Graphs in the `gRbase` package

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Contents

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 `graphNEL`s 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 0 1
g 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 <- dag(~a + b*a + c*a*b + d*c*e + e*a + g*f)
> dag12 <- dag("a", c("b","a"), c("c","a","b"), c("d","c","e"),
+               c("e","a"),c("g","f"))
> dag13 <- dag(~a, ~b*a,  ~c*a*b, ~d*c*e, ~e*a, ~g*f)
```

```
> 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")

  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 0 1
g 0 0 0 0 0 1 0

> as(as(as(ug11,"igraph"),"matrix"),"graphNEL")

A graphNEL graph with undirected edges
Number of Nodes = 7
Number of Edges = 7
```

4 Plotting graphs

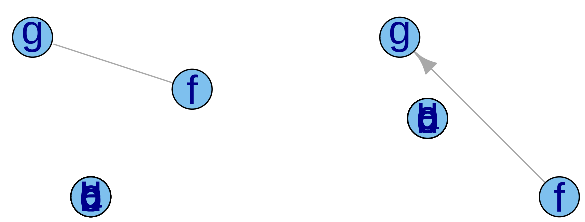
Graphs represented as `graphNEL`: Graphs (represented as `graphNEL` objects) are displayed with `plot()`, but this requires that 1) the `Rgraphviz` package is installed and also 2) that the `Graphviz` program is installed.

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

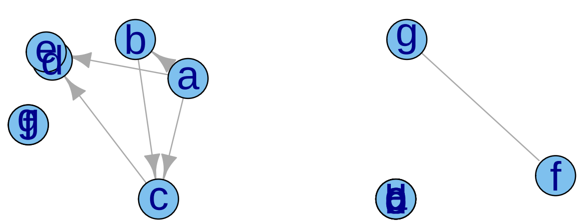
```
> args(querygraph)

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)
```



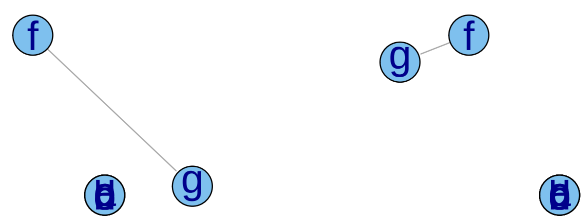
Testing for whether a graph is triangulated is based on Maximum Cardinality Search. If `character(0)` is returned the graph is not triangulated. Otherwise a linear ordering of the nodes is returned.

```
> 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    0.34

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

   user  system elapsed
   0.03    0.00    0.03
```

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
   0.12    0.00    0.13

> 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] 135

> object.size(g1)

90992 bytes

> object.size(as.adjMAT(g1))

47448 bytes

> ## More dense graph
> ##
> g1 <- randomGraph(V, M, 0.2)
> length(edgeList(g1))

[1] 1591

> object.size(g1)

766248 bytes

> object.size(as.adjMAT(g1))

47448 bytes

> ## Even more dense graph
> ##
> g1 <- randomGraph(V, M, 0.5)
> length(edgeList(g1))

[1] 4744

> object.size(g1)

2229096 bytes

> object.size(as.adjMAT(g1))

47448 bytes
```