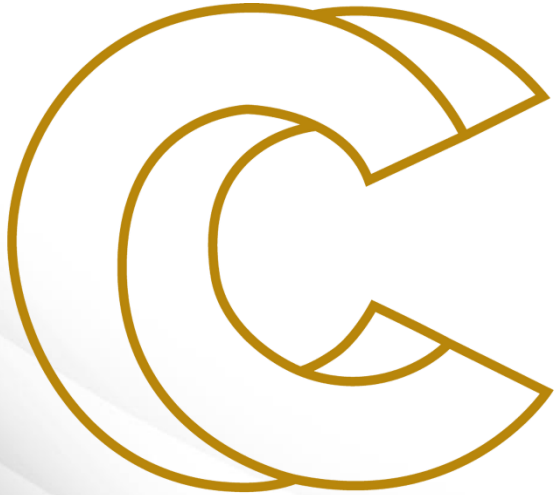
Sabancı Üniversitesi

TÜBİTAK



EURO 4SEE

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

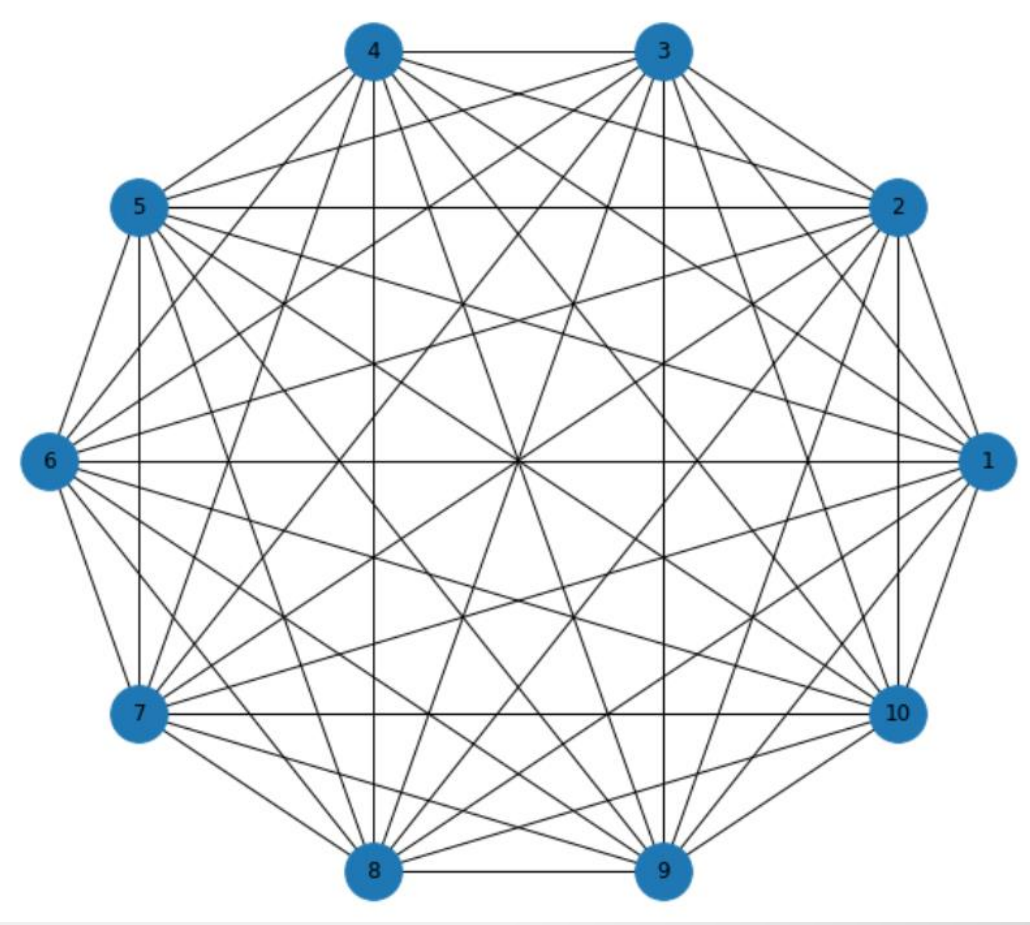
Tandac Furkan Guclu
Sabancı University

ncc@ulakbim.gov.tr

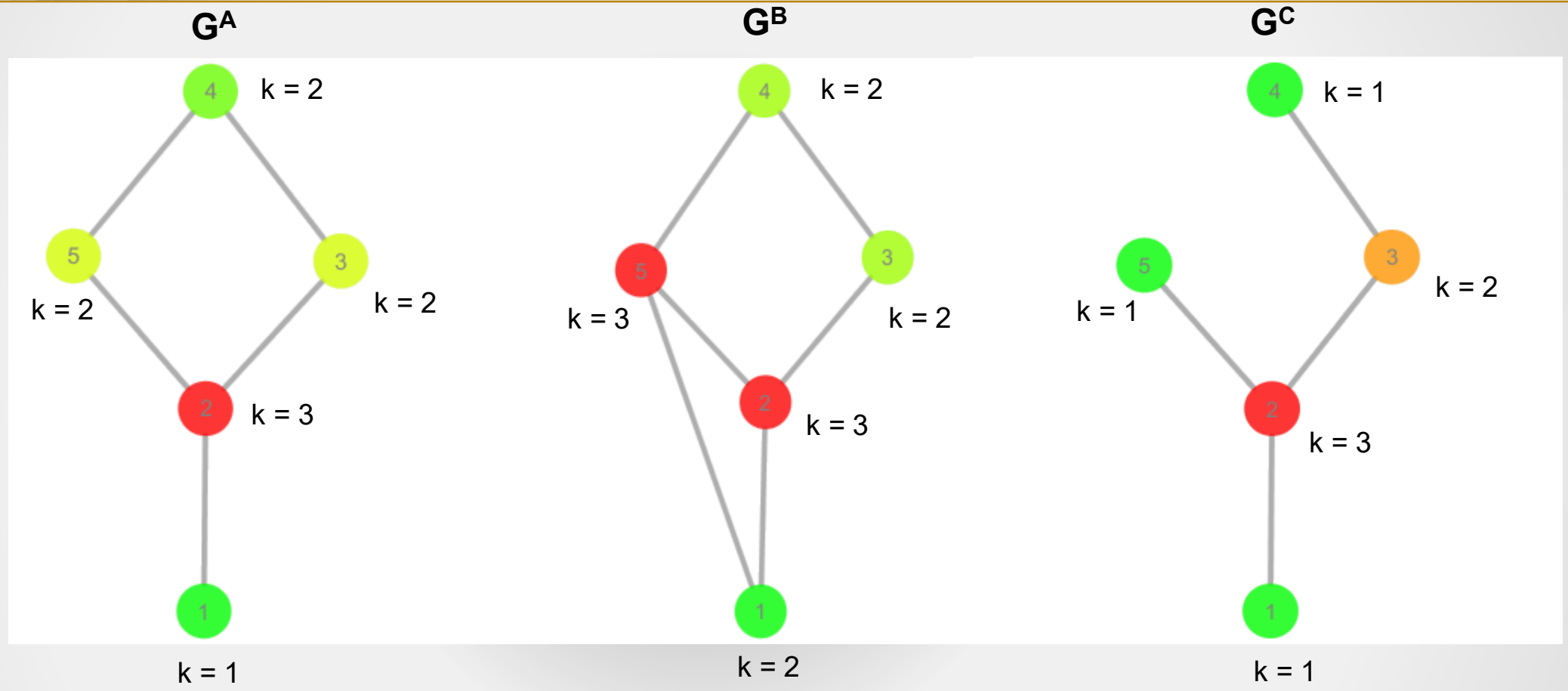
Lesson 1: Introduction to graphs and measures

Graph or network

- Consists of vertices (nodes) and edges (links)
- Nodes and edges may be weighted
- Stored as adjacency matrix or edge/node list
- Here our graphs are
  - Undirected
  - Unweighted
  - No self-loops
  - No parallel edges
- Parameters we use
  - Degree or number of neighbors (*k*)
  - Average shortest path length (<*L*>)
  - Clustering coefficient (*C*)
  - Betweenness centrality (BC)



Degree or number of neighbors (*k*)



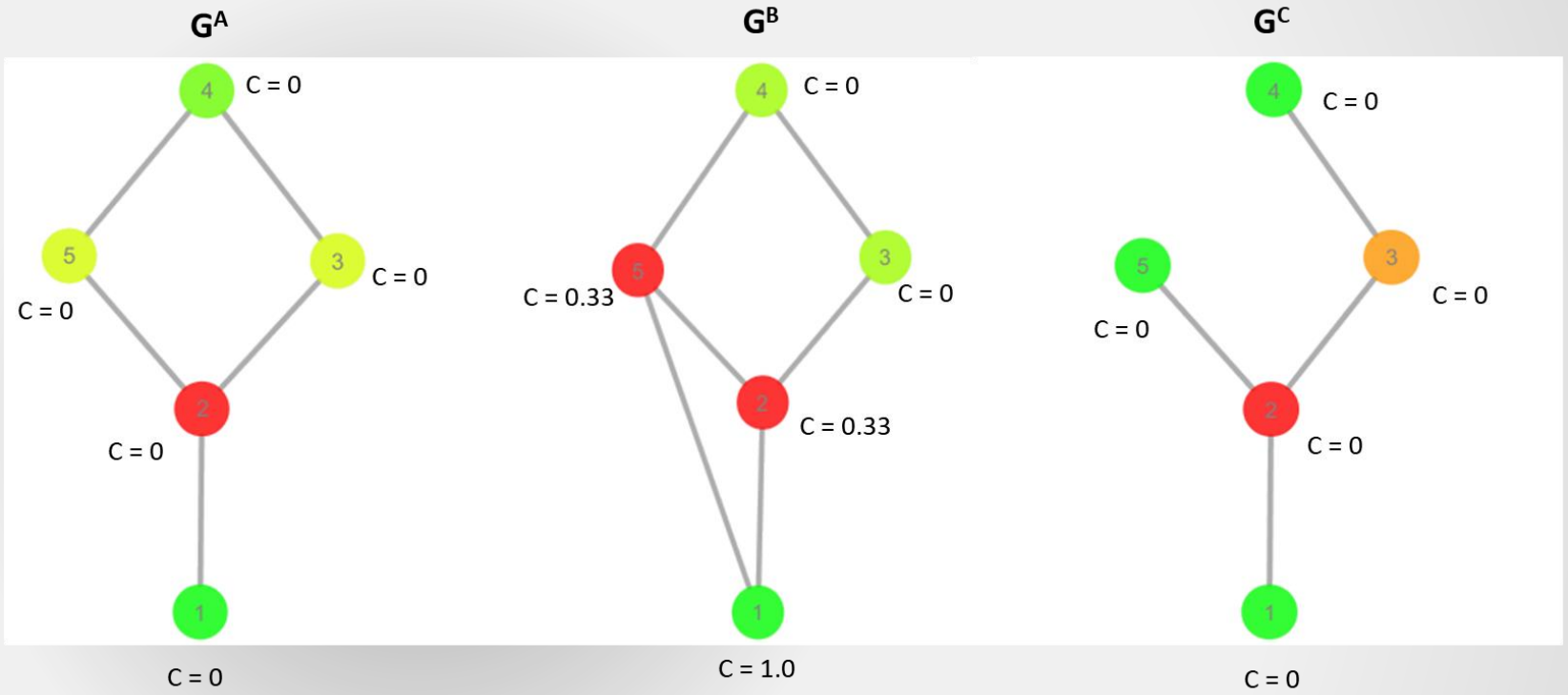
Local information about network.

