



# Towards Ecological Network Analysis with Gromov-Wasserstein Distances

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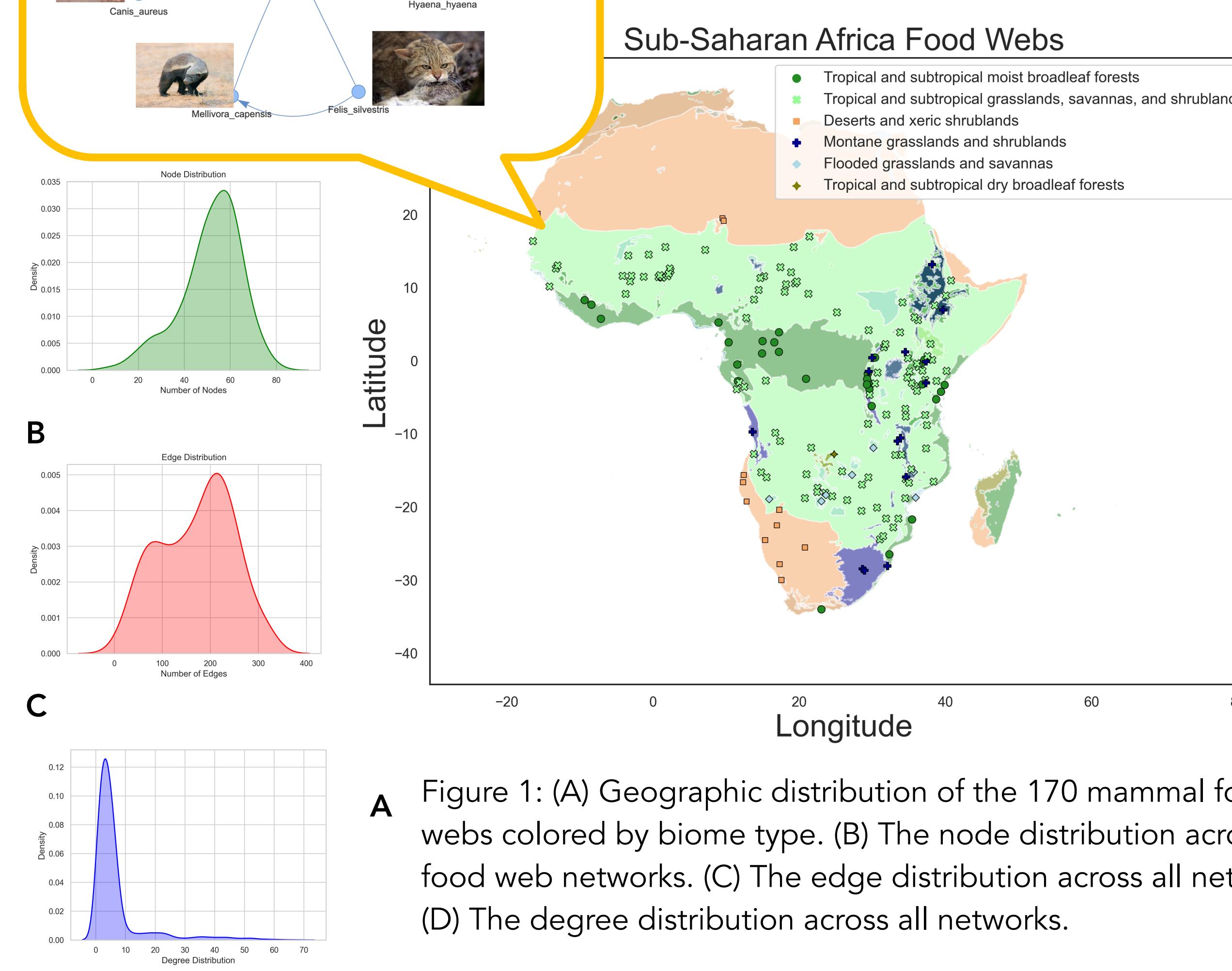
## Background

- Predator-prey interactions in **food webs** play a critical role in maintaining biodiversity.
- Climate change causes species to shift their geographic ranges to track preferred preys.
- Understanding **changes among food webs** can thus inform local impact of climate change.

