Graphs in the **gRbase** package

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Contents

1 Introduction

For the `R` community, the packages `graph`, `RBGL`, `Rgraphviz` and `igraph` 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 in one of the following forms:[1]

   - A `graphNEL` object (the default),
   - A dense adjacency matrix. By this we mean a "standard" matrix in `R`.
   - A sparse adjacency matrix. By this we mean a `dgCMatrix` from the `Matrix` package.

2. Some graph algorithms are implemented in **gRbase**. These can be applied to graphs represented as `graphNEL`s and matrices. The most important algorithms are:

   - `moralize()`, (moralize a directed acyclic graph)
   - `mcs()`,(maximum cardinality search for undirected graph)
   - `triangulate()`, (triangulate undirected graph)
   - `rip()`, (RIP ordering of cliques of triangulated undirected graph)
   - `getCliques()`, (get the (maximal) cliques of an undirected graph)
   - `minimalTriang()` (minimal triangulation of undirected graph)[2]
   - `mpd()` (maximal prime subgraph decomposition of undirected graph)[3]

   The general scheme is the following: There is a `mcs()` function and `mcs()` methods for `graphNEL`s and for the two matrix types. The workhorse is the function `mcsMAT()` and the various methods coerces the graph to a (sparse) matrix and invokes `mcsMAT()`.

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.

2.1 Undirected graphs

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

[1] There is a fourth form: `igraph` objects. These, however, will probably not be supported in the future.
[2] Needs more work
[3] Needs more work

As `graphNEL`: The following specifications are equivalent (notice that ":" and "*" can be used interchangably):

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

```
R> ug11
```

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

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

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

```
R> 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
```

```
R> ug11M <- ug(~a*b*c + c*d + d*e + a*e + f*g, result="Matrix")
R> ug12M <- ug(c("a","b","c"),c("c","d"),c("d","e"),c("a","e"),c("f","g"),
              result="Matrix")
```

```
R> ug11M
```

```
7 x 7 sparse Matrix of class "dgCMatrix"
  a b c d e f g
a . 1 1 . 1 . .
b 1 . 1 . . . .
c 1 1 . 1 . . .
d . . 1 . 1 . .
e 1 . . 1 . . .
f . . . . . . 1
g . . . . . 1 .
```

2.2 Directed acyclic graphs (DAGs)

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

As `graphNEL`: The following specifications are equivalent (notice that ":" and "*" can be used interchangably):

```
R> dag11 <- dag(~a + b:a + c:a:b + d:c:e + e:a + g:f)
R> dag11 <- dag(~a + b*a + c*a*b + d*c*e + e*a + g*f)
R> dag12 <- dag("a", c("b","a"), c("c","a","b"), c("d","c","e"),
                c("e","a"),c("g","f"))
R> dag13 <- dag(~a, ~b:a,  ~c:a:b, ~d:c:e, ~e:a, ~g:f)
R> dag13 <- dag(~a, ~b*a,  ~c*a*b, ~d*c*e, ~e*a, ~g*f)
```

```
R> 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".

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

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

```
R> dag11m
```

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

```
R> dag11M <- dag(~a + b:a + c:a:b + d:c:e + e:a + g:f, result="Matrix")
R> dag12M <- dag("a", c("b","a"), c("c","a","b"), c("d","c","e"),
                c("e","a"),c("g","f"), result="Matrix")
```

```
R> dag11M
```

```
7 x 7 sparse Matrix of class "dgCMatrix"
  a b c d e g f
a . 1 1 . 1 . .
b . . 1 . . . .
c . . . 1 . . .
d . . . . . . .
e . . . 1 . . .
g . . . . . . .
f . . . . . 1 .
```

2.3 Graph coercion

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

```
R> as(ug11,"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
```

```
R> as(as(ug11,"matrix"),"dgCMatrix")
```

```
7 x 7 sparse Matrix of class "dgCMatrix"
  a b c d e f g
a . 1 1 . 1 . .
b 1 . 1 . . . .
c 1 1 . 1 . . .
d . . 1 . 1 . .
e 1 . . 1 . . .
f . . . . . . 1
g . . . . . 1 .
```

```
R> as(as(as(ug11,"matrix"),"dgCMatrix"),"graphNEL")
```

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

```
R> as(as(as(as(ug11,"matrix"),"Matrix"),"graphNEL"),"igraph")
```

```
IGRAPH UNW- 7 7 --
+ attr: name (v/c), label (v/c), weight (e/n)
```

NOTICE! There is one thing to notice when coercing a dense matrix to a sparse matrix. Consider this

