Network analysis with Cytoscape

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in lecture on systems bioinformatics

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Outline

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Introduction I

. . . why should we care about glycolysis and gluconeogeneses

Introduction II

. . . basic setup of our two networks ... how we modelled them and what did not work (CellDesigner) ...

Outline

Plugin for calculation of Katz's Index

Definition (Katz's Index)

...

We considered two cases: α small and $\alpha = \frac{1}{\lambda_{max}}$.

Plugin for calculation of Katz's Index - α small

Listing 1: Necessary import statements

```
1  package katz.plugin;
2
3  import java.util.List;
4  import java.awt.event.ActionEvent;
5  import javax.swing.JOptionPane;
6  import java.text.DecimalFormat;
7
8  import cytoscape.plugin.CytoscapePlugin;
9  import cytoscape.util.CytoscapeAction;
10 import cytoscape.Cytoscape;
11 import cytoscape.CyNetwork;
12 import cytoscape.CyEdge;
13 import cytoscape.view.CyNetworkView;
14
15 import Jama.Matrix;
```

Plugin for calculation of Katz's Index - α small

Listing 2: Basic class definition

```
16 public class KatzPlugin extends CytoscapePlugin {
17
18     public KatzPlugin() {
19         KatzPlugin.MolbiPluginAction action = new KatzPlugin.MolbiPluginAction();
20         action.setPreferredMenu("Plugins.Molbi");
21         Cytoscape.getDesktop().getCyMenus().addAction(action);
22     }
23
24     public String describe() {
25         return "Plugin to calculate the topological Katz Index for networks";
26     }
27
28     public class MolbiPluginAction extends CytoscapeAction {
29
30         public MolbiPluginAction() {
31             super("Katz's Index (alpha = 0.1)");
32         }
33
34         @Override
35         public void actionPerformed(ActionEvent ae) {
36             run();
37         }
```

Plugin for calculation of Katz's Index - α small

Listing 3: Run method (I)

```
38          private void run() {
39
40              CyNetwork network = Cytoscape.getCurrentNetwork();
41              CyNetworkView view = Cytoscape.getCurrentNetworkView();
42              int N = network.getNodeCount() + 1;
43
44              if (N == 1) {
45                  JOptionPane.showMessageDialog(view.getComponent(), "No network/view
                        loaded.");
46                  return;
47              }
48
49              double[][] A = new double[N][N];
50              for (double[] row : A) Arrays.fill(row, 0.0);
51
52              for (CyEdge edge : (List<CyEdge>) network.edgesList()) {
53                  int i = Math.abs(edge.getSource().getRootGraphIndex());
54                  int j = Math.abs(edge.getTarget().getRootGraphIndex());
55                  A[i][j] = 1;
56              }
```

Plugin for calculation of Katz's Index - α small

Listing 4: Run method (II)

```
57                Matrix M = new Matrix(A);
58                Matrix I = Matrix.identity(N, N);
59                Matrix IVec = new Matrix(N, 1, 1.0);
60
61                double alpha = 0.1; // emulates degree centrality
62                double[][] values = ((I.minus(M.transpose().times(alpha))).inverse()).
                        minus(I).times(IVec).getArrayCopy();
63
64                StringBuilder sb = new StringBuilder();
65                DecimalFormat df = new DecimalFormat("#0.000");
66
67                for (int i = 1; i < N; i++) {
68                    if (i % 10 == 0) sb.append("\n");
69                    sb.append("C(").append(i).append("): ").append(df.format(values[i
                            ][0])).append("    ");
70                }
71
72                JOptionPane.showMessageDialog(view.getComponent(), "All done.\n" + sb);
73                view.redrawGraph(false, true);
74            }
75        }
76    }
```