## 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



A 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?

$$d(\text{graph}_1, \text{graph}_2) = ?$$

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

## Gromov-Wasserstein Distance

**Definition 1:** Given a graph  $G = (V, E)$ , we define its **measure network** as  $M_G = (p_G, w_G)$  where  $p_G$  is the node distribution and  $w_G : V \times V \rightarrow \mathbb{R}$  is a bounded edge weight function.

**Definition 2:** Given two measure networks  $M_{G_1}$  and  $M_{G_2}$ , we define the **discrete network Gromov-Wasserstein (GW) distance** by

$$d_{gw}(G_1, G_2) := \min_{\substack{T \in \mathbb{R}_{\geq 0}^{n_1 \times n_2}, \\ T\mathbf{1} = p_{G_1}, \\ T^T\mathbf{1} = p_{G_2}}} \left\{ \sum_{u, u' \in V_1} \sum_{v, v' \in V_2} |w_{G_1}(u, u') - w_{G_2}(v, v')| T_{u,v} T_{u',v'} \right\}$$

where  $T \in \mathbb{R}_{\geq 0}^{n_1 \times n_2}$  is an optimal transport (OT) plan between  $M_{G_1}$  and  $M_{G_2}$ .

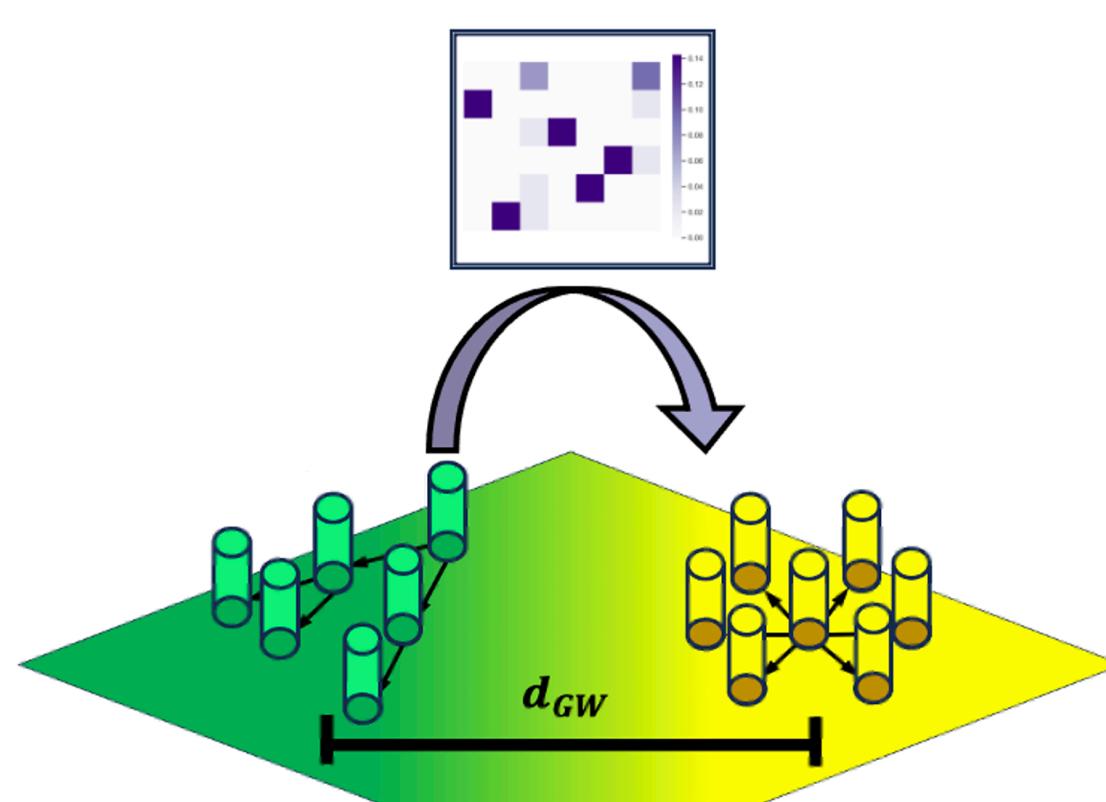


Figure 2: Conceptual illustration for the space characterized by  $d_{gw}$ .

