Package ‘mwcsr’

July 12, 2022

Title Solvers for Maximum Weight Connected Subgraph Problem and Its Variants

Version 0.1.6


Depends R (>= 3.5)

Imports methods, igraph, Rcpp

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

SystemRequirements C++11, Java (>=8)

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Encoding UTF-8

LazyData true

RoxygenNote 7.1.2

VignetteBuilder knitr

URL https://github.com/ctlab/mwcsr

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

LinkingTo Rcpp

NeedsCompilation yes

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Date/Publication  2022-07-12 17:50:02 UTC

R topics documented:

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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 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 mwcs_solver

See Also

rnc_solver will probably be a better choice with minimal tuning necessary
### bionet_example

*Example MWCS instance obtained from BioNet package tutorial*

**Description**

Example MWCS instance obtained from BioNet package tutorial

**Usage**

`bionet_example`

**Format**

An object of class `igraph` of length 10.

---

### gam_example

*GAM instance for MWCS problem*

**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**

Example of graph from which an SGMWCS instance can be obtained

Description
The graph is based on gatom package

Usage

gatom_example

Format
An object of class igraph of length 10.

Check the type and the validity of an MWCS instance

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_mwcsp 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 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 10.
**gmwcs_small_instance**

Small example of GMWCS instance for demonstration purposes.

**Usage**

```
gmwcs_small_instance
```

**Format**

An object of class `igraph` of length 10.

---

**mwcs_example**

Example MWCS instance

**Description**

Instance is based on gatom package.

**Usage**

```
mwcs_example
```

**Format**

An object of class `igraph` of length 10.

---

**gmwcs_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 `igraph` of length 10.
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**

```r
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**

```r
data("gatom_example")
normalize_sgmwcs_instance(gatom_example)
```
parameters

---

The method returns all parameters supported by specific solver

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

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
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.
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://scip.zib.de/).

**Details**

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

**References**


**Examples**

```r
## Not run:
data("bionet_example")
s SCIP <- scipjack_solver(scipstp_bin="/path/to/scipoptsuite/build/bin/applications/scipstp")
sol <- solve_mwcsp(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**

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>solver</td>
<td>a solver</td>
</tr>
<tr>
<td>...</td>
<td>listed parameter names and values assigned to them</td>
</tr>
</tbody>
</table>

**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 10.

---

**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 10.
solve_mwcsp  Solves a MWCS instance.

Description

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

Usage

solve_mwcsp(solver, instance, ...)

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

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

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

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

## S3 method for class 'scipjack_solver'
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 necessary attributes.

Value

An object of class mwcsp_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

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,  # a path to dir containing cplex_bin and cplex_jar, setting this to NULL sets mst`` param to TRUE'
  threads = parallel::detectCores(),
  timelimit = NULL,
  penalty = 0,
  memory = "2G",
  log = 0,
  cplex_bin = NULL,
  cplex_jar = NULL,
  mst = FALSE
)
```

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

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.
**virgo_solver**

**Value**

An object of class `mwcs_solver`.

**References**


**Examples**

```r
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)
```
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