ComponentGrapher User Guide

February 2019 / version 1.11

Table of contents

[Table of contents 3](#_Toc513496463)

[1. Pre-requisites 4](#_Toc513496464)

[2. Quickstart 4](#_Toc513496465)

[2.1 Input files 5](#_Toc513496466)

[2.2 Command-line and options 6](#_Toc513496467)

[2.3 Output files 8](#_Toc513496468)

[2.3.1 Network files (\_complete.txt, \_1.txt, \_2.txt, \_3.txt, \_4.txt) 10](#_Toc513496469)

[2.3.2 Node identification (\_id.txt) 10](#_Toc513496470)

[2.3.3 Summary files 10](#_Toc513496471)

[2.3.4 Triplets file (triplets.txt) 14](#_Toc513496472)

[2.3.5 Graphml files (\_graphml.txt) 14](#_Toc513496473)

[3. Miscellaneous 15](#_Toc513496474)

[3.1 External node annotation file 15](#_Toc513496475)

[3.2 Compiling the source code 16](#_Toc513496476)

[4. References 17](#_Toc513496477)

[5. Abbreviations and mathematical formulas 18](#_Toc513496478)

ComponentGrapher is a multi-platform java program which eases the creation of character-states networks from character matrices in NEXUS or PHYLIP format. This command-line tool also allows the characterization of the resulting networks by searching for global and local articulation points, the numbers of complexes (connect components), betweenness, and other network related statistics. The software and its source code are provided at https://github.com/etiennelord/ComponentGrapher using a GPL3 license. This work was developed as a collaboration between the Université de Montréal (UdeM), Université du Québec à Montréal (UQAM) and Sorbonne Université, Université Pierre et Marie Curie, UPMC Paris 6.

# 1. Pre-requisites

The software ComponentGrapher is implemented as a multi-platform java program. It requires Java SE8 (JDK 8) or later versions of Java. For large matrices (>1000 characters), a fair amount of RAM is required, and should be specified before launching the tool. The *results*, if no output option is specified, will be found in the **results directory**.

**Example for large matrices with allocation of 6 gb of memory [-Xmx6g]:**

java -Xmx6g -jar ComponentGrapher.jar sample/matrix.txt

# 2. Quickstart

The ComponentGrapher software is to be run as a **command-line utility.** Given an input matrix (section 2.1), the software ComponentGrapher will generate character state networks *i.e.* for each state (e.g. 0,1) of a character, a new node is created (see also table 1 - section 2.3). The created edges will then reflect some characteristics between the character-state nodes (see also table 2 - section 2.3). For example, given a matrix with one character (C*har.1*) and two states (0,1), this will result in 2 nodes (character state):

i 0

Taxa **m,n,o**

1|1

j 0

k 0

l 0

Taxa i,j,k,l,p

1|0

**m** 1

**n** 1

**o** 1

p 0

*Note*: refer to the published paper for more information and section 2.3.

The edges represent the link between pair of nodes. For example, four types of edges can exist if we add another character to this matrix.

*Note*: the **complete network** is then composed of the link of types 1, 2 and 3.

### 2.1 Input files

The software requires as input either a character matrix either in Phylip format [1] or a character matrix in NEXUS format [2] with **only one** morphological MATRIX tag.

Phylip format (sample/Sample.phy) :

5 6

A 110110

B 110000

C 100110

D 001001

E 001110

Nexus format (sample/Sample.nex):

#NEXUS

[Note: this is a sample matrix]

begin data;

dimensions ntax=5;

dimensions nchar=6;

format datatype=standard gap=- missing=? Interleave=no;

MATRIX

A 110110

B 110000

C 100100

D 001001

E 001110

;

end;

\*Note that multiple states at one position in the matrix are supported (*e.g.* {0,1}, (0 1), (0,1,2,3) ) as well as interleaves for the NEXUS format. Also note that **undefined states symbol** (*e.g.* ?, -, \*) **are not processed in this version**. For the NEXUS format, column and specific states information can be specified using the CHARSTATELABELS, STATELABELS or CHARLABELS annotation specific to NEXUS format [2].

Nexus format (Sample matrix with multiple states and annotations):

#NEXUS

[Note: this is a sample matrix]

begin data;

dimensions ntax=5;

dimensions nchar=6;

format datatype=standard gap=- missing=? Interleave=no;

CHARSTATELABELS

1 Mouth / present, absent, 2 'eyes'/ two, eight, 3 hands / two,

'more than 2', 4 hairs / present, absent, 5 'eye color' / blue,

brown, 6 nose / red, normal

;

MATRIX

A 110110

B 1{0,1}0000

C 100100

D 00100{0,1}

E 001110

;

end;

