Package 'rang'

October 8, 2023

```
Title Reconstructing Reproducible R Computational Environments
```

Version 0.3.0

```
Description Resolve the dependency graph of R packages at a specific time point based on the information from various 'R-hub' web services <a href="https://blog.r-hub.io/">https://blog.r-hub.io/</a>. The dependency graph can then be used to reconstruct the R computational environment with 'Rocker' <a href="https://rocker-project.org">https://rocker-project.org</a>.
```

```
License GPL (>= 3)
Encoding UTF-8
RoxygenNote 7.2.3
URL https://github.com/gesistsa/rang
BugReports https://github.com/gesistsa/rang/issues
Suggests knitr, rmarkdown, testthat (>= 3.0.0)
Config/testthat/edition 3
Imports parsedate, fastmap, jsonlite, memoise, pkgsearch, remotes,
      utils, httr, vctrs, renv, here
Depends R (>= 3.5.0)
VignetteBuilder knitr
LazyData true
NeedsCompilation no
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apptainerize

Create an Apptainer/Singularity Definition File of The Resolved Result

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Description

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This function exports the result from resolve() to an Apptainer/Singularity definition file. For R version \geq 3.1.0, the file is based on the versioned Rocker Docker image. For R version \leq 3.1.0, the Apptainer/Singularity definition is based on Debian and it compiles R from source.

Usage

```
apptainerize(
  rang,
  output_dir,
 materials_dir = NULL,
  post_installation_steps = NULL,
  image = c("r-ver", "rstudio", "tidyverse", "verse", "geospatial"),
  rang_as_comment = TRUE,
  cache = FALSE,
  verbose = TRUE,
  lib = NA,
  cran_mirror = "https://cran.r-project.org/",
  check_cran_mirror = TRUE,
  bioc_mirror = "https://bioconductor.org/packages/",
  no_rocker = FALSE,
  debian_version = c("lenny", "squeeze", "wheezy", "jessie", "stretch"),
  skip_r17 = TRUE,
  insert_readme = TRUE,
  copy_all = FALSE
```

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```
apptainerize_rang(...)
    apptainerise(...)
    apptainerise_rang(...)
    singularize(...)
    singularize_rang(...)
    singularise(...)
    singularise_rang(...)
Arguments
    rang
                      output from resolve()
                      character, where to put the Apptainer/Singularity definition file and associated
    output_dir
                      content
    materials_dir
                      character, path to the directory containing additional resources (e.g. analysis
                      scripts) to be copied into output_dir and in turn into the Apptainer/Singularity
                      container
    post_installation_steps
                      character, additional steps to be added before the in the end of %post section the
                      Apptainer/Singularity definition file, see an example below
                      character, which versioned Rocker image to use. Can only be "r-ver", "rstudio",
    image
                      "tidyverse", "verse", "geospatial" This applies only to R version >= 3.1
    rang_as_comment
                      logical, whether to write resolved result and the steps to reproduce the file to
                      path as comment
    cache
                      logical, whether to cache the packages now. Please note that the system re-
                      quirements are not cached. For query with non-CRAN packages, this option
                      is strongly recommended. For query with local packages, this must be TRUE
                      regardless of R version. For R version < 3.1, this must be also TRUE if there is
                      any non-CRAN packages.
    verbose
                      logical, pass to install.packages(), the negated value is also passed as quiet
                      to both install.packages() and download.file().
    lib
                      character, pass to install.packages(). By default, it is NA (to install the
                      packages to the default location)
                      character, which CRAN mirror to use
    cran_mirror
```

logical, whether to skip using Rocker images even when an appropriate version is available. Please keep this as TRUE unless you know what you are doing

logical, whether to check the CRAN mirror

character, which Bioconductor mirror to use

check_cran_mirror

bioc_mirror

no_rocker

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debian_version	when Rocker images are not used, which EOL version of Debian to use. Can only be "lenny", "etch", "squeeze", "wheezy", "jessie", "stretch". Please keep this as default "lenny" unless you know what you are doing
skip_r17	logical, whether to skip R 1.7.x. Currently, it is not possible to compile R 1.7.x (R 1.7.0 and R 1.7.1) with the method provided by rang. It affects snapshot_date from 2003-04-16 to 2003-10-07. When skip_r17 is TRUE and snapshot_date is within the aforementioned range, R 1.8.0 is used instead
insert_readme	logical, whether to insert a README file
copy_all	logical, whether to copy everything in the current directory into the container. If inst/rang is detected in output_dir, this is coerced to TRUE.
	arguments to be passed to apptainerize

