Network analysis with Cytoscape

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in lecture on systems bioinformatics

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Outline

Outline

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  }
```

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

```java
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 lRandic = 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                    lRandic += Math.pow(network.getDegree(node), -0.5);
53
54            JOptionPane.showMessageDialog(view.getComponent(), "All done.\nRandic
                    Index " + lRandic);
55            view.redrawGraph(false, true);
56        }
57    }
58 }
```
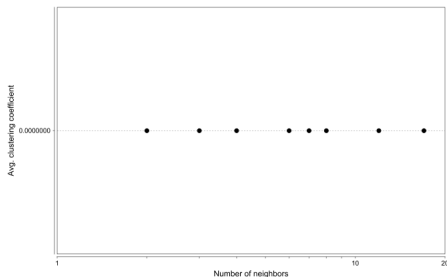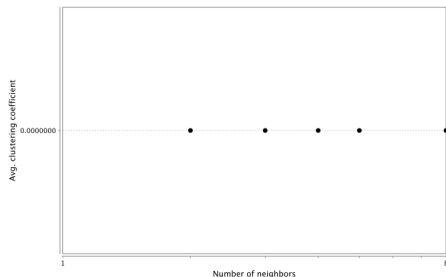
Outline

Results I
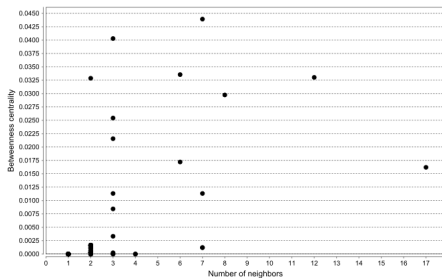
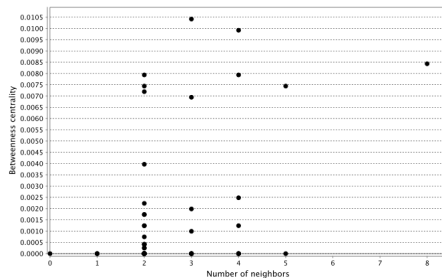...give example results from network 1 and network2

(a) Glyco1

(b) Glyco2

Fig. 1: Avgerage Clustering Coefficient Centrality

(a) Glyco1

(b) Glyco2

Fig. 2: Betweeness Centrality

Results . . .

. . . more results . . .

Differences

To other groups

. . .

Problems

To other groups
...

Outline

Conclusion

Benefits of cytoscape
...

Outline

Resources

Git repository

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