Clustering coefficient (C)

For G^B:

$$C = \frac{2T(u)}{\mathrm{k}(u)(\mathrm{k}(u)-1)}$$

$$C_{Node2} = \frac{2 \times 1}{3 \times 2} = 0.33$$



Connectivity of the neighbors of a node, semi-local information about connectivity.

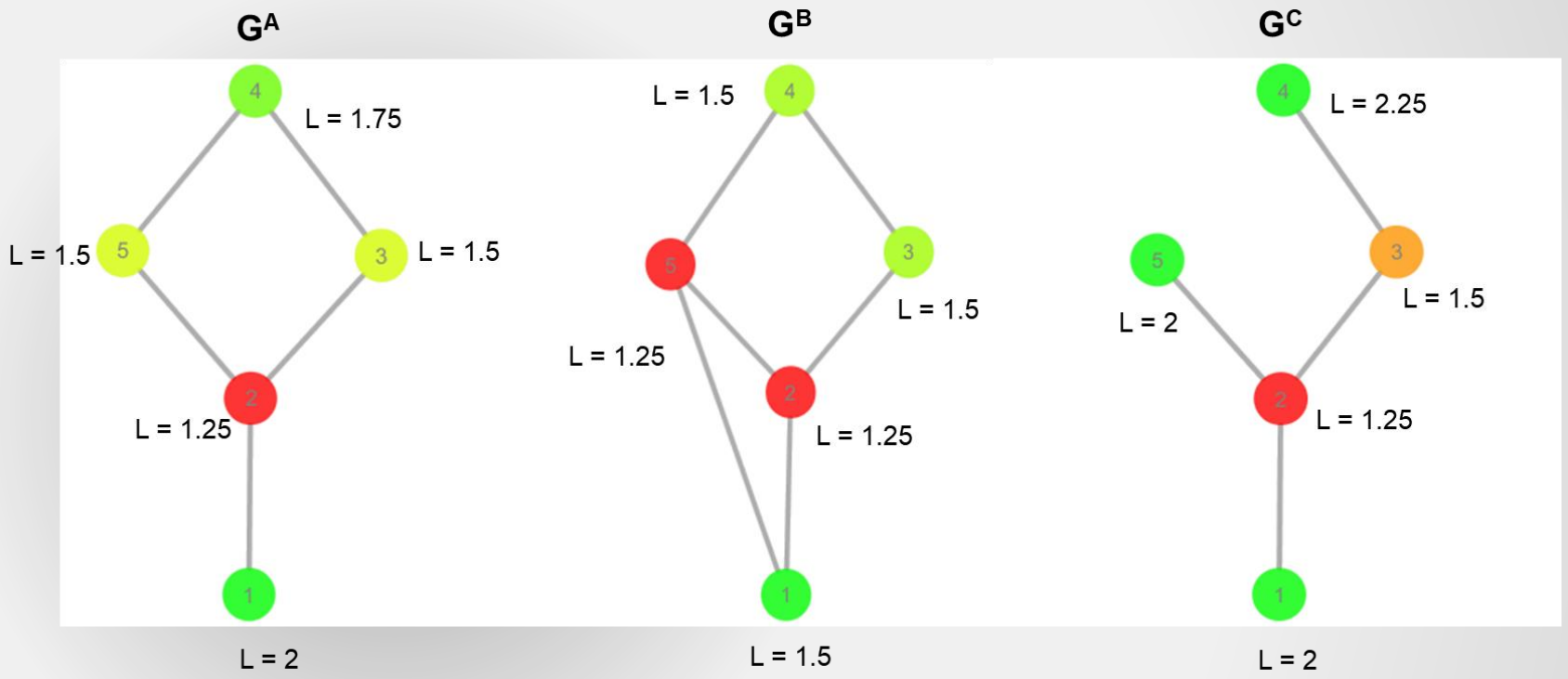
Average Shortest Path Length (<L>)

For G^A:

$$< L_i >= \frac{1}{n-1}\sum_{i}^{n} L_{ij}$$

$$< L >_{Node\ 2} = \frac{L_{21} + L_{25} + L_{23} + L_{24}}{N}$$

$$< L >_{Node\ 2} = \frac{1+1+1+2}{4} = 1.25$$



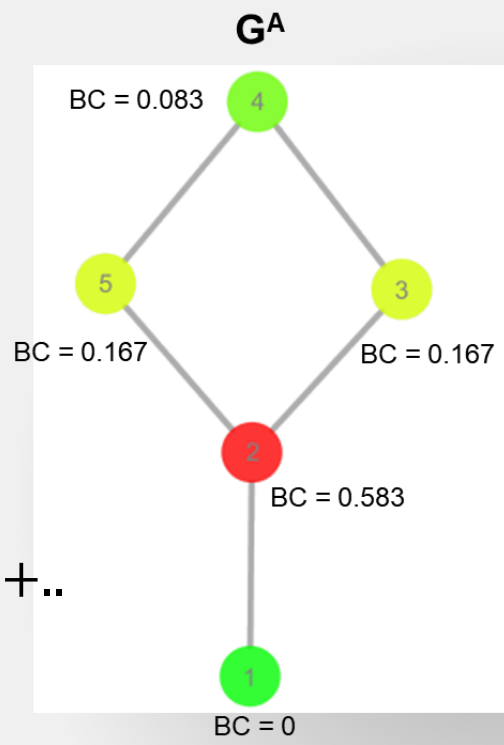
Information about the accessibility of a node in units of edges.

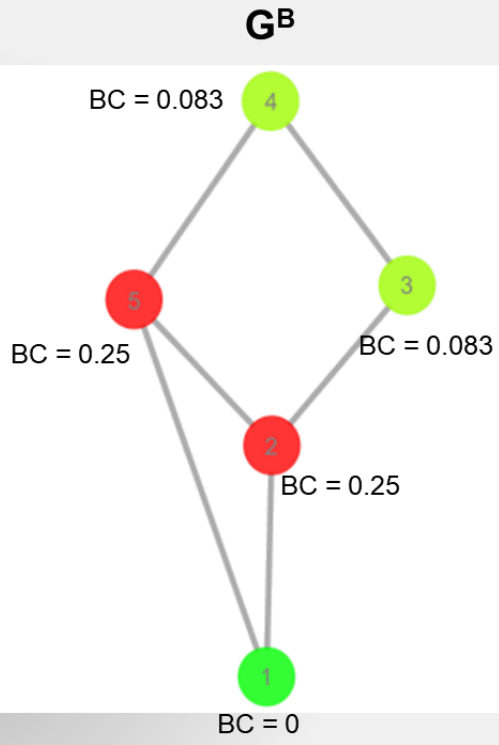
Betweenness centrality (BC)

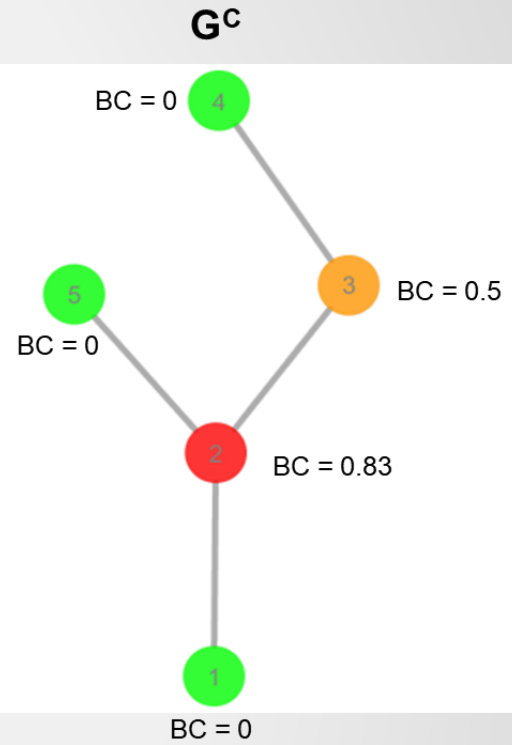
For G^A:

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

$$BC_{Node\ 2} = \frac{P_{13}(2)}{P_{13}} + \frac{P_{15}(2)}{P_{15}} + \frac{P_{14}(2)}{P_{14}} + ..$$





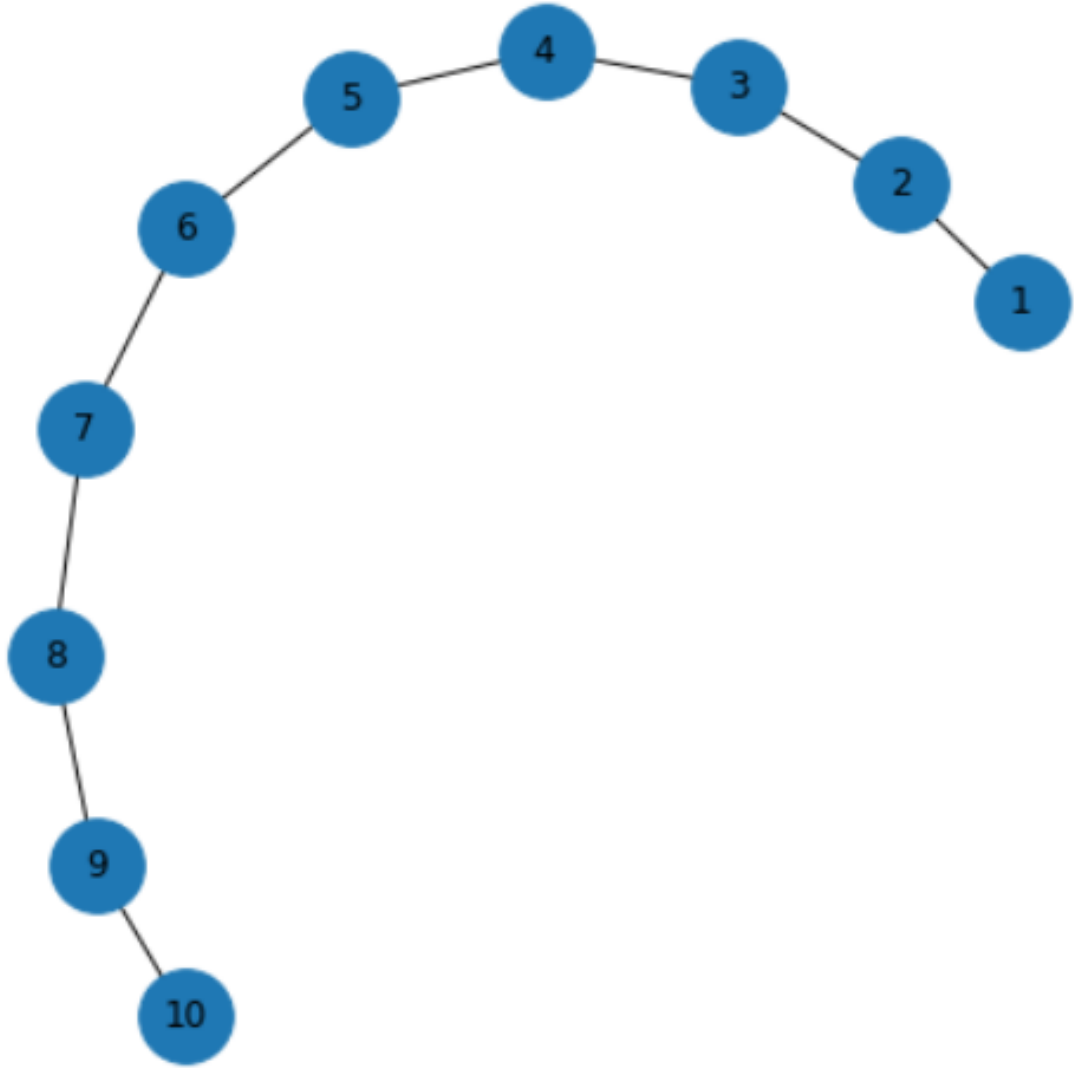


$$BC_{Node\ 2} = \frac{1}{1} + \frac{1}{1} + \frac{2}{2} + 0 + \frac{1}{2} + 0 = 3.5$$

