A Graph Theory Package for Maple, Part II: Graph Coloring, Graph Drawing, Support Tools, and Networks.

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1 Introduction

This is the second paper detailing a new Maple package for graph theory, called `GraphTheory`, [1], that is being developed at Simon Fraser University as part of our MITACS research project.

The package is intended for both research and teaching. It supports directed and undirected graphs, weighted and unweighted graphs, and networks, but not multi-graphs. The package includes procedures for drawing graphs in 2 and 3 dimensions. To make the package easy to use we have added 'context menus'.

In this paper we describe new functionality added to support graph input, storing of arbitrary information about edges and vertices, importing graphs from and exporting graphs to other software, including support for MetaPost for use with LaTeX.

We describe a graph drawing algorithm that models a graph as a physical system that leads to a system of second order differential equations that needs to be solved. This approach gives very good drawings of graphs. It is limited in that its complexity is inherently $O(n^2)$ where n is the number of vertices in the graph. Our implementation is effective for n up to about 100.

We also describe the facilities for graph coloring and for networks.

2 Defining Graphs

2.1 The `Graph` and `Digraph` commands

The commands `Graph` and `Digraph` are used to construct a graph or digraph by specifying its parameters. Here we give a description of how the `Graph` command is used.

The following parameters of the graph can be given *in any order* as arguments of the `Graph` command: number of vertices, vertex labels, edges/arcs, the adjacency matrix, the weight matrix, the keywords `directed`, `undirected`, `weighted`, and `unweighted`.

Vertex labels are specified in a list (in a fixed order). Each label can be either an integer, a symbol, or a string.

Edges are of the form `{x,y}` and arcs are of the form `[x,y]` where `x` and `y` are valid vertex labels. A convenient solution for entering the edges of a graph is to use trails. For example `Trail(1,2,3,4,2,3,5)` for an undirected graph is short for the edges {{1,2},{2, 3},{3,4},{2,4},{3,5}}.

If the graph to be constructed is weighted, then the weights of edges/arcs can be given in a weight matrix, or in the set of edges in the form `[e,w]`, where `e` is an edge/arc and `w` is the weight of `e`. If no weight is assigned to an edge, it is assigned the weight `1` by default. In the following we present some examples.

```
> G := Graph(5);
```

Graph 1 : *an undirected unweighted graph with* 5 *vertices and* 0 *edge(s)*

```
> Vertices(G), Edges(G);
```

$[1, 2, 3, 4, 5], \{\}$

```
> Graph([a,b,c,d,e], {{a,b}, {b,c}, {c,e}, {a,c}});
```

Graph 2 : *an undirected unweighted graph with* 5 *vertices and* 4 *edge(s)*

```
> Graph({{a,b}, {b,c}, {c,e}, {a,c}});
```

Graph 3 : *an undirected unweighted graph with* 5 *vertices and* 4 *edge(s)*

```
> G := Graph([a,b,c,d,e], Trail(c,a,b,c,e));
```

G := *Graph* 5 : *an undirected unweighted graph with* 5 *vertices and* 4 *edge(s)*

```
> Edges(G);
```

$\{\{c, a\}, \{c, b\}, \{c, e\}, \{a, b\}\}$

```
> W := Matrix(6, {(1,2)=2,(2,3)=4,(2,6)=7,(3,4)=6,(3,5)=5,(4,5)=3},
        shape=symmetric):
> G := Graph([$1..6], W):
```

```
> Edges(G, weights);
```

$\{[\{1, 2\}, 2], [\{2, 3\}, 4], [\{2, 6\}, 7], [\{3, 4\}, 6], [\{3, 5\}, 5], [\{4, 5\}, 3]\}$

```
> A := Matrix([[0,1,1,1],[1,0,1,0],[1,1,0,1],[1,0,1,0]]);
```

```
> Edges( Graph([a,b,c,d], A) );
```

