

# Package ‘mwcsr’

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**Title** Solvers for Maximum Weight Connected Subgraph Problem and Its Variants

**Version** 0.1.11

**Description** Algorithms for solving various Maximum Weight Connected Subgraph Problems, including variants with budget constraints, cardinality constraints, weighted edges and signals. The package represents an R interface to high-efficient solvers based on relax-and-cut approach (Álvarez-Miranda E., Sinnl M. (2017) <[doi:10.1016/j.cor.2017.05.015](https://doi.org/10.1016/j.cor.2017.05.015)>) mixed-integer programming (Loboda A., Artyomov M., and Sergushichev A. (2016) <[doi:10.1007/978-3-319-43681-4\\_17](https://doi.org/10.1007/978-3-319-43681-4_17)>) and simulated annealing.

**Depends** R (>= 3.5)

**Imports** methods, igraph, Rcpp

**Suggests** knitr, rmarkdown, mathjaxr, testthat, BioNet, roxygen2, DLBCL

**SystemRequirements** Java (>=8)

**License** MIT + file LICENSE

**Encoding** UTF-8

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**VignetteBuilder** knitr, rmarkdown

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**BugReports** <https://github.com/ctlab/mwcsr/issues>

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## Contents

annealing_solver . . . . .	2
bionet_example . . . . .	4
gam_example . . . . .	4
gatom_example . . . . .	5
get_instance_type . . . . .	5
get_weight . . . . .	6
gmwcs_example . . . . .	6
gmwcs_small_instance . . . . .	7
mwcs_example . . . . .	7
mwcs_small_instance . . . . .	7
normalize_sgmwcs_instance . . . . .	8
parameters . . . . .	9
rmwcs_solver . . . . .	9
rnc_solver . . . . .	11
scipjack_solver . . . . .	12
set_parameters . . . . .	12
sgmwcs_example . . . . .	13
sgmwcs_small_instance . . . . .	13
solve_mwmsp . . . . .	14
timelimit<- . . . . .	15
virgo_solver . . . . .	16
<b>Index</b>	<b>18</b>

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annealing_solver	<i>Construct an annealing solver</i>
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## Description

Simulated annealing is a heuristic method of solving optimization problems. Typically, it allows to find some good solution in a short time. This implementation doesn't compute any upper bound on solution, so there is no guarantee of optimality of solution provided.

**Usage**

```
annealing_solver(  
    schedule = c("fast", "boltzmann"),  
    initial_temperature = 1,  
    final_temperature = 1e-06,  
    verbose = FALSE  
)
```

**Arguments**

schedule	boltzmann annealing or fast annealing
initial_temperature	initial value for the temperature
final_temperature	final value for the temperature
verbose	whether be verbose or not

**Details**

Algorithm maintains connected subgraph starting with empty subgraph. Each iteration one random action is considered. It may be a removal of a vertex or an edge which does not separate graph or addition of an extra vertex or an edge neighboring existing graph. If the subgraph is empty all vertices are considered as candidates to form a subgraph. After candidate is chosen two subgraph scores are considered: for a new subgraph and for an old one. Simulated annealing operates with a notion of temperature. The candidate action is accepted with probability:  $p(S'|S) = \exp(-E / T)$ , where  $E$  is weight difference between subgraphs and  $T$  is current temperature.

Temperature is calculated in each iteration. in `mwcsr` there are two temperature schedules supported. So called Boltzmann annealing uses the formula:  $T(k) = T_0 / (\ln(1 + k))$ , while in case of fast annealing this one is used:  $T(k) = T_0 / k$ , where  $k$  is iteration number.

To tune the algorithm it is useful to realize how typical changes in the goal function for single actions are distributed. Calculating the acceptance probabilities at initial temperature and final temperatures may help to choose schedule and temperatures.

**Value**

An object of class `mwcs_solver`

**See Also**

[rnc\\_solver](#) will probably be a better choice with minimal tuning necessary

---

bionet_example	<i>Example MWCS instance obtained from BioNet package tutorial</i>
----------------	--

---

**Description**

Example MWCS instance obtained from BioNet package tutorial

**Usage**

bionet\_example

**Format**

An object of class igraph of length 2559.

