Clustering and Applications to Biodiversity

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Problem

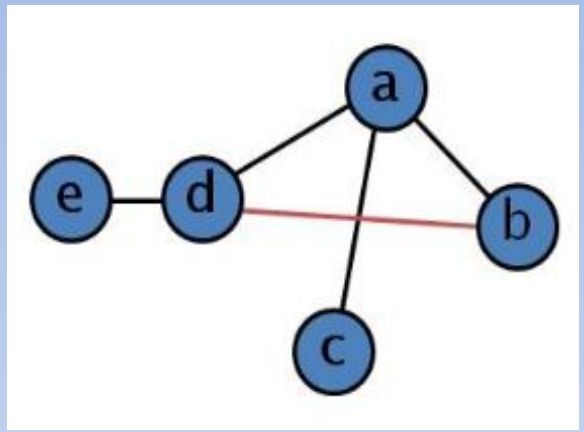
- *Given the competition graph G = (V,E), is it possible to partition the competition graph G into two sub-graphs G_A and G_B using a combination of Fiedler order and linkage-based refinements to minimize cut(A,B) while maximizing W(A) and W(B) at the same time?*
- *Note: The strength between two nodes is given by their edge weight W_{ij} and the strength between two clusters A and B is given by* : cut(A,B) =W(A,B) where:

$$W(A,B) = \sum W_{ij} \quad i \in A \quad j \in B$$

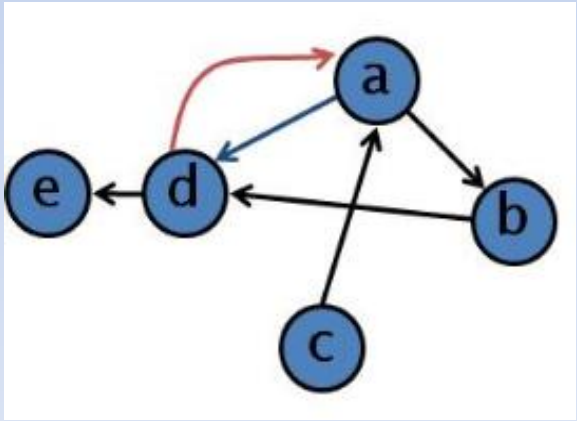
Adjacency Matrix

- An adjacency matrix is an *n x n* matrix where the *ij*-th entry takes the value of 1 if there is an edge between vertices *i* and *j*. Otherwise, the element is 0.

$$A = \begin{cases} 1 & if \quad i \sim j \\ 0 & Otherwise \end{cases}$$



0	1	1	1	0
1	0	0	1	0
1	0	0	0	0
1	1	0	0	1
0	0	0	1	0



0	1	0	1	0
0	0	0	1	0
1	0	0	0	0
1	0	0	0	1
0	0	0	0	0

Spectral Clustering

Uses information obtained from the Eigen-values and eigenvectors of the Laplacian matrix for partitioning of graphs;

Laplacian

- Given A, the Laplacian matrix L is defined as:
- $$L = D - A$$

$$L = \begin{cases} \deg(v_i) & if \quad i = j \\ -1 & if \quad i \neq j \quad and \quad v_i \sim v_j \\ 0 & otherwise \end{cases}$$

Normalized Laplacian

- Given A, the normalize Laplacian L is define as:

$$L = \begin{cases} 1 \quad if \quad i = j \quad and \quad \deg(v_i) \neq 0 \\ -\dfrac{1}{\sqrt{\deg(v_i)\deg(v_2)}} \qquad if \quad i \neq j \quad and \quad v_i \sim v_j \\ 0 \quad otherwise \end{cases}$$

Basic spectral bi-clustering algorithm

- Partitions a graph into two clusters
- Nodes within the same cluster, vertices are more connected to each other than with those in the other cluster.

Input: Weighted Laplacian Matrix

Find the eigenvector *v* corresponding to the second smallest eigenvalue for one of the following problems:
L*v* = λ*v* (L: Laplacian),
L''*v* = λ*v* (L'': Normalized Laplacian).