Plugin for calculation of Katz's Index - $\alpha = \frac{1}{\lambda_{max}}$

Listing 5: Run method (II)

```
57                  Matrix M = new Matrix(A);
58                  Matrix I = Matrix.identity(N, N);
59                  Matrix IVec = new Matrix(N, 1, 1.0);
60
61                  double[] eigs = M.eig().getRealEigenvalues();
62                  double alpha;
63                  Arrays.sort(eigs);
64
65                  if (eigs[eigs.length - 1] == 0) alpha = 1.0;
66                  else alpha = 1.0 / eigs[eigs.length - 1];
67
68                  double[][] values = ((I.minus(M.transpose().times(alpha))).inverse()).
                        minus(I).times(IVec).getArrayCopy();
69                  StringBuilder sb = new StringBuilder();
70                  DecimalFormat df = new DecimalFormat("#0.000");
71
72                  for (int i = 1; i < N; i++) {
73                      if (i % 10 == 0) sb.append("\n");
74                      sb.append("C(").append(i).append("): ").append(df.format(values[i
                            ][0])).append("    ");
75                  }
76
77                  JOptionPane.showMessageDialog(view.getComponent(), "All done.\n" + sb);
78                  view.redrawGraph(false, true);
79              }
80          }
81      }
```

Plugin for calculation of Randic's Index

Definition (Randics's Index)

...

Plugin for calculation of Randic's Index

Listing 6: Necessary import statements

```
1  package katz.plugin;
2
3  import java.util.List;
4  import java.awt.event.ActionEvent;
5  import javax.swing.JOptionPane;
6  import java.text.DecimalFormat;
7
8  import cytoscape.plugin.CytoscapePlugin;
9  import cytoscape.util.CytoscapeAction;
10 import cytoscape.Cytoscape;
11 import cytoscape.CyNetwork;
12 import cytoscape.CyEdge;
13 import cytoscape.view.CyNetworkView;
14
15 import Jama.Matrix;
```

Plugin for calculation of Randic's Index

Listing 7: Basic class definition

```
16 public class RandicPlugin extends CytoscapePlugin {
17
18     public RandicPlugin() {
19         RandicPlugin.MolbiPluginAction action = new RandicPlugin.MolbiPluginAction();
20         action.setPreferredMenu("Plugins.Molbi");
21         Cytoscape.getDesktop().getCyMenus().addAction(action);
22     }
23
24     public String describe() {
25         return  "Plugin to calculate the Index of Randic for networks";
26     }
27
28     public class MolbiPluginAction extends CytoscapeAction {
29
30         public MolbiPluginAction() {
31             super("Randic's Index");
32         }
33
34         @Override
35         public void actionPerformed(ActionEvent ae) {
36             run();
37         }
```

Plugin for calculation of Randic's Index

Listing 8: Run method

```
38          private void run() {
39              CyNetwork network = Cytoscape.getCurrentNetwork();
40              CyNetworkView view = Cytoscape.getCurrentNetworkView();
41              int N = network.getNodeCount();
42
43              if (N == 0) {
44                  JOptionPane.showMessageDialog(view.getComponent(), "No network/view
                        loaded.");
45                  return;
46              }
47
48              Double IRandic = 0.0;
49              for (CyNode node : (List<CyNode>) network.nodesList())
50                  // otherwise Randic's Index will be +infinity!
51                  if (network.getDegree(node) != 0)
52                    IRandic += Math.pow(network.getDegree(node), -0.5);
53
54              JOptionPane.showMessageDialog(view.getComponent(), "All done.\nRandic
                     Index " + IRandic);
55              view.redrawGraph(false, true);
56          }
57      }
58  }
```

Outline

Results - Centralities

- determine the relative importance of a vertex within a graph
- centraltity concepts were first developed in social network analysis

  –> e.g. how influential a person is within a social network

Definition (Four measures of centrality)

1. degree centrality
2. eccentricity centrality
3. closeness centrality
4. betweeness centrality