---

gam_example	<i>GAM instance for MWCS problem</i>
-------------	--------------------------------------

---

**Description**

A dataset containing some real-world instances appeared in network enrichment analysis tool Shiny GAM ([doi:10.1093/nar/gkw266](https://doi.org/10.1093/nar/gkw266)).

**Usage**

gam\_example

**Format**

A vector of named vertex-weighted igraph instances

**Source**

<http://dimacs11.zib.de/instances/MWCS-GAM.zip>

---

gatom_example	<i>Example of graph from which an SGMWCS instance can be obtained</i>
---------------	---

---

**Description**

The graph is based on gatom package

**Usage**

```
gatom_example
```

**Format**

An object of class `igraph` of length 194.

---

get_instance_type	<i>Check the type and the validity of an MWCS instance</i>
-------------------	--

---

**Description**

Check the type and the validity of an MWCS instance

**Usage**

```
get_instance_type(instance)
```

**Arguments**

`instance` `igraph` object, containing an instance to be checked

**Value**

A list with members `type` containing the type of the instance, `valid` – boolean flag indicating whether the instance is valid or not, `errors` – a character vector containing the error messages

A list with two fields: the type of the instance with which it will be treated by `solve_mwscsp` function and boolean showing validness of the instance.

**Examples**

```
data(mwcs_example)
get_instance_type(mwcs_example)
```

`get_weight`                    *Calculate weight of the solution. MWCS, GMWCS and SGMWCS instances are supported*

---

**Description**

Calculate weight of the solution. MWCS, GMWCS and SGMWCS instances are supported

**Usage**

```
get_weight(solution)
```

**Arguments**

`solution`                    Either `mwcs_solution` or `'igraph'` object representing the solution

**Value**

Weight of the subgraph

---

`gmwcs_example`                    *Example GMWCS instance*

---

**Description**

Instance is based on `gatom` package.

**Usage**

```
gmwcs_example
```

**Format**

An object of class `igraph` of length 194.

---

gmwcs\_small\_instance    *Small example of GMWCS instance for demonstration purposes.*

---

**Description**

Small example of GMWCS instance for demonstration purposes.

**Usage**

gmwcs\_small\_instance

**Format**

An object of class igrph of length 5.

---

mwcs\_example            *Example MWCS instance*

---

**Description**

Instance is based on gatom package.

**Usage**

mwcs\_example

**Format**

An object of class igrph of length 194.

---

mwcs\_small\_instance    *Small example of MWCS instance for demonstration purposes.*

---

**Description**

Small example of MWCS instance for demonstration purposes.

**Usage**

mwcs\_small\_instance

**Format**

An object of class igrph of length 5.

---

```
normalize_sgmwcs_instance
```

*Helper function to convert an igraph object into a proper SGMWCS instance*

---

### Description

This function generates new igraph object with additional signals field added. The way the instance is constructed is defined by the function parameters. Nodes and edges are grouped separately, grouping columns are defined by `nodes.group.by` and `edges.group.by` arguments. `group.only.positive` param specifies whether to group only positive-weighted (specified by `nodes/edges.weight.column`) nodes and edges.

### Usage

```
normalize_sgmwcs_instance(
  g,
  nodes.weight.column = "weight",
  edges.weight.column = "weight",
  nodes.group.by = "signal",
  edges.group.by = "signal",
  group.only.positive = TRUE
)
```

### Arguments

```
g           Graph to convert
nodes.weight.column  Nodes column name (e.g. weight, score, w) for scoring
edges.weight.column  Edges column name for scoring
nodes.group.by  Nodes grouping column (e.g. signal, group, class)
edges.group.by  Edges grouping column
group.only.positive  Whether to group only positive-scored nodes/edges#'
```

### Value

An igraph object with proper attributes set.

### Examples

```
data("gatom_example")
normalize_sgmwcs_instance(gatom_example)
```

---

parameters	<i>The method returns all parameters supported by specific solver</i>
------------	---

---

**Description**

The method returns all parameters supported by specific solver

**Usage**

```
parameters(solver)
```

**Arguments**

solver            a solver object

**Value**

A table containing parameter names and possible values for each parameter.