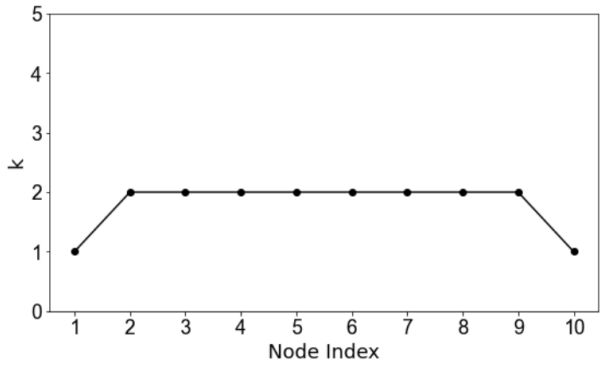
Further normalized by (n-1)(n-2)/2

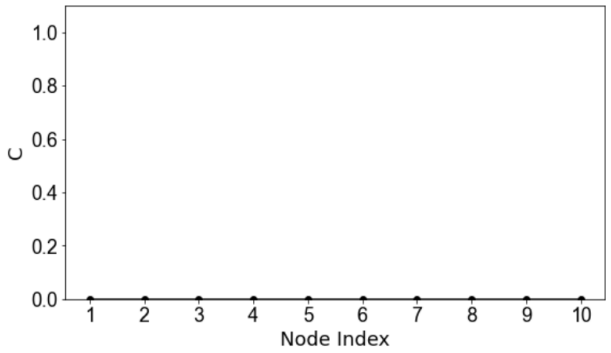
$$BC_{Node\ 2} = \frac{3.5}{6} = 0.583$$

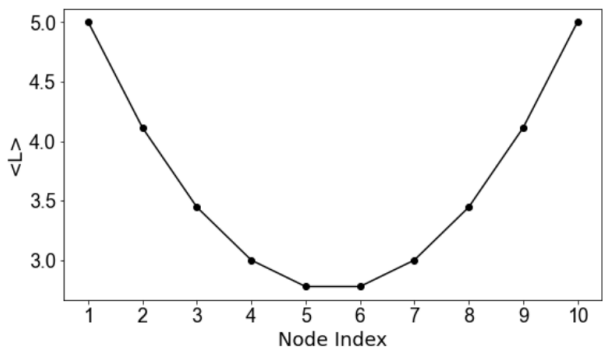
More toy graphs…

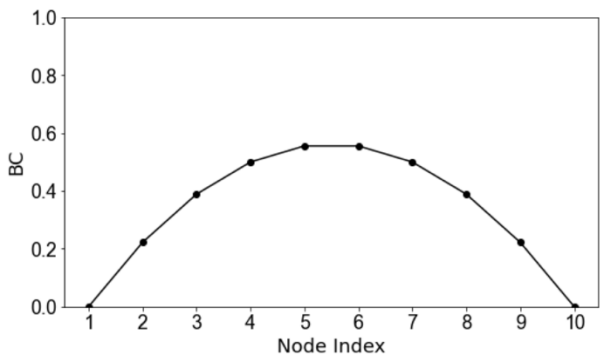


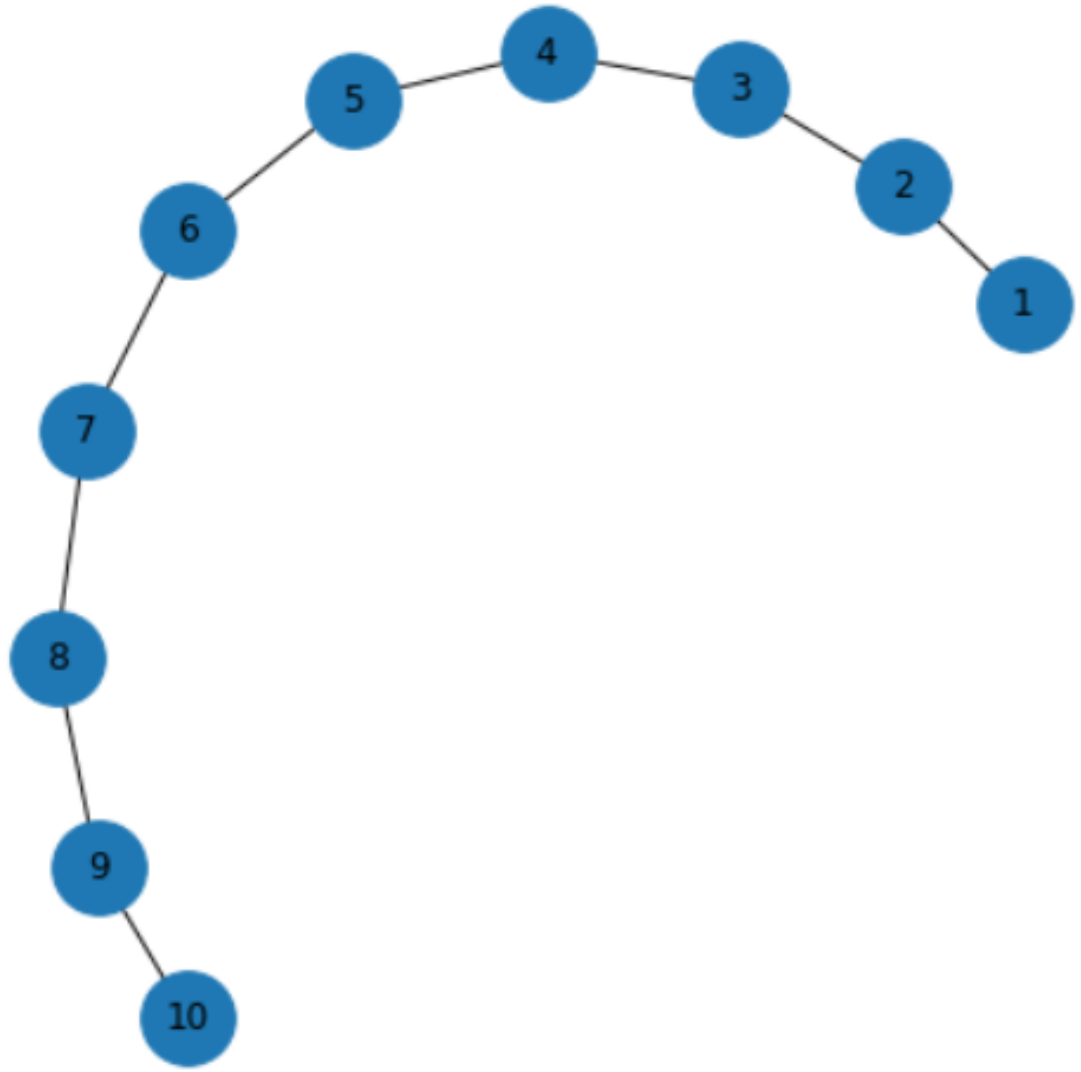
Number of nodes: 10
Number of edges: 9
Average degree: 1.8











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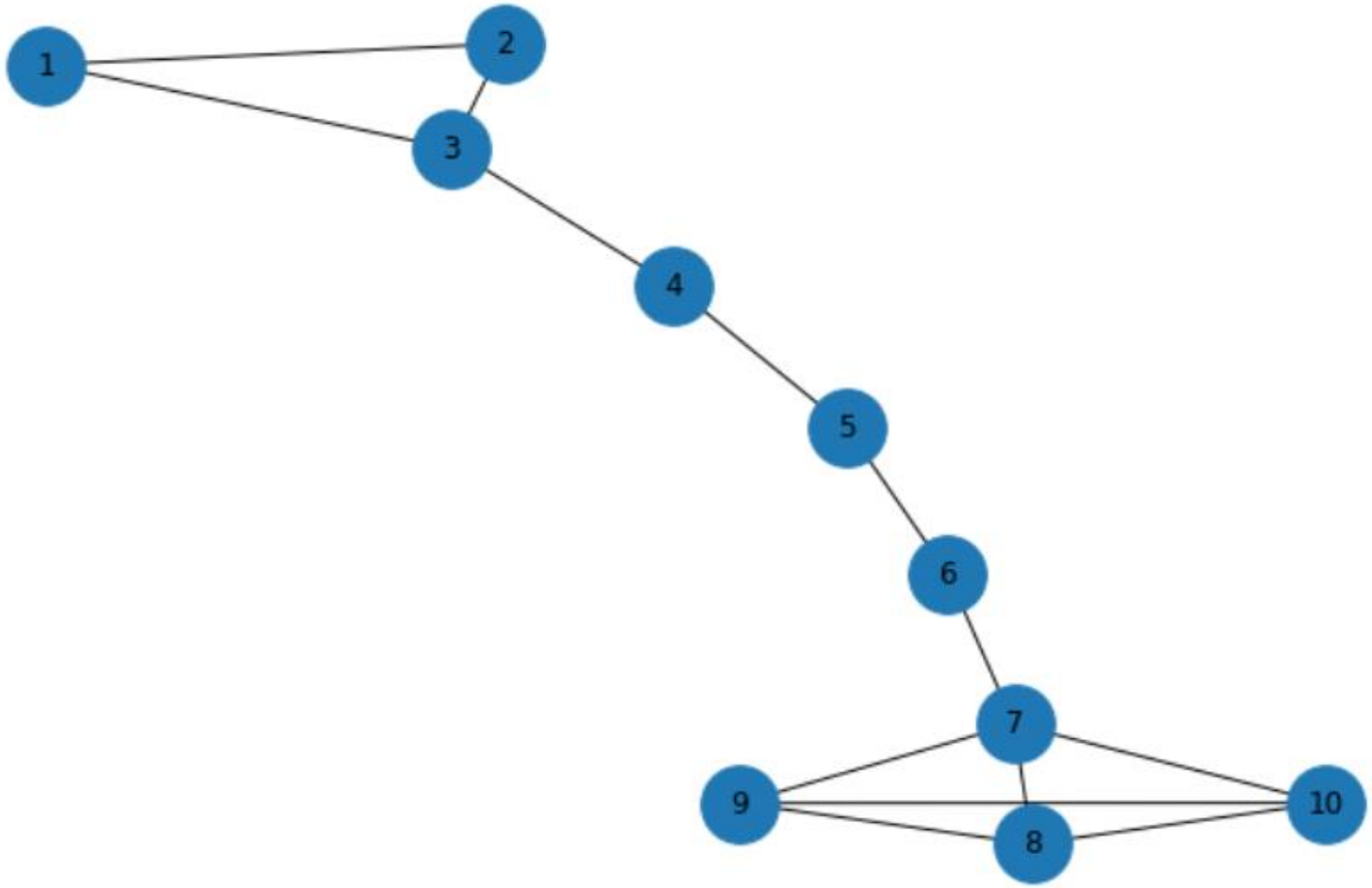
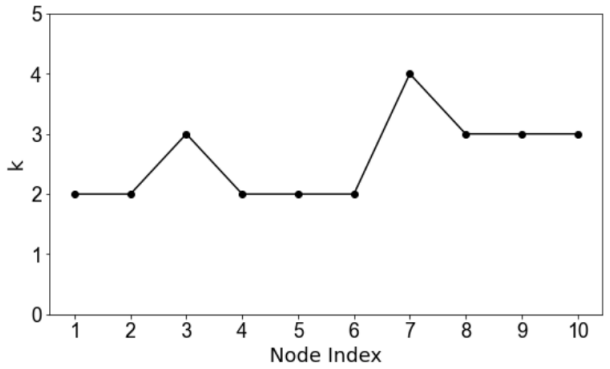
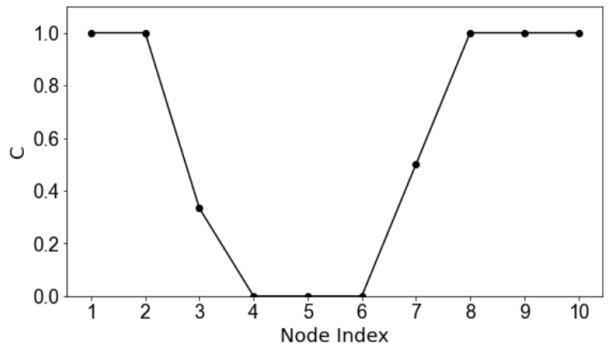
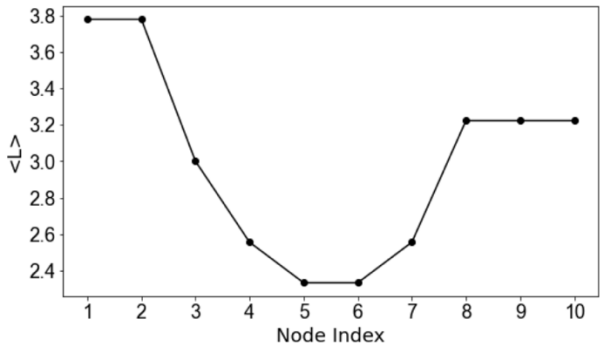