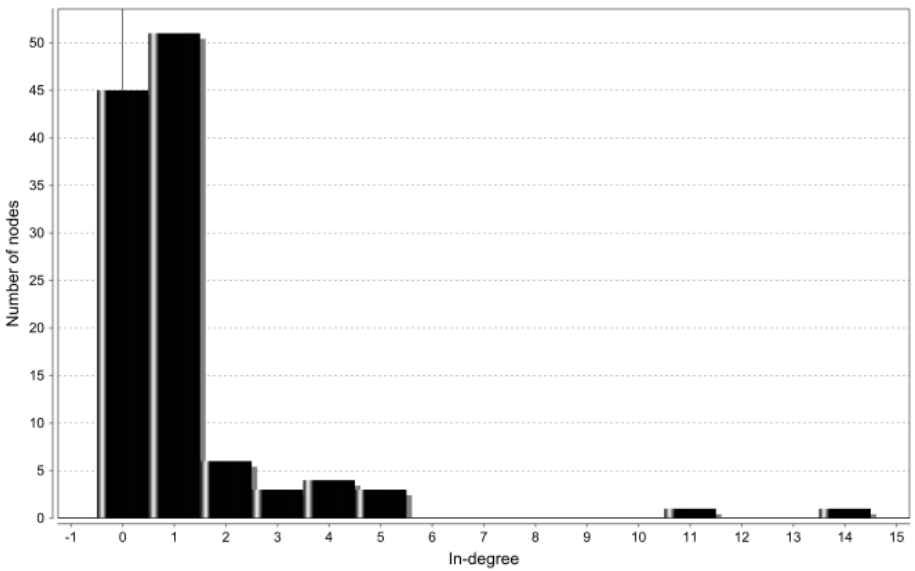
Results - Degree Centrality

Definition (Degree Centrality)

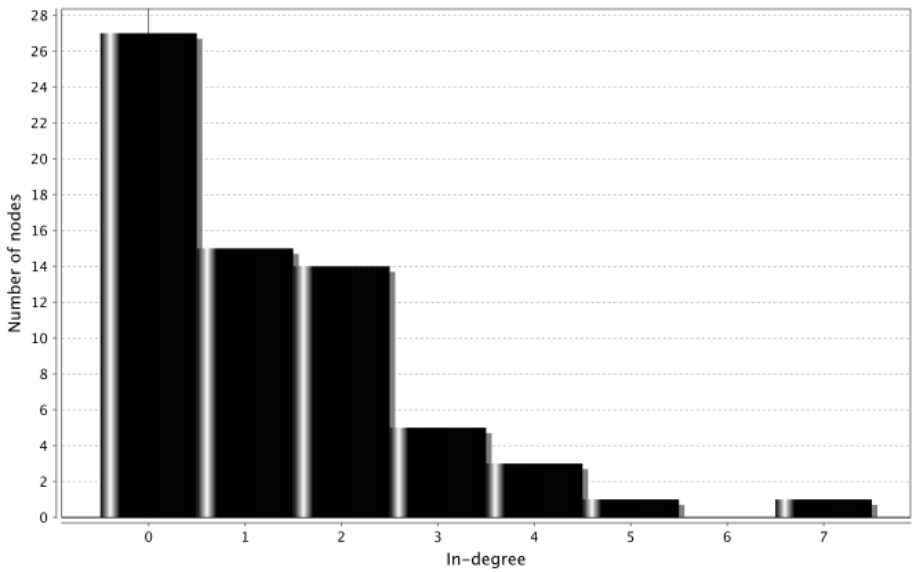
$C_{deg}(v) = \{e | e \in E \text{ and } v \in e\}$

- counts the number of edges attached to a vertex
- a local centrality measure
  -> only direct neighborhood considered
- directed graphs:
  -> indegree (interpreted as "popularity")
  -> outdegree (interpreted as "gregariousness")