Details

The idea behind this is to determine the installation order of R packages locally. Then, the installation script can be deployed to another fresh R session to install R packages. dockerize() and apptainerize() are more reasonable ways because a fresh R session with all system requirements is provided. The current approach does not work in R < 2.1.0.

Value

```
output_dir, invisibly
```

References

Apptainer / Singularity

Kurtzer, G. M., Sochat, V., & Bauer, M. W. (2017) Singularity: Scientific containers for mobility of compute. PLOS ONE, 12(5):e0177459. doi:10.1371/journal.pone.0177459

The Rocker Project

Ripley, B. (2005) Packages and their Management in R 2.1.0. R News, 5(1):8–11.

See Also

```
resolve(), export_rang(), use_rang()
```

Examples

```
if (interactive()) {
    graph <- resolve(
        pkgs = c("openNLP", "LDAvis", "topicmodels", "quanteda"),
        snapshot_date = "2020-01-16"
    )
    apptainerize(graph, ".")
    ## An example of using post_installation_steps to install quarto
    install_quarto <- c("apt-get install -y curl git && \\
    curl -LO https://quarto.org/download/latest/quarto-linux-amd64.deb && \\
    dpkg -i quarto-linux-amd64.deb && \\</pre>
```

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```
quarto install tool tinytex")
apptainerize(graph, ".", post_installation_steps = install_quarto)
}
```

as_pkgrefs

Convert Data Structures into Package References

Description

This generic function converts several standard data structures into a vector of package references, which in turn can be used as the first argument of the function resolve(). This function guessimates the possible sources of the packages. But we strongly recommend manually reviewing the detected packages before using them for resolve().

Usage

```
as_pkgrefs(x, ...)
## Default S3 method:
as_pkgrefs(x, ...)
## S3 method for class 'character'
as_pkgrefs(x, bioc_version = NULL, no_enhances = TRUE, no_suggests = TRUE, ...)
## S3 method for class 'sessionInfo'
as_pkgrefs(x, ...)
```

Arguments

Х,	currently supported data structure(s) are: output from $sessionInfo()$, a character vector of package names
,	not used
bioc_version	character. When x is a character vector, version of Bioconductor to search for package names. NULL indicates not search for Bioconductor.
no_enhances	logical, when parsing DESCRIPTION, whether to ignore packages in the "Enhances" field
no_suggests	logical, when parsing DESCRIPTION, whether to ignore packages in the "Suggests" field

Value

a vector of package references

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Examples

```
as_pkgrefs(sessionInfo())
if (interactive()) {
    require(rang)
    graph <- resolve(as_pkgrefs(sessionInfo()))
    as_pkgrefs(c("rtoot"))
    as_pkgrefs(c("rtoot", "S4Vectors")) ## this gives cran::S4Vectors and is not correct.
    as_pkgrefs(c("rtoot", "S4Vectors"), bioc_version = "3.3") ## This gives bioc::S4Vectors
}</pre>
```

convert_edgelist

Convert Data Structures to rang edgelist

Description

This generic function converts several data structures provided by rang into an edgelist of package dependencies.

Usage

```
convert_edgelist(x, ...)
## Default S3 method:
convert_edgelist(x, ...)
## S3 method for class 'ranglet'
convert_edgelist(x, ...)
## S3 method for class 'rang'
convert_edgelist(x, ...)
```

Arguments

```
x, supported data structures are rang and ranglet S3 objects ..., not used
```

Details

the resulting data frame can be converted to an igraph object for plotting and analysis via the function igraph::graph_from_data_frame()

Value

a data frame of directed edges of dependencies

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Examples

create_turing

Create executable research compendium according to the Turing Way

Description

This usethis-style function creates an executable research compendium according to the Turing Way.

Usage