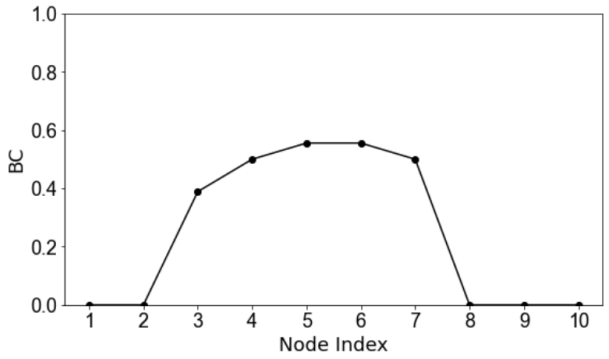
Number of nodes: 10
Number of edges: 13
Average degree: 2.6

[1,3]
[8,10]
[7,10]
[7,9]









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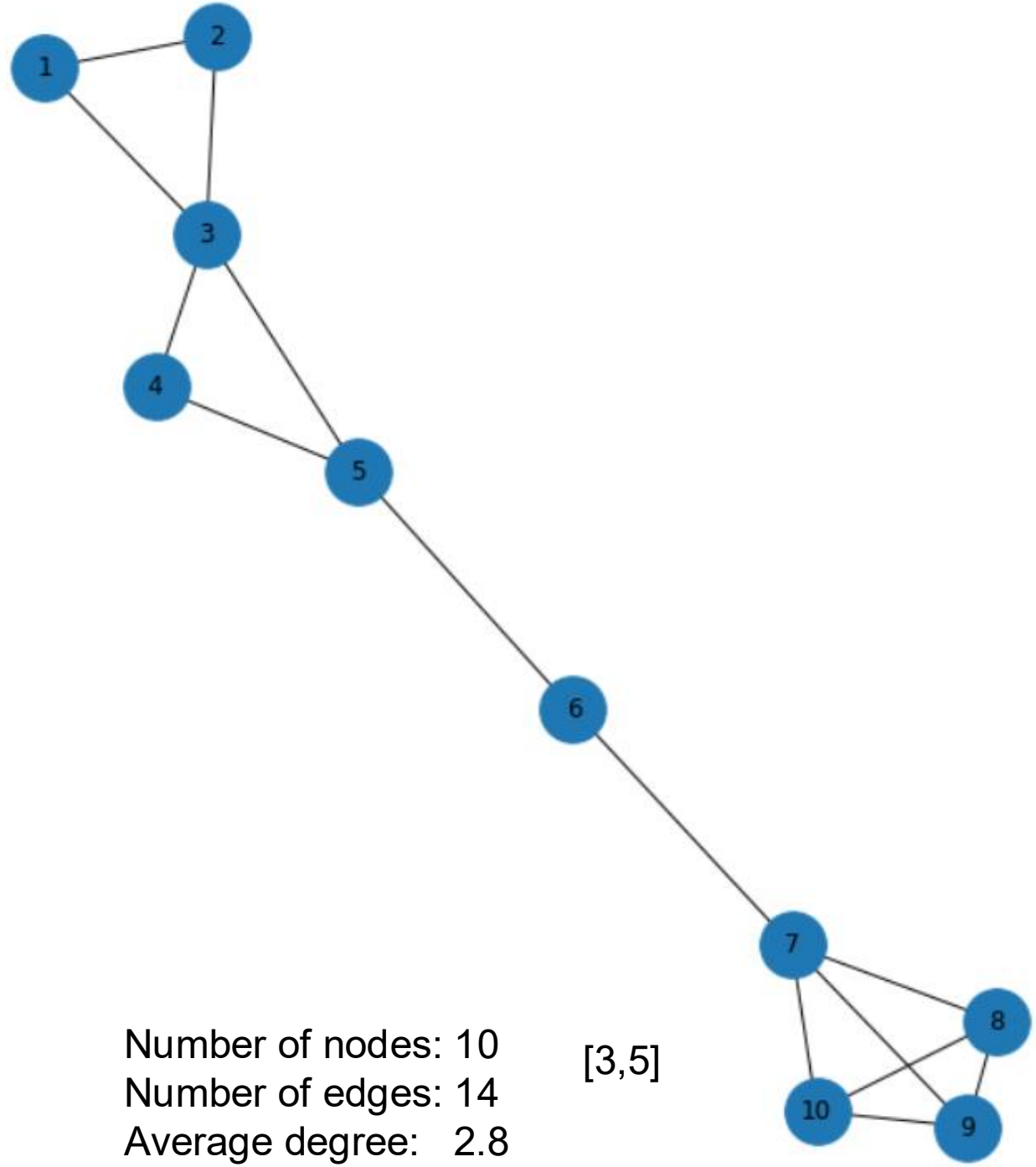
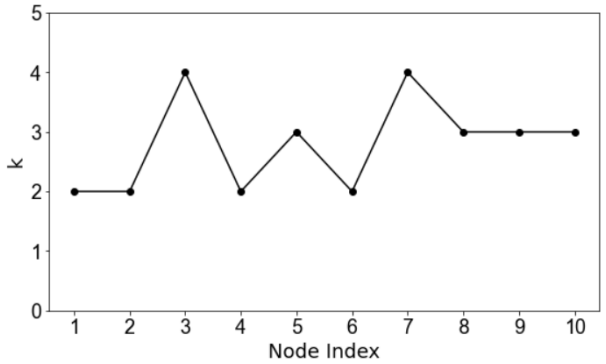
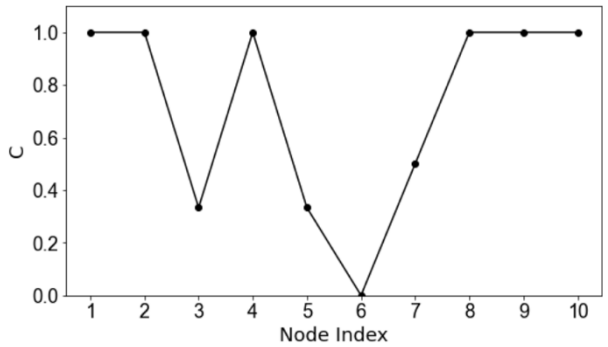
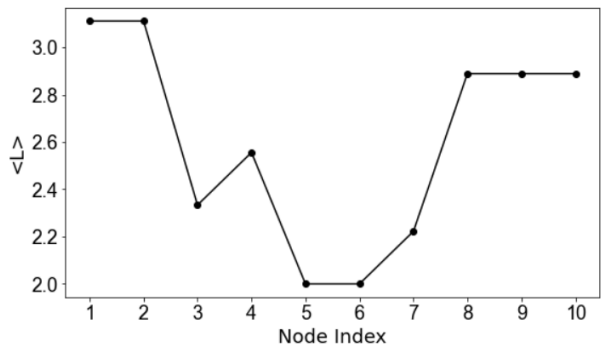


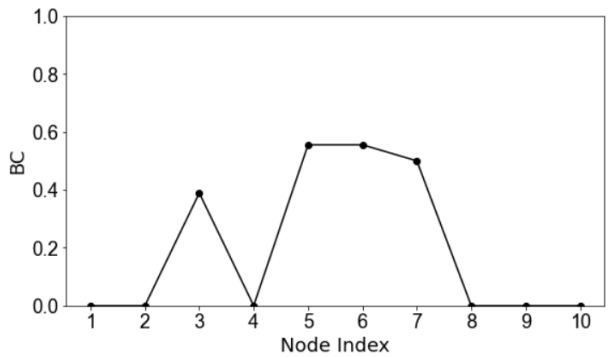
Number of nodes: 10
Number of edges: 14
Average degree: 2.8

