Open Science / Research w/ R featuring rOpenSci

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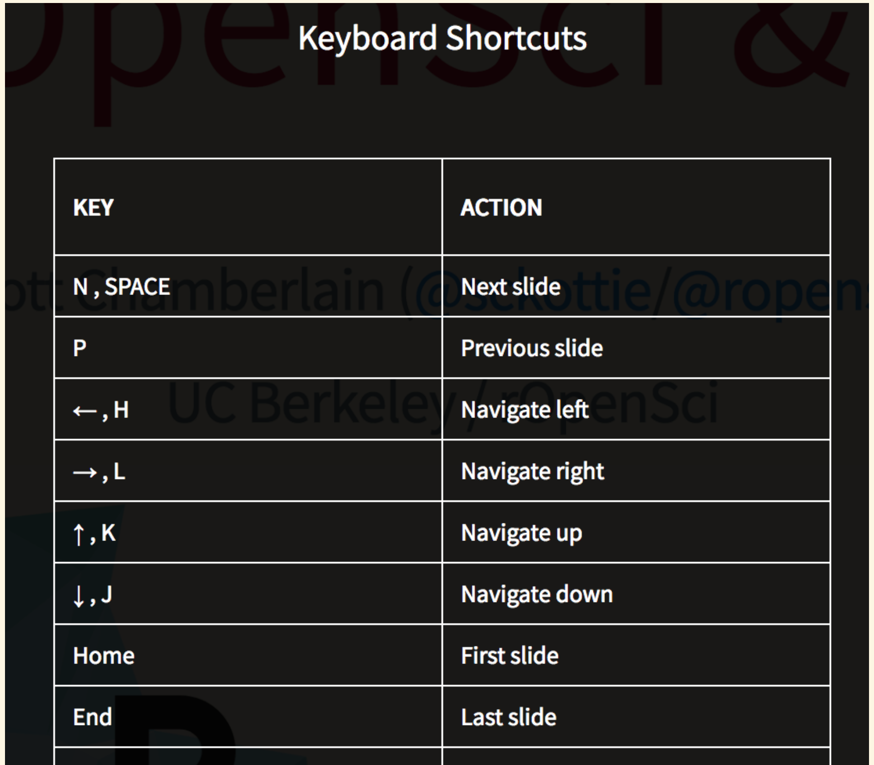
HELMSLEY
CHARITABLE TRUST