Output: Clusters $A = \{j; v_j >= 0\}$ *and* $A' = \{j; v_j < 0\}$

Min-max cut

- Given a weighted graph G=G(E,V) with node set V, edge set E and weight W partition G into two sub-graphs A, B using the min-max clustering principle.
- Minimize similarity between sub-graphs.
- Maximize similarity within sub-graph.
- Similarity between sub-graphs A, B is the cut size: cut(A,B)=W(A,B) where:

$$w(A,B) = \sum_{u \in A, v \in B} w_{uv} \qquad w(A) \equiv w(A,A) \qquad w(B) \equiv w(B,B)$$

The Mcut Function

- Minimize cut(A,B) while maximizing W(A) and W(B) at the same time.
- Objective function to be minimized:

$$Mcut = \frac{cut(A,B)}{W(A)} + \frac{cut(A,B)}{W(B)}$$

Fiedler vector

- Eigenvector associated with the second smallest eigen-value.
- Believed to provide the best linear search order for finding the optimum cut.
- However, it is possible to have nodes sharing higher linkage to the other cluster than the one they are currently assigned to by using only the information of Fiedler order.

$$cut(A,B) = \sum_{e_{uv} \in E} \frac{(x_u - x_v)^2}{4} w_{uv} = \frac{x^T (D - W) x}{2}$$

$$(D - W)\, x = \lambda x$$

Linkage-based refinement

- Identify the nodes near the cut.
- Define linkage l as a similarity measure between two sub-graphs:

$$l(A,B) = \frac{W(A,B)}{W(A)W(B)}$$

- Linkage between a node and a sub-graph:

$$l(A,u) = \frac{W(A,u)}{W(A)} \qquad l(B,u) = \frac{W(B,u)}{W(B)}$$

Linkage difference

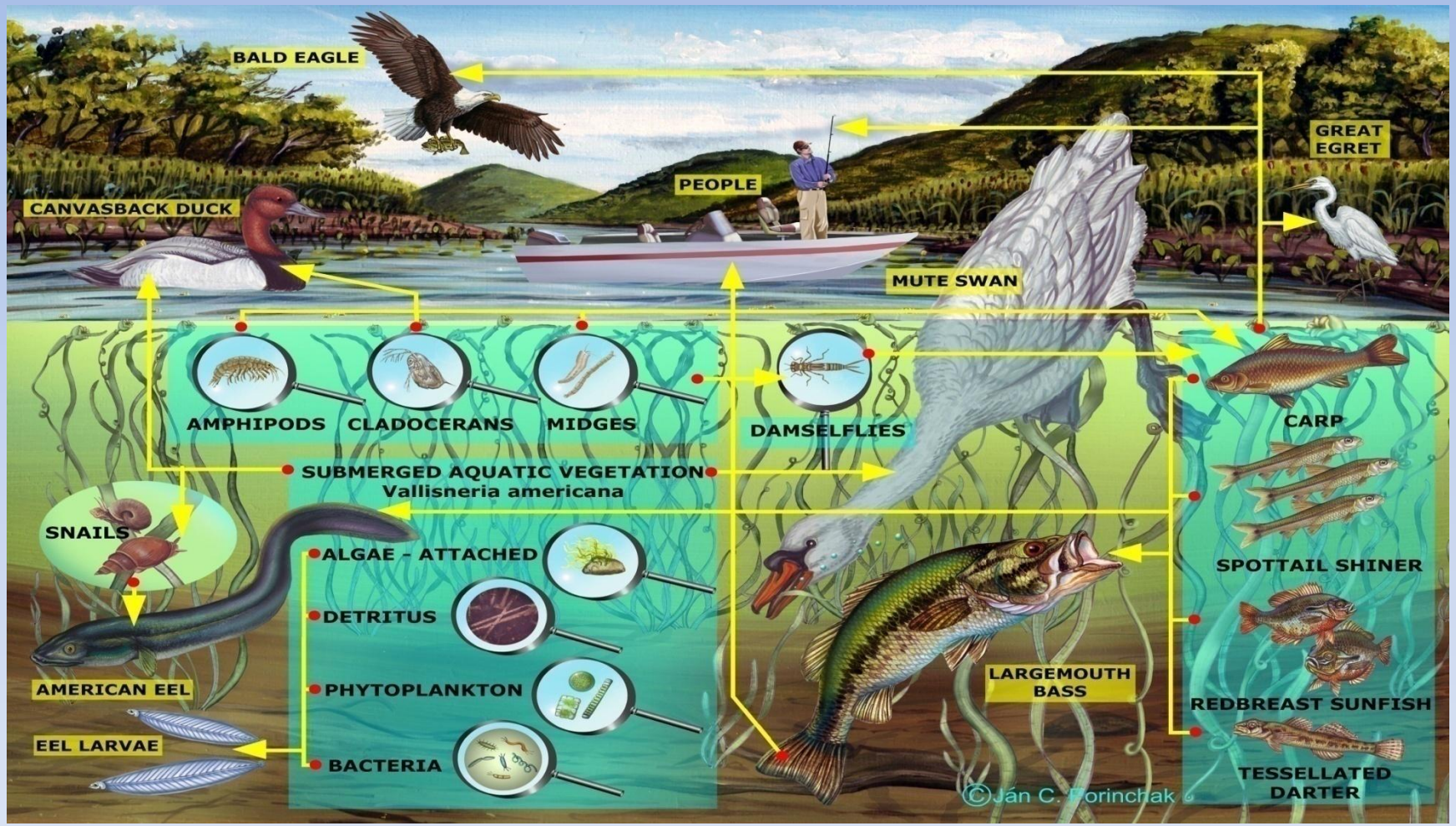
- The linkage difference: $\Delta l(u) = l(A,U) - l(B,U)$
- If u is well inside A we expect $\Delta l(u) \succ 0$
- If u is well inside B we expect $\Delta l(u) \prec 0$
- If u is near the cut we expect $\Delta l(u) \approx 0$
  - In this case it might be a possible candidate to move to a different cluster if the objective function Mcut is reduced