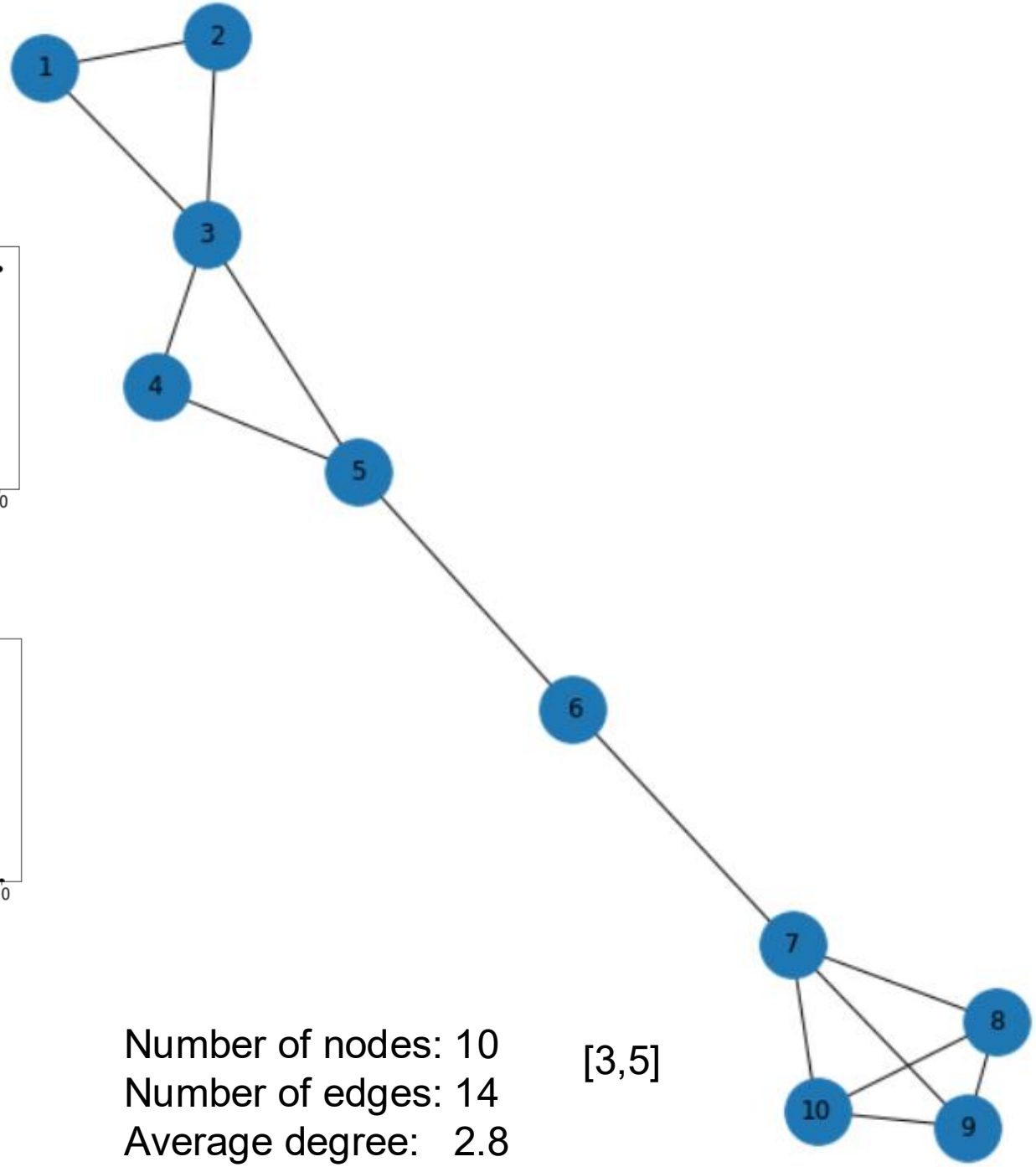
[3,5]





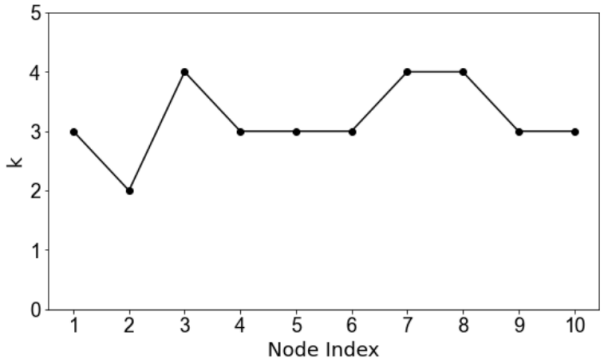


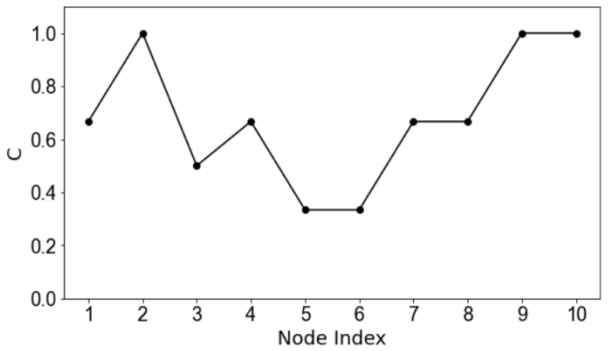


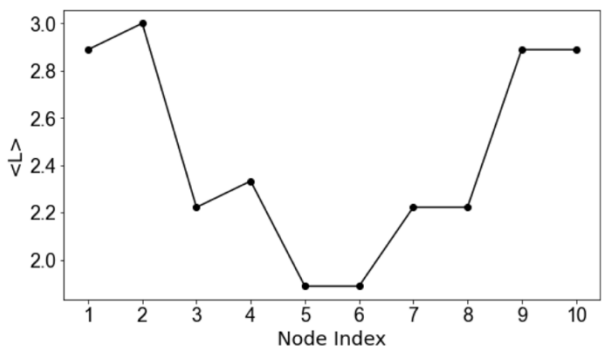


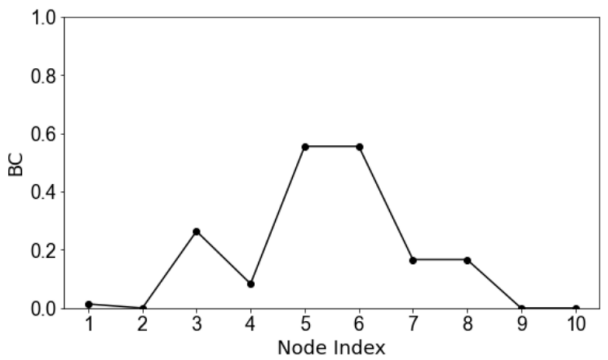
Number of nodes: 10
Number of edges: 14
Average degree: 2.8

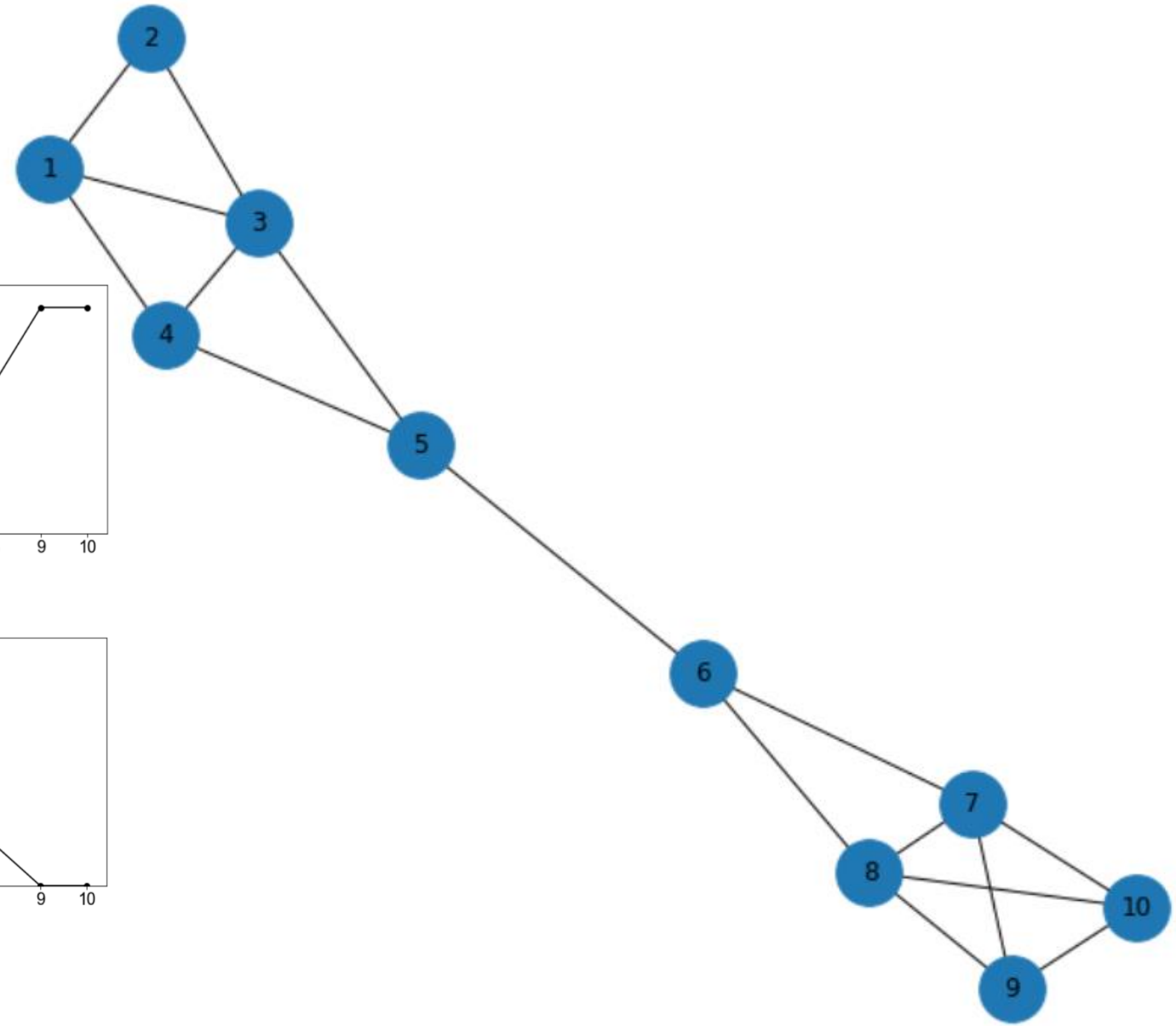
[3,5]





