Graphs in the gRbase package

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1 Introduction

For the R community, the packages igraph, graph, RBGL and Rgraphviz are extremely useful tools for graph operations, manipulation and layout. The gRbase package adds some additional tools to these fine packages. The most important tools are:

1. Undirected and directed acyclic graphs can be specified using formulae or an adjacency list using the functions ug() and dag(). This gives graphs represented as graphNEL objects (the default), as igraphs or as adjacency matrices.

2. Some graph algorithms are implemented in gRbase. These can be applied to graphs represented as graphNELs or as matrices.

The most important algorithms are: mcs(),(maximum cardinality search) moralize(), (moralization of directed acyclic graph), rip(), (RIP ordering of cliques of triangulated undirected graph), triangulate(), (triangulate undirected graph).

Furthermore corresponding to some of the functions in the graph and RBGL packages there are corresponding matrix versions of these implemented in gRbase. These are: maxCliqueMAT().

2 Graphs

Undirected graphs can be created by the ug() function and directed acyclic graphs (DAGs) by the dag() function.

The graphs can be specified either using formulae or a list of vectors; see examples below.

The representation of a graph can be as a graphNEL object, as an igraph object or as an adjacency matrix.

2.1 Undirected graphs

An undirected graph is created by the ug() function.

As graphNEL: The following specifications are equivalent:

```
> ug11 <- ug(~a*b*c + c*d + d*e + a*e + f*g)
> ug12 <- ug(c("a","b","c"),c("c","d"),c("d","e"),c("a","e"),c("f","g"))
> ug13 <- ug(~a*b*c, ~c*d, ~d*e + a*e + f*g)
```

Notice that a ":" can be used instead of "*" in the formula specifications above.

```
> ug11

A graphNEL graph with undirected edges

Number of Nodes = 7

Number of Edges = 7
```

As igraph: A representation as an **igraph** object can be obtained with one of the following equivalent specifications:

```
> ug11i <- ug(~a*b*c + c*d + d*e + a*e + f*g, result="igraph")
> ug12i <- ug(c("a","b","c"),c("c","d"),c("d","e"),c("a","e"),c("f","g"),
+ result="igraph")
```

```
> ug11i

Vertices: 7
Edges: 7
Directed: FALSE
Edges:

[0] 'a' -- 'b'
[1] 'a' -- 'c'
[2] 'a' -- 'e'
[3] 'b' -- 'c'
[4] 'c' -- 'd'
[5] 'd' -- 'e'
[6] 'f' -- 'g'
```

As adjacency matrix: A representation as an adjacency matrix can be obtained with one of the following equivalent specifications:

```
> ug11m <- ug(~a*b*c + c*d + d*e + a*e + f*g, result="matrix")
> ug12m <- ug(c("a", "b", "c"), c("c", "d"), c("d", "e"), c("a", "e"), c("f", "g"),
+ result="matrix")
```

```
> ug11m

a b c d e f g
a 0 1 1 0 1 0 0
b 1 0 1 0 0 0 0
c 1 1 0 1 0 0 0
d 0 0 1 0 1 0 0
e 1 0 0 1 0 0 0
f 0 0 0 0 0 1 0
```

2.2 Directed acyclic graphs (DAGs)

A directed acyclic graph is created by the dag() function.

As graphNEL: The following specifications are equivalent:

```
> dag11
A graphNEL graph with directed edges
Number of Nodes = 7
Number of Edges = 7
```

Here ~a means that "a" has no parents while ~d*b*c means that "d" has parents "b" and "c". Notice that a ":" can be used instead of "*" the specification.

As igraph: A representation as an igraph object can be obtained with

```
> dag11i <- dag(~a + b*a + c*a*b + d*c*e + e*a + g*f, result="igraph")
> dag12i <- dag("a", c("b", "a"), c("c", "a", "b"), c("d", "c", "e"),
+ c("e", "a"), c("g", "f"), result="igraph")
```

As adjacency matrix: A representation as an adjacency matrix can be obtained with

```
> dag11m <- dag(~a + b*a + c*a*b + d*c*e + e*a + g*f, result="matrix")
> dag12m <- dag("a", c("b", "a"), c("c", "a", "b"), c("d", "c", "e"),
+ c("e", "a"), c("g", "f"), result="matrix")
```

3 Graph coercion

Graphs can be coerced between differente representations using as(); for example

```
> as(ug11,"igraph")
Vertices: 7
Edges: 7
Directed: FALSE
Edges:
[0] 'a' -- 'b'
[1] 'a' -- 'c'
[2] 'a' -- 'e'
[3] 'b' -- 'c'
[4] 'c' -- 'd'
[5] 'd' -- 'e'
[6] 'f' -- 'g'
> as(as(ug11, "igraph"), "matrix")
  abcdefg
a 0 1 1 0 1 0 0
b 1 0 1 0 0 0 0
c 1 1 0 1 0 0 0
d 0 0 1 0 1 0 0
e 1 0 0 1 0 0 0
f 0 0 0 0 0 0 1
g 0 0 0 0 0 1 0
> as(as(ug11,"igraph"),"matrix"),"graphNEL")
A graphNEL graph with undirected edges
Number of Nodes = 7
Number of Edges = 7
```

4 Plotting graphs

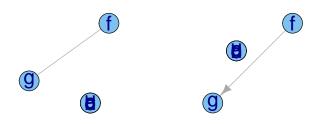
Graphs represented as graphNEL: Graphs (represented as graphNEL objects) are displayed with plot(), but this requires that 1) the Rgraphviz package is installed and also 2) that the Graphviz program is installed.