```
R> m <- matrix(1:4,nrow=2)
R> as(m, "Matrix")
```

```
2 x 2 Matrix of class "dgeMatrix"
     [,1] [,2]
[1,]    1    3
[2,]    2    4
```

```
R> as(m, "dgCMatrix")
```

```
2 x 2 sparse Matrix of class "dgCMatrix"

[1,] 1 3
[2,] 2 4
```

In the first case, the matrix coercion method will, based on properties of the matrix, impose a specific type on the result. The graph algorithms in **gRbase** are based on the `dgCMatrix` form and hence the latter case is more safe. Coercion to a `dgCMatrix` can be made much faster with the following function from **gRbase**:

```
R> asdgCMatrix(m)
```

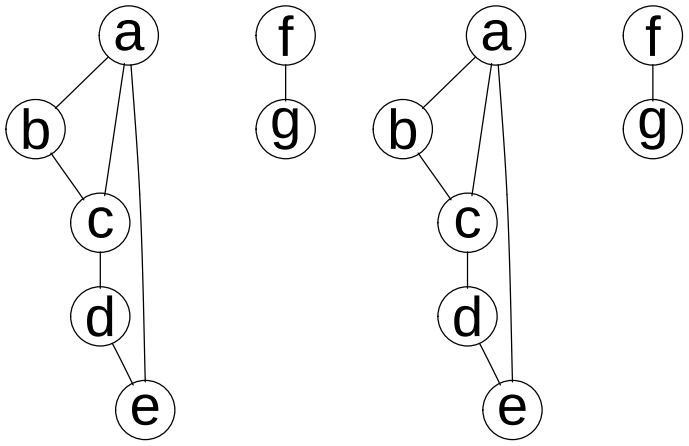
```
2 x 2 sparse Matrix of class "dgCMatrix"

[1,] 1 3
[2,] 2 4
```

2.4 Plotting graphs

Graphs represented as `graphNEL` objects are displayed with `plot()`. There is no `plot()` method for graphs represented as adjacency matrices, so here coercion is one option:

```
R> par(mfrow=c(1,2))
R> plot(ug11)
R> plot(as(ug11m,"graphNEL"))
```



An alternative for adjacency matrices is the `gplot()` function in the **sna** package:

```
R> par(mfrow=c(1,2))
R> library(sna)
R> gplot(ug11m, label=colnames(ug11m),gmode="graph")
R> gplot(dag11m, label=colnames(dag11m))
```

3 Advanced graph operations

3.1 Moralization

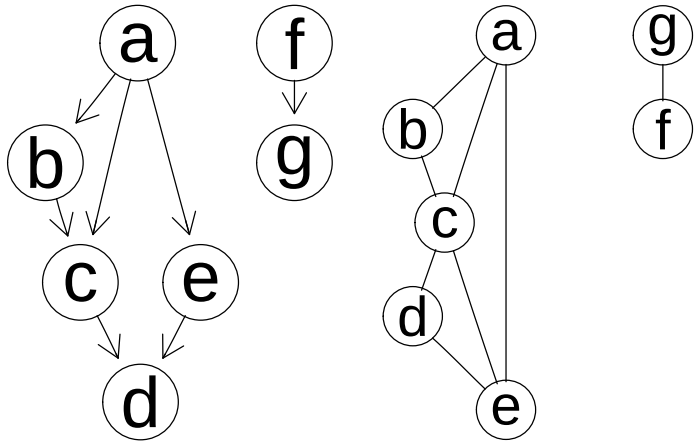
```
R> apropos("^moralize\\.")
```

```
[1] "moralize.graphNEL" "moralize.igraph"   "moralize.matrix"
[4] "moralize.Matrix"
```

A moralized directed acyclic graph is obtained with

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

```
R> par(mfrow=c(1,2))
R> plot(dag11)
R> plot(dag11.mor)
```



For the alternative representations

```
R> moralize(dag11m)
```

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

```
R> moralize(dag11M)
```

```
7 x 7 sparse Matrix of class "dgCMatrix"
  a b c d e g f
a . 1 1 . 1 . .
b 1 . 1 . . . .
c 1 1 . 1 1 . .
```

```
d . . 1 . 1 . .
e 1 . 1 1 . . .
g . . . . . . 1
f . . . . . 1 .
```

3.2 Topological sort

A topological ordering of a directed graph is a linear ordering of its vertices such that, for every edge (u->v), u comes before v in the ordering. A topological ordering is possible if and only if the graph has no directed cycles, that is, if it is a directed acyclic graph (DAG). Any DAG has at least one topological ordering.