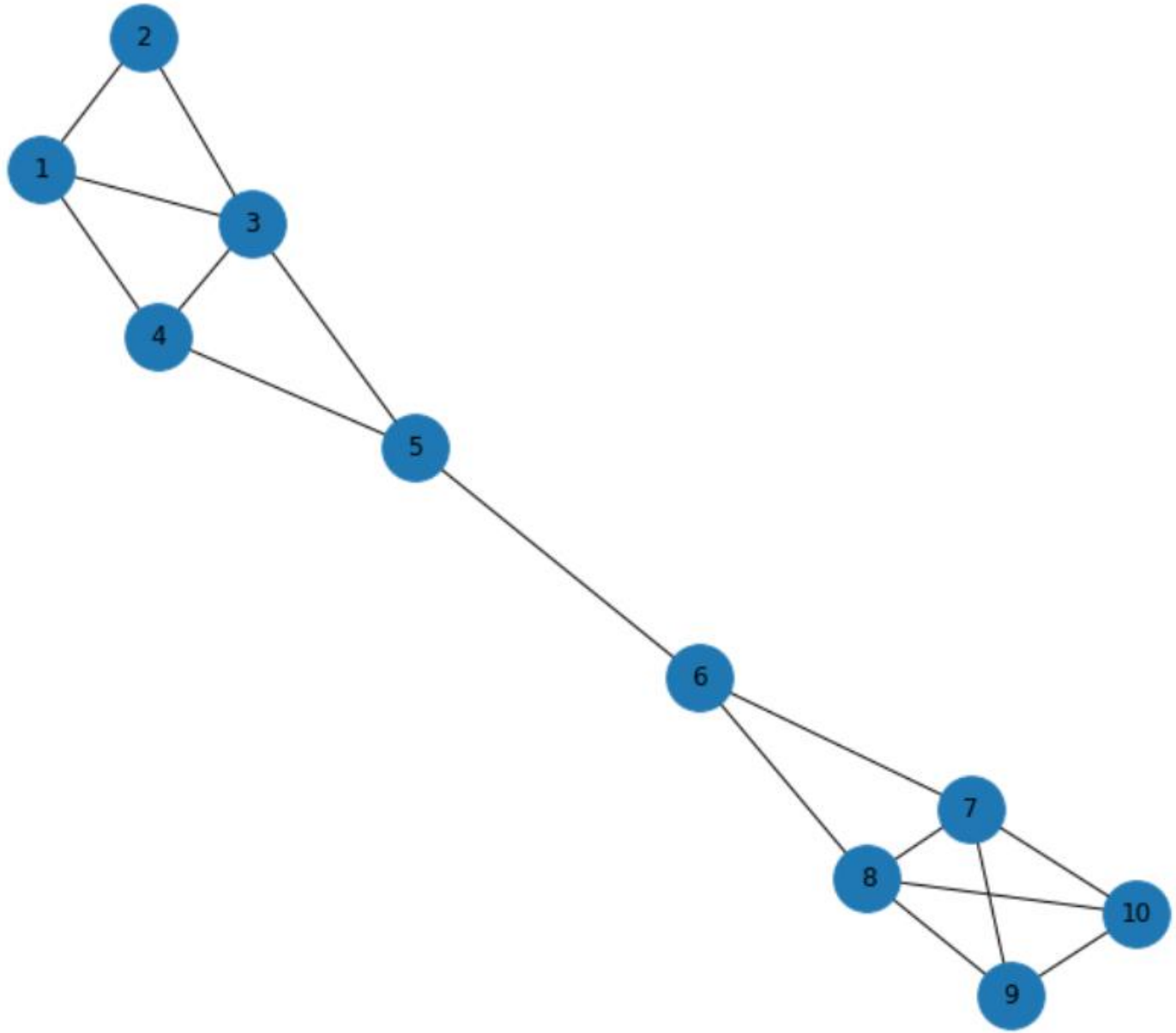






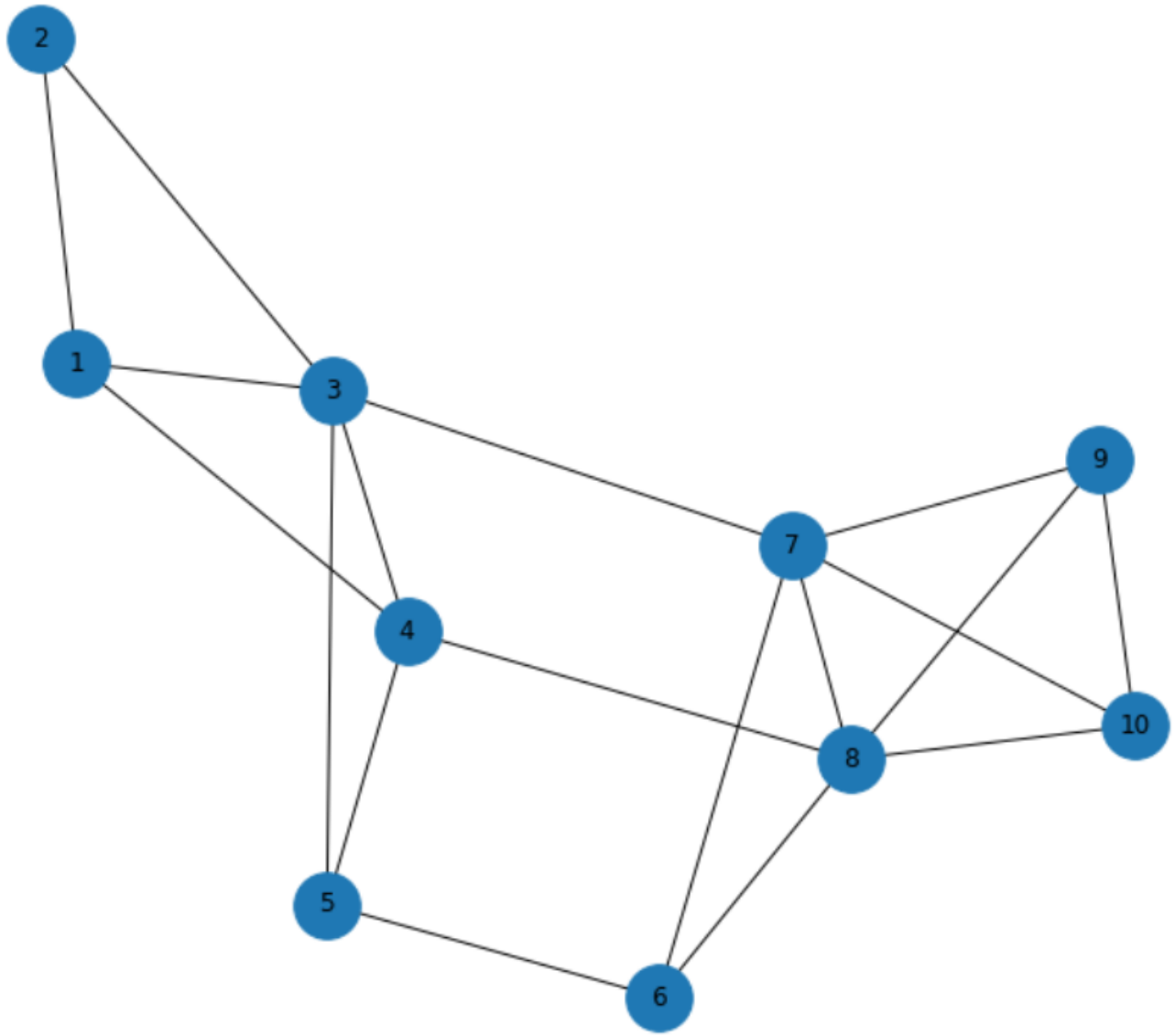
Number of nodes: 10
Number of edges: 16
Average degree: 3.2

[1,4]
[6,8]

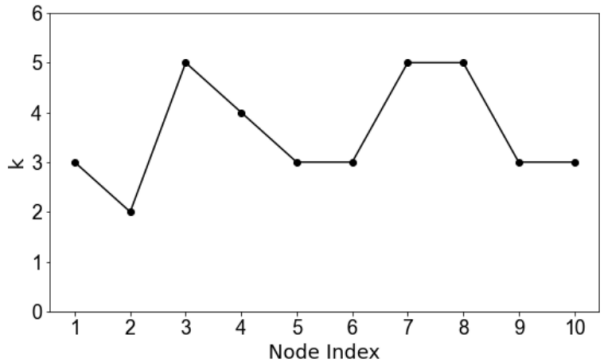


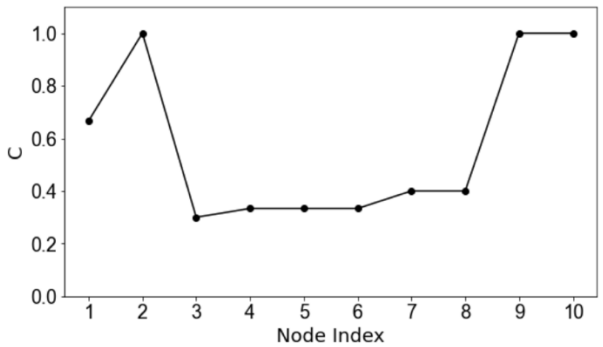
Number of nodes: 10
Number of edges: 16
Average degree: 3.2

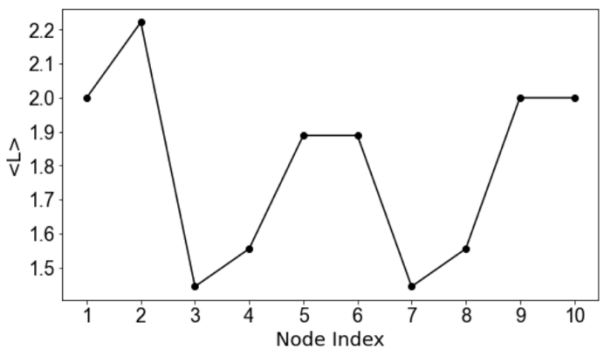
[1,4]
[6,8]

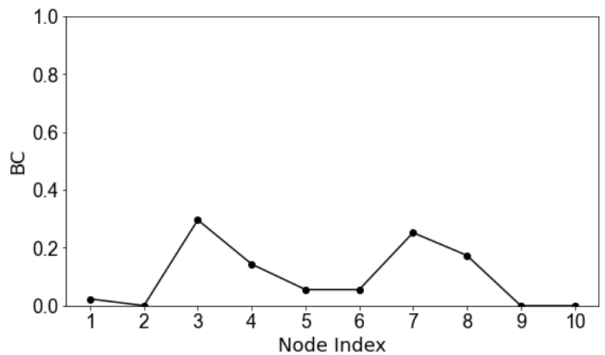


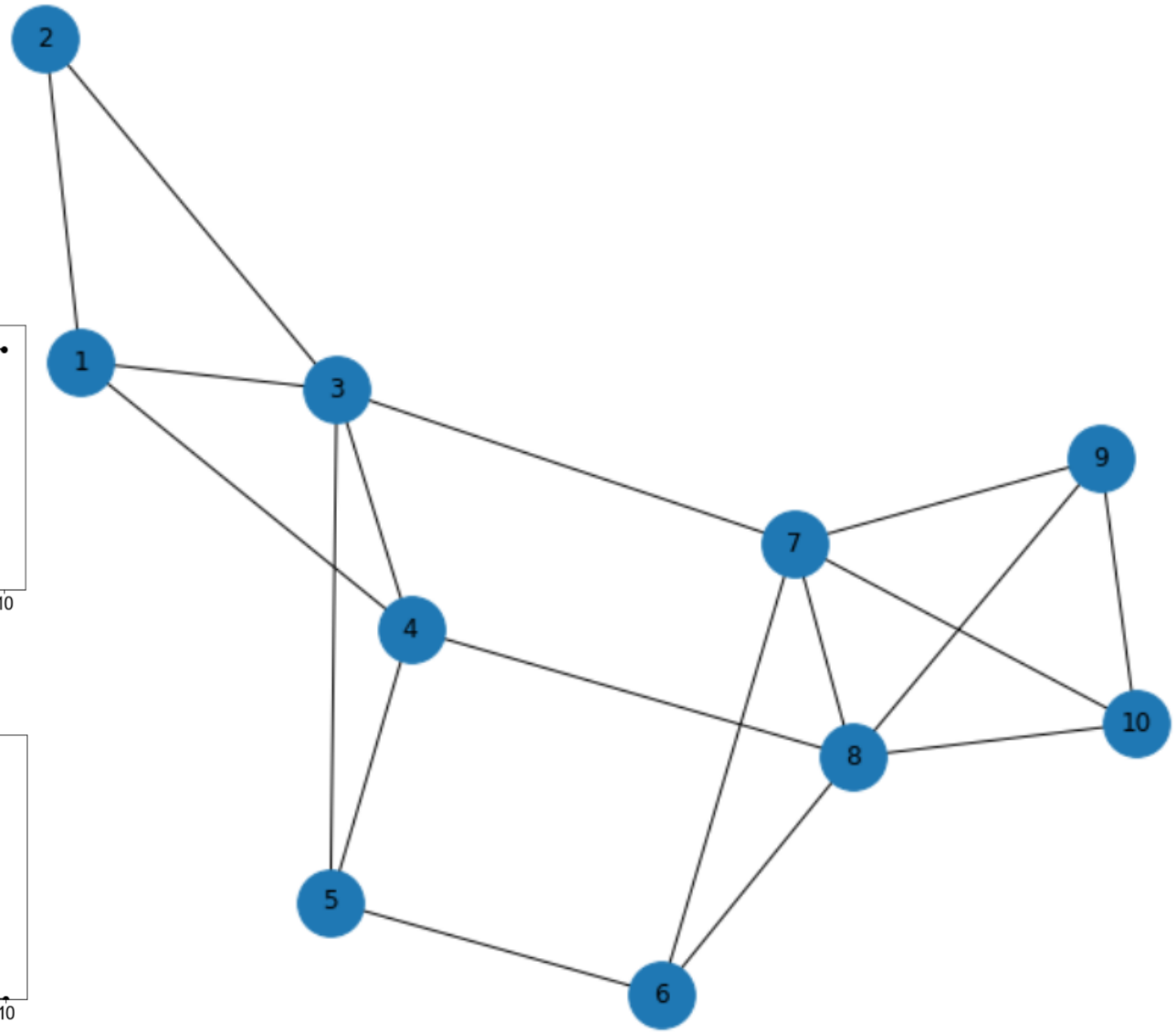
Number of nodes: 10 [3,7]
Number of edges: 18 [4,8]
Average degree: 3.6