$\{\{a,b\},\{a,c\},\{a,d\},\{b,c\},\{c,d\}\}$

A graph may also be defined by specifying its list of neighborhoods. This argument must be of type `list` or `Array`. For example:

```
> A := Array([{2,3}, {1,3,4,5}, {1,2,4,5}, {2,3}, {2,3}]);
> Edges( Graph([v1,v2,v3,v4,v5], A) );
```

$\{\{v1,v2\},\{v1,v3\},\{v2,v3\},\{v2,v4\},\{v2,v5\},\{v3,v4\},\{v3,v5\}\}$

2.2 The data structure

The `GraphTheory` package stores graphs in Maple as functions. The following is the general form of a graph generated by the `GraphTheory` package:

```
GRAPHLN(dir, wt, vlist, listn, ginfo, ewts)
```

In this structure, `dir` and `wt` are symbols indicating whether the graph is `directed` or `undirected` and whether it is `weighted` or `unweighted`. The argument `vlist` is the list of vertex labels of the graph. Each label can be of type `integer`, `string` or `symbol`. Internally, the vertices are labelled by numbers $1, 2, \ldots, n$ where n is the number of vertices of the graph. The adjacency structure of the graph is stored in `listn` which is an `Array` of sets. The ith entry in `listn` is the set of neighbors of the ith vertex. If the graph is weighted, the edge weights are stored in `ewts` which is of type `Matrix`. Additional information such as vertex positions and vertex and edge information will be stored in `ginfo` which is a of type `table`.

The choice of 'list of neighbors' as the graph data structure provides ease of modification of adjacency information (the edges of the graph) while adding/removing vertices is more expensive. Another restriction of the list of neighbors as the graph structure is that multiple edges are not supported.

2.3 Vertex/edge attributes

Attributes are used to store arbitrary information for the vertices and/or edges of a graph. Each attribute is an equation of the form `tag = value`. For example

```
> G := Graph( Trail(a, b, c, d, b) ):
> SetVertexAttribute(G, b, msg="text");
> SetVertexAttribute(G, c, [msg="message", timesvisited=10]);
> GetVertexAttribute(G, b);
```

$[msg = "text"]$

```
> GetVertexAttribute(G, c, timesvisited);
```

10

```
> GetVertexAttribute(G, b, timesvisited);
```

FAIL

```
> SetEdgeAttribute(G, {a,b}, msg="weak edge");
> SetEdgeAttribute(G, {c,d}, [tag=fake,visited=true,cost=3]);
> DiscardEdgeAttribute(G, {c,d}, tag);
> GetEdgeAttribute(G, {c,d});
```

$$[visited = true, cost = 3]$$

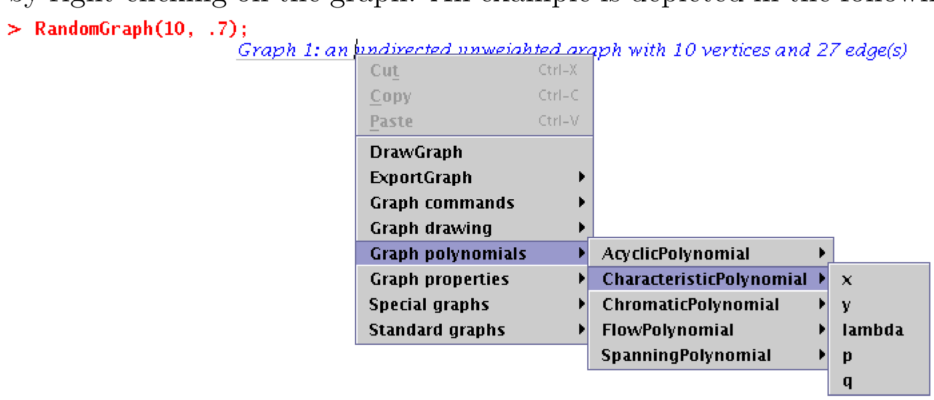
2.4 Special graphs

The defenitions of some special graphs are included in the submodule `SpecialGraphs` of the `GraphTheory` package. The following is a list of these special graphs.