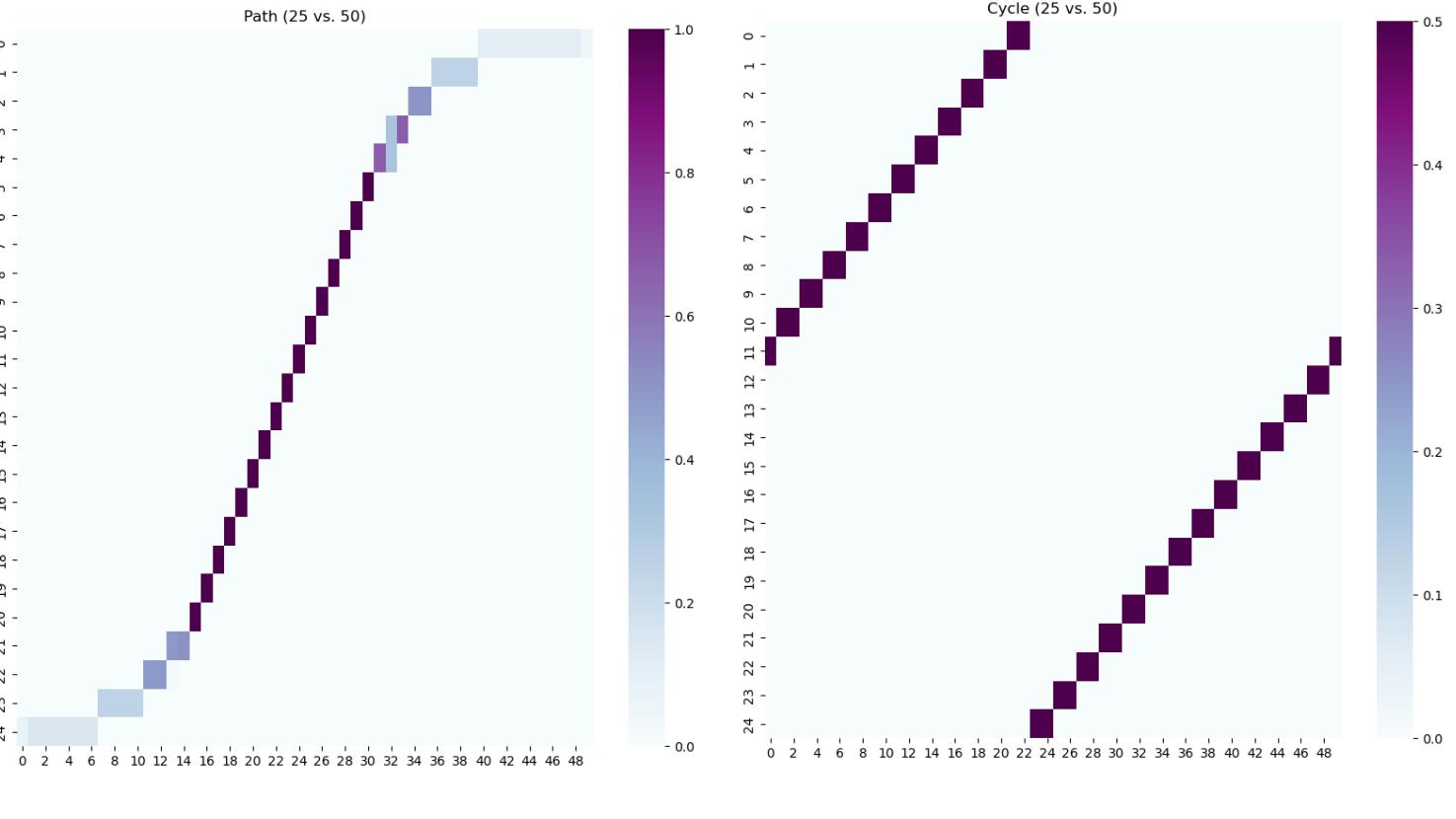


Figure 3: The optimal transport maps between (A) a 25-path and 50-path graph, and (B) a 25-cycle and 50-cycle graph.