```
create_turing(
  path,
  add_rang = TRUE,
  add_makefile = TRUE,
  add_here = TRUE,
  verbose = TRUE,
  force = FALSE,
  apptainer = FALSE
)
```

Arguments

path	character, path to the project root
add_rang	logical, whether to run use_rang() to path
add_makefile	logical, whether to insert a barebone Makefile in the project root.
add_here	logical, whether to insert a hidden . here file in the project root
verbose	logical, whether to print out messages
force	logical, whether to overwrite files (inst/rang/update.R, Makefile, .here) if they exist.
apptainer	logical, whether to use apptainer. FALSE indicates using Docker

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Details

According to the Turing Way, an executable research compendium should have the following properties

- 1. Files should be organized in a conventional folder structure;
- 2. Data, methods, and output should be clearly separated;
- 3. The computational environment should be specified.

We use the structure suggested by the Turing Way:

- data_raw: a directory to hold the raw data
- data_clean: a directory to hold the processed data
- code: a directory to hold computer code
- CITATION: a file holding citation information
- paper.Rmd: a manuscript This function provides the a clearly separated organizational structure. Components can be changed. For example, the manuscript can be in another format (e.g. quarto, sweave) or even optional. With add_rang, the computational environment can be recorded and reconstructed later.

Value

path, invisibly

References

The Turing Way: Research Compendia Gorman, KB, Williams TD. and Fraser WR (2014). Ecological Sexual Dimorphism and Environmental Variability within a Community of Antarctic Penguins (Genus Pygoscelis). PLoS ONE 9(3):e90081. doi:10.1371/journal.pone.0090081

See Also

use_rang()

dockerize

Dockerize The Resolved Result

Description

This function exports the result from resolve() to a Docker file. For R version >= 3.1.0, the Dockerfile is based on the versioned Rocker image. For R version < 3.1.0, the Dockerfile is based on Debian and it compiles R from source.

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Usage

```
dockerize(
  rang,
  output_dir,
 materials_dir = NULL,
 post_installation_steps = NULL,
  image = c("r-ver", "rstudio", "tidyverse", "verse", "geospatial"),
  rang_as_comment = TRUE,
  cache = FALSE,
  verbose = TRUE,
  lib = NA,
  cran_mirror = "https://cran.r-project.org/",
  check_cran_mirror = TRUE,
  bioc_mirror = "https://bioconductor.org/packages/",
  no_rocker = FALSE,
  debian_version = c("lenny", "squeeze", "wheezy", "jessie", "stretch"),
  skip_r17 = TRUE,
  insert_readme = TRUE,
  copy_all = FALSE
)
dockerize_rang(...)
dockerise(...)
dockerise_rang(...)
```

Arguments

rang output from resolve()

output_dir character, where to put the Docker file and associated content

materials_dir character, path to the directory containing additional resources (e.g. analysis

scripts) to be copied into output_dir and in turn into the Docker container

post_installation_steps

character, additional steps to be added before the CMD part of the Dockerfile, see

an example below

image character, which versioned Rocker image to use. Can only be "r-ver", "rstudio",

"tidyverse", "verse", "geospatial" This applies only to R version >= 3.1

rang_as_comment

logical, whether to write resolved result and the steps to reproduce the file to

path as comment

cache

logical, whether to cache the packages now. Please note that the system requirements are not cached. For query with non-CRAN packages, this option is strongly recommended. For query with local packages, this must be TRUE regardless of R version. For R version < 3.1, this must be also TRUE if there is

any non-CRAN packages.

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verbose logical, pass to install.packages(), the negated value is also passed as quiet

to both install.packages() and download.file().

lib character, pass to install.packages(). By default, it is NA (to install the

packages to the default location)

cran_mirror character, which CRAN mirror to use

check_cran_mirror

logical, whether to check the CRAN mirror

bioc_mirror character, which Bioconductor mirror to use

no_rocker logical, whether to skip using Rocker images even when an appropriate version

is available. Please keep this as TRUE unless you know what you are doing

debian_version when Rocker images are not used, which EOL version of Debian to use. Can

only be "lenny", "etch", "squeeze", "wheezy", "jessie", "stretch". Please keep

this as default "lenny" unless you know what you are doing

skip_r17 logical, whether to skip R 1.7.x. Currently, it is not possible to compile R 1.7.x

(R 1.7.0 and R 1.7.1) with the method provided by rang. It affects snapshot_date from 2003-04-16 to 2003-10-07. When skip_r17 is TRUE and snapshot_date

is within the aforementioned range, R 1.8.0 is used instead

insert_readme logical, whether to insert a README file

copy_all logical, whether to copy everything in the current directory into the container. If

inst/rang is detected in output_dir, this is coerced to TRUE.

... arguments to be passed to dockerize

Details

The idea behind this is to determine the installation order of R packages locally. Then, the installation script can be deployed to another fresh R session to install R packages. dockerize() and apptainerize() are more reasonable ways because a fresh R session with all system requirements is provided. The current approach does not work in R < 2.1.0.

Value