`ClebschGraph`	`GridGraph`	`PappusGraph`
`CompleteBinaryTree`	`GrinbergGraph`	`PathGraph`
`CompleteGraph`	`GrotzschGraph`	`PayleyGraph`
`CompleteKaryTree`	`HeawoodGraph`	`PetersenGraph`
`CycleGraph`	`HerschelGraph`	`PrismGraph`
`DesarguesGraph`	`HypercubeGraph`	`ShrikhandeGraph`
`DodecahedronGraph`	`IcosahedronGraph`	`SoccerBallGraph`
`DoubleStarSnark`	`KneserGraph`	`SzekeresSnark`
`DyckGraph`	`LCFGraph`	`TetrahedronGraph`
`FlowerSnark`	`LeviGraph`	`TorusGridGraph`
`FosterGraph`	`MobiusKantorGraph`	`WebGraph`
`GeneralizedPetersenGraph`	`OctahedronGraph`	`WheelGraph`
`GoldbergSnark`	`OddGraph`	

2.5 Context menu

The context menu is a convenient way to access some of the `GraphTheory` package commands. The context menu of a graph can be accessed in the Maple graphical user interface by right-clicking on the graph. An example is depicted in the following figure.



3 Drawing Graphs

The `GraphTheory` package provides a command `DrawGraph` for drawing graphs and digraphs. If a graph doesn't contain drawing information, it is checked for being a tree or a bipartite graph in which cases it is drawn with respect to those structures. Otherwise the vertices are positioned on a circle. To force a style of drawing, one may specify a second argument which is of the form `style=`$\cdots$ In the remainder of this section we describe one of these styles, namely the `spring` style. The spring method may be used to generate 2-dimensional or 3-dimensional drawings of a graph. The default dimension is 2 and an extra argument `dimension=3` can be used to generate a 3D drawing. Once a drawing is generated it will be stored in the memory for future reference. To force generation of a new drawing, which is useful for the spring method which uses random initial positions, one may use the option `redraw` in the `DrawGraph` command.

Let G be a connected graph with n vertices V and m edges E. We want our algorithm to find an aesthetic layout of the graph that clearly conveys its structure and assign a location for each vertex and a route for each edge, so that the resulting drawing is 'nice'. The method we use models a graph as a physical system that leads to a system of second order differential equations that needs to be solved. Starting from random initial position for the vertices, the algorithm finds a local minimal total energy of the system.

We model edges in the graph with springs with zero rest length. We model vertices as electrically charged particles which repel each other. And we add damping to the physical system to dampen oscillations.

Thus we construct a system of second order differential equations where the equation for vertex i is the following:

$$\frac{d^2}{dt^2} X_i(t) = \sum_{j \in \mathrm{N}(i)} (X_i(t) - X_j(t)) \ - \ \frac{d}{dt} X_i(t) \ + \ \sum_{j \in \mathrm{V}} \frac{|X_i(t) - X_j(t)|}{(X_i(t) - X_j(t))^3}$$

where V is the set of vertices of G, $N(i)$ are the vertices adjacent to vertex i, and X_i is the position of vertex i, a vector. Thus if there are n vertices in the graph and we model the system in 2 dimensions, there are $2n$ second order differential equations in $2n$ unknowns. For the initial values, we set initial velocities to 0 and choose initial positions at random inside the unit square (in 2 dimensions) and unit box (in 3 dimensions).

We solve this system by the Fehlberg fourth-fifth order Runge-Kutta method (RKF45) with degree four interpolant. This is done in Maple by using the `dsolve[numeric]` command which is adaptive.

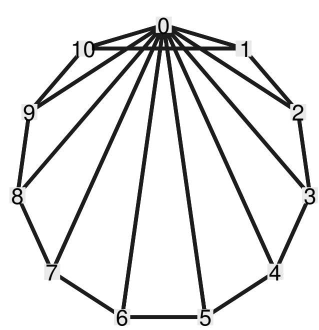
While graph drawing is a complicated problem in general, an advantage of this approach is that it requires no special knowledge about the structure of the graph such as whether it has articulation points or not. It also gives very good drawings of graphs. It is limited in that the complexity is inherently $O(n^2)$. This is because the model of vertices being charged particles repelling each other means each differential equation has n non-zero terms in it. Our implementation can treat graphs with n up to 100 in a few seconds.

