A Gromov-Wasserstein Approach for African Food Web Network Analysis

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Background

- Predator-prey interactions in **food webs** play a critical role in maintaining biodiversity.
- Human-induced **habitat loss** threatens these interactions and overall ecosystem health.
- Understanding mammal food webs can inform **conservation efforts.**

Data

Our group curated 170 mammal food web networks of Sub-Saharan Africa from literature. Attributes include but are not limited to:

- Geographic coordinates
- Network topology
  - Species names
  - Predator-prey relationships
- Primary productivity
- Fragmentation

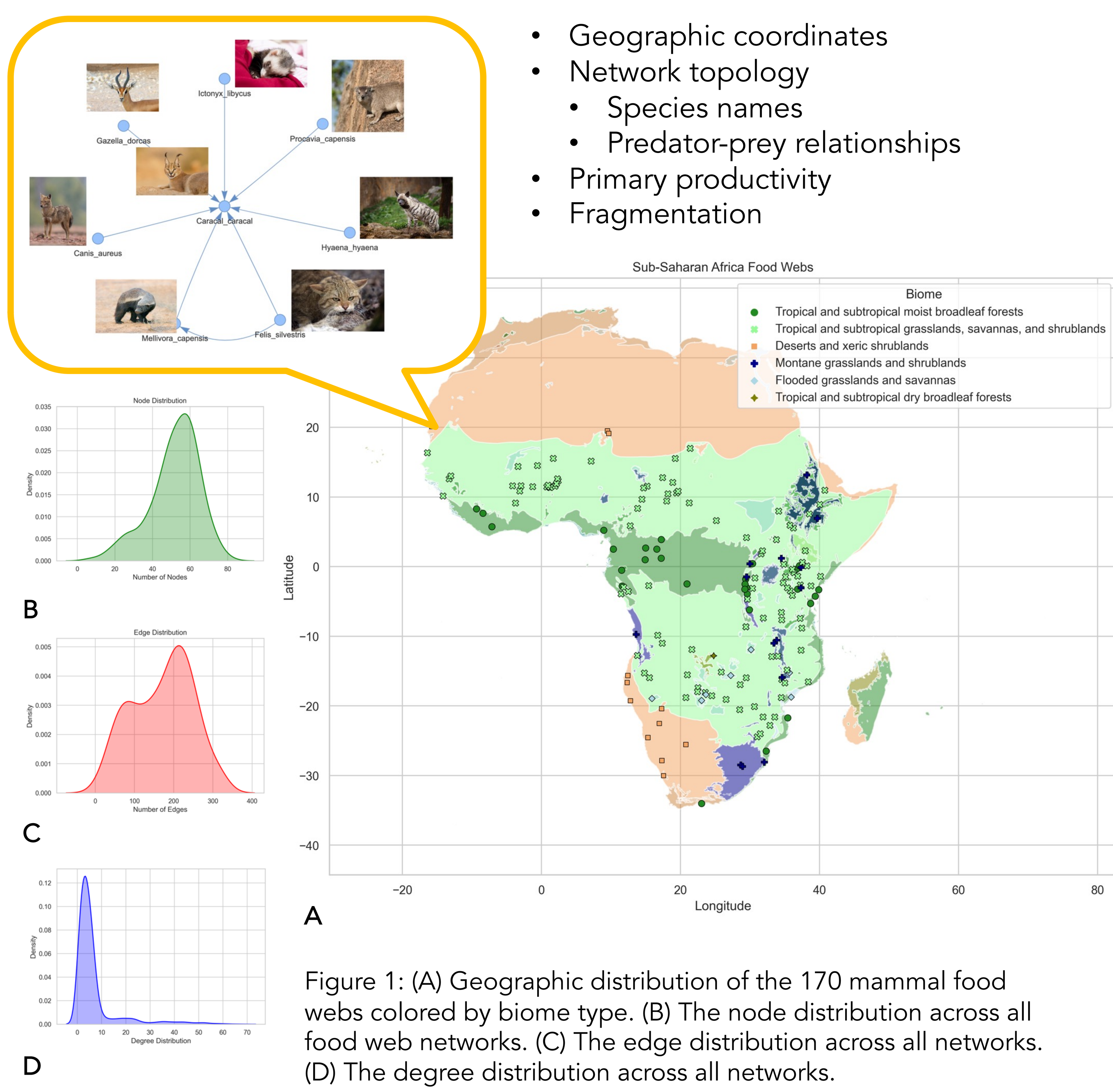
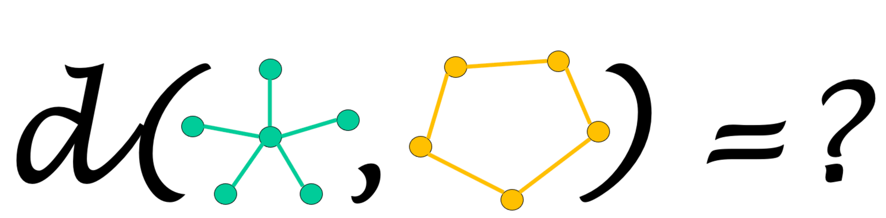