```
output_dir, invisibly
```

References

The Rocker Project Ripley, B. (2005) Packages and their Management in R 2.1.0. R News, 5(1):8–11.

See Also

```
resolve(), export_rang(), use_rang()
```

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Examples

export_rang

Export The Resolved Result As Installation Script

Description

This function exports the results from resolve() to an installation script that can be run in a fresh R environment.

Usage

```
export_rang(
  rang,
  path,
  rang_as_comment = TRUE,
  verbose = TRUE,
  lib = NA,
  cran_mirror = "https://cran.r-project.org/",
  check_cran_mirror = TRUE,
  bioc_mirror = "https://bioconductor.org/packages/")
```

Arguments

```
rang output from resolve()

path character, path of the exported installation script

rang_as_comment

logical, whether to write resolved result and the steps to reproduce the file to

path as comment

verbose logical, pass to install.packages(), the negated value is also passed as quiet

to both install.packages() and download.file().

lib character, pass to install.packages(). By default, it is NA (to install the

packages to the default location)
```

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```
cran_mirror character, which CRAN mirror to use
check_cran_mirror
logical, whether to check the CRAN mirror
bioc_mirror character, which Bioconductor mirror to use
```

Details

The idea behind this is to determine the installation order of R packages locally. Then, the installation script can be deployed to another fresh R session to install R packages. dockerize() and apptainerize() are more reasonable ways because a fresh R session with all system requirements is provided. The current approach does not work in R < 2.1.0.

Value

```
path, invisibly
```

References

```
Ripley, B. (2005) Packages and their Management in R 2.1.0. R News, 5(1):8–11.
```

See Also

```
generate_installation_order()
```

Examples

export_renv

Export The Resolved Result As a renv Lockfile

Description

This function exports the results from resolve() to a renv lockfile that can be used as an alternative to a docker container.

Usage

```
export_renv(rang, path = ".")
```

Arguments

```
rang output from resolve()
path character, path of the exported renv lockfile
```

Details

A renv lockfile is easier to handle than a docker container, but it cannot always reliably reproduce the exact computational environment, especially for very old code.

Value

```
path, invisibly
```

Examples

generate_installation_order

Create a Data Frame of The Resolved Result This function exports the results from resolve() to a data frame, which each row represents one installation step. The order of rows is the installation order. By installing packages in the specified order, one can install all the resolved packages without conflicts.

Description

Create a Data Frame of The Resolved Result This function exports the results from resolve() to a data frame, which each row represents one installation step. The order of rows is the installation order. By installing packages in the specified order, one can install all the resolved packages without conflicts.

Usage

```
generate_installation_order(rang)
```

Arguments

```
rang output from resolve()
```

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Value

A data frame ordered by installation order.

References

```
Ripley, B. (2005) Packages and their Management in R 2.1.0. R News, 5(1):8–11.
```

Examples

query_sysreqs

Query for System Requirements

Description

This function takes an S3 object returned from resolve() and (re)queries the System Requirements.