Combination of the two methods

It is observed that a ***linkage differential order*** provides a better ordination than the **Fiedler order** therefore we implement a combination of Fiedler order with linkage differential order to get a better result on minimizing the cut between cluster while maximizing W(A) and W(B) at the same time.

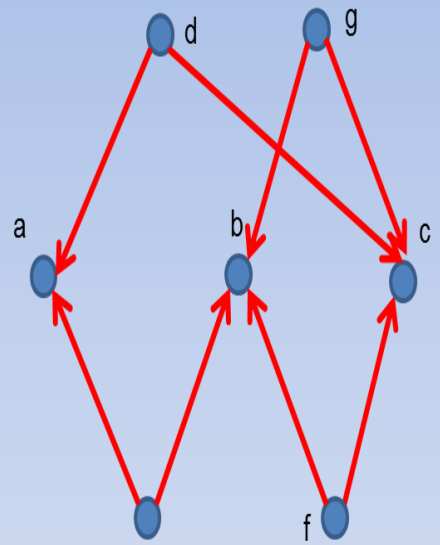
Application

Hudson River Food Web

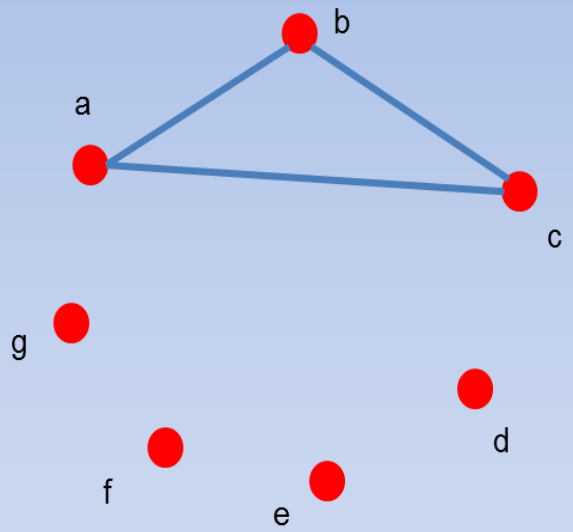


Competition graph for Hudson River Food Web

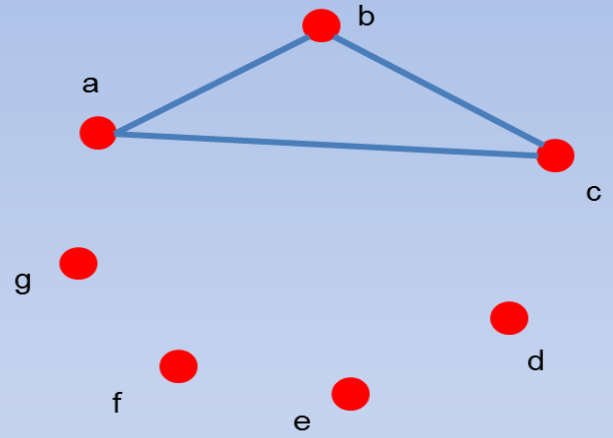
- A **competition graph** is a graph where the vertices are species in the ecosystem and there is an edge between two vertices if they have a common prey. If vertices are isolated, they either do not have any prey in common with the other species of the ecosystem or they are primary producers. For example, in our Hudson River Competition Graph, the isolated vertices are bacteria, phytoplankton, polychates, algae, water celery, eel larvae, spartina alterniflora, typha, phragmites, snapping turtle and great blue heron.