Figure 1: (A) Geographic distribution of the 170 mammal food webs colored by biome type. (B) The node distribution across all food web networks. (C) The edge distribution across all networks. (D) The degree distribution across all networks.

Problem of Interest

A Topological Data Analysis Toolkit for Food Webs

But… how do we compare networks?



Existing methods (ex. graph kernels, graph neural networks) are either computationally intensive, difficult to interpret, applicable only to a singular network, or does not apply to networks with different sizes.

Optimal Transport

Definition 1: Let (X, ω_X, μ_X) and (Y, ω_Y, μ_Y) be two measure networks, we define the **network Gromov-Wasserstein (GW) distance**[1] as

$$d_{gw}(X,Y) := \min_{\mu \in \mathcal{L}(\mu_X,\mu_Y)} \int_{X\times X}\int_{Y\times Y} |\omega_X(x,x') - \omega_Y(y,y')| d\mu(x,y) d\mu(x',y')$$

where $\mathcal{L}(\mu_x, \mu_y)$ is the set of measure couplings between μ_X and μ_Y.

Theorem 1: The network GW distance is a pseudo-metric on the space of networks $\mathcal{N}$

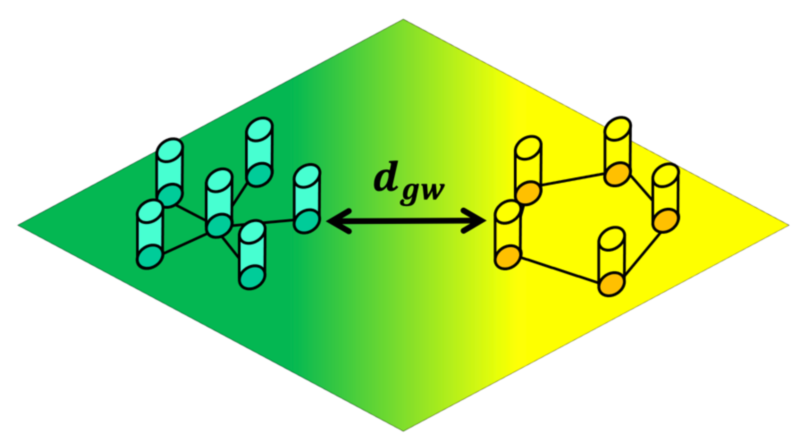


Figure 2: Conceptual illustration of the metric space of networks characterized by d_{gw}.

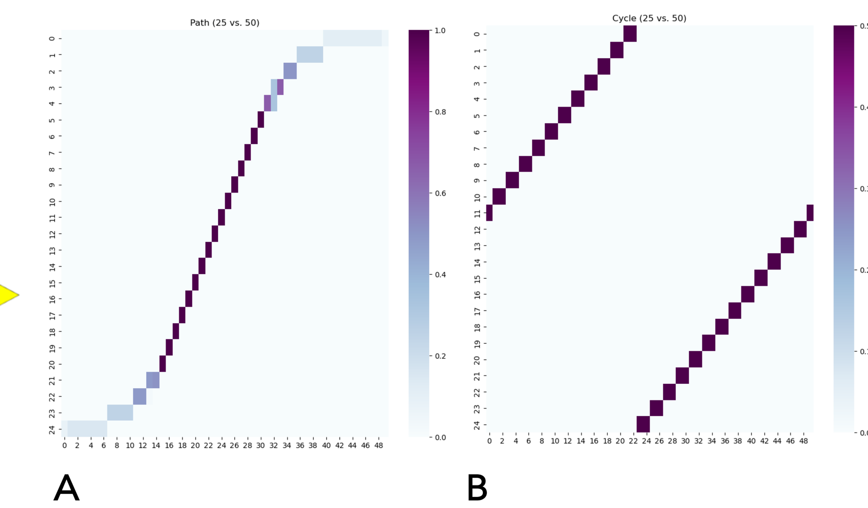


Figure 3: The optimal transport maps between (A) a 25-path and 50-path graph, and (B) a 25-cycle and 50-cycle graph.