scotttalks.info/cdc18

Keyboard shortcuts: press `?`



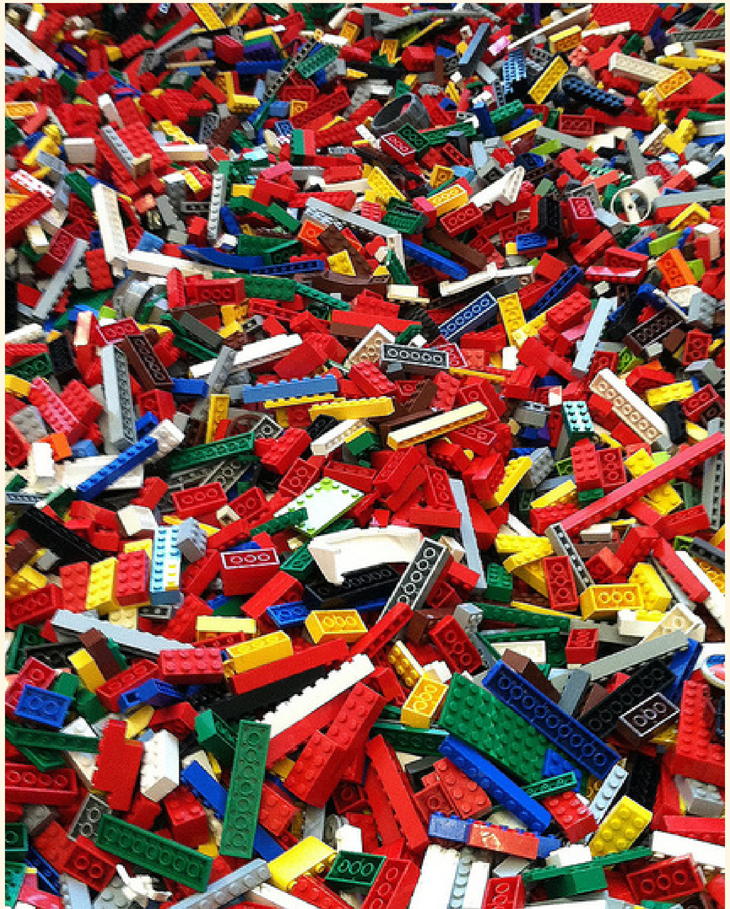
Keyboard Shortcuts

KEY	ACTION
N , SPACE	Next slide
P	Previous slide
← , H	Navigate left
→ , L	Navigate right
↑ , K	Navigate up
↓ , J	Navigate down
Home	First slide
End	Last slide

open science/research

🔓🧪

Open science as a lego set



Open science as a lego set

open science may be hard to do

but - you can work on different components

and - individual components are worth learning

Open Data

(at least within your organization)