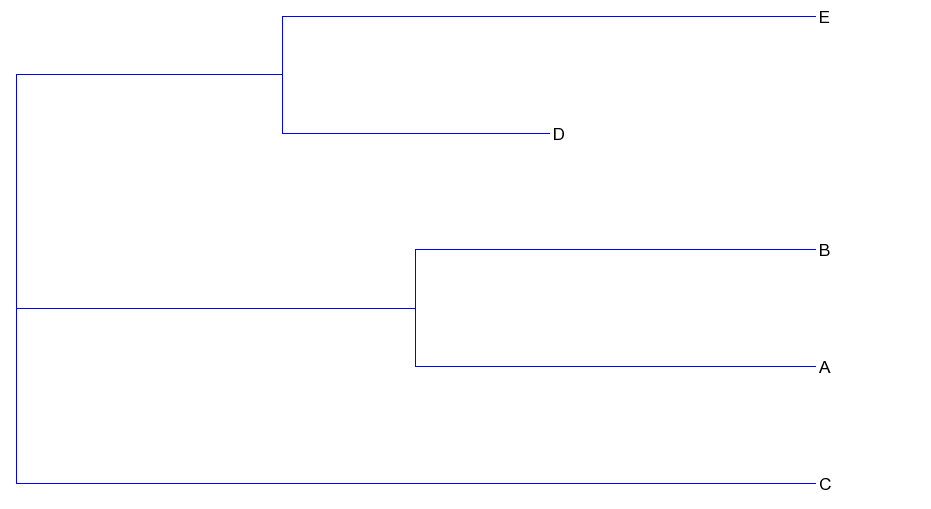
Note: Phylogenetic trees in nexus datasets are not currently supported if phylogenetic permutations are performed (*see below*).

If phylogenetic permutations [-tree] are performed, a tree in the newick format is required.

Newick format (sample/Sample\_tree.newick):

((A:1.5,B:1.5):1.5,C:3.0,(D:1.0,E:2.0):1.0);

Visualisation of this phylogenetic tree using the trex webserver (**http://www.trex.uqam.ca**)



### 2.2 Command-line and options

**Base command-line**

java -jar ComponentGrapher.jar matrixfile

java -jar ComponentGrapher.jar matrixfile -tree=treefile

**Command-line options**

**-tree=file.newick**

Specify the phylogenetic tree in newick format used for the character permutations.

**-perm=100**

Specify the number of permutations to perform.

Important note: ff no permutation is specified, the default number of permutation is defined as the total number of possible nodes divided by 0.05 (i.e. the *p*-value significance limit).

**-permmode=0**

0 : Equiprobable permutation (default option). This results in a random permutation in the state in each columns.

1 : Probabilistic permutation. This result in a permutation of the states in each column proportional to the number of each character found in this column.

2 : Phylogeny (default if -tree option is used). Perform the phylogenetic permutation defined in the article of *Lapointe and Garland (2001)* [4].

3 : Equiprobable of undefined states. Perform the equiprobable permutation but only change the

undefined states in the matrix.

4 : Probabilistic of undefined states. Perform the probabilistic permutation but only change the

undefined states in the matrix.

Important: Please specify a random seed using the **-seed** option for better randomness.

**-k=2.0**

Specify the *PhyloPermute* *k* parameter. See the article of Lapointe and Garland(2001) [4].

The default value is 2.0.

**-filter=…,…**

Filter some nodes from the created networks based on the “*state*” of those nodes. For example, ones might want to remove from the created networks all the nodes containing the state: **absent** indicating that only the present states should be considered. A list separated with commas can be given.

For example, the option -filter=absent,not\_present,? will remove all nodes with absent, not\_present or ? states.

**-threads=10**

Specify the number of concurrent threads to be used during the computation. Defaults is 2.

**-edges=0**

Specify edge's inference mode

0 : Treat all edges (default)

1 : Absolute Majority

2 : Majority Rule

>10 : Minimum percent to consider the edge

**-undefined**

Remove columns containing undefined states (e.g.?,\*)

**-multiple**

Remove columns containing multiple states (e.g.[1,2}).

**-bipartite**

Specify that we want to output bipartite files.

**-graphml**

Specify the output of graphml files (Gephi[3] or Cytoscape[10] compatibles, see section 2.3.5).

**-nodeid=file**

Provide a node identification file (see section 2.3.2).

**-output=dir**

Specify output directory. The default is ../results/[matrixfile].

**-triplets**

Specify to output the triplets file (triplets.txt, see section 2.3.4).

**-seed=42**

Specify the random seed for the random number generator.

**2.2.1 Base analysis with sample file**

java -jar ComponentGrapher.jar sample/Sample.phy

Results will be located in the [Base component-grapher directory]/results/Sample\_phy directory.

**2.2.2 Analysis without columns containing multiple states and with specified output file [-multiple, -output]**

java -jar ComponentGrapher.jar matrixfile -multiple -output=result

**2.2.3 Analysis with a phylogenetic permutations**

java -jar ComponentGrapher.jar sample/Sample.phy -tree=sample/Sample\_tree.newick

Important note: the supplied phylogenetic tree must be in newick format.