### MDS of Synthetic Block Graphs

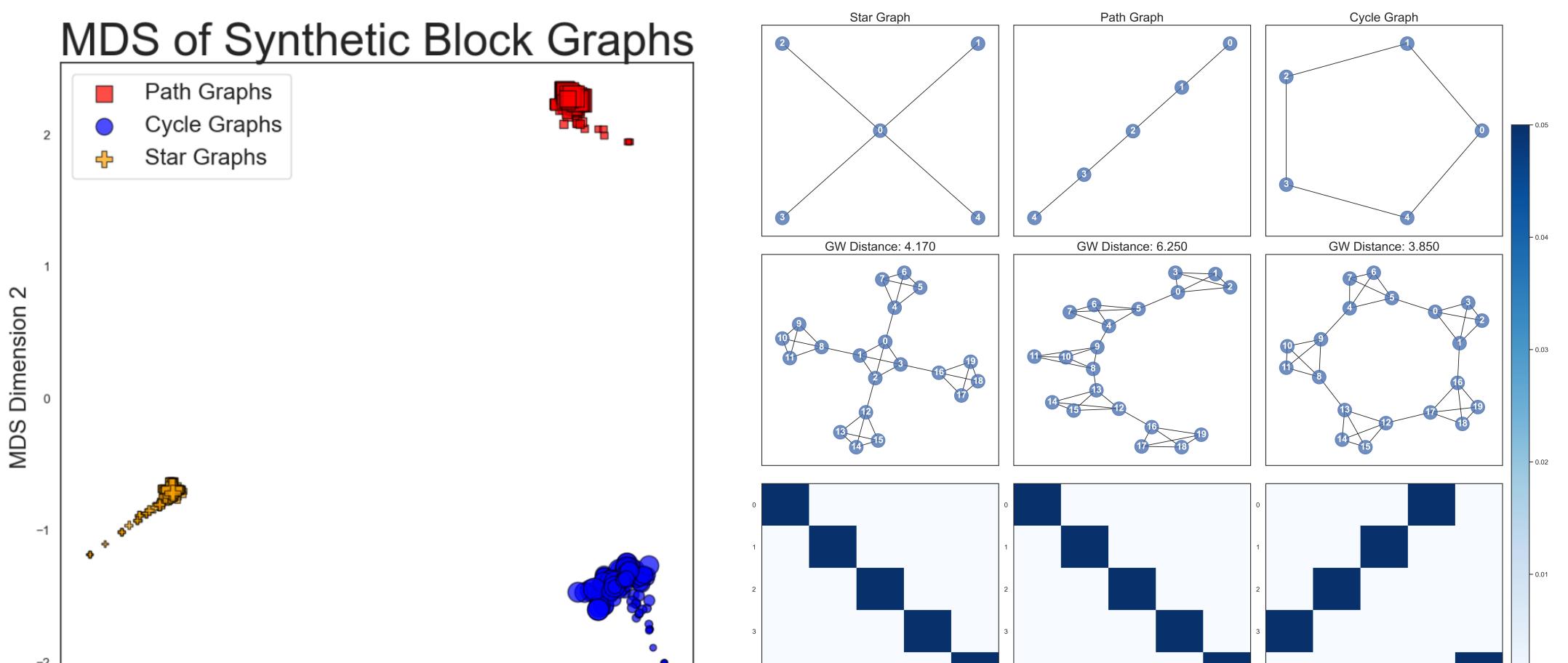


Figure 4: Numerical experiments for GW distance between block graphs of different sizes. (Left) MDS visualization. (Right) OT plans between select graphs.