Results - Degree Centrality



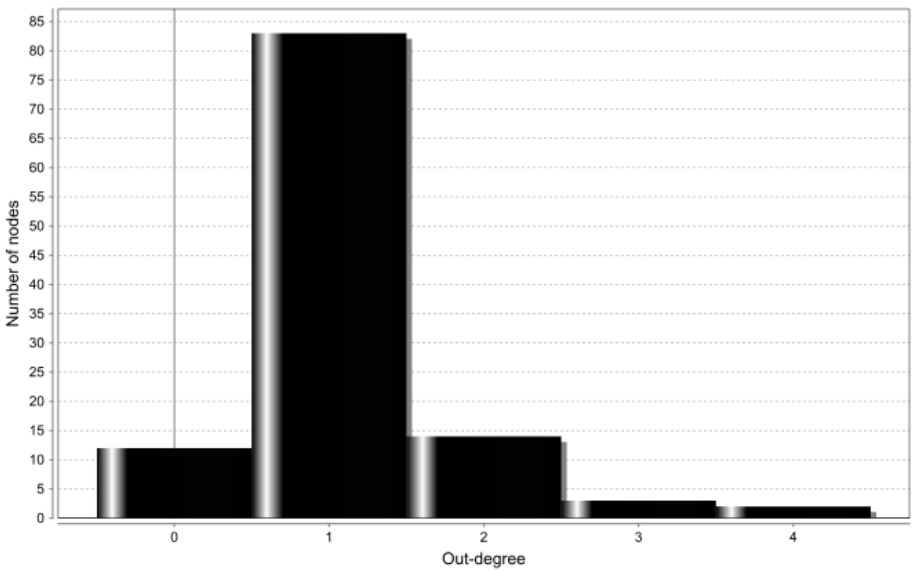
(a) Glyco1



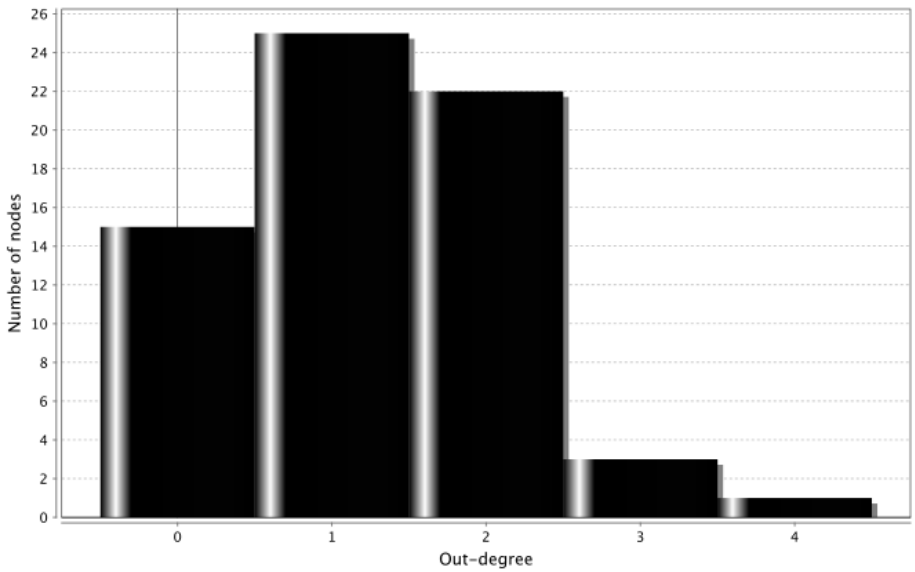
(b) Glyco2

Fig. 1: Indegree Centrality

Results - Degree Centrality



(a) Glyco1



(b) Glyco2

Fig. 2: Outdegree Centrality

Results - Eccentricity Centrality

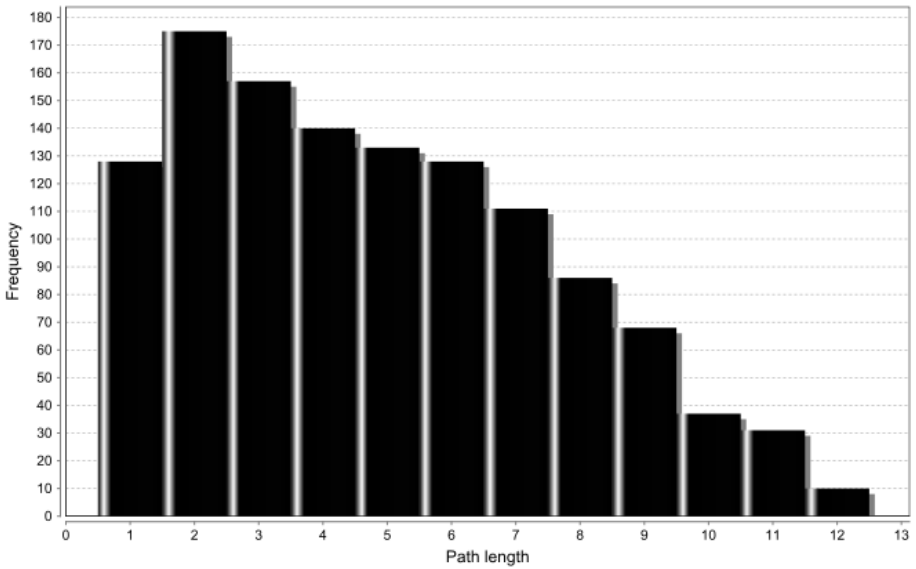
Definition (Eccentricity Centrality)