funders/journals often requiring this anyway

future self will thank you

Versioning: code/data/text

xkcd.com/1597

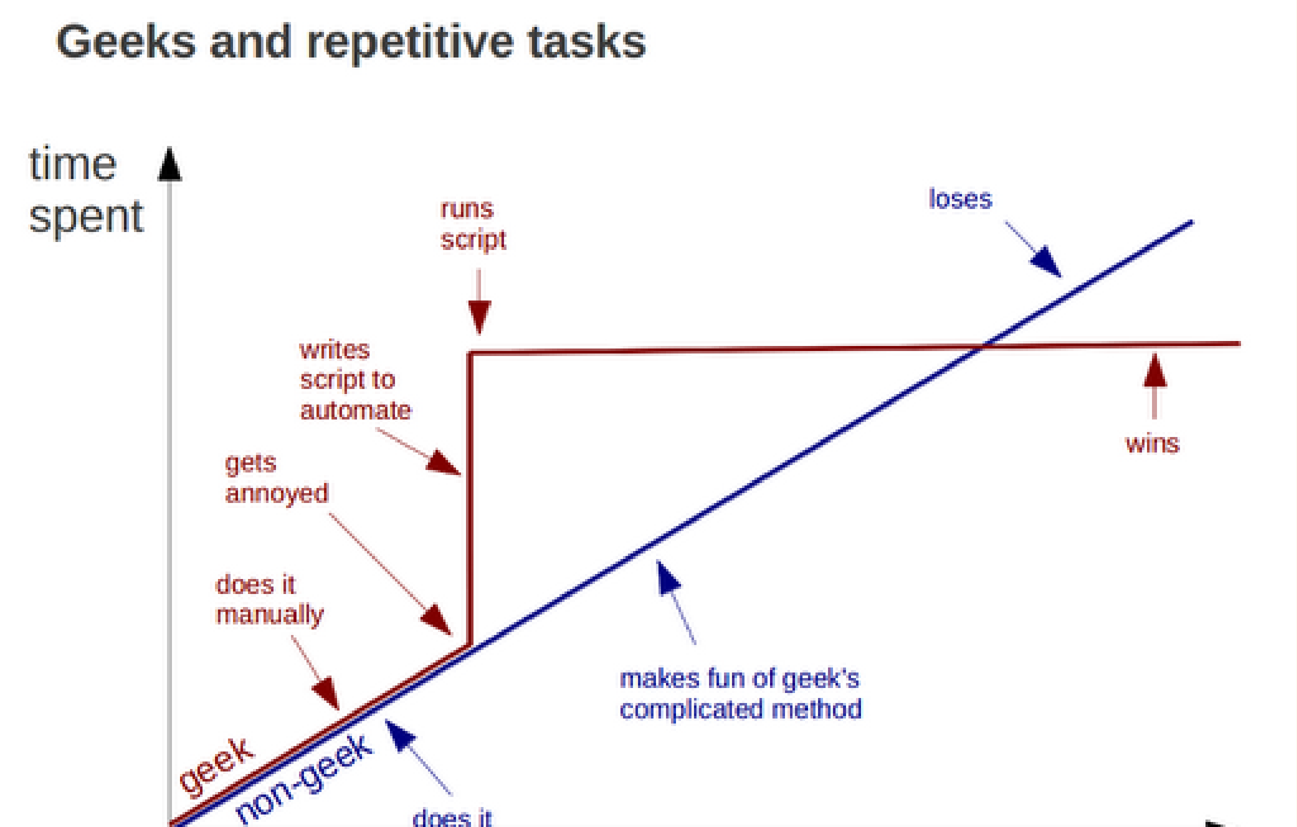
Versioning: code/data/text

failure proofs your work

experiment freely!

makes collaboration easier

Do all work programatically



Do all work programatically

Key to reproduciblity

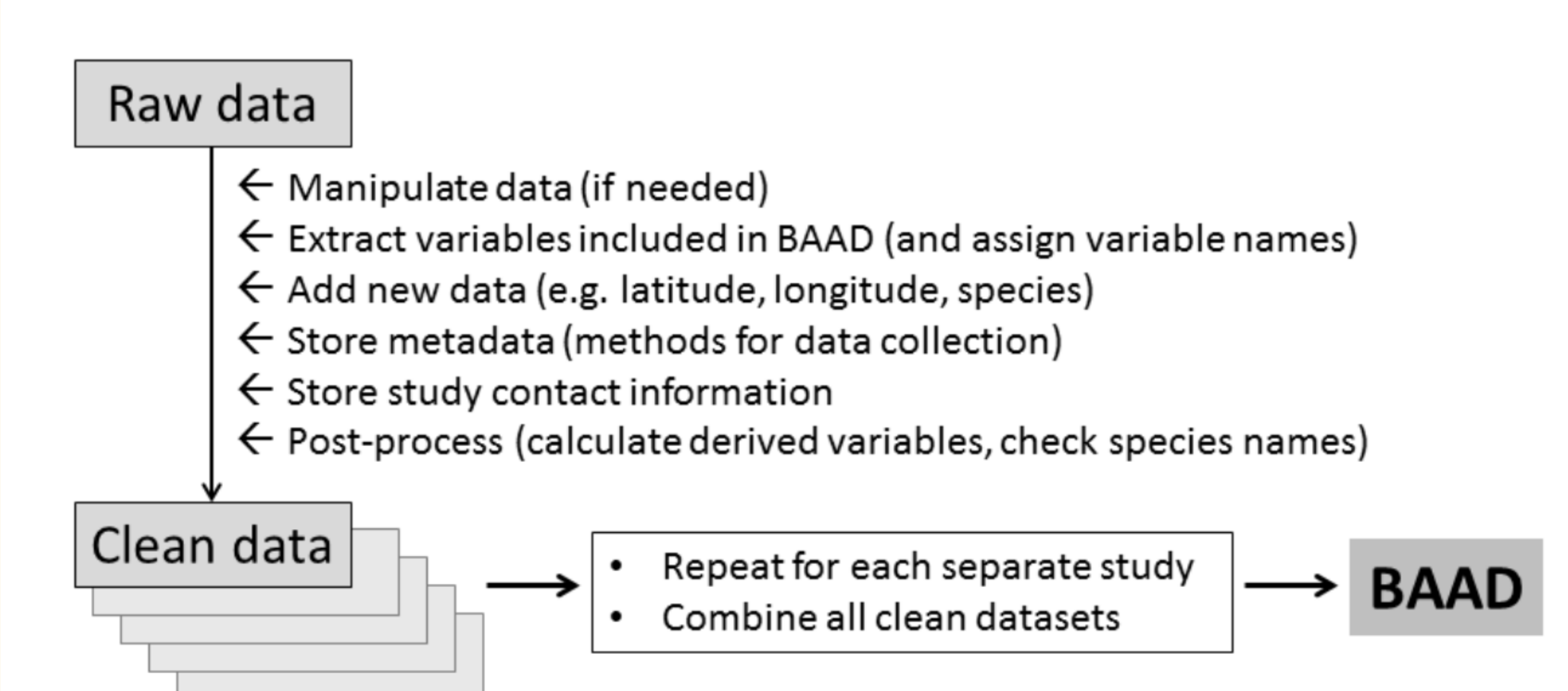
Most important person that wants to reproduce your work is you!

