EURO⁴SEE

Residue Networks: Understanding the Time Evolution and Mutations of Proteins from a Graph Theoretical Perspective

Tandac Furkan Guclu

Sabancı University

ncc@ulakbim.gov.tr

BC revisited

- A central node/edge has an impact on information flow in a network

- A common centrality measure is BC

- The ratio for the number of the shortest paths travelled through an arbitrary element and the number of all shortest path between those nodes, calculated for all node pairs.

$$BC(X) = \sum \left(\frac{P(a, b|X)}{P(a, b)} \right)$$

Freeman et *al.*, Sociometry 1977.
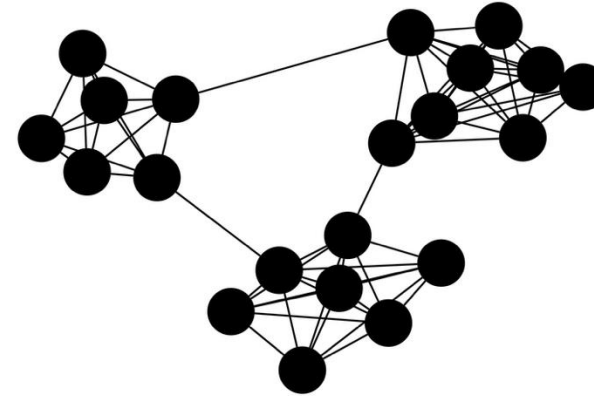
BC revisited

- A central node/edge has an impact on information flow in a network

- A common centrality measure is BC

- The ratio for the number of the shortest paths travelled through an arbitrary element and the number of all shortest path between those nodes, calculated for all node pairs

- High BC residues are important for protein function
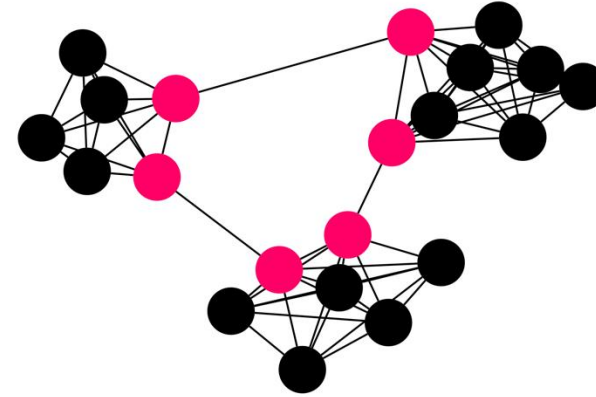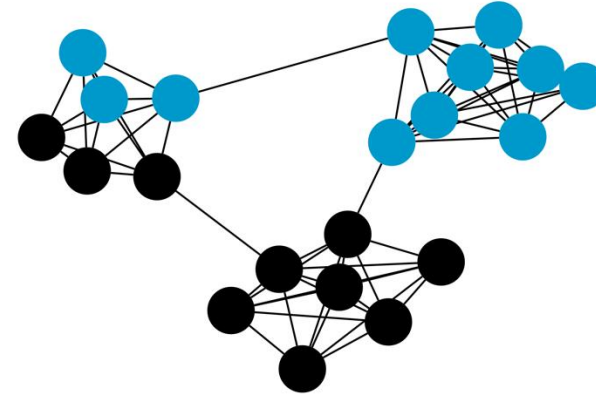
$$BC(X) = \sum \left(\frac{P(a,b|X)}{P(a,b)} \right)$$

Sheik Amamuddy *et al.*, J Chem Inf Model 2020.
Penkler *et al.*, J Chem Inf Model 2018.
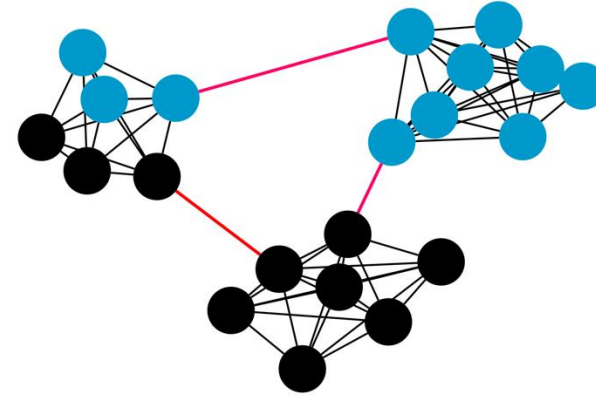Ozbaykal *et al.*, Proteins 2015.

Community detection

- Community analysis shows close-knit groups in a network

- A community is a group of nodes that connected to each other, without an edge to outer nodes

- Girvan-Newman algorithm removes the most central (highest BC) edge one-by-one and searches for communities

1. Calculate edge BC

2. Remove the edge with highest BC

3. Check for emergence of new communities

4. Return to step 1 and iterate

Girvan et *al.*, PNAS 2002.

Community detection

- Community analysis shows close-knit groups in a network

- A community is a group of nodes that connected to each other, without an edge to outer nodes

- Girvan-Newman algorithm removes the most central (highest BC) edge one-by-one and searches for communities

1. Calculate edge BC

2. Remove the edge with highest BC

3. Check for emergence of new communities

4. Return to step 1 and iterate

Girvan *et al.,* PNAS 2002.

Community composition

- Assessing the composition of communities and scoring the structural origins of members shed light on communication between the segments
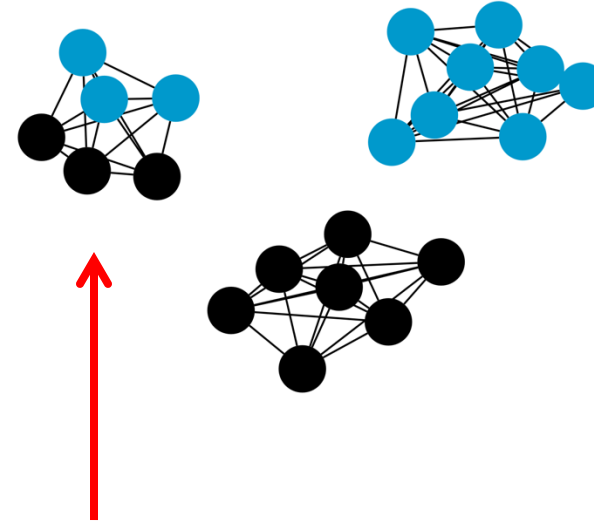
Blue and Black together in a community in this instance so the score is 1.

Thanks!