$$C_{ecc}(s) = \frac{1}{max\{d_{st} | t \in V\}}$$

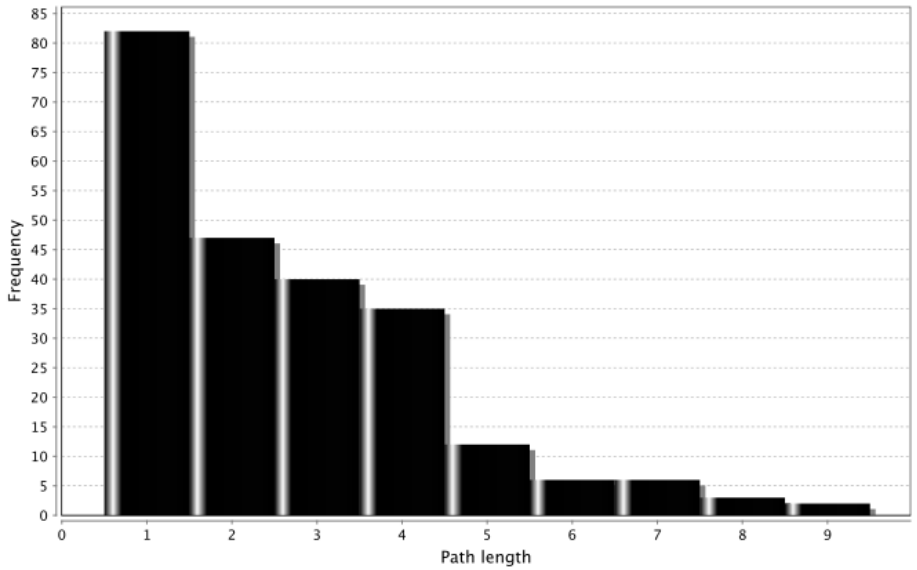
- determine the maximum distance between every two vertices
- central vertices get low values
- centralities require high centrality values