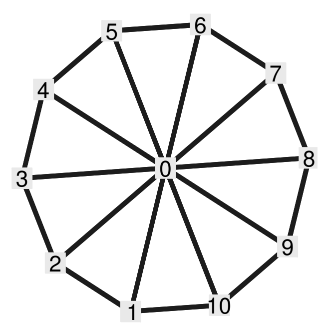
Damping Constants

In order to reconstruct good graphs from the randomly positioned initial vertices it is important that the spring model is neither over damped nor under damped. Since we are solving the system of differential equations numerically, in case of over damped or under damped, reaching to the local minimum is almost impossible. To correct this we choose the damping constant, spring constant, and repelling constants carefully. After experimenting with different graphs we have concluded that a dynamic model with respect to different graphs is required.

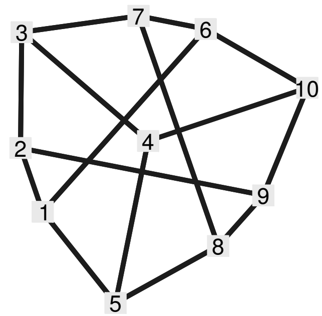
We suggest that the value of damping constant be proportional to the degree of each node. For example if we have a node with three edges connected to it then there is more damping required for that node. We suggest that the value of the spring constant and also repulsion constant be directly related. For example if we increase the strength of the spring then we need to have stronger repulsion force. However the relation between the spring and repulsion constant is not linear. We suggest the ratio $\frac{A}{B} = \sqrt{n}$ where A is the repulsion constant and B is the spring constant. On the other hand if we have a vertex with high degree then the repulsion force should be small on this vertex and consequently less force for our spring. In summary $A = \frac{\sqrt{n}}{d_i}$ and $B = \frac{1}{d_i}$ where d_i is the degree of vertex i.

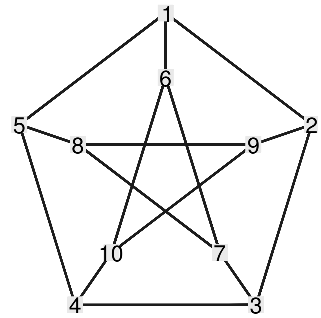
The first example shows that the algorithm recovers the 'wheel graph'. The graph on the left was constructed by placing all vertices in a circle using the command `DrawGraph(G,style=circle)`. The graph on the right is using the algorithm. The command is `DrawGraph(G,style=spring)`.



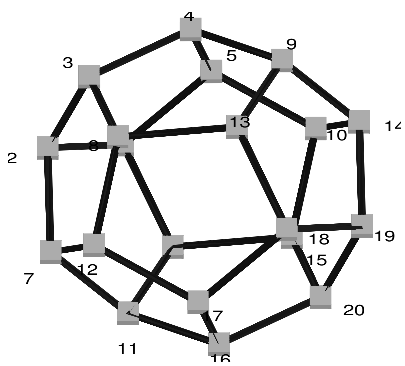


In this second example, we have constructed the Petersen graph. The graph on the right below is the default output of the `DrawGraph` command. This is usual way of drawing the Petersen graph. To obtain this output, the GraphTheory package stores the vertex positions for this special graph. The graph on the left is the output of the spring algorithm. It is another symmetric drawing of the Petersen graph.

