

Package ‘mwcsr’

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Title Solvers for Maximum Weight Connected Subgraph Problem and Its Variants

Version 0.1.7

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)

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VignetteBuilder knitr

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

LinkingTo Rcpp

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annealing_solver	<i>Construct an annealing solver</i>
------------------	--------------------------------------

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>
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Description

A dataset containing some real-world instances appeared in network enrichment analysis tool [Shiny GAM](#)

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>
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Description

This solver requires STP extension of **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. Parameters list is accessible at [Official SCIP website](#).

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](#)

Examples

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

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

`timelimit<-` *Sets time limitation for a solver*

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(approx_vs, sgmwcs_example)

## End(Not run)
```

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