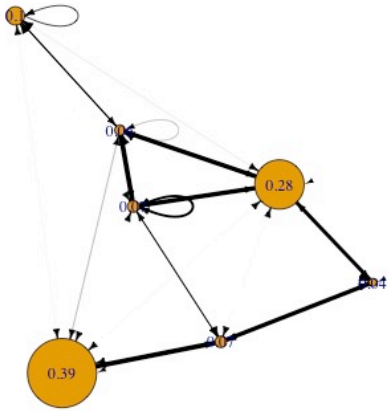
Cluster 1



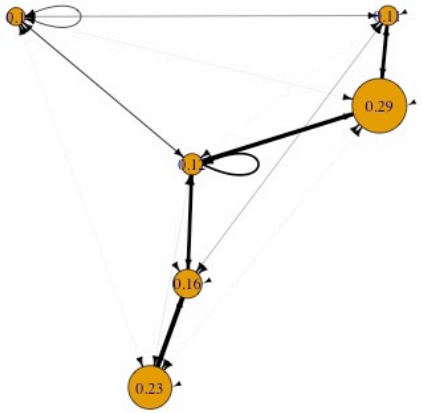
Cluster 2



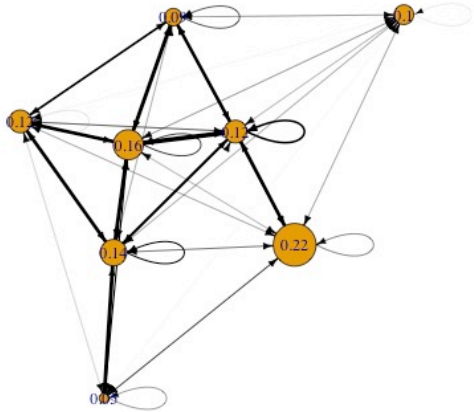
Cluster 3



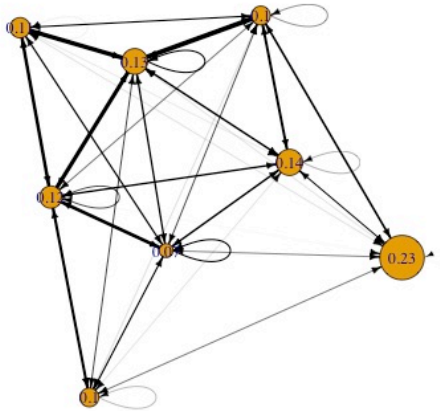
Cluster 4



Cluster 8



Cluster 10



Conclusion & perspectives I

Hierarchical algorithm

- better scalability than EM-type algorithms
- automatic search of the best number of clusters
- cluster hierarchy (dendrogram)
- interpretable output (SBM parameters)

Conclusion & perspectives II

Opens many questions on foodwebs

- interpretation of the network organizations
- analysis of species
- analysis of individual networks
- outlier detection (climate change)
- prediction of the cluster of a new network
- variants of SBM (varying intensity, varying group proportions etc.)
- include covariables

Bibliography

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Poisot, T., Bergeron, G., Cazelles, K., Dallas, T., Gravel, D., Macdonald, A., Mercier, B., Violet, C., and Vissault, S. (2020). Environmental biases in the study of ecological networks at the planetary scale. *bioRxiv*.