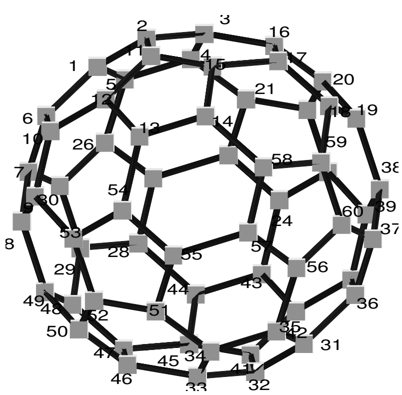




The final two examples are in three dimensions. The spring algorithm is easy to generalize to higher dimensions. In three dimensions, it is possible that the orientation of the result, of say the wheel graph, would end up showing as a line. To prevent this from happening, we rotate the graph through various angles and choose the orientation which maximizes the area of the convex hull of the vertices when projected onto the viewing plane. The first example is a docdecahedron. This graph has 20 vertices and 30 edges.



The second example is a graph of a soccer ball. The surface of a soccer ball consists of pentagons and hexagons. There are 60 vertices and 90 edges. The spring algorithm recovered the soccer ball in 0.546 seconds on an AMD 64 bit Opteron running at 2.2 GHz.



4 Graph Coloring

There are several commands implemented in the `GraphTheory` package for dealing with graph coloring problems. Since coloring problems are NP-Complete in general, the commands usually use brute-force search methods.

The two commands `ChromaticNumber` and `ChromaticIndex` return the chromatic number and the chromatic index (edge chromatic number) of a graph respectively. These commands also return an optimal coloring. To speed up the search, these commands calculate upper and lower bounds on the chromatic number of the given graph. The upper bound is obtained from a greedy coloring of the graph while the lower bound is the maximum of $\omega(G)$ and $\frac{n}{\alpha(G)}$ for a graph G where n is the number of vertices, $\omega(G)$ is the clique number, and $\alpha(G)$ is the independence number of G. The call `ChromaticNumber(G, bound)` calculates and returns the bounds without searching for the chromatic number. The commands `IsKColorable` and `IsKEdgeColorable` can be used to check if a graph is k-colorable or edge k-colorable for a fixed number k.

Circular colorings of graphs are also supported in the `GraphTheory` package. The commands `CircularChromaticNumber` and `CircularChromaticIndex` return the circular chromatic number and the circular edge chromatic number of a given graph along with the corresponding optimal circular colorings. The commands `IsKDColorable` and `IsKDEdgeColorable` are used to check (k, d)-colorability or edge (k, d)-colorability for a fixed pair (k, d) of integers.

From König's theorem we know that the chromatic index of every bipartite graph is equal to the maximum degree of a vertex in the graph. This theorem gives a polynomial-time algorithm for obtaining an optimal edge coloring of a bipartite graph. This algorithm is based on the maximum bipartite matching algorithm implemented in the `GraphTheory` package in the command `BipartiteMatching`. The `ChromaticIndex` command uses this method to obtain optimal edge colorings of bipartite graphs in polynomial time.

These commands along with the `ImportGraph` and `ExportGraph` commands, and definitions of some families of snarks in `SpecialGraphs`, provide a good collection of tools for teaching and research in graph coloring.

5 Networks

There are four commands in the `GraphTheory` package for dealing with networks. They are `IsNetwork`, `RandomNetwork`, `MaxFlow` and `DrawNetwork`.

Here we define a network to be a directed graph with at least one source and one sink. A source is a vertex of the network with no incoming arcs and a sink is a vertex with no outgoing arcs.

5.1 Network Test

The command IsNetwork is used to test whether a graph is a network or not. The command can also be used to determine whether a graph with two specified sets of vertices as sources and sinks is a network or not.

```
> N := Digraph({[a,b], [c,d], [b,d], [d,e]});
```
$N := \mathit{Graph}\ 1 : \mathit{a\ directed\ unweighted\ graph\ with}\ 5\ \mathit{vertices\ and}\ 4\ \mathit{arc(s)}$
```
> IsNetwork(N);
```
$\mathit{true}, \{c, a\}, \{e\}$
```
> IsNetwork(N, a, d);
```
false
```
> IsNetwork(N, c, e);
```
true

5.2 Generating Random Networks

The command RandomNetwork can be used to create a random network with specified set or number of vertices. The generated Network has exactly one source and one sink.

We partition the vertices of the network into *levels*. The source and sink are in the first and last levels respectively. If u and v are two vertices in the network, if there is an arc from u to v and u belongs to the ith level then v must be in the $(i+1)$st level.