There is also an iplot() function which converts a graphNEL to an igraph and plots this. To use iplot(), no additional software must be installed. There is a lot of room for improvement of the iplot() function.

Graphs represented as igraph: Graphs (represented as igraph objects) are displayed with plot().

Graphs represented as adjacency matrices: There is no plot method for graphs represented as adjacency matrices.

```
> par(mfrow=c(1,2))
> iplot(ug11)
> iplot(dag11)
```



5 Graph queries

The graph and RBGL packages implement various graph operations for graphNEL objects. See the documentation for these packages. The gRbase implements a few additional functions, see Section 1. An additional function in gRbase for graph operations is querygraph(). This function is intended as a wrapper for the various graph operations available in gRbase, graph and RBGL. There are two main virtues of querygraph():

1) querygraph() operates on any of the three graph representations described above and 2) querygraph() provides a unified interface to the graph operations. The general syntax is

```
> args(querygraph)
function (object, op, set = NULL, set2 = NULL, set3 = NULL)
NULL
```

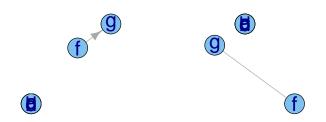
6 More advanced graph operations

A moralized directed acyclic graph is obtained with

```
> dag11.mor <- moralize(dag11)
```

```
> par(mfrow=c(1,2))
> iplot(dag11)
```

> iplot(dag11.mor)



Testing for whether a graph is triangulated is based on Maximum Cardinality Search. If character(0) is returned the graph is not triangulated. Otherwise a linear ordering of the nodes is returned.

```
> mcs(ug11)
character(0)
```

Triangulate an undirected graph by adding extra edges to the graph:

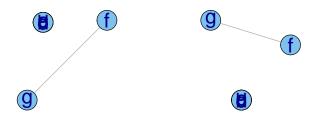
```
> tug11<-triangulate(ug11)

A graphNEL graph with undirected edges

Number of Nodes = 7

Number of Edges = 8
```

```
> par(mfrow=c(1,2))
> iplot(ug11)
> iplot(tug11)
```



A RIP ordering of the cliques of a triangulated graph can be obtained as:

```
> r <- rip(tug11)
> r
cliques
 1 : c a b
 2 : e a c
 3 : d c e
 4 : g f
separators
 1:
  2 : a c
  3 : c e
  4:
parents
 1:0
  2:1
  3:2
  4:0
```

7 Time and space considerations

7.1 Space

It is worth noticing that working with graphs representated as graphNEL objects is somewhat slower working with graphs represented as adjacency matrices. On the other hand, graph

Consider for example coerction from a graphNEL object. This can be obtained with as() as shown above or by using as.adjMAT() from gRbase. The timings are:

```
> system.time({for (ii in 1:200) as(ug11, "matrix")})

user system elapsed
0.35  0.00  0.35

> system.time({for (ii in 1:200) as.adjMAT(ug11)})

user system elapsed
0.01  0.00  0.01
```

Similarly, consider finding the cliques of an undirected graph represented as a graphNEL object or as a matrix:

```
> system.time({for (ii in 1:200) maxClique(ug11)})

user system elapsed
0.11  0.00  0.10

> system.time({for (ii in 1:200) maxCliqueMAT(ug11m)})

user system elapsed
0.01  0.00  0.01
```

7.2 Space

On the other hand, the graphNEL representation is – at least – in principle more economic in terms of space requirements than the adjacency matrix representation (because the adjacency matrix representation uses a 0 to represent a "missing edge". However, in practice the picture is not so clear. Consider the following examples

```
> V <- 1:100
> M <- 1:10
> ## Sparse graph
> ##
> g1 <- randomGraph(V, M, 0.05)
> length(edgeList(g1))
[1] 175
> object.size(g1)
109496 bytes
> object.size(as.adjMAT(g1))
47448 bytes
> ## More dense graph
> ##
> g1 <- randomGraph(V, M, 0.2)
> length(edgeList(g1))
[1] 2200
> object.size(g1)
1048680 bytes
> object.size(as.adjMAT(g1))
47448 bytes
> ## Even more dense graph
> ##
> g1 <- randomGraph(V, M, 0.5)
> length(edgeList(g1))
[1] 4772
> object.size(g1)
2242088 bytes
> object.size(as.adjMAT(g1))
47448 bytes
```