```
R> topoSort(dag11)
```

```
[1] "a" "b" "c" "e" "f" "d" "g"
```

```
R> topoSort(dag11m)
```

```
[1] "a" "b" "c" "e" "f" "d" "g"
```

```
R> topoSort(dag11M)
```

```
[1] "a" "b" "c" "e" "f" "d" "g"
```

The `dag()` function actually allows specification of a directed graph with cycles (a check can be imposed with `forceCheck=TRUE`). Below is a directed graph with a cycle

```
R> topoSort(dag(~a:b+b:c+c:a))
```

```
character(0)
```

3.3 Getting cliques

I graph theory, a clique is often a complete subset of a graph. A maximal clique is a clique which can not be enlarged. In statistics (and that is the convention we follow here) a clique is usually understood to be a maximal clique.

Finding the cliques of a general graph is an NP complete problem. Finding the cliques of triangualted graph is linear in the number of cliques.

```
R> str(getCliques(ug11))
```

```
List of 5
 $ : chr [1:3] "a" "b" "c"
 $ : chr [1:2] "a" "e"
 $ : chr [1:2] "d" "c"
 $ : chr [1:2] "d" "e"
 $ : chr [1:2] "f" "g"
```

```
R> str(getCliques(ug11m))
```

```
List of 5
 $ : chr [1:3] "a" "b" "c"
 $ : chr [1:2] "a" "e"
 $ : chr [1:2] "d" "c"
 $ : chr [1:2] "d" "e"
 $ : chr [1:2] "f" "g"
```

```
R> str(getCliques(ug11M))
```

```
List of 5
 $ : chr [1:3] "a" "b" "c"
 $ : chr [1:2] "a" "e"
 $ : chr [1:2] "d" "c"
 $ : chr [1:2] "d" "e"
 $ : chr [1:2] "f" "g"
```

3.4 Maximum cardinality search

```
R> apropos("^mcs\\.")
```

```
[1] "mcs.graphNEL" "mcs.igraph"   "mcs.matrix"   "mcs.Matrix"
```

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.

```
R> mcs(ug11)
```

```
character(0)
```

```
R> mcs(ug11m)
```

```
character(0)
```

```
R> mcs(ug11M)
```

```
character(0)
```

```
R> mcs(dag11.mor)
```

```
[1] "a" "b" "c" "e" "d" "g" "f"
```

```
R> mcs(as(dag11.mor,"matrix"))
```

```
[1] "a" "b" "c" "e" "d" "g" "f"
```

```
R> mcs(as(dag11.mor,"Matrix"))
```

```
[1] "a" "b" "c" "e" "d" "g" "f"
```

```
R> mcs(dag11)
```

```
character(0)
```

3.5 Triangulation

```
R> apropos("^triangulate\\.")
```

```
[1] "triangulate.graphNEL" "triangulate.igraph"   "triangulate.matrix"
[4] "triangulate.Matrix"
```

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

```
R> (tug11<-triangulate(ug11))
```

```
A graphNEL graph with undirected edges
Number of Nodes = 7
Number of Edges = 8
```

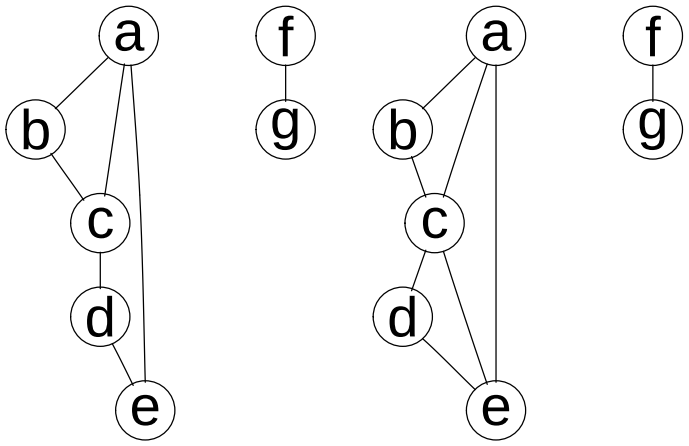
```
R> (tug11m<-triangulate(ug11m))
```