---

rmwcs_solver	<i>Generate a rmwcs solver</i>
--------------	--------------------------------

---

**Description**

The method is based on relax-and-cut approach and allows to solve Maximum Weight Subgraph Problem and its budget and cardinality variants. By constructing lagrangian relaxation of MWCS problem necessary graph connectivity constraints are introduced in the objective function giving upper bound on the weight of the optimal solution. On the other side, primal heuristic uses individual contribution of the variables to lagrangian relaxation to find possible solution of the initial problem. The relaxation is then optimized by using iterative subgradient method.

**Usage**

```
rmwcs_solver(
  timelimit = 1800L,
  max_iterations = 1000L,
  beta_iterations = 5L,
  separation = "strong",
  start_constraints = TRUE,
  pegging = TRUE,
  max_age = 10,
  sep_iterations = 10L,
  sep_iter_freeze = 50L,
  heur_iterations = 10L,
  subgradient = "classic",
  beta = 2,
  verbose = FALSE
)
```

**Arguments**

timelimit	Timelimit in seconds
max_iterations	Maximum number of iterations
beta_iterations	Number of nonimproving iterations until beta is halved
separation	Separation: "strong" or "fast"
start_constraints	Whether to add flow-conservation/degree constraints at start
pegging	variable fixing
max_age	number of iterations in aging procedure for non-violated cuts
sep_iterations	Frequency of separating cuts (in iterations)
sep_iter_freeze	Number of iterations when a newly separated cut is unaffected by subgradient algorithm.
heur_iterations	Frequency of calling heuristic method (in iterations)
subgradient	Subgradient: "classic", "average", "cft"
beta	Initial step size of subgradient algorithm
verbose	Should the solving progress and stats be printed?

**Details**

One iteration of algorithm includes solving lagrangian relaxation and updating lagrange multipliers. It may also contain cuts (or connectivity constraints) separation process, run of heuristic method, variable fixing routine. The initial step size for subgradient method can be passed as beta argument. If there is no improvement in upper bound in consecutive beta\_iterations iterations the step size is halved. There are three possible strategies for updating multipliers. See the references section for the article where differences are discussed.

Some initial cuts are added at the start of the algorithm if start\_constraints is set to TRUE. Other constraints are separated on the fly and are unaffected in the next sep\_iter\_freeze iterations of the subgradient method. Then the corresponding lagrange multipliers are updated from iteration to iteration. Aging procedure for cuts is incorporated in the algorithm meaning constraint multipliers are updated for non-violated cuts for up to max\_age iterations from the point where a cut was violated last time. There are two separation methods implemented: fast and strong, where the latter is supposed to minimize number of variables used in generated constraint while in the former case there is no need to explore whole graph to construct a constraint.

A variant of MST approximation of PCSTP is used as Primal Heuristic. See references for more details.

The frequencies of running separation process and heuristic are specified in sep\_iterations and heur\_iterations.

**Value**

An object of class mwcs\_solver.

## References

Álvarez-Miranda E., Sinnl M. (2017) "A Relax-and-Cut framework for large-scale maximum weight connected subgraph problems" [doi:10.1016/j.cor.2017.05.015](https://doi.org/10.1016/j.cor.2017.05.015)

---

rnc\_solver

*Construct relax-and-cut SGMWCS solver*

---

## Description

The solver is based on the same approach as rmwcs solver. Modifications to the original scheme are introduced to tackle problems arising with introduction of edge weights and signals. It is recommended to use rmwcs solver to solve MWCS problems, while due to differences in primal heuristic it may be a good practice to run both solvers on the same problem.

## Usage

```
rnc_solver(  
  max_iterations = 1000L,  
  beta_iterations = 50L,  
  heur_iterations = 10L,  
  sep_iterations = 10L,  
  verbose = FALSE  
)
```

## Arguments

max_iterations	Maximum number of iterations
beta_iterations	Number of nonimproving iterations until beta is halved
heur_iterations	Frequency of calling heuristic method (in iterations)
sep_iterations	Frequency of separating cuts (in iterations)
verbose	Should the solving progress and stats be printed?