The user can specify the number of levels in the generated network with an argument p which is a number between 0 and 1. The larger p is, the larger the number of levels will be. For example for $p = 1$ the number of levels would be exactly the number of vertices and the ith level will only has the ith vertex as its member.

There is also an optional argument q which determines the probability of having an arc between each pair of vertices. The generated network can be forced to be weighted or acyclic by adding each of these terms in the list of arguments.

```
> N := RandomNetwork(10, 0.3);
> IsNetwork(N);
```
$\mathit{true}, \{1\}, \{10\}$
```
> N := RandomNetwork(10, 0.3, acyclic, weighted);
> IsNetwork(N);
```
$\mathit{true}, \{1\}, \{10\}$
```
> MaxFlow(N, 1, 10);
```
1.119382241

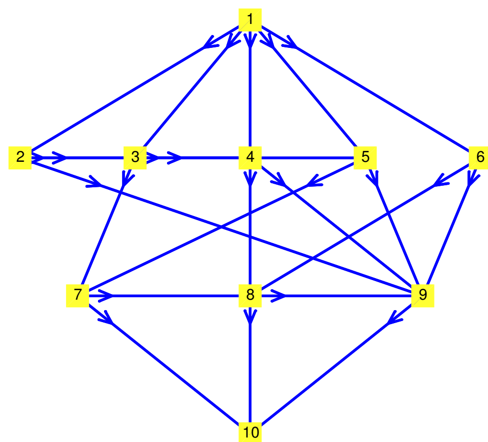
5.3 Drawing Networks

The `GraphTheory` package includes a command named `DrawNetwork` for displaying networks. The user can specify the set of vertices for sources and sinks of the network, otherwise the sets of **all** possible sources and sinks will be chosen. The user can also choose the network to be displayed either horizontally or vertically.

```
> N := RandomNetwork(10, 0.3, .4, acyclic);
```

$N := \mathit{Graph}\ 2 : \mathit{a\ directed\ unweighted\ graph\ with}\ 10\ \mathit{vertices\ and}\ 34\ \mathit{arc(s)!}$

```
> DrawNetwork(N);
```



6 The `ImportGraph` and `ExportGraph` Commands

The `ImportGraph` and `ExportGraph` commands provide a way to read graphs from files into the `GraphTheory` package and to output graphs to files in some formats. One format is used in the DIMACS graph coloring challenge. For example the command

```
ExportGraph(SpecialGraphs:-CycleGraph(5), "C5.col", dimacs)
```

generates a file `C5.col` in the current working directory with the following contents:

```
c Generated by the Maple GraphTheory package
p edge 5 10
e 2 3
e 3 2
e 1 2
e 2 1
e 3 4
e 4 3
```

```
e 1 5
e 5 1
e 4 5
e 5 4
```

This file may be read into the `GraphTheory` package using the command

`ImportGraph("C5.col", dimacs).`

Another format supported by the `ImportGraph` and `ExportGraph` commands is the format used by the Mathematica package “Combinatorica”.

`ExportGraph` also supports export to MetaPost. The resulting file may be compiled using the `mpost` command (in Unix systems, for other systems refer to your LaTeXmanual). Figure 1 shows the final result of the following commands.

```
> G := SpecialGraphs:-DoubleStarSnark();
> ExportGraph(G, "dblstar.mp", metapost);
```