### 2.3 Output files

With a matrix as input, the ComponentGrapher software will generate five network files (Table 3 - below) for each evaluated matrix in either an *edge list* or *graphml* (Gephi [3] and Cytoscape [10] compatible) format, statistics files and a node identification file. In this analysis, each node corresponds to a character-state meaning that each state of a particular character, column in the matrix, will be present in the complete network.

For example, processing the Sample.phy will result in the following nodes (Table 1):

Command-line: java -jar ComponentGrapher.jar sample/Sample.phy

Sample.phy

5 6

A **1**10110

B **1**10000

C **1**00110

D **0**01001

E **0**01110

**Table 1. Generated nodes found in Sample.phy\_summary\_statistics.tsv1**

|  |  |  |  |
| --- | --- | --- | --- |
| **Node ID** | **Character-state** | **Character (column)** | **Associated taxa** |
| **0** | **char. 1|1** | **char. 1** | **A,B,C** |
| **1** | **char. 1|0** | **char. 1** | **D,E** |
| 2 | char. 2|1 | char. 2 | A,B |
| 3 | char. 2|0 | char. 2 | C,D,E |
| 4 | char. 3|0 | char. 3 | A,B,C |
| 5 | char. 3|1 | char. 3 | D,E |
| 6 | char. 4|1 | char. 4 | A,C,E |
| 7 | char. 4|0 | char. 4 | B,D |
| 8 | char. 5|1 | char. 5 | A,C,E |
| 9 | char. 5|0 | char. 5 | B,D |
| 10 | char. 6|0 | char. 6 | A,B,C,E |
| 11 | char. 6|1 | char. 6 | D |

1In bold, the nodes created for the first state column.

The different files generated correspond to the types of edges (1, 2, 3, or 4) found between each nodes (Table 2).

**Table 2. Type of links (*see first section for details*)**

|  |  |  |  |
| --- | --- | --- | --- |
| **Edge type** | **Directed**  **/Undirected** | **Link types** | **Meaning** |
| 1 | Undirected | Co-existence /  identical | Same taxa found in both nodes |
| 2 | Directed | Inclusion | One group of taxa is included in the other group of taxa |
| 3 | Undirected | Overlap | Overlap between the group of taxa in each node |
| 4\* | Undirected | Disjoint | No overlap between the group of taxa for both nodes |

\*Note: the disjoint edges (type 4) are not included in the *complete network*.

The generated files for a matrix file **without multiple states** (*e.g.* more than one possible state per position in the matrix) are shown in Table 3.

**Table 3. Generated networks, node identification and statistics files for a matrix without multiple states.**

|  |  |
| --- | --- |
| **Generated files** | **Content** |
| Filename\_summary.txt1 | Screen output of the simulation (log) |
| Filename\_complete.txt | Edge types: 1,2,3 (complete network/section 2.3.1) |
| Filename\_1.txt | Edge types: 1 (network/section 2.3.1) |
| Filename\_2.txt | Edge types: 2 (network/section 2.3.1) |
| Filename\_3.txt | Edge types: 3 (network/section 2.3.1) |
| Filename\_4.txt | Edge types: 4 (network/section 2.3.1) |
| Filename\_id.txt | Node identification file for the resulting networks (section 2.3.2) |
| Filename\_network\_statistics.tsv | Final results for the computed network (section 2.3.3) |
| Filename\_nodes\_statistics.tsv | Final results of the computed network nodes |
| Filename\_summary\_statistics.tsv | Other statistics for the generated networks (table 5) |
|  | **Note: for the generated files, see section 5 for the abbreviations used.** |
| **Other generated files** | |
| *Randomization\_\*.json* | *Internal serialization of the network and statistics during simulation* |
| *Replicate\_matrix\_\*.txt* | *The permutated matrices used for the permutation* |
| *Replicate\_matrix\_\*\_charstates.txt* | *The nodes identification for the replicated matrices* |

**1Filename refers to the original matrix *e.g.* Sample.phy\_summary.txt**

### 2.3.1 Network files (\_complete.txt, \_1.txt, \_2.txt, \_3.txt, \_4.txt)

The result edge list files are zero-based *tab-separated value* (.tsv) files. Each line corresponds to one edge with a source id (src\_id), destination id (dest\_id), the edge type and the number of common taxa between each node:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Source  node ID | Destination  node ID | Type of edge | Number of common taxa | Percent of common taxa |

#src\_id(tab)dest\_id(tab)edge\_type(tab)number\_common\_taxa(tab) percent

2 0 2 2 1.0

0 3 3 1 0.5

0 4 1 3 1.0

0 6 3 2 0.75

...

\*Note: that there is no fourth and fifth columns (Number of common taxa, percent of common taxa) for the type 4 network.

### 2.3.2 Node identification (\_id.txt)

The result node identification file (*tab-separated values*) contains information about each node in the networks.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Node ID | Name | Char.  Label | State  label | Encoded  State | Edge  count | In  edge  count | Out  edge  count | Number of taxa | Taxa |

0 char.1|1 char.1 1 1 8 1 7 3 A,B,C

1 char.1|0 char.1 0 0 8 1 7 2 D,E

...