Let D be a Digraph with node set $V(D) = 7$



$\{v_i, v_j\} = 1$, If $\exists\ v_k \mid (v_i, v_k) \cap (v_j, v_k)$ are directed edges in $E(D)$



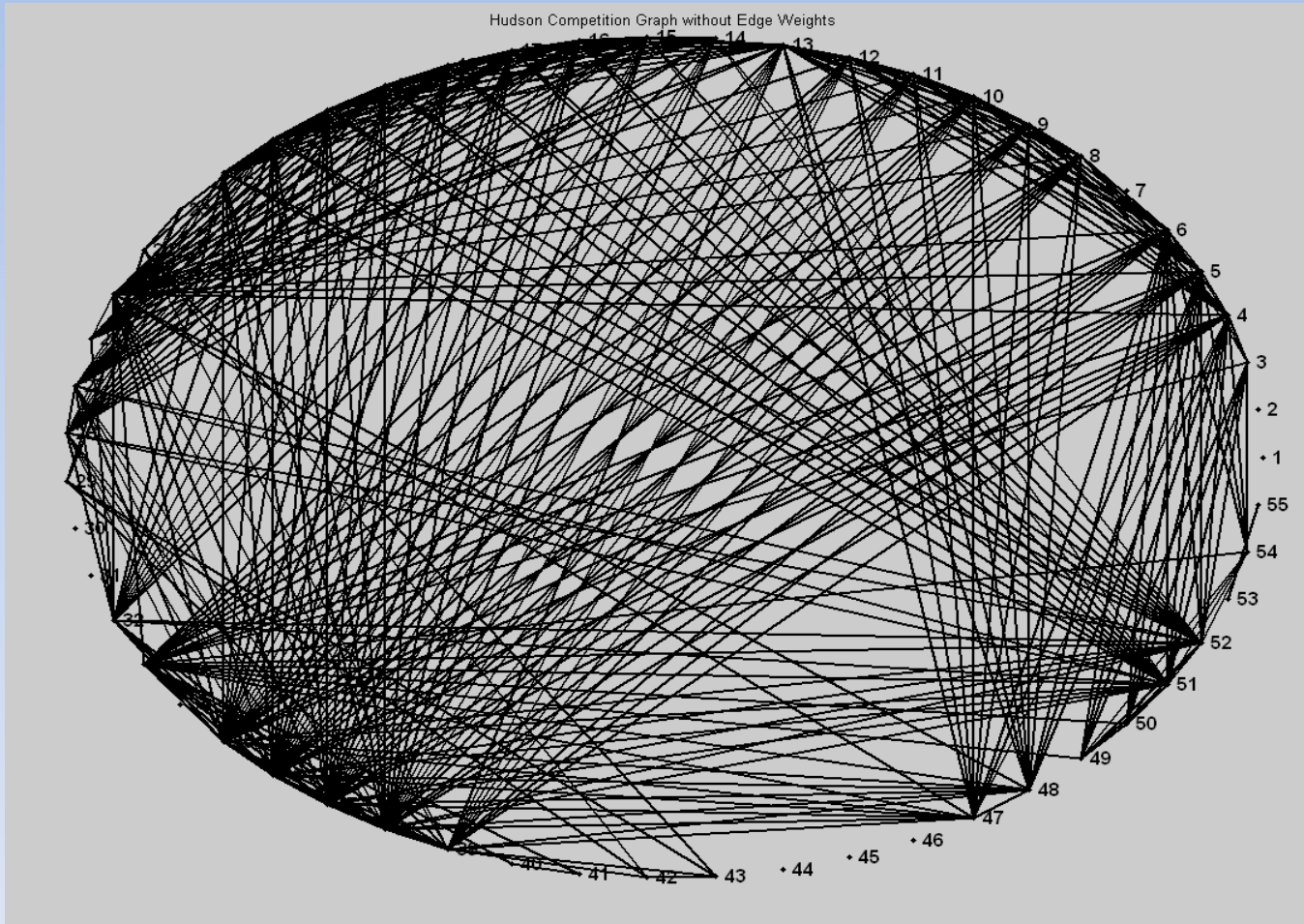
Weighted Competition Graph

Adjacency matrix
Hudson Competition

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55
1	Bacteria	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	Phyto-plankton	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	Detritus	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	Mud Worms	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0	0	0	0
5	Midges	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0	0	0	0
6	Amphipods	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0	0	0
7	Polychaetes	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	Cladocerans	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	Copepods	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	Crab larvae	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	Rotifers	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	Rangia Clam	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	Opossum Shrimp	1	1	1	0	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	Blue Crab	0	0	0	1	1	1	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	Blueback Herring	0	0	0	1	1	1	1	0	1	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	Bay Anchovy	0	0	0	1	1	1	1	0	1	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	Bluefish	0	0	0	1	1	1	1	0	1	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	Shad	0	0	0	1	1	1	1	1	1	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	White Perch	0	0	0	1	1	1	1	0	1	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	Atlantic Tomcod	0	0	0	1	1	1	1	0	1	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21	Striped Bass	0	0	0	1	1	1	1	0	1	1	1	0	0	0	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	Sturgeon	0	0	0	1	1	1	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23	Cormorant	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	1	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	People	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	1	1	0	0	0	0	0	0	1	0	0	0	0	0	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	Zebra Mussels	1	1	1	0	0	0	0	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26	Striped Bass Larvae	0	0	0	0	0	0	0	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	Striped Bass Juvenile	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28	Catfish	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	Largemouth Bass	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	Algae	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31	Water Celery	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32	Damselfly	0	0	0	0	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33	Snails	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	0	0	0	0	0	0	0