Do all work programatically

you and yourself

- one week from now
- two months from now
- & so on

An example to shoot for



Raw data

← Manipulate data (if needed)
← Extract variables included in BAAD (and assign variable names)
← Add new data (e.g. latitude, longitude, species)
← Store metadata (methods for data collection)
← Store study contact information
← Post-process (calculate derived variables, check species names)

Clean data

- Repeat for each separate study
- Combine all clean datasets

BAAD

important (higher level) scientific programming languages

python

R

julia

R language

- used widely in biology, psychology, medicine, etc.
- rapidly growing user base, companies surrounding it
- includes all tools for open science workflow
- though work to be done ...

Open science ecosytsem

Open Data
(e.g., GBIF,
Dataverse)

Open Science Training
(e.g., Software
Carpentry)

Open Access
Publishers
(e.g., eLife, PeerJ)

Researcher

Software
(e.g., rOpenSci,
Jupyter, etc.)

Infrastructure
(e.g., Crossref,
Datacite, Zenodo)

ROpenSci

rOpenSci Does

👥 </> 📖 ☑

rOpenSci Staff

ropensci.org/about/#team

- ~5 full time
- leadership team
- advisory board

Community stats

- ~ 400 code contributors
- ~ 490 Github repositories (most are R packages)
- ~ 45,000 commits
- ~ 160 published R packages on CRAN (another ~100 not on CRAN)

rOpenSci Unconference

unconf18.ropensci.org

Nominations (including self) close Mar. 8th

rOpenSci Unconf

May 21 - 22 2018 • Seattle • WA

What data do you use in your research?