## Value

An object of class `mwcs_solver`

## See Also

[rmwcs\\_solver](#)

---

scipjack_solver	<i>Construct a SCIP-jack solver</i>
-----------------	-------------------------------------

---

### Description

This solver requires the STP extension of the SCIP-jack solver. To use this class you first need to download and build SCIP-jack and SCIPSTP application.

### Usage

```
scipjack_solver(scipstp_bin, config_file = NULL)
```

### Arguments

scipstp_bin	path to scipstp binary.
config_file	scipstp-formatted file. Parameter names and values follow the SCIP configuration format.

### Details

You can access solver directly using `run_scip` function. See example.

### References

Rehfeldt D., Koch T. (2019) "Combining NP-Hard Reduction Techniques and Strong Heuristics in an Exact Algorithm for the Maximum-Weight Connected Subgraph Problem." [doi:10.1137/17M1145963](https://doi.org/10.1137/17M1145963)

### Examples

```
## Not run:
data("bionet_example")
scip <- scipjack_solver(scipstp_bin='/path/to/scipoptsuite/build/bin/applications/scipstp')
sol <- solve_mwcsp(scip, bionet_example)

## End(Not run)
```

---

set_parameters	<i>Sets values of specific parameters</i>
----------------	---

---

### Description

Sets values of specific parameters

### Usage

```
set_parameters(solver, ...)
```

**Arguments**

solver            a solver  
 ...                listed parameter names and values assigned to them

**Value**

The solver with parameters changed.

---

sgmwcs\_example        *Example SGMWCS instance*

---

**Description**

Instance is based on gatom package.

**Usage**

sgmwcs\_example

**Format**

An object of class igraph of length 194.

---

sgmwcs\_small\_instance    *Small example of SGMWCS instance for demonstration purposes.*

---

**Description**

Small example of SGMWCS instance for demonstration purposes.

**Usage**

sgmwcs\_small\_instance

**Format**

An object of class igraph of length 6.

---

solve_mwesp	<i>Solves a MWCS instance.</i>
-------------	--------------------------------

---

### Description

Generic function for solving MWCS instances using solvers collected in the package.

### Usage

```
solve_mwesp(solver, instance, ...)

## S3 method for class 'virgo_solver'
solve_mwesp(solver, instance, ...)

## S3 method for class 'rmwesp_solver'
solve_mwesp(solver, instance, max_cardinality = NULL, budget = NULL, ...)

## S3 method for class 'rnc_solver'
solve_mwesp(solver, instance, ...)

## S3 method for class 'simulated_annealing_solver'
solve_mwesp(solver, instance, warm_start, ...)

## S3 method for class 'scipjack_solver'
solve_mwesp(solver, instance, ...)
```

### Arguments

<code>solver</code>	a solver object returned by <code>rmwesp_solver</code> , <code>annealing_solver</code> , <code>rnc_solver</code> or <code>virgo_solver</code> .
<code>instance</code>	an MWCS instance, an <code>igraph</code> object with problem-related vertex, edge and graph attributes. See details.
<code>...</code>	other arguments to be passed.
<code>max_cardinality</code>	integer maximum number of vertices in solution.
<code>budget</code>	numeric maximum budget of solution.
<code>warm_start</code>	warm start solution, an object of the class <code>mwesp_solution</code> .

### Details

MWCS instance here is represented as an undirected graph, an `igraph` object. The package supports four types of instances: Simple MWCS, Generalized MWCS, Budget MWCS, signal MWCS problems. All the necessary weights and costs are passed by setting vertex and edge attributes. See [get\\_instance\\_type](#) to check if the `igraph` object is a correct MWCS instance. For Simple MWCS problem numeric vertex attribute `weight` must be set. For generalized version weights can be provided for edges. For budget version of the problem in addition to vertex weights it is required that `igraph` object would have `budget_cost` vertex attribute with positive numeric values.

Signal MWCS instance is quite different. There is no `weight` attribute for neither vertices nor edges. Instead, vertex and edge attribute `signal` should be provided with signal names. A numeric vector containing weights for the signals should be assigned to graph attribute `signals`.

See vignette for description of the supported problems. See `igraph` package documentation for more details about getting/setting necessary attributes.