Results: Gromov-Wasserstein Distance

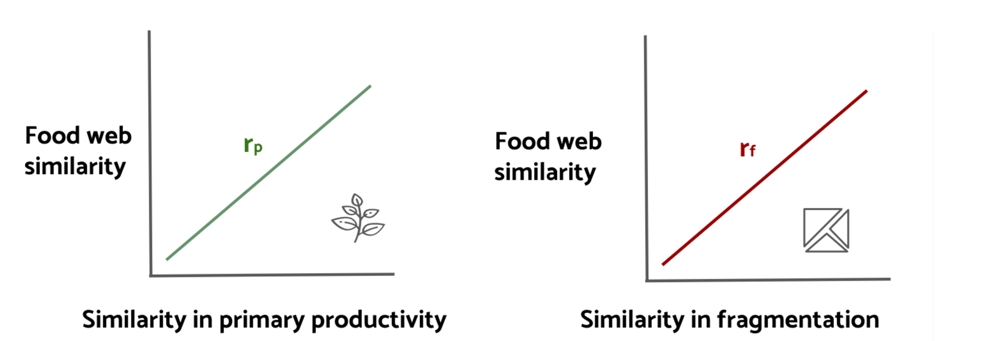


Figure 4: Positive correlations between change in d_{gw} and primary productivity (deserts and grasslands) as well as fragmentation (tropical rainforest) with a partial mantel test.

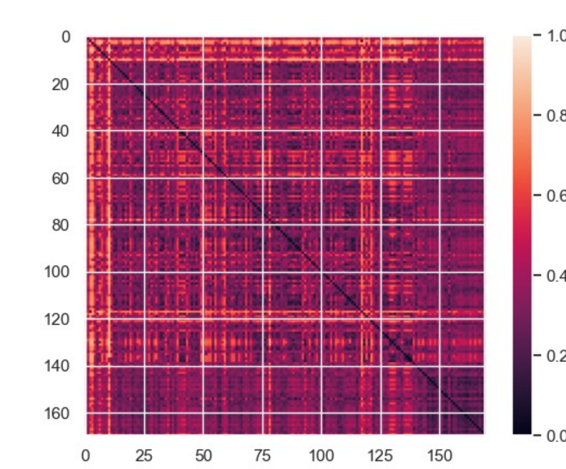


Figure 5: Heatmap of pairwise d_{gw}

Results: Gromov-Wasserstein Barycenter

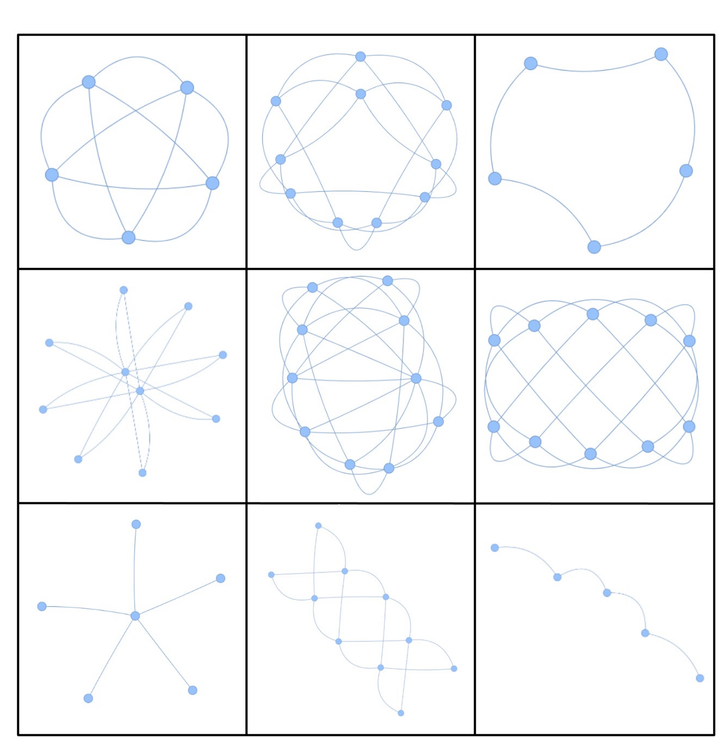


Figure 6: GW barycenter of complete graph (top-left), cycle graph (top-right), star graph (bottom-left), and path graph (bottom-right).