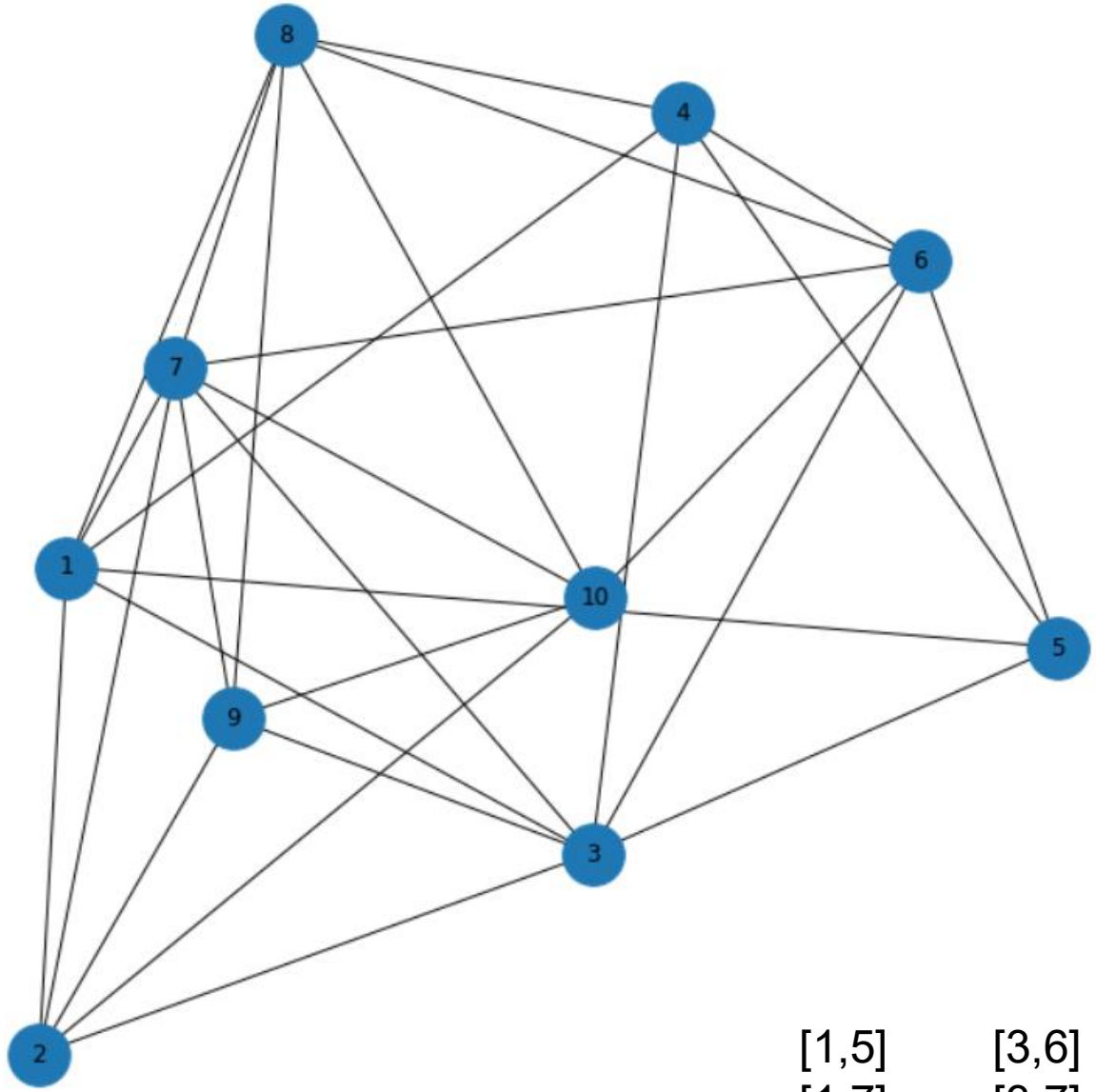






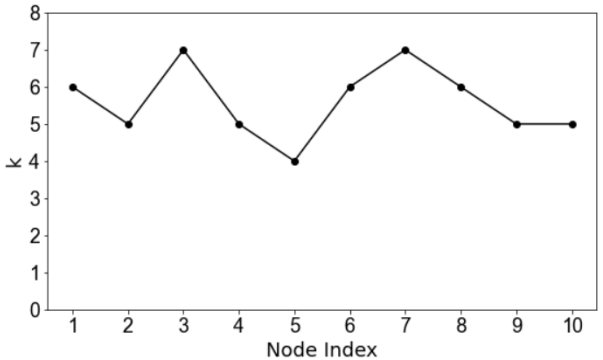


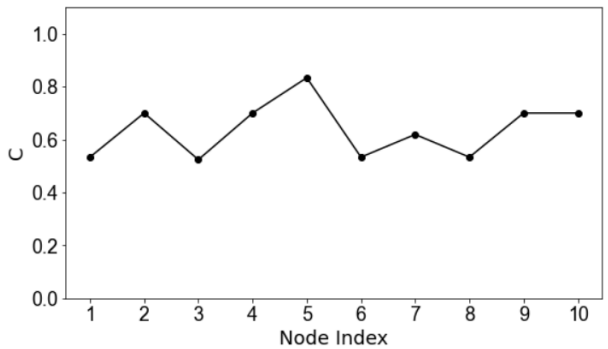
Number of nodes: 10 [3,7]
Number of edges: 18 [4,8]
Average degree: 3.6

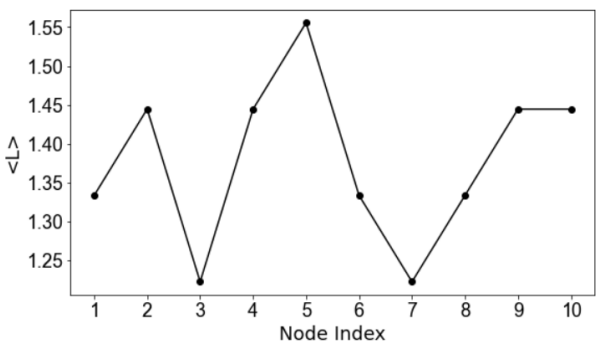


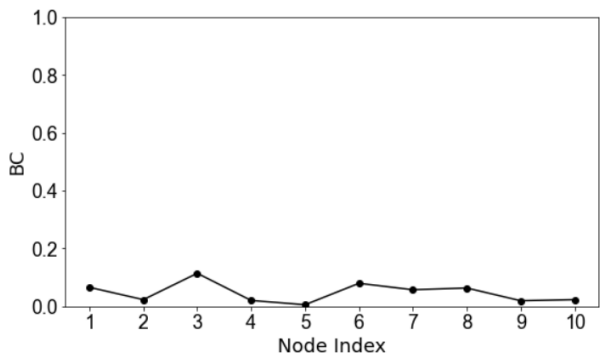
Number of nodes: 10
Number of edges: 28
Average degree: 5.6

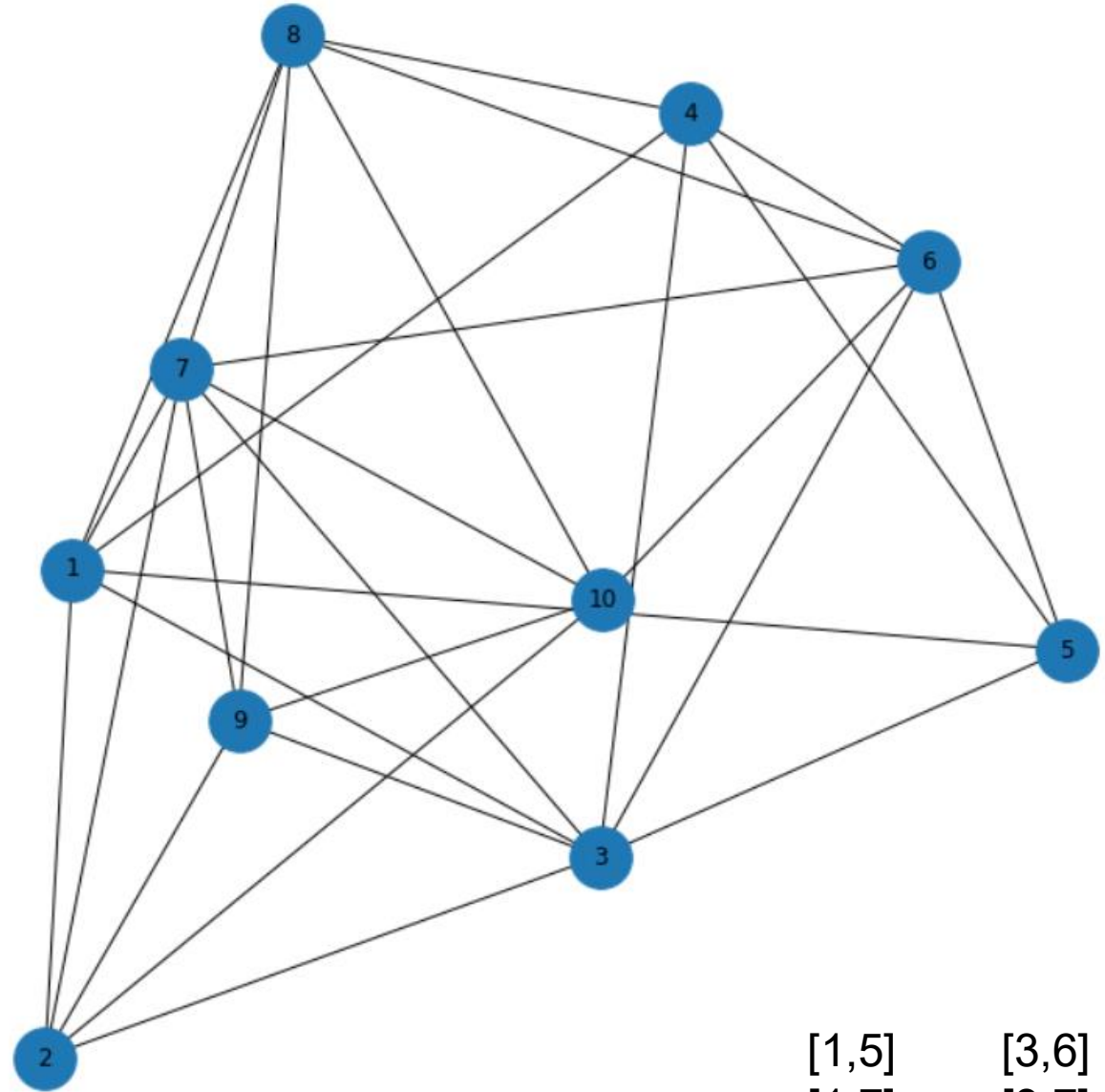
[1,5]
[1,7]
[1,8]
[2,7]
[2,9]
[2, 10]
[3,6]
[3,7]
[3,9]
[4,6]
[6,10]