34	Eel Larvae	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35	Carp	1	1	1	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36	Spottail Shiner	1	1	1	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	Redbreast Sunfish	1	1	1	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	Tessellated Darter	1	1	1	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39	American Eel	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40	Mute Swan	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	Canvasback Duck	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42	Great Egret	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43	Bald Eagle	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44	Spartina Alterniflora	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45	Typha	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46	Phragmites	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47	Microbes	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48	Fungi	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49	Killifish	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0
50	Mouse	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0
51	Marsh Wren	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0
52	Red-wing Blackbird	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0
53	Great Blue Heron	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0
54	Muskrat	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0
55	Snapping Turtle	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0

Bipartition

Hudson Weighted Competition Graph



Fiedler Vector corresponding to the smallest non-zero Eigen Value for 44 nodes

- Eigen-value 1.0191
- Node 35 and 35 less connected

0.0291
0.0296
0.0296
0.0295
0.0305
0.0305
0.0305
0.0305
0.0305
0.0315
0.0336
0.0335
0.0335
0.0335
0.0335
0.0335
0.0335
0.0340
0.0336
0.0448
0.0439
0.0314
0.0348
0.0338
0.0340
0.0443
0.0339
0.0132
0.0316
0.0316
0.0316
0.0316
0.0334
-0.6904
-0.6904
0.0443
0.0443
0.0318
0.0318
0.0291
0.0291
0.0318
0.0318
0.0291

Fiedler Vector corresponding to the smallest non-zero Eigen Value For 42 nodes

- Eigen-value 3.7991

```
 0.0874
 0.0503
 0.0503
 0.0488
 0.0463
 0.0463
 0.0463
 0.0463
 0.0463
 0.0508
 0.0631
 0.0616
 0.0616
 0.0616
 0.0616
 0.0616
 0.0616
 0.0432
 0.0631
-0.3337
-0.4089
 0.0506
 0.0701
 0.0648
 0.0562
-0.4363
 0.0658
 0.0534
 0.0515
 0.0515
 0.0515
 0.0515
-0.0658
-0.4443
-0.4443
 0.0554
 0.0554
 0.0874
 0.0874
 0.0679
 0.0679
 0.0874
```

Fiedler order
+
Linkage based refinements

- Algorithm

1. Computer the Fiedler Vector. Sort the nodal values to obtain the Fiedler order
2. Search for optional cut point corresponding to the lowest Mcut based on the Fiedler order.
3. Do linkage-based refinements