  –> reciprocal is used as centrality value
- only for CONNECTED networks

Results - Eccentricity Centrality



(a) Glyco1



(b) Glyco2

Fig. 3: Eccentricity Centrality

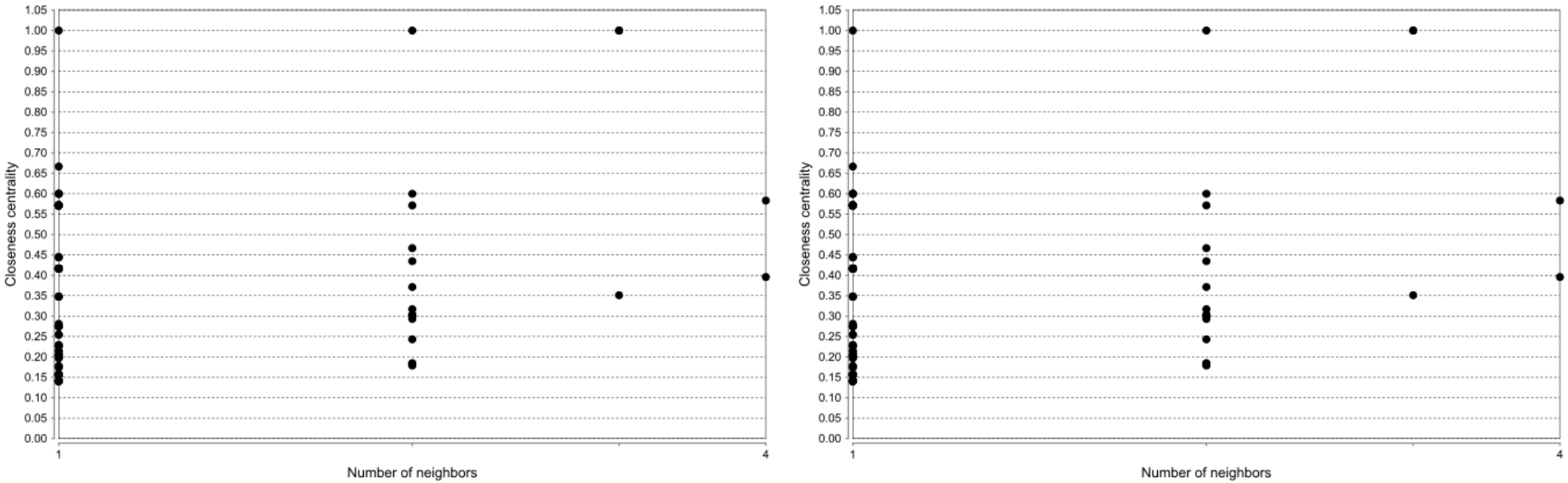
Results - Closeness Centrality

Definition (Closeness Centrality)

$$C_{clo}(s) = \frac{1}{\sum_{t \in V} d_{st}}$$

- C_{clo} of a vertex s is the sum of shortest path form s to all other vertices
- degree of interaction in the network
- the closer a point is to all the rest, the more effective and independent he can reach them

Results - Closeness Centrality



(a) Glyco1

(b) Glyco2

Fig. 4: Closeness Centrality

Results - Betweenness Centrality

Definition (Betweenness Centrality)

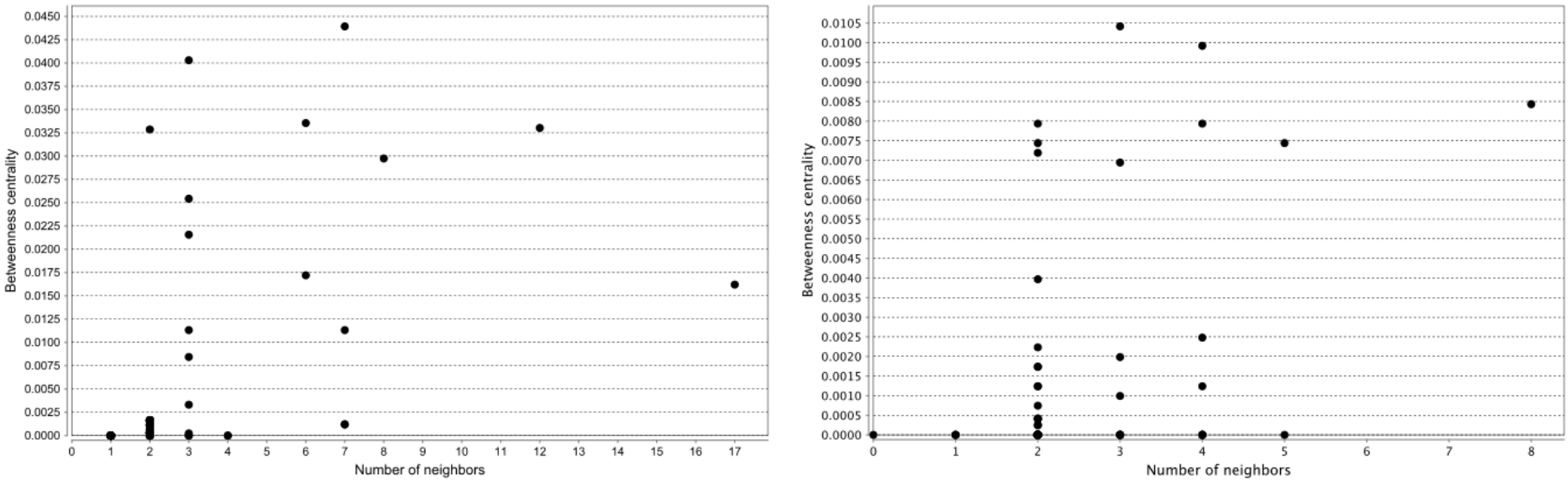
$$C_{spb}(v) = \sum_{s \in V \text{ and } s \neq v} \sum_{t \in V \text{ and } s \neq v} \delta_{st}(v)$$

- center of attention: indirect relationships

  $->$ Control of interaction

- v is the more powerful the more shortest paths between other vertices it can interrupt

Results - Betweenness Centrality



(a) Glyco1

(b) Glyco2

Fig. 5: Closeness Centrality

Outline

Conclusion

Benefits of cytoscape

...

Outline

Resources

Git repository

git://gitorious.org/cytoscape-plugins/cytoscape-plugins.git