Definition 2: Let $\{C_s, p_s\}_{s=1}^{S}$ be S pairs of cost matrices C_s and node distribution p_s. The **Gromov-Wasserstein Barycenter**[2] $\mathcal{B}$ of $\{C_s, p_s\}_{s=1}^{S}$ is defined as

$$\mathcal{B} := \min_{C \in \mathbb{R}^{n\times n}} \sum_{s} \lambda_s d_{gw}(C, C_s, p, p_s)$$

where λ_s is the weight of (C_s, p_s).

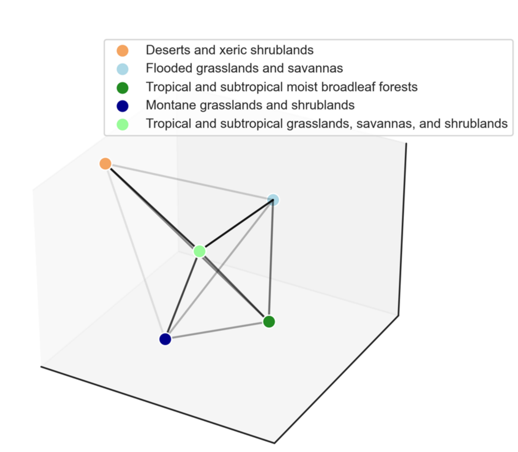


Figure 7: Distance between Barycenters of different biomes. Edge strength scaled with d_{gw}.

Results: Graph Factorization

Definition 3: Let $\{U_k, \lambda_k\}_{k=1}^{K}$ be K pairs of cost matrix and weight for the support networks. The **Gromov-Wasserstein Factorization (GWF)**[3] framework for I observed networks is defined by

$$\min_{0 \le U_{1:K} \le 1, \lambda_{1:I} \in \Delta^K} \sum_{i=1}^{I} d(B(U_{1:K}, \lambda_i, d_{gw}), C_i)$$

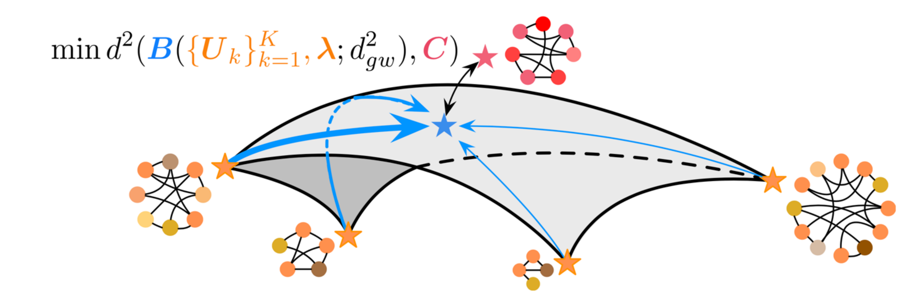


Figure 8: Conceptual illustration of the GWF framework. Courtesy of Xu, et al.