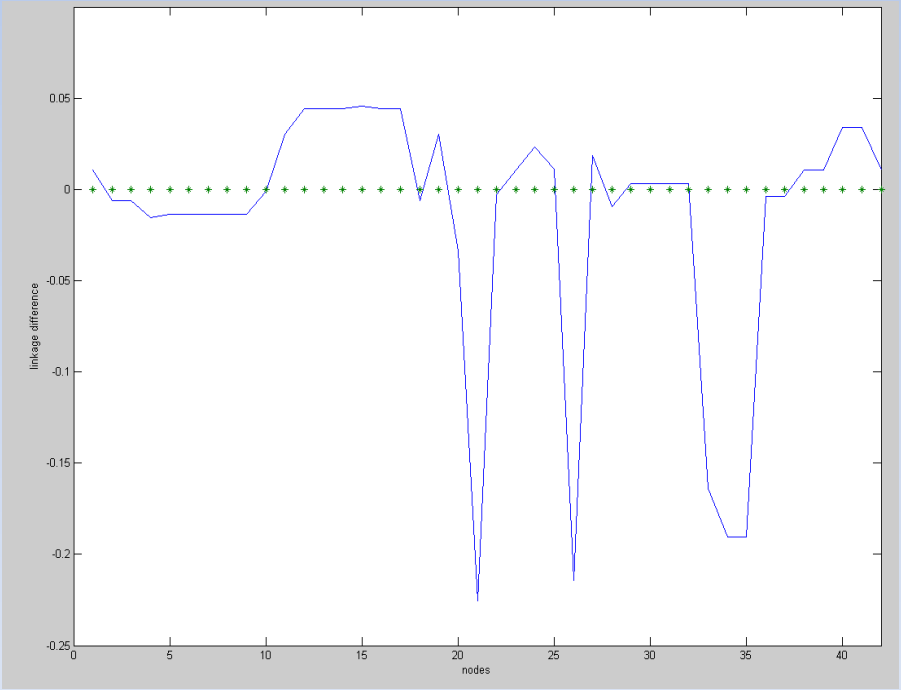
Objective Function

Mcut = 3.3746

Cluster A 36 nodes

Cluster B 6 nodes

The linkage difference of all nodes



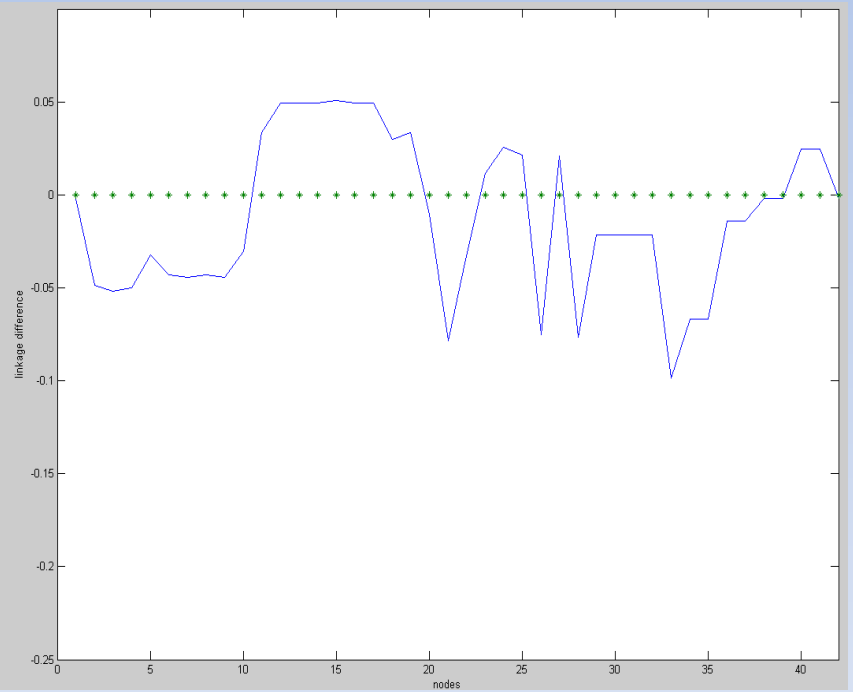
Improvement
Results, Analyses

Mcut = 2.0986

Cluster A 32 Nodes

Cluster B 10 Nodes

The linkage difference of all nodes



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