the research workflow

Data acquisition +

data manipulation/analysis/viz +

writing +

publish

the research workflow

Data acquisition +

data manipulation/analysis/viz +

writing +

publish

the research workflow

Data acquisition ☁ +

data manipulation/analysis/viz 📊
+

writing ✎ +

publish ☁

the research workflow

Data acquisition ☁ +

data manipulation/analysis/viz 📊 +

writing ✎ +

publish ☁

the research workflow

Data acquisition ☁ ➕

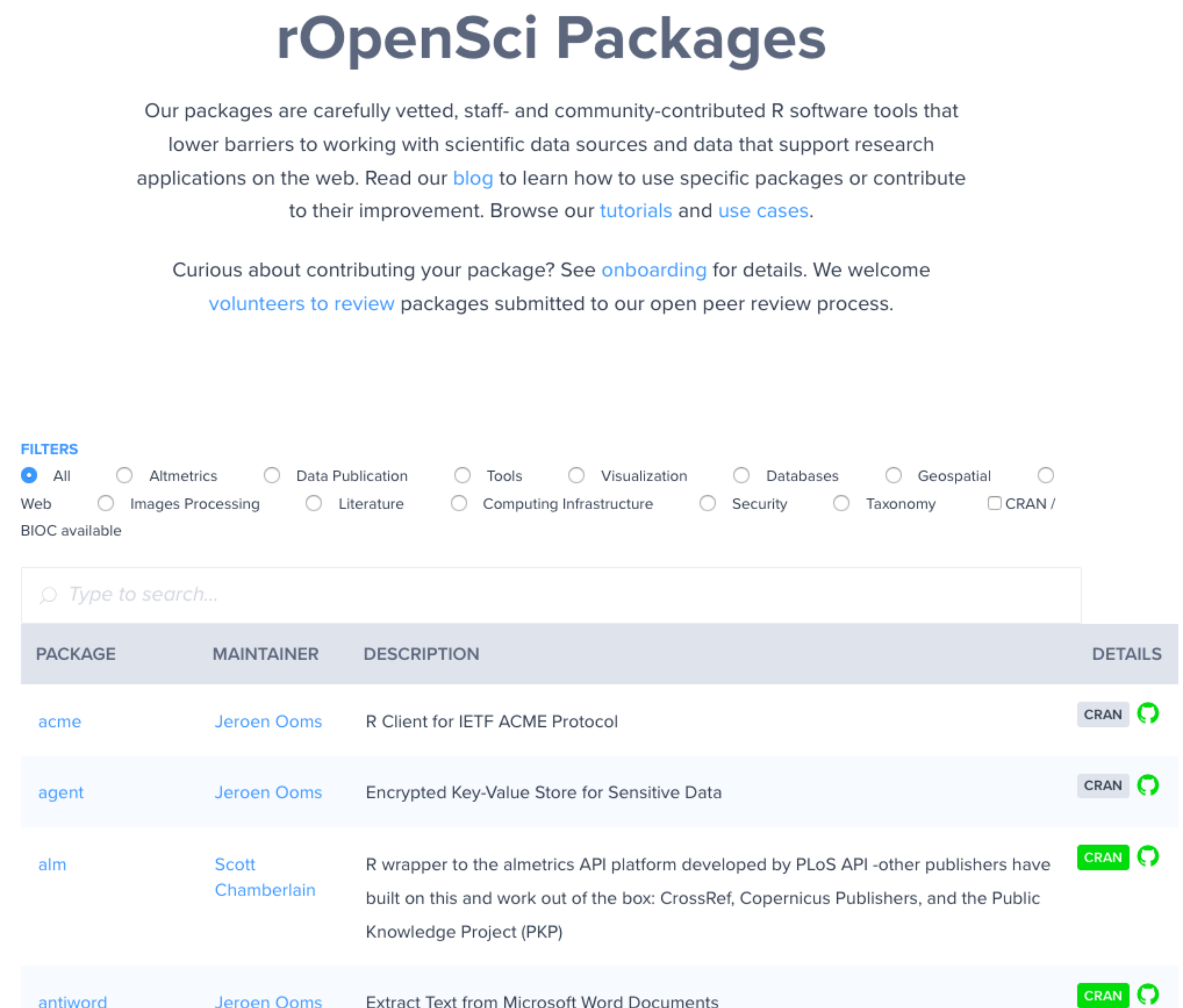
data manipulation/analysis/viz 📊 ➕

writing ✎ ➕

publish ☁

rOpenSci Tools

ropensci.org/packages



rOpenSci Packages

Our packages are carefully vetted, staff- and community-contributed R software tools that lower barriers to working with scientific data sources and data that support research applications on the web. Read our blog to learn how to use specific packages or contribute to their improvement. Browse our tutorials and use cases.

Curious about contributing your package? See onboarding for details. We welcome volunteers to review packages submitted to our open peer review process.

FILTERS

● All ○ Altmetrics ○ Data Publication ○ Tools ○ Visualization ○ Databases ○ Geospatial ○ Web ○ Images Processing ○ Literature ○ Computing Infrastructure ○ Security ○ Taxonomy ☐ CRAN / BIOC available

Type to search...

