

ComponentGrapher User Guide

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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

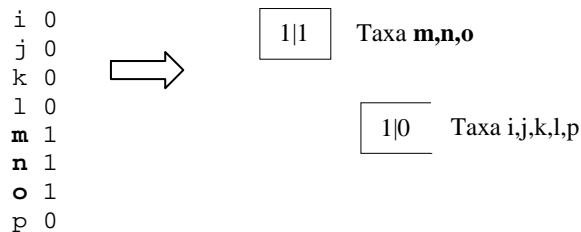
The software ComponentGrapher is implemented as a multi-platform java program. It requires Java SE8 (JDK 8) or later versions of Java. For large matrices (>1000 characters), a fair amount of RAM is required, and should be specified before launching the tool. The *results*, if no output option is specified, 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 (*Char.1*) and two states (0,1), this will result in 2 nodes (character state):



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.

	Type I Identical		Type II Inclusion		Type III Overlap		Type IV Disjoint	
	A2	B2	C2	D2	E2	F2	A2	F2
i	-	-	-	-	-	+	-	+
j	-	-	-	-	-	+	-	+
k	-	-	-	+	+	+	-	+
l	-	-	-	+	+	+	-	+
m	+	+	+	+	+	-	+	-
n	+	+	+	+	+	-	+	-
o	+	+	+	+	+	-	+	-
p	-	-	-	+	+	-	-	-

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;
```

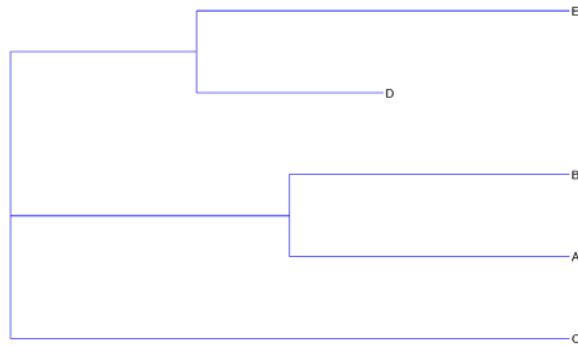
Note: Phylogenetic trees in nexus datasets are not currently supported if phylogenetic permutations are performed (*see below*).

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: If 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    110110
B    110000
C    100110
D    001001
E    001110
```

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.txt ¹	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 permuted 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	Associated taxa
#src_id(tab)dest_id(tab)edge_type(tab)associated_taxa			
2	0	2	2
0	3	3	1
0	4	1	3
0	6	3	2
...			

*Note: the number of associated taxa refers for: type I edges to the number of common taxa (3, below); type II edges the number of included taxa (D2, below); type III the overlapping taxa (2, below) and for the type IV, the number of taxa with dissimilar traits (7, below).

Type I Identical			Type II Inclusion			Type III Overlap			Type IV Disjoint		
	A2	B2		C2	D2		E2	F2		A2	F2
i	-	-	i	-	-	i	-	+	i	-	+
j	-	-	j	-	-	j	-	+	j	-	+
k	-	-	k	-	+	k	+	+	k	-	+
l	-	-	l	-	+	l	+	+	l	-	+
m	+	+	m	+	+	m	+	-	m	+	-
n	+	+	n	+	+	n	+	-	n	+	-
o	+	+	o	+	+	o	+	-	o	+	-
p	-	-	p	-	+	p	+	-	p	-	-

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_typeB	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
<hr/>										
NodeID_1	Char.	l l								
Statistics	Ref	p-value Sign.	N	Mean	STD	Min	Max	5%	95%	
<hr/>										

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 permuted dataset.
G	Maximum value found in the permuted dataset.
H	Mean value found in the permuted dataset.
I	Standard deviation found in the permuted dataset.
J	5% percentile value found in the permuted dataset.
K	95% percentile value found in the permuted 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:

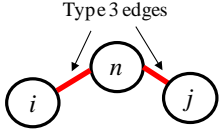
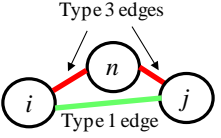
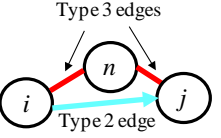
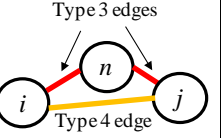
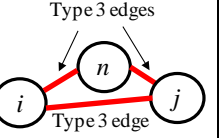
Column	Descriptions
Nodeid	Node numbering (zero-based)
Name	Node name
Found in type 1 network	Node is found in type 1 network (Presence indicate by a x)
Found in type 2 network	Node is found in type 2 network (Presence indicate by a x)
Found in type 3 network	Node is found in type 3 network (Presence 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 (Node 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
 <p>Nodes <i>i</i> and <i>j</i> are not connected. Central node <i>n</i> is linked with type 3 edges.</p>	 <p>Nodes <i>i</i> and <i>j</i> are connected by a type 1 edge. Central node <i>n</i> is linked with type 3 edges</p>	 <p>Nodes <i>i</i> and <i>j</i> are connected by a type 2 edge. Central node <i>n</i> is linked with type 3 edges</p>	 <p>Nodes <i>i</i> and <i>j</i> are connected by a type 4 edge. Central node <i>n</i> is linked with type 3 edges</p>	 <p>Nodes <i>i</i> and <i>j</i> are connected by a type 4 edge. Central node <i>n</i> is linked with type 3 edges (e.g. it forms a <i>triangle</i>)</p>

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' />
  <node id='6_0'>
    <data key='k0'>10</data>
    <data key='k3'>Char. 6</data>
    <data key='k6'>10</data>
    <data key='k7'>6</data>
    <data key='k8'>Char. 6</data>
    <data key='k9'>0</data>
    <data key='k10'>0</data>
    <data key='k61'>10</data>
    <data key='k62'>0</data>
    <data key='k11'>4</data>
  </node>
  <edge directed='true' source='1_0' target='6_0'>
    <data key='k1'>2</data>
    <data key='k2'>2</data>
    <data key='k13'>inclusion</data>
  </edge>
</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
<u>Sample_nodeid.txt</u>					
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] Saryüce, 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 density ¹ (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.

$$B(v) = \sum_{s \neq v \neq t \in V} \frac{\sigma_{st}(v)}{\sigma_{st}}.$$

Where σ_{st} denotes the number of shortest paths from $s \in V$ to $t \in V$, where V is the vertices (nodes) of a graph. The symbol $\sigma_{st}(v)$ then indicate the number of shortest paths from s to t that some $v \in V$ 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 $d_G(v, t)$ denote the distance between the nodes s and t .

Formula 2.

$$C_c(v) = \frac{1}{\sum_{t \in V} d_G(v, t)}.$$

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.