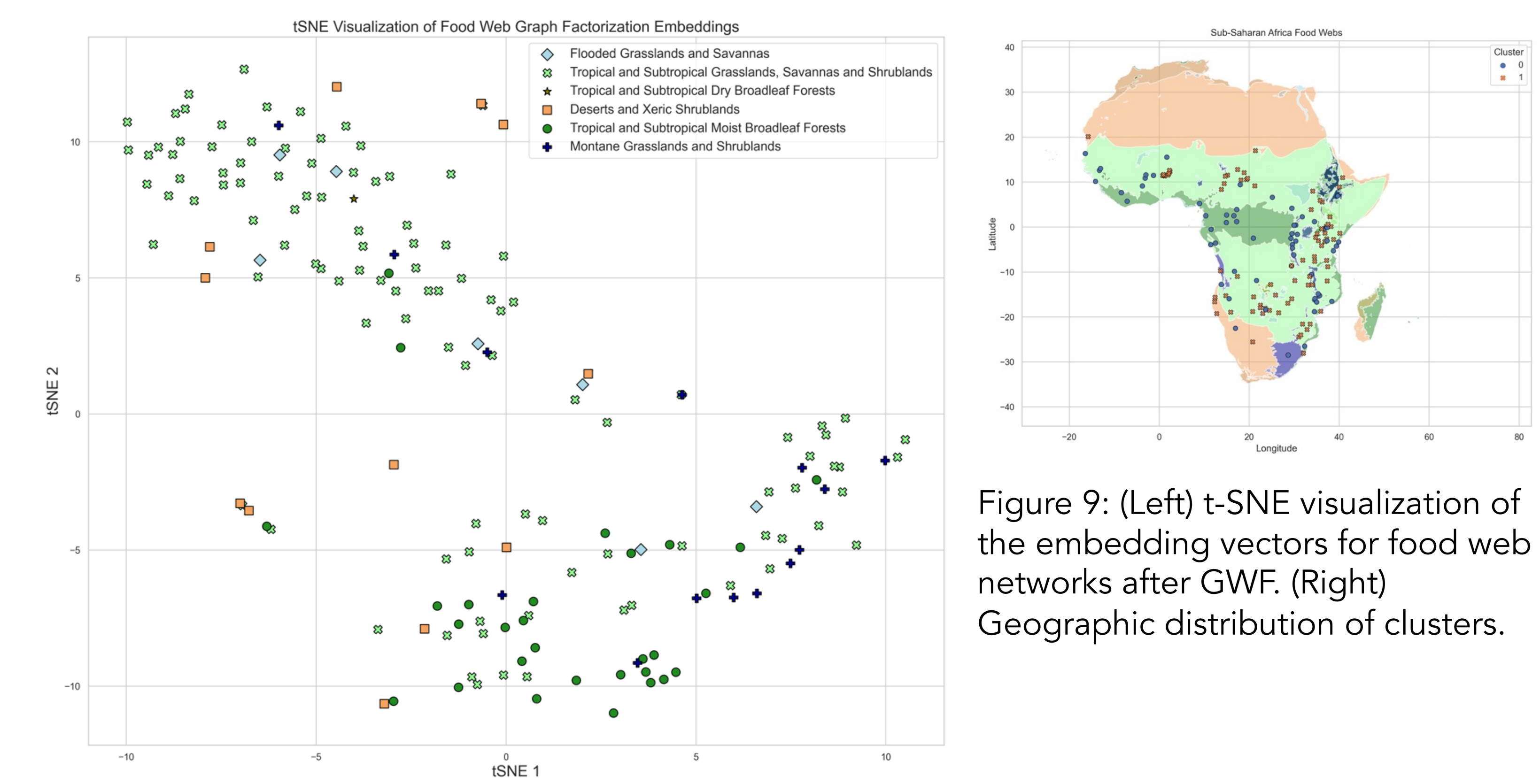


Figure 9: (Left) t-SNE visualization of the embedding vectors for food web networks after GWF. (Right) Geographic distribution of clusters.

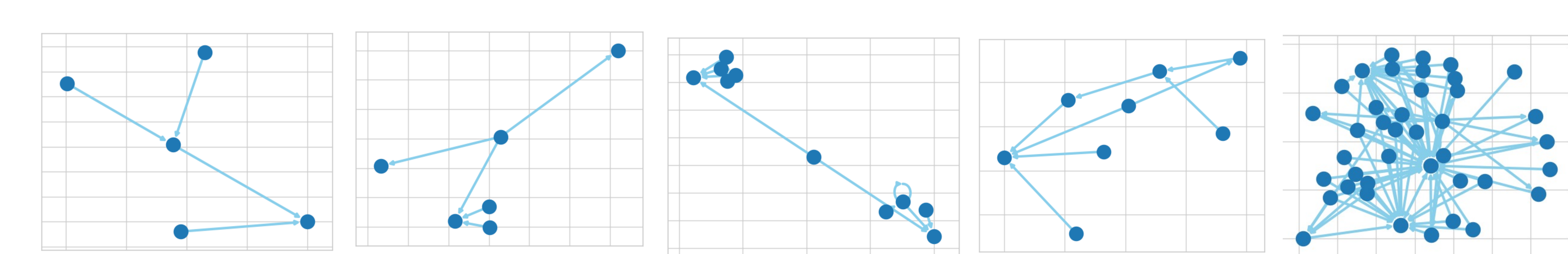


Figure 10: Sample of top-weighted learned support networks across the observed clusters.

Future Works

- Endow the food web networks with node distributions based on the **flow of energy** within an ecosystem.
- Incorporate features beyond network topology via the **Fused Gromov-Wasserstein distance**.
- Conduct a **theoretical analysis** of the growth in d_{gw} as a function of difference in network sizes.

References

1. Samir Chowdhury and Facundo Mémoli. The Gromov-Wasserstein distance between networks and stable network invariants. 2019
2. Peyré, G., Cuturi, M., and Solomon, J. Gromov-Wasserstein averaging of kernel and distance matrices. In Proceedings of the 33rd International Conference on Machine Learning, 2016.
3. Xu, H., Liu, J., Lu, D., and Carin, L. Representing graphs via gromov-wasserstein factorization. IEEE Transactions on Pattern Analysis and Machine Intelligence, 2022.

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