## Gromov-Wasserstein Barycenter

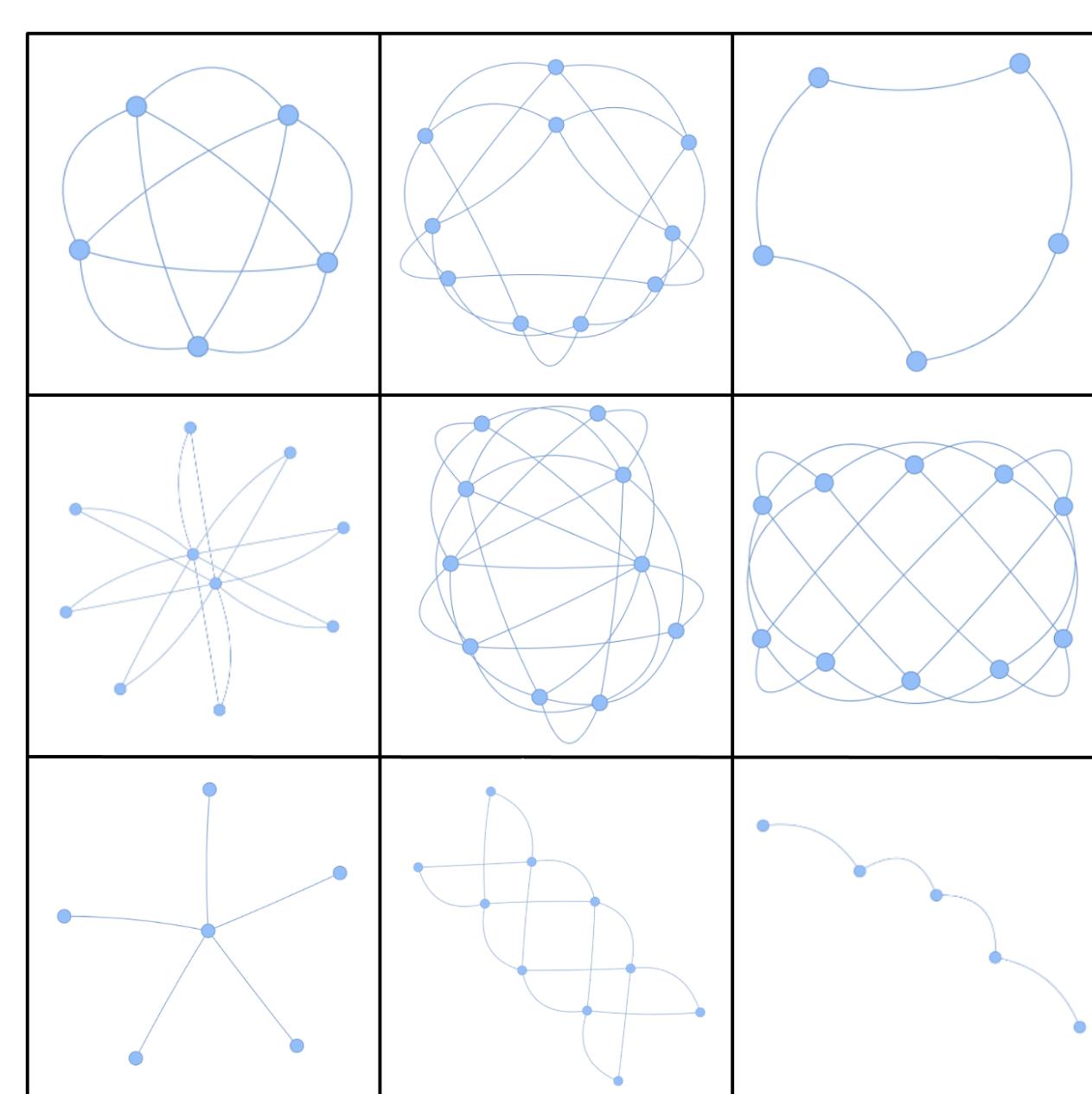


Figure 5: GW barycenter of complete graph (top-left), cycle graph (top-right), star graph (bottom-left), and path graph (bottom-right).

**Definition 3:** 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**<sup>2</sup>  $\mathcal{B}$  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  $\lambda_s$  is the weight of  $(C_s, p_s)$ .