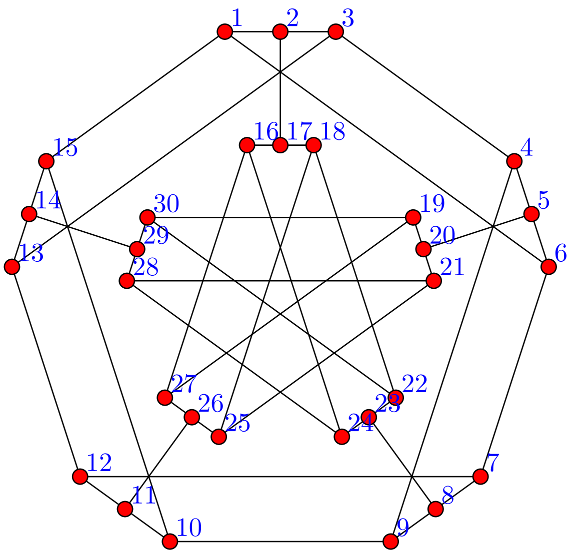


Figure 1: The double-star snark exported to MetaPost

The MetaPost file generated by `ExportGraph` may be edited to customize the result. For example one may remove some vertex labels or change the size of the vertices.

7 List of Commands

`AcyclicPolynomial`
`AddArc`
`GetVertexPositions`
`Girth`
`MakeDirected`
`MakeWeighted`

AddEdge
AddVertex
AdjacencyMatrix
AllPairsDistance
Arrivals
ArticulationPoints
BiconnectedComponents
BipartiteMatching
Blocks
CartesianProduct
CharacteristicPolynomial
ChromaticIndex
ChromaticNumber
ChromaticPolynomial
CircularChromaticIndex
CircularChromaticNumber
CircularEdgeChromaticNumber
CliqueNumber
ClosedNeighborhood
CompleteGraph
ConnectedComponents
Contract
CopyGraph
CycleBasis
CycleGraph
Deck
Degree
DegreeSequence
DeleteArc
DeleteEdge
DeleteVertex
Departures
Diameter
Digraph
DiscardEdgeAttribute
DiscardVertexAttribute
Distance
DrawGraph
DrawNetwork
EdgeChromaticNumber
EdgeConnectivity
Graph
GraphComplement
GraphDifference
GraphJoin
GraphPolynomial
GraphPower
GraphRank
GraphSpectrum
GraphSum
GraphUnion
GreedyColor
Head
HighlightEdge
HighlightVertex
ImportGraph
InDegree
IncidenceMatrix
IncidentEdges
IndependenceNumber
InducedSubgraph
Internal
IsAcyclic
IsBiconnected
IsBipartite
IsClique
IsConnected
IsCutSet
IsDirected
IsEulerian
IsForest
IsGraphicSequence
IsHamiltonian
IsIntegerGraph
IsKColorable
IsKDColorable
IsKDEdgeColorable
IsKEdgeColorable
IsNetwork
IsPlanar
IsRegular
IsStronglyConnected
MaxFlow
MaximumClique
MaximumDegree
MaximumIndependentSet
MinimalSpanningTree
MinimumDegree
Mycielski
Neighbors
NumberOfEdges
NumberOfSpanningTrees
NumberOfVertices
OptimalEdgeColoring
OptimalVertexColoring
OutDegree
PermuteVertices
PrimsAlgorithm
RandomBipartiteGraph
RandomDigraph
RandomGraph
RandomNetwork
RandomTournament
RandomTree
RankPolynomial
RelabelVertices
SeidelSpectrum
SeidelSwitch
SequenceGraph
SetEdgeAttribute
SetEdgeWeight
SetVertexAttribute
SetVertexPositions
ShortestPath
SpanningPolynomial
SpanningTree
StronglyConnectedComponents
Subdivide
Subgraph
Tail
TopologicalSort
TravelingSalesman
TreeHeight

`Edges`	`IsTree`	`TuttePolynomial`
`ExportGraph`	`IsTwoEdgeConnected`	`TwoEdgeConnectedComponents`
`FlowPolynomial`	`IsWeighted`	`UnderlyingGraph`
`FundamentalCycle`	`Join`	`VertexConnectivity`
`GetEdgeAttribute`	`KruskalsAlgorithm`	`Vertices`
`GetEdgeWeight`	`LineGraph`	`WeightMatrix`
`GetVertexAttribute`		

References

[1] J. Farr, M. Khatirinejad, S. Khodadad, M. Monagan, A Graph Theory Package for Maple, Proceedings of the 2005 Maple Conference, pp. 260-271, Maplesoft, 2005.