Usage

```
query_sysreqs(rang, os = "ubuntu-20.04")
```

Arguments

rang output from resolve()

os character, which OS to query for system requirements

Value

```
a rang S3 object with the following items
```

call original function call

ranglets List of dependency graphs of all packages in pkgs

snapshot_date snapshot_date
no_enhances no_enhances
no_suggests no_suggests
unresolved_pkgsrefs

Packages that can't be resolved

sysreqs System requirements as Linux commands r_version The latest R version as of snapshot_date

os os

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See Also

```
resolve()
```

Examples

recipes

Recipes for Building Container Images

Description

A list containing several useful recipes for container building. Useful for the post_installation_steps argument of dockerize(). Available recipes are:

- texlive: install pandoc and LaTeX, useful for rendering RMarkdown
- texlivefull: Similar to the above, but install the full distribution of TeX Live (~ 3GB)
- quarto: install quarto and tinytex
- clean: clean up the container image by removing cache
- make: install GNU make

Usage

recipes

Format

An object of class list of length 5.

Examples

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resolve

Resolve Dependencies Of R Packages

Description

This function recursively queries dependencies of R packages at a specific snapshot time. The dependency graph can then be used to recreate the computational environment. The data on dependencies are provided by R-hub.

Usage

```
resolve(
  pkgs = ".",
  snapshot_date,
  no_enhances = TRUE,
  no_suggests = TRUE,
  query_sysreqs = TRUE,
  os = "ubuntu-20.04",
  verbose = FALSE
)
```

Arguments

pkgs

pkgs can be 1) a character vector of R packages to resolve, 2) a path to a renv lockfile, or 3) a data structure that as_pkgrefs() can convert to a character vector of package references. For 1) pkgs can be either in shorthands, e.g. "rtoot", "ropensci/readODS", or in package references, e.g. "cran::rtoot", "github::ropensci/readODS". Please refer to the Package References documentation of pak for details. Currently, this package supports only cran and github packages. For 2) as_pkgrefs() support the output of sessionInfo(), a renv lockfile or a single directory. If it is a single directory, all R scripts are scanned for R packages used using renv::dependencies(). Currently, the default is to scan the R scripts in the current working directory. Please also note that this scanning only assumes there are CRAN and Bioconductor packages. We strongly recommend checking whether this is really the case (see example below).

snapshot_date Snapshot date, if not specified, assume to be a month ago no_enhances logical, whether to ignore packages in the "Enhances" field logical, whether to ignore packages in the "Suggests" field

query_sysreqs logical, whether to query for System Requirements. Important: Archived CRAN

can't be queried for system requirements. Those packages are assumed to have

no system requirement.

os character, which OS to query for system requirements

verbose logical, whether to display messages

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Value

```
a rang S3 object with the following items
call
                 original function call
ranglets
                 List of dependency graphs of all packages in pkgs
snapshot_date
                 snapshot_date
no_enhances
                 no_enhances
no_suggests
                 no_suggests
unresolved_pkgsrefs
                 Packages that can't be resolved
sysreqs
                 System requirements as Linux commands
r_version
                 The latest R version as of snapshot_date
os
                 os
```

References

Package References

See Also

```
dockerize()
```

Examples

18 use_rang

use_rang Setup rang for a directory

Description

This usethis-style function adds the infrastructure in a directory (presumably with R scripts and data) for (re)constructing the computational environment. Specifically, this function inserts inst/rang into the directory, which contains all components for the reconstruction. Optionally, Makefile and . here are also inserted to ease the development of analytic code. By default, (re)running this function does not overwrite any file. One can change this by setting force to TRUE.

Usage

```
use_rang(
  path = ".",
  add_makefile = TRUE,
  add_here = TRUE,
  verbose = TRUE,
  force = FALSE,
  apptainer = FALSE
)
```

Arguments

path character, path to the project root

add_makefile logical, whether to insert a barebone Makefile in the project root.

add_here logical, whether to insert a hidden .here file in the project root

verbose logical, whether to print out messages

force logical, whether to overwrite files (inst/rang/update.R, Makefile, .here) if

they exist.

apptainer logical, whether to use apptainer. FALSE indicates using Docker

Details

The infrastructure being added to your path consists of:

- inst/rang directory in the project root
- update. R file inside the directory
- .here in the project root (if add_here is TRUE)
- Makefile in the project root (if add_makefile is TRUE) You might need to edit update.R manually. The default is to scan the whole project for used R packages and assume they are either on CRAN or Bioconductor. If you have used other R packages, you might need to edit this manually.

Value

path, invisibly

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