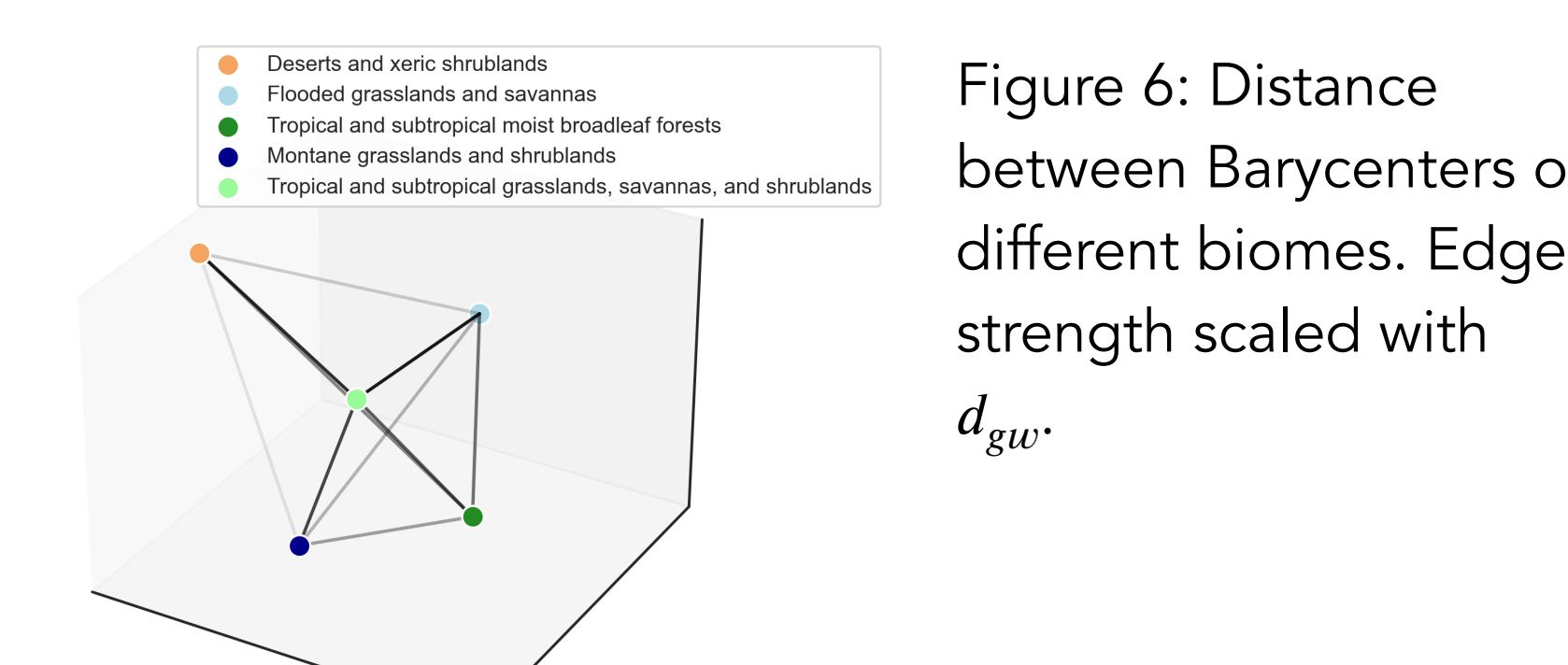


Figure 6: Distance between Barycenters of different biomes. Edge strength scaled with  $d_{gw}$ .