### 2.3.3 Summary file (.summary.txt, summary\_statistics.tsv, network\_statistics.tsv and nodes\_statistics.tsv)

The software will compute some statistics for each resulting networks and save them in the **results** **directory**. During operation, the software will also output some statistics (*see below*). Additionally, statistic files are generated for each network. The file ending with "*\_summary.txt*" contains the command-line arguments for this particular run and the screen output, as well as some results such as the number of edges in each network, the number of total nodes and other network statistics (Table 5). The network and nodes statistic files are also available separately in the file "\_*network\_statistics.tsv*" and "*\_nodes\_statistics.tsv*". Finally, a *"\_summary\_statistics.tsv*" is also available and contains some node-specific informations (*see below*).

**Default screen output when executing the software. This output is also found in the \_summary.txt file.**

COMPONENT-GRAPHER v1.0.11

Etienne Lord, Jananan Pathmanathan, Vladimir Makarenkov,

François-Joseph Lapointe, Éric Bapteste

=============================== PARAMETERS ====================================

Command line options : sample/sample.phy -perm=10 -graphml -triplets

Input : sample/sample.phy

Output directory : results/sample\_phy

N taxa : 5 (rows)

N characters : 6 (columns)

Total number of multistate characters: 0

Total number of possible variations\* : 1

Total variations tested : 1

Permutations statistics : 10

Suggested permutations\*\* : 240

Remove multiple state columns : false

Remove undefined columns : false

Total column : 6

Total undefined column(s) : 0

Total multiple column(s) : 0

Total treated column : 6

Total undefined char : 0

Total multiple char : 0

Total possible nodes : 12

Edges selection mode : treat all edges (default)

Permutations mode : equiprobable (default)

Seed : 1001

PhyloPermute k : 2.0

Number of threads : 2

===============================================================================

\* Indicate the number of state variation for polymorphic characters.

\*\* Indicate the minimum number of permutations for significant p-values.

===============================================================================

Total permutations (N replicate) : 0

Total time : 949ms

===============================================================================

Trying to allocate memory for 66 possible edges.

===============================================================================

Current iteration : 1/1

States variations :

(saving to: results/sample\_phy/sample.phy\_\_complete.txt)

===============================================================================

6 / 66 ( 0ms )

12 / 66 ( 5ms )

18 / 66 ( 9ms )

24 / 66 ( 13ms )

30 / 66 ( 17ms )

36 / 66 ( 21ms )

42 / 66 ( 24ms )

48 / 66 ( 28ms )

54 / 66 ( 32ms )

60 / 66 ( 35ms )

66 / 66 ( 39ms )

===============================================================================

Computing statistics:

===============================================================================

(50%) Creating and analyzing intermediate networks ( 11ms ).

(60%) Shortest paths complete network ( 11ms ).

(80%) Shortest paths type 3 network ( 12ms ).

(100%) Done statistics ( 33ms ).

===============================================================================

===============================================================================================

Network statistics (See manual for descriptions)

===============================================================================================