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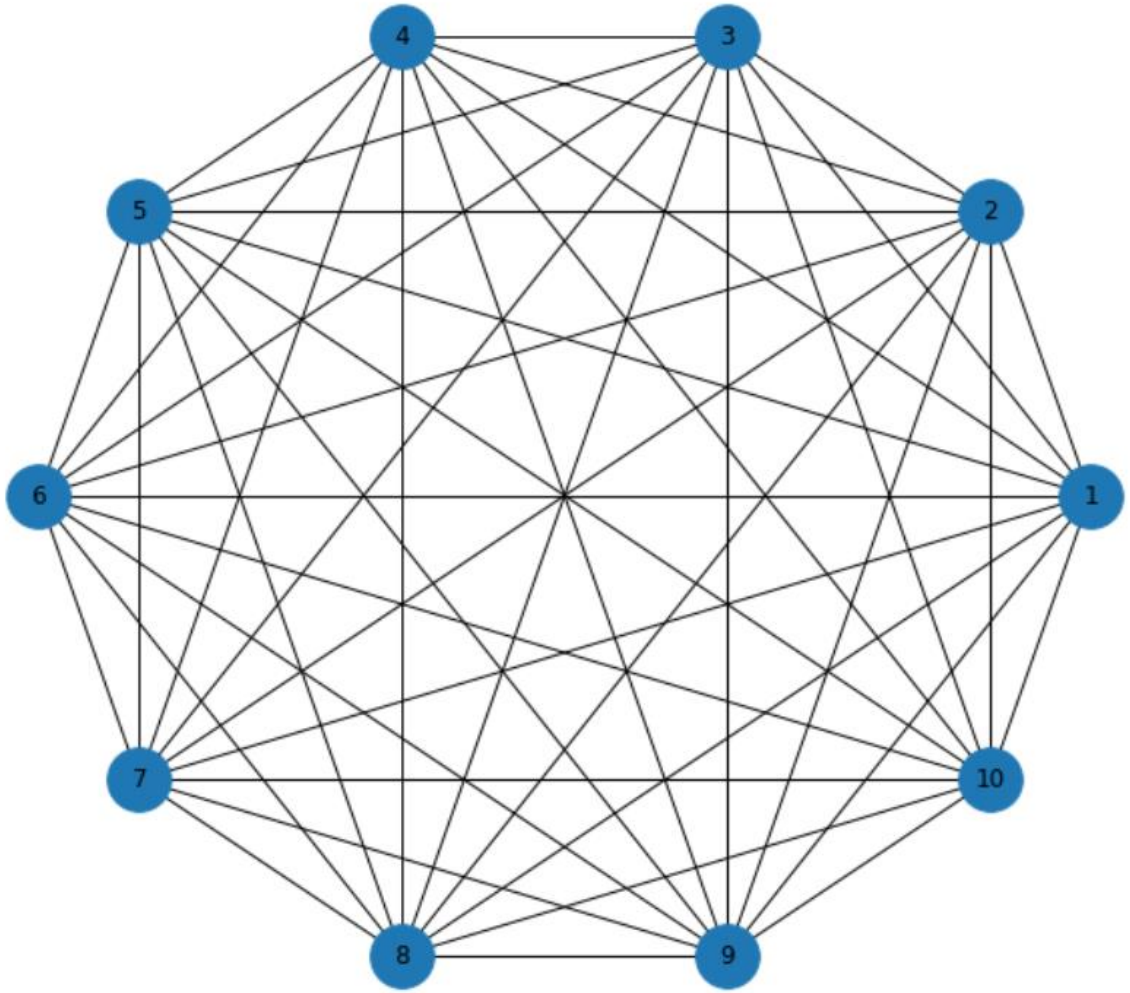
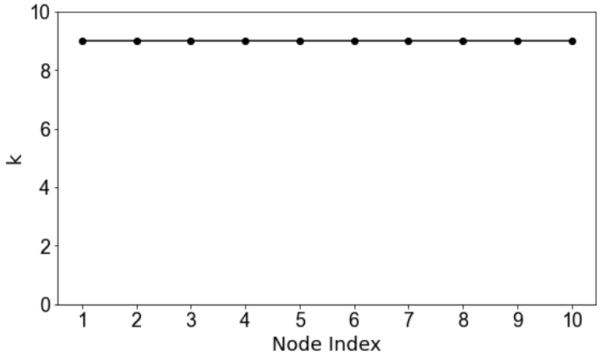
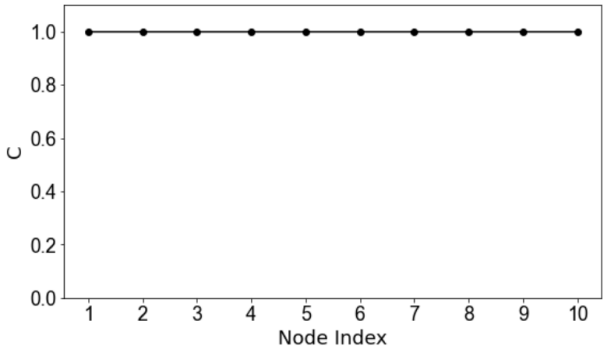
[1,5]
[1,7]
[1,8]
[2,7]
[2,9]
[2, 10]
[3,6]
[3,7]
[3,9]
[4,6]
[6,10]

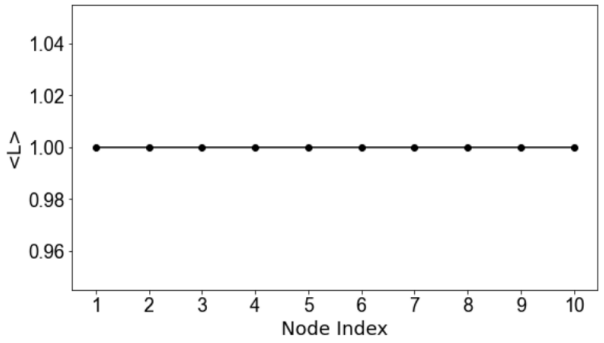


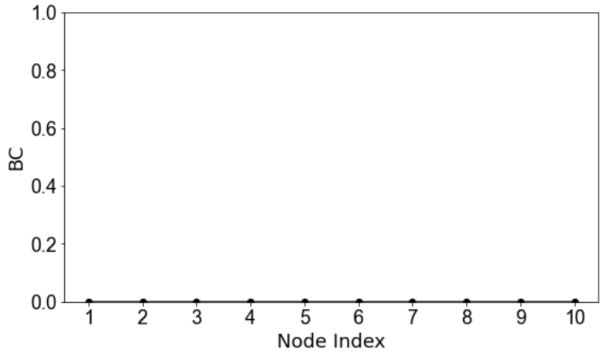
Number of nodes: 10
Number of edges: 45
Average degree: 9

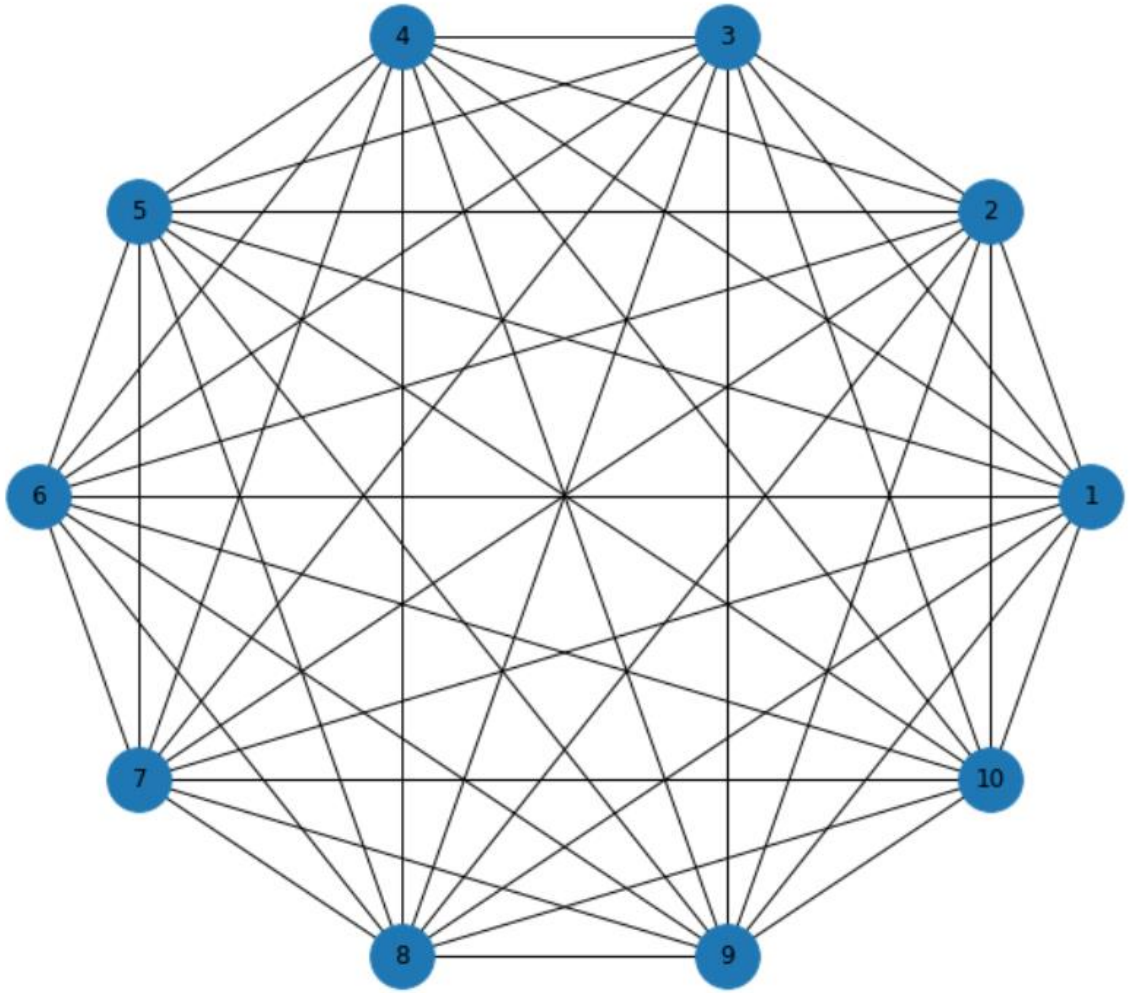
Complete network











Number of nodes: 10
Number of edges: 45
Average degree: 9

Complete network

Next lecture

Code for these toy graphs…

EURO 4SEE

Thanks!

Co-funded by
the European Union

EuroHPC
Joint Undertaking

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