## Gromov-Wasserstein on Food Webs

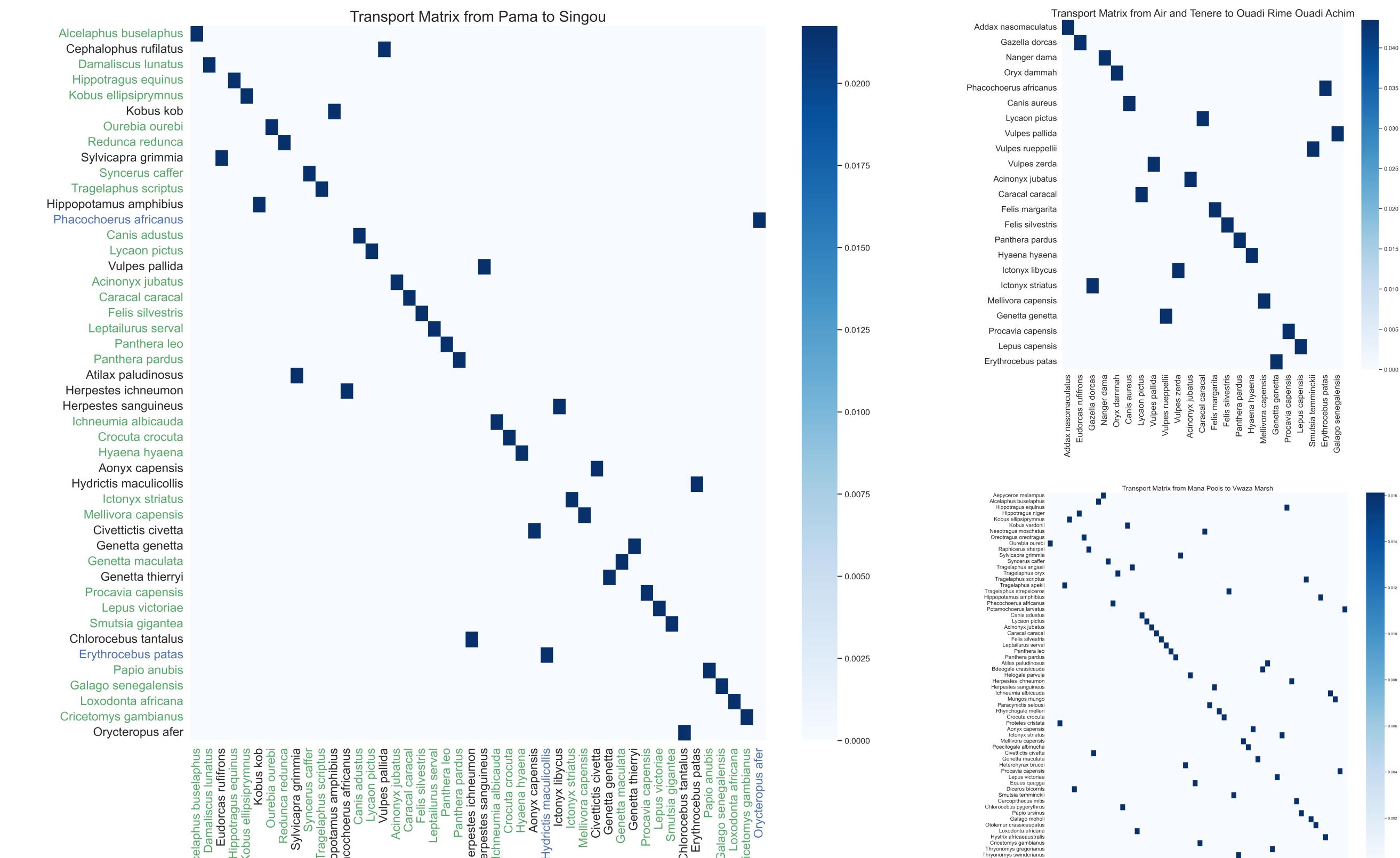


Figure 7: OT plan between mammal communities at Pama and Singou in Sub-Saharan Africa. Green highlights denote mass transported between shared species. Blue highlights surprising basal species mappings.

Site 1	Site 2	$d_{gw}$
Pama	Singou	1414.01
	Tamou	1414.02
Pama	Tamou	1886.60
Air and Tenere	Ouadi Rime Ouadi Achim	1886.60
Mana Pools	Vwaza Marsh	2595.25
Loddalga	Mago	2772.26
Banhine	Mudumu	2865.89
Mudumu	Okavango Delta	3726.56
Kourtiagou	Madjoari	3773.17

Table 1: Top 9 most similar food webs under  $d_{gw}$ .