Statistics Ref p-value sign. N Mean STD Min Max 5% 95%

CC\_type1 4.0 0.182 10 1.8 1.135 0.0 4.0 0.0 4.0

CC\_type3 1.0 1.0 10 1.0 0.0 1.0 1.0 1.0 1.0

CC\_complete 1.0 1.0 10 1.0 0.0 1.0 1.0 1.0 1.0

total\_ap\_compl. 0.0 1.0 10 0.0 0.0 0.0 0.0 0.0 0.0

n\_edge\_type1 4.0 0.182 10 1.8 1.135 0.0 4.0 0.0 4.0

n\_edge\_type2 14.0 0.364 10 16.6 3.534 12.0 22.0 12.0 22.0

n\_edge\_type3 31.0 0.545 10 31.5 6.276 19.0 38.0 19.0 38.0

n\_edge\_type4 11.0 0.545 10 10.1 2.331 8.0 15.0 8.0 15.0

n\_edge\_compl. 49.0 0.545 10 49.9 2.331 45.0 52.0 45.0 52.0

total\_ap\_type3 0.0 1.0 10 0.0 0.0 0.0 0.0 0.0 0.0

local\_ap\_type3 7.0 0.091 10 2.5 2.273 0.0 6.0 0.0 6.0

local\_ap\_compl. 0.0 1.0 10 0.0 0.0 0.0 0.0 0.0 0.0

triplet\_type3 107.0 0.091 10 77.8 16.369 39.0 93.0 39.0 93.0

convergence 0.6944 0.364 10 0.623 0.085 0.471 0.72 0.471 0.72

loop4\_type3 84.3333 0.545 10 101.267 53.835 23.667 166.333 23.667 166.333

len4\_type3 84.3333 0.545 10 101.267 53.835 23.667 166.333 23.667 166.333

den\_complete 0.7424 0.545 10 0.756 0.035 0.682 0.788 0.682 0.788

density\_type1 0.1429 0.364 10 0.248 0.143 0.0 0.333 0.0 0.333

density\_type2 0.2121 0.364 10 0.252 0.054 0.182 0.333 0.182 0.333

density\_type3 0.5636 0.545 10 0.591 0.084 0.473 0.691 0.473 0.691

density\_type4 0.2444 0.455 10 0.282 0.057 0.222 0.393 0.222 0.393

triangle\_type3 14.0 0.182 10 30.8 13.653 10.0 46.0 10.0 46.0

prop\_triangle 0.0848 0.091 10 0.193 0.075 0.097 0.279 0.097 0.279

triplet\_typeA 107.0 0.091 10 77.8 16.369 39.0 93.0 39.0 93.0

triplet\_typeB 23.0 0.091 10 7.8 4.894 0.0 13.0 0.0 13.0

triplet\_typeC 32.0 0.455 10 34.2 8.967 16.0 50.0 16.0 50.0

triplet\_typeD 28.0 0.091 10 12.6 4.427 4.0 18.0 4.0 18.0

triangle 42.0 0.182 10 92.4 40.959 30.0 138.0 30.0 138.0

time/net. (ms) 12.0 0.091 10 3.0 0.943 2.0 5.0 2.0 5.0

\* Some statistic are not available for each permutations, resulting in smaller sample size (N).

===============================================================================================

Nodes statistics

===============================================================================================

-----------------------------------------------------------------------------------------------

NodeID 0 Char. 1|0

Statistics Ref p-value Sign. N Mean STD Min Max 5% 95%

-----------------------------------------------------------------------------------------------

in\_degree2 1.0 0.091 10 0.3 0.483 0.0 1.0 0.0 1.0

out\_degree2 1.0 0.727 10 2.0 1.155 0.0 4.0 0.0 4.0

in\_degree3 5.0 0.545 10 4.7 2.541 0.0 9.0 0.0 9.0

in\_degree1 1.0 0.091 10 0.5 0.527 0.0 1.0 0.0 1.0

closeness\_type3 0.0667 0.909 10 0.062 0.024 0.0 0.091 0.0 0.091

between\_type3' 1.6429 0.273 10 1.803 3.201 0.0 10.7 0.0 10.7

%triplet type3 7.48 0.364 10 7.414 8.924 0.0 31.17 0.0 31.17

triplet\_typeA 8.0 0.273 10 6.1 6.919 0.0 24.0 0.0 24.0

triplet\_typeB 2.0 0.091 10 0.4 0.843 0.0 2.0 0.0 2.0

triplet\_typeC 2.0 0.273 10 2.3 3.653 0.0 12.0 0.0 12.0

triplet\_typeD 2.0 0.182 10 1.2 1.874 0.0 6.0 0.0 6.0

triangle 2.0 0.727 10 5.5 4.17 0.0 12.0 0.0 12.0

-----------------------------------------------------------------------------------------------

NodeID 1 Char. 1|1

Statistics Ref p-value Sign. N Mean STD Min Max 5% 95%

-----------------------------------------------------------------------------------------------

…

**Table 5. The network and node statistics files: [Filename]\_network\_statistics.tsv and [Filename]\_nodes\_statistics.tsv display the following information:**

|  |  |
| --- | --- |
| **Columns** | **Descriptions** |
| **A** | Statistics (refer to section 5 for descriptions) |
| **B** | Reference value. The value associated with the computed original network. |
| **C** | The calculated p-value |
| **D** | Significance of the *p*-value. This indicate if the *p*-value should be considered significant. If no star (\*) is present, the value should not be considered statistically different. Legend:  \* *p* < 0.05  \*\* *p* < 0.01  \*\*\* *p* < 0.001 |
| **E** | Number of permutation performed. |
| **F** | Minimum value found in the permutated dataset. |
| **G** | Maximum value found in the permutated dataset. |
| **H** | Mean value found in the permutated dataset. |
| **I** | Standard deviation found in the permutated dataset. |
| **J** | 5% percentile value found in the permutated dataset. |
| **K** | 95% percentile value found in the permutated dataset. |

Example:

**Columns: A B C D E F G H I J K**

Statistics Ref. p-value sign. N Mean STD Min Max 5% 95%

================================================================================================================