### Value

An object of class `mwcs_solution` consisting of resulting subgraph, its weight and other information about solution provided.

### Examples

```
library(igraph)

# for a MWCS instance

data(mwcs_example)
head(V(mwcs_example)$weight)

# for a GMWCS instance
data(gmwcs_example)
head(E(gmwcs_example)$weight)

# for a SGMWCS instance
data(sgmwcs_example)
head(V(sgmwcs_example)$signal)
head(E(sgmwcs_example)$signal)

head(sgmwcs_example$signals)
```

---

<code>timelimit&lt;-</code>	<i>Sets time limitation for a solver</i>
-----------------------------	--

---

### Description

Sets time limitation for a solver

### Usage

```
timelimit(x) <- value
```

### Arguments

<code>x</code>	a variable name.
<code>value</code>	a value to be assigned to <code>x</code> .

**Value**

The solver with new timelimit set.

---

virgo_solver	<i>Construct a virgo solver</i>
--------------	---------------------------------

---

**Description**

This solver uses reformulation of MWCS problem in terms of mixed integer programming. The later problem can be efficiently solved with commercial optimization software. Exact version of solver uses CPLEX and requires it to be installed. CPLEX 12.7.1 or higher is required.

**Usage**

```
virgo_solver(
  cplex_dir,
  threads = parallel::detectCores(),
  timelimit = NULL,
  penalty = 0,
  memory = "2G",
  log = 0,
  cplex_bin = NULL,
  cplex_jar = NULL,
  mst = FALSE,
  dryrun = FALSE,
  jvmargs = NULL
)
```

**Arguments**

cplex_dir	a path to dir containing cplex_bin and cplex_jar, setting this to NULL sets mst param to TRUE
threads	number of threads for simultaneous computation
timelimit	maximum number of seconds to solve the problem
penalty	additional edge penalty for graph edges
memory	maximum amount of memory(-Xmx flag)
log	verbosity level
cplex_bin	a path to cplex binary dir
cplex_jar	a path to cplex jar file
mst	whether to use approximate MST solver, no CPLEX files required with this parameter is set to TRUE
dryrun	if set to TRUE only prints the solver command, without actually running it
jvmargs	character vector with additional arguments for Java Virtual Machine

**Details**

The solver currently does not support repeated negative signals, i.e. every negative signal should be present only once among all edges and vertices.

You can access solver directly using `run_main` function. See example.

**Value**

An object of class `mwcs_solver`.

**References**

Loboda A., Artyomov M., and Sergushichev A. (2016) "Solving generalized maximum-weight connected subgraph problem for network enrichment analysis" [doi:10.1007/9783319436814\\_17](https://doi.org/10.1007/9783319436814_17)

**Examples**

```
data("sgmwcs_small_instance")
approx_vs <- virgo_solver(mst=TRUE, threads = 1)
approx_vs$run_main("-h")
sol <- solve_mwvsp(approx_vs, sgmwcs_small_instance)
## Not run:
vs <- virgo_solver(cplex_dir='/path/to/cplex')
sol <- solve_mwvsp(vs, sgmwcs_example)

## End(Not run)
```

# Index

## \* datasets

- bionet\_example, 4
- gam\_example, 4
- gatom\_example, 5
- gmwcs\_example, 6
- gmwcs\_small\_instance, 7
- mwcs\_example, 7
- mwcs\_small\_instance, 7
- sgmwcs\_example, 13
- sgmwcs\_small\_instance, 13

annealing\_solver, 2

bionet\_example, 4

gam\_example, 4

gatom\_example, 5

get\_instance\_type, 5, 14

get\_weight, 6

gmwcs\_example, 6

gmwcs\_small\_instance, 7

mwcs\_example, 7

mwcs\_small\_instance, 7

normalize\_sgmwcs\_instance, 8

parameters, 9

rmwcs\_solver, 9, 11

rnc\_solver, 3, 11

scipjack\_solver, 12

set\_parameters, 12

sgmwcs\_example, 13

sgmwcs\_small\_instance, 13

solve\_mwvsp, 14

timelimit<-, 15

virgo\_solver, 16