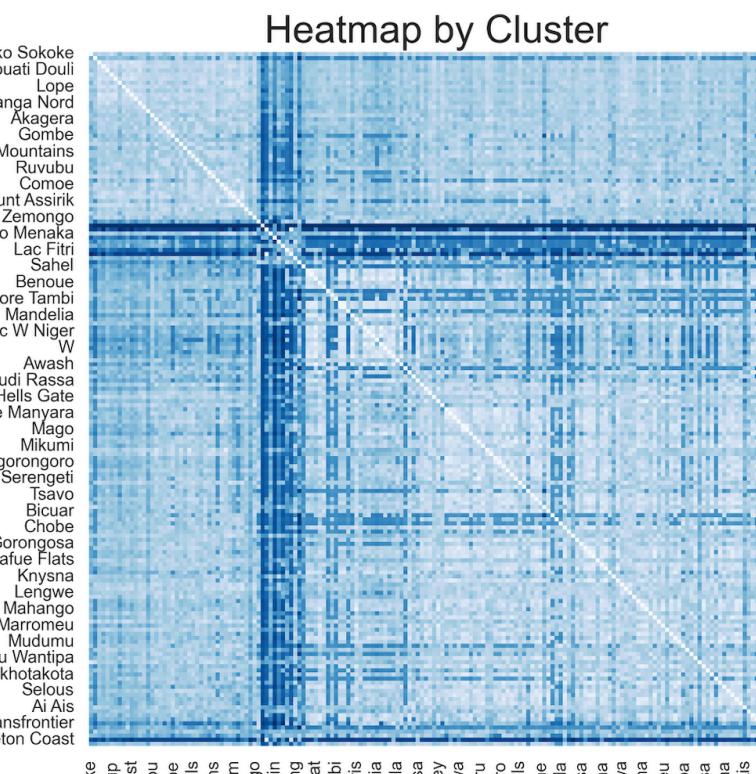


Figure 8: OT Plans for the top 3 similar webs from outside of the tropical and subtropical grasslands, savanna, and shrublands biome.

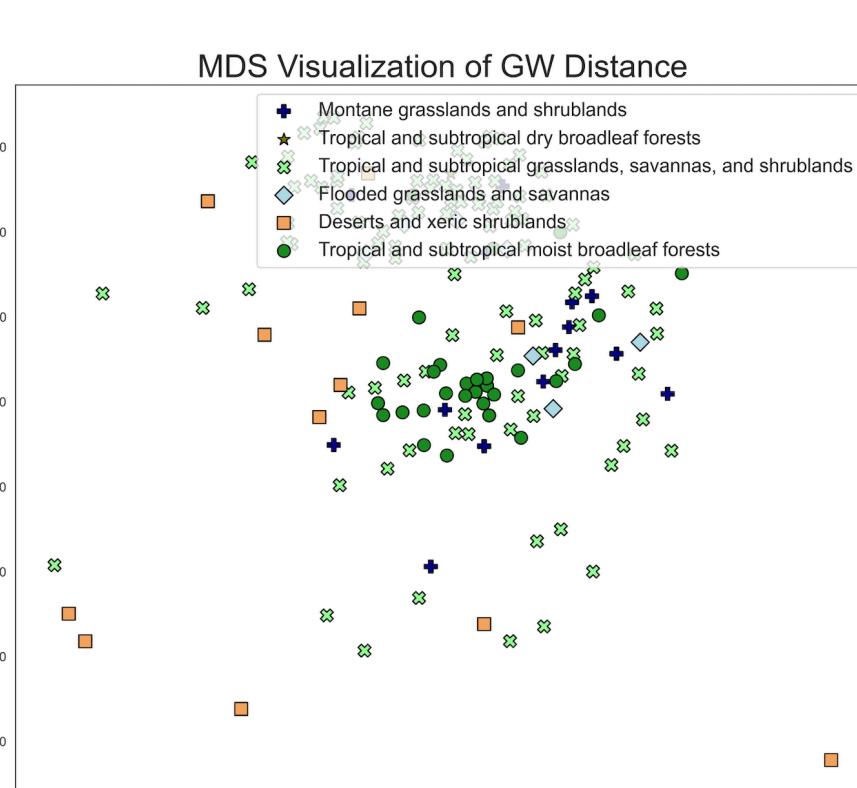


Figure 9: Heatmap of pairwise  $d_{gw}$  ordered by Sorenson-Dice cluster groups.

Figure 10: MDS over food webs.

## Future Works

- Incorporate features beyond network topology via the **Fused Gromov-Wasserstein distance**.

## References

- Samir Chowdhury and Facundo Mémoli. The Gromov-Wasserstein distance between networks and stable network invariants. 2019
- 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.

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