CC\_type1 4.0 0.12 \* 30 1.46 1.27 0.0 4.0 0.0 4.0

CC\_type3 1.0 1.0 30 1.0 0.0 1.0 1.0 1.0 1.0

CC\_complete 1.0 1.0 30 1.0 0.0 1.0 1.0 1.0 1.0

total\_ap\_compl. 0.0 1.0 30 0.0 0.0 0.0 0.0 0.0 0.0

…

**Note: *p-*values are not calculated if the reference value is either absent (NA) or equal to zero.**

**The file [Filename]\_summary\_statistics.tsv contains 21 fields in the following order:**

|  |  |
| --- | --- |
| Column | Descriptions |
| Nodeid | Node numbering (zero-based) |
| Name | Node name |
| Found in type 1 network | Node is found in type 1 network  (Presence indicate by a x) |
| Found in type 2 network | Node is found in type 2 network  (Presence indicate by a x) |
| Found in type 3 network | Node is found in type 3 network  (Presence indicate by a x) |
| Found in complete network | Node is found in complete network  (Presence indicate by a x) |
| Column | Column in the matrix (starting at index 1) |
| Encoded state | Encoded state in the matrix (*e.g.* 0,1) |
| Character | If provided in the matrix, the full description of this character and its associated state (e.g. red nose | present) |
| Connected component type 1 network | The connected component associated with this node in the type 1 network |
| Connected component complete network | The connected component associated with this node in the complete network |
| Local articulation point type 3 network | In the type 3 network, is this node a local articulation point? If present, indicated as a x. |
| Global articulation point type 3 network | In the type 3 network, is this node a global articulation point? If present, indicated as a x. |
| Local articulation point in complete network | In the complete network, is this node a local articulation point? If present, indicated as a x. |
| Global articulation point in complete network | In the complete network, is this node a global articulation point? If present, indicated as a x. |
| Indegree type 2 network | This node "in" degree in the directed type 2 network. |
| Normalized indegree type 2 network | This node normalized "in" degree in the directed type 2 network. |
| Betweenness type 3 network | Betweenness centrality of node in type 3 network. |
| Closeness type 3 network | Closeness centrality of node in type 3 network |
| Numbers of triplet type 3 network | Number of triplets in the type 3 network containing this node. Here, triplet stands for a linear series of 3 nodes where the terminal nodes are unconnected. |
| Percent(%) triplet type 3 network | Percent of those triplets over the total number of triplets in the type 3 network. |

### 

### 2.3.4 Triplets file (triplets.txt)

If the [-triplets] option is selected, the software will compute the triplets and generate the file triplets.txt. In this file each line corresponds to one triplet with the first node (node 1), the second node which is in the middle of the triplet (central node), the third node (Nod**e** 3) and the triplet type (Table 6):

|  |  |  |  |
| --- | --- | --- | --- |
| Node 1 | Central node | Node 3 | Type |

7 0 6 Type A

8 0 6 Type A

8 0 6 Type B

8 0 7 Type A

9 0 6 Type A

…

**Table 6: The different types of identified triplets are described in the following table.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Triplet type A** | **Triplet type B** | **Triplet type C** | **Triplet type D** | **Triplet type E** |
|  |  |  |  |  |
| Nodes *i* and *j* are not connected. Central node *n* is linked with type 3 edges. | Nodes *i* and *j* are connected by a type 1 edge. Central node *n* is linked with type 3 edges | Nodes *i* and *j* are connected by a type 2 edge. Central node *n* is linked with type 3 edges | Nodes *i* and *j* are connected by a type 4 edge. Central node *n* is linked with type 3 edges | Nodes *i* and *j* are connected by a type 4 edge. Central node *n* is linked with type 3 edges (e.g. it forms a *triangle*) |

### 2.3.5 Graphml files (\_graphml.txt)

If the [-graphml] option is selected, the software will generate a graphml file for each network and compatible with Gephi and Cytoscape, e.g. sample.phy\_\_1.graphml (network type 1) :

<?xml version='1.0' encoding='UTF-8' standalone='no'?>

<graphml>

<key id='k2' for='edge' attr.name='type' attr.type='double'/>

<key id='k1' for='edge' attr.name='total\_shared\_taxa' attr.type='double'/>

<key id='k3' for='node' attr.name='fullname' attr.type='string'/>

<key id='k4' for='node' attr.name='number\_of\_taxa' attr.type='double'/>

<key id='k5' for='node' attr.name='partition' attr.type='string'/>

<key id='k6' for='node' attr.name='total\_edges' attr.type='double'/>

<key id='k61' for='node' attr.name='in\_edges' attr.type='double'/>

<key id='k62' for='node' attr.name='out\_edges' attr.type='double'/>

<key id='k7' for='node' attr.name='associated\_character\_column' attr.type='double'/>

<key id='k8' for='node' attr.name='charlabel' attr.type='string'/>

<key id='k9' for='node' attr.name='statelabel' attr.type='string'/>

<key id='k10' for='node' attr.name='statematrix' attr.type='string'/>

<key id='k11' for='node' attr.name='total\_taxa' attr.type='double'/>

<key id='k12' for='node' attr.name='taxa\_id' attr.type='string'/>

<graph edgedefault='undirected' id=''>

...

</graph>

</graphml>

# 3. Miscellaneous

## 3.1 External node annotation file

If needed, you can supply a list of character-state annotation if none is provided in the NEXUS matrix or if you use a Phylip matrix file. To do so, include a list of node character-states with the [-nodeid=] option.