```
  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 1 0 0
d 0 0 1 0 1 0 0
e 1 0 1 1 0 0 0
f 0 0 0 0 0 0 1
g 0 0 0 0 0 1 0
```

```
R> (tug11M<-triangulate(ug11M))
```

```
7 x 7 sparse Matrix of class "dgCMatrix"
  a b c d e f g
a . 1 1 . 1 . .
b 1 . 1 . . . .
c 1 1 . 1 1 . .
d . . 1 . 1 . .
e 1 . 1 1 . . .
f . . . . . . 1
g . . . . . 1 .
```

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



3.6 RIP ordering / junction tree

```
R> apropos("^rip\\.")
```

```
[1] "rip.graphNEL" "rip.igraph"   "rip.matrix"   "rip.Matrix"
```

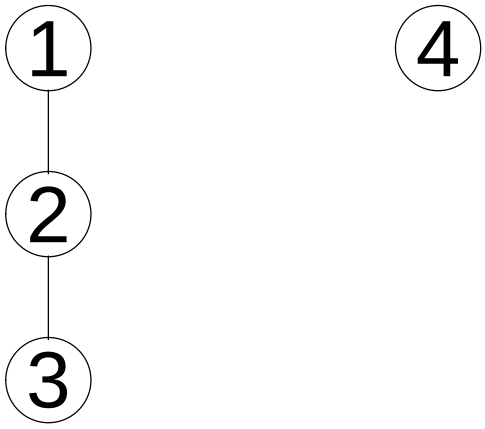
A RIP ordering of the cliques of a triangulated graph can be obtained as:

```
R> rr <- rip(tug11)
R> rr
```

```
cliques
  1 : c a b
  2 : c a e
  3 : c d e
  4 : f g
separators
  1 :
  2 : c a
  3 : c e
  4 :
parents
  1 : 0
  2 : 1
  3 : 2
  4 : 0
```

```
R> rr <- rip(tug11m)
R> rr <- rip(tug11M)
```

```
R> plot(rr)
```



3.7 Minimal triangulation and maximum prime subgraph decomposition

An undirected graph uG is triangulated (or chordal) if it has no cycles of length >= 4 without a chord which is equivalent to that the vertices can be given a perfect ordering. Any undirected graph can be triangulated by adding edges to the graph, so called fill-ins which gives the graph TuG. A triangulation TuG is minimal if no fill-ins can be removed without breaking the property that TuG is triangulated. A related concept is the minimum triangulation, which is the the graph with the smallest number of fill-ins. The minimum triangulation is unique. Finding the minimum triangulation is NP-hard.

4 Time and space considerations

4.1 Time

It is worth noticing that working with graphs representated as `graphNEL` objects is somewhat slower working with graphs represented as adjacency matrices. Consider finding the cliques of an undirected graph represented as a `graphNEL` object or as a matrix:

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

   user  system elapsed
   0.10    0.00    0.09

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

   user  system elapsed
   0.02    0.00    0.02
```

Working with sparse matrices rather than standard matrices slows indexing down:

```
R> system.time({for (ii in 1:2000) ug11m[2,]})

   user  system elapsed
      0       0       0

R> system.time({for (ii in 1:2000) ug11M[2,]})

   user  system elapsed
   0.92    0.00    0.94
```

However, **gRbase** has some functionality for indexing sparse matrices quickly:

```
R> system.time({for (ii in 1:2000) sp_getXj(ug11M,2)})

   user  system elapsed
   0.04    0.00    0.03
```

4.2 Space

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". The sparse matrix representation is clearly only superior to the standard matrix representation if the graph is sparse:

```
R> V <- 1:100
R> M <- 1:10
R> ## Sparse graph
R> ##
R> g1 <- randomGraph(V, M, 0.05)
R> length(edgeList(g1))

[1] 112

R> c(NEL=object.size(g1),
  mat=object.size(as(g1, "matrix")),
  Mat=object.size(as.adjMAT(g1, "Matrix")))

  NEL   mat   Mat
80216 47448 11116

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

[1] 4640

R> c(NEL=object.size(g1),
  mat=object.size(as(g1, "matrix")),
  Mat=object.size(as.adjMAT(g1, "Matrix")))

    NEL     mat     Mat
2180840   47448  119788
```

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[4] and 2) `querygraph()` provides a unified interface to the graph operations. The general syntax is

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

[4]Actually not quite yet, but it will be so in the future.