Package ‘mwcsr’

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Title Solvers for Maximum Weight Connected Subgraph Problem and Its Variants

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R topics documented:

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_mwesp .................................................. 14	timelimit<- .................................................. 15
virgo_solver .................................................. 16

Index 18

annealing_solver Construct an annealing solver

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 staring 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 subgaph. 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 \texttt{mwcsr} there are two temperature schedules supported. So called Boltmann 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 \texttt{mwcs_solver}

See Also

\texttt{rnc_solver} will probably be a better choice with minimal tuning necessary
<table>
<thead>
<tr>
<th>bionet_example</th>
<th>Example MWCS instance obtained from BioNet package tutorial</th>
</tr>
</thead>
</table>

**Description**

Example MWCS instance obtained from BioNet package tutorial

**Usage**

bionet_example

**Format**

An object of class igraph of length 2559.

<table>
<thead>
<tr>
<th>gam_example</th>
<th>GAM instance for MWCS problem</th>
</tr>
</thead>
</table>

**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
Example of graph from which an SGMWCS instance can be obtained

**Description**

The graph is based on gatom package

**Usage**

```r
gatom_example
```

**Format**

An object of class igraph of length 194.

Check the type and the validity of an MWCS instance

**Description**

Check the type and the validity of an MWCS instance

**Usage**

```r
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_mwcsp function and boolean showing validness of the instance.

**Examples**

```r
data(mwcs_example)
get_instance_type(mwcs_example)
```
get_weight

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

Usage
get_weight(solution)

Arguments
solution Either mwcsp_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

**Description**

Small example of GMWCS instance for demonstration purposes.

**Usage**

```r
gmwcs_small_instance
```

**Format**

An object of class `igraph` of length 5.

---

### mwcs_example

**Description**

Example MWCS instance

**Usage**

```r
mwcs_example
```

**Format**

An object of class `igraph` of length 194.

---

### gmwcs_small_instance

**Description**

Small example of MWCS instance for demonstration purposes.

**Usage**

```r
mwcs_small_instance
```

**Format**

An object of class `igraph` 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

The method returns all parameters supported by specific solver.

**Usage**

```r
parameters(solver)
```

**Arguments**

- **solver** — a solver object

**Value**

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

### rmwcs_solver

Generate a rmwcs solver.

**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**

```r
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

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

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

---

**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**

```r
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

Construct a SCIP-jack solver

#### 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

```r
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](https://scipopt.org). 

#### Details

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

#### References


#### Examples

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

## End(Not run)
```

### set_parameters

Sets values of specific parameters

#### Description

Sets values of specific parameters

#### Usage

```r
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_mwcsp**

Solves a MWCS instance.

---

**Description**

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

**Usage**

```r
solve_mwcsp(solver, instance, ...)
```

## S3 method for class 'virgo_solver'
```r
solve_mwcsp(solver, instance, ...)
```

## S3 method for class 'rmwcs_solver'
```r
solve_mwcsp(solver, instance, max_cardinality = NULL, budget = NULL, ...)
```

## S3 method for class 'rnc_solver'
```r
solve_mwcsp(solver, instance, ...)
```

## S3 method for class 'simulated_annealing_solver'
```r
solve_mwcsp(solver, instance, warm_start, ...)
```

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

**Arguments**

- `solver`: a solver object returned by rmwcs_solver, annealing_solver, rnc_solver or virgo_solver.
- `instance`: an MWCS instance, an igraph 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 mwcsp_solution.

**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 necesasry attributes.

Value

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

Examples

```r
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**

- `x` a variable name.
- `value` a value to be assigned to `x`.  

Value

The solver with new timelimit set.

---

Construct a virgo solver

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

```r
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**


**Examples**

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

get_instance_type, 5, 14

gatom_example, 5

get_weight, 6

gmwcs_example, 6

normalize_sgmwcs_instance, 8

parameters, 9

rmwcs_solver, 9, 11

rnc_solver, 3, 11

scipjack_solver, 12

set_parameters, 12

sgmwcs_example, 13

solve_mwcsp, 14

timelimit<-, 15

virgo_solver, 16