**Example command-line with the sample.phy matrix**

java -jar COMPONENTGRAPHER.jar sample/Sample.phy -nodeid=sample/Sample\_nodeid.txt

This file should be a *tab-separated value* with four columns: column number (character position starting at 1), encoded state, new character label, new state label:

|  |  |  |  |
| --- | --- | --- | --- |
| Column | State | Character label | State label |

Sample\_nodeid.txt

|  |  |  |  |
| --- | --- | --- | --- |
| 1 | 0 | Mouth opening orientation | Terminal |
| 1 | 1 | Mouth opening orientation | Ventral |
| 2 | 0 | Pre-oral chamber | Absent |
| 2 | 1 | Pre-oral chamber | Present |
| 3 | 0 | Radially arranged circumoral structures | Absent |
| 3 | 1 | Radially arranged circumoral structures | Present |
| 4 | 0 | Differentiated circumoral structures | undifferentiated plates |
| 4 | 1 | Differentiated circumoral structures | three or four enlarged plates |
| 5 | 0 | Pharynx differentiated from midgut | not differentiated |
| 5 | 1 | Pharynx differentiated from midgut | differentiated |
| 6 | 0 | Pharynx reversible | permanently inverted |
| 6 | 1 | Pharynx reversible | completely reversible |

These annotations will be reflected in the **node identification file** (\_id.txt) and in the **summary file** (\_summary.txt) as well as in the general screen output:

**Without the nodeid file**

-----------------------------------------------------------------------------------------NodeID 0 Char. 1|0

Statistics Ref p-value Sign. N Mean STD Min Max 5% 95%

-----------------------------------------------------------------------------------------

**With the nodeid file**

-----------------------------------------------------------------------------------------NodeID 0 **Mouth opening orientation|terminal**

Statistics Ref p-value Sign. N Mean STD Min Max 5% 95%

-----------------------------------------------------------------------------------------

## 3.2 Compiling the source code

The java source code provided is a **Netbeans** **project** (https://netbeans.org). To compile the source code, download the Netbeans IDE, open the project file and build the project. The required libraries are listed below:

**SSJ(https://github.com/umontreal-simul/ssj)**

The SSJ library is used for BitVector calculations and for computing random uniform distribution. The`ssj.jar` archive (version 3.2.0) is included in the COMPONENT-GRAPHER distribution and it must be in the CLASSPATH environment variable.

**Apache Commons Mathematics Library (http://commons.apache.org/proper/commons-math/)**

The Apache common mathematics library is used for distribution and *p*-value calculations. The `commons-math3-3.6.1.jar` archive is included in the COMPONENT-GRAPHER distribution and it must be in the CLASSPATH environment variable.

**Google gson (https://github.com/google/gson)**

The Google gson library is used for serialization/deserialization of the datasets. The `gson-2.6.2.jar` archive is included in the COMPONENT-GRAPHER distribution and it must be in the CLASSPATH environment variable.

**Forester.jar (https://sites.google.com/site/cmzmasek/home/software/forester)**

Forester is a collection of open source libraries for phylogenomics and evolutionary biology research created by Christian Zmasek. The `forester.jar` archive is included in the COMPONENT-GRAPHER distribution and it must be in the CLASSPATH environment variable.

# 4. References

[1] Felsenstein, J. 2005. PHYLIP (Phylogeny Inference Package) version 3.6. Distributed by the author. Department of Genome Sciences, University of Washington, Seattle.

[2] Maddison DR, Swofford DL, Maddison WP. 1997. NEXUS: an extensible file format for systematic information. Syst Biol. 46(4):590-621.

[3] Bastian M., Heymann S., Jacomy M. 2009. Gephi: an open source software for exploring and manipulating networks. International AAAI Conference on Weblogs and Social Media.

[4] Lapointe, F. J., & Garland Jr, T. 2001. A generalized permutation model for the analysis of cross-species data. Journal of Classification, 18(1), 109-127.

[5] Brandes, U. (2001). A faster algorithm for betweenness centrality. Journal of mathematical sociology, 25(2), 163-177.

[6] Brandes, U. (2008). On variants of shortest-path betweenness centrality and their generic computation. Social Networks, 30(2), 136-145.

[7] Sarıyüce, A. E., Kaya, K., Saule, E., & Catalyürek, U. V. (2013, October). Incremental algorithms for closeness centrality. In IEEE International Conference on BigData.

[8] Anthonisse, J. M. (1971). The rush in a directed graph. Stichting Mathematisch Centrum. Mathematische Besliskunde, (BN 9/71).

[9] Freeman, L. C. (1977). A set of measures of centrality based on betweenness. *Sociometry*, 35-41.

[10] Shannon, P., Markiel, A., Ozier, O., Baliga, N. S., Wang, J. T., Ramage, D. & Ideker, T. (2003). Cytoscape: a software environment for integrated models of biomolecular interaction networks. *Genome research*, *13*(11), 2498-2504.

[11] Cormen, T. H., Leiserson, C. E., Rivest, R. L., & Stein, C. (2009). Introduction to algorithms. MIT press.

[12] Schank, T, and Wagner, D. (2005) Finding, counting and listing all triangles in large graphs, an experimental study. International Workshop on Experimental and Efficient Algorithms. Springer Berlin Heidelberg, 2005.

# 5. Abbreviations and mathematical formulas

Some abbreviations can be found in the software outputs.

|  |  |
| --- | --- |
| **Abbreviations** | **Descriptions** |
| **N** | Number of permutations (replicates) |
| **%triplet type3** | Number of time (in percent) that this node is central in a triplet |
| **between\_type3** | Node betweenness centrality [5,8-9] in type3 network |
| **between\_type3'** | Betweenness centrality [5,8-9] of node (type 3 network) |
| **CC\_complete** | Number of complexes (complete network composed of type 1, 2, and 3 edges) |
| **CC\_type1** | Number of complexes (type 1 network) |
| **CC\_type3** | Number of complexes (type 3 network) |
| **closeness\_type3** | Closeness centrality [5,7] of node (type 3 network) |
| **den\_complete** | Network density1 (complete network composed of type 1, 2, and 3 edges) |
| **density\_type1** | Network density (type 1 network) |
| **density\_type2** | Network density (type 2 network) |
| **density\_type3** | Network density (type 3 network) |
| **density\_type4** | Network density (type 4 network) |
| **in\_degree1** | Degree of nodes (type 1 network, undirected) |
| **in\_degree2** | In-degree of nodes (type 2 network) |
| **in\_degree3** | Degree of nodes (type 3 network, undirected) |
| **loop4\_type3** | Total loop of length 4 (quad) in (type 3 network (undirected) |
| **len4\_type3** | Total paths of length 4 in (type 3 network (undirected) |
| **n\_edges\_complete** | Number of edges  (complete network composed of type 1, 2, and 3 edges) |
| **n\_edges\_type1** | Number of edges  (type 1 network) |
| **n\_edges\_type2** | Number of edges  (type 2 network) |
| **n\_edges\_type3** | Number of edges  (type 3 network) |
| **n\_edges\_type4** | Number of edges  (type 4 network) |
| **out\_degree2** | Out-degree of nodes (type 2 network) |
| **prop\_triangle** | Proportion of triangles (type 3 network, over the total number of possible triangles in a complete graph) |
| **sign.** | Significance of p-value from the permutation statistics and Bonferronicorrection for  multiple tests (\* p<0.05, \*\* p<0.01, \*\*\* p<0.001) |
| **time/net. (ms)** | Time to process a network (in milliseconds) |
| **total\_ap\_compl.** | Number of global articulation points (complete network composed of type 1, 2, and 3 edges) |
| **total\_ap\_type3** | Number of global articulation points (type 3 network) |
| **local\_ap\_compl.** | Number of local articulation points (complete network composed of type 1, 2, and 3 edges) |
| **local\_ap\_type3** | Number of local articulation points (type 3 network) |
| **triangle\_type3** | Number of triangles (type 3 network) |
| **triplet\_type3** | Number of non-transitive triplets (type 3 network) |
| **triplet\_typeA** | Number of triplets of type A. For a node n, the triplet is in the form  i -3- n -3- j  where i and j are other nodes connected to n with a type 3 edge and i and j are not connected) |
| **triplet\_typeB** | Number of triplets of type B. For a node n, the triplet is in the form  i -3- n -3- j  where i and j are other nodes connected to n with a type 3 edge and i and j are connected with a type 1 edge) |
| **triplet\_typeC** | Number of triplets of type C. For a node n, the triplet is in the form  i -3- n -3- j  where i and j are other nodes connected to n with a type 3 edge and i and j are connected with a type 2 edge) |
| **triplet\_typeD** | Number of triplets of type D. For a node n, the triplet is in the form  i -3- n -3- j  where i and j are other nodes connected to n with a type 3 edge and i and j are connected with a type 4 edge) |
| **triangle** | Triangle where node n is present (type 3 network) |

1The ratio of the number of edges to the number of possible edges in the network.

Some information about the calculated network statistics. The number of **connected components** are computed using the depth-first search algorithm [11]. The nodes **betweenness centrality** [5,8-9] is calculated using formula 1 [5] and the algorithm of Brandes (2008) [6]

**Formula 1.**

Where denotes the number of shortest paths from to , where is the vertices (nodes) of a graph. The symbol then indicate the number of shortest paths from to that some lies on (Brandes, 2001[5]). For **closeness centrality**, the algorithm used was from Sarıyüce *et al.* (2013 [7]) and calculated using formula 2. In this later formula [5], the symbol denote the distance between the nodes and .

**Formula 2.**

To calculate the **number of triangles** in each network, the fast procedure of Schank and Wagner (2005) [11] was used. All the source code can be found in the graph.java source code.