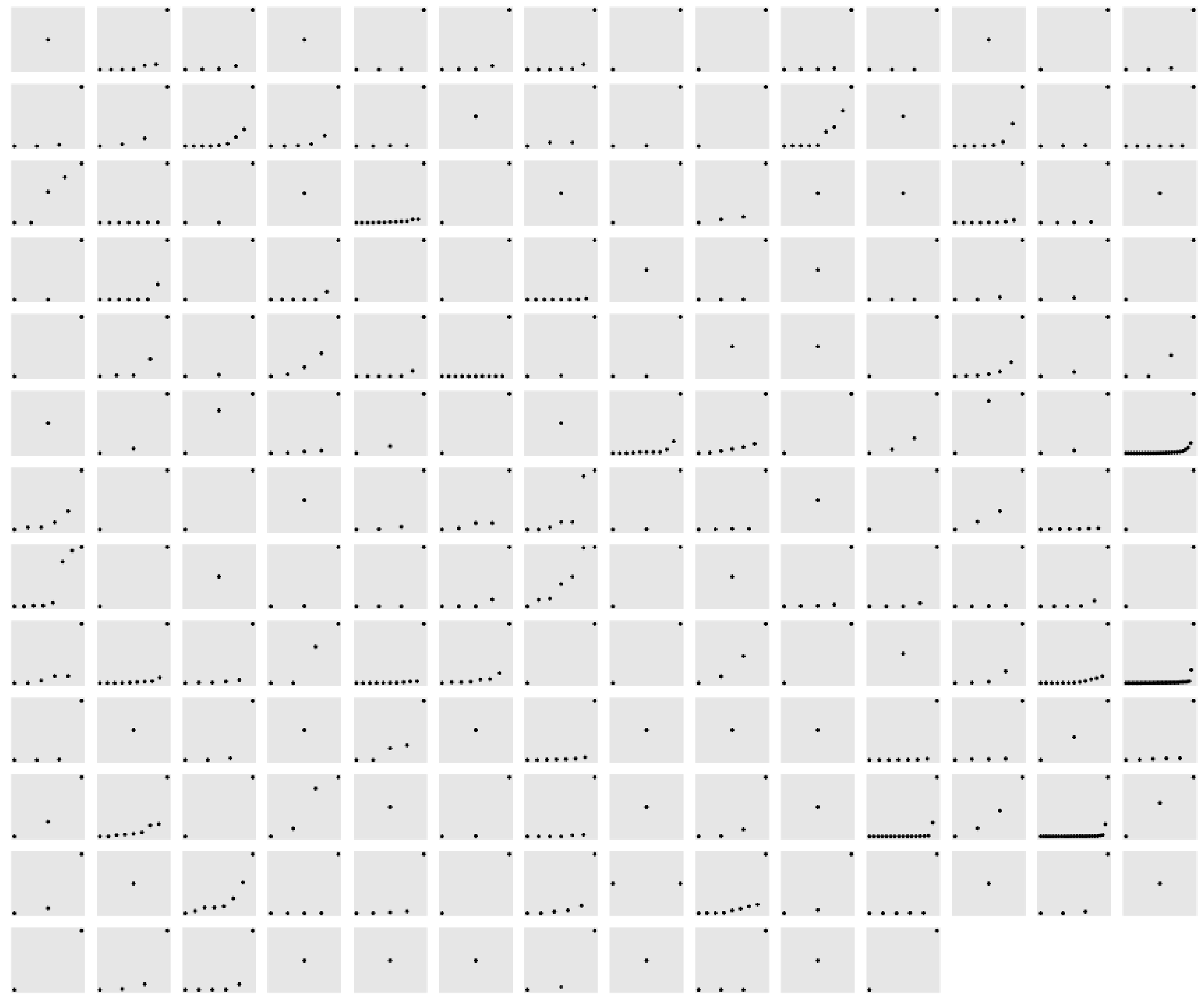
PACKAGE	MAINTAINER	DESCRIPTION	DETAILS
acme	Jeroen Ooms	R Client for IETF ACME Protocol	CRAN
agent	Jeroen Ooms	Encrypted Key-Value Store for Sensitive Data	CRAN
alm	Scott Chamberlain	R wrapper to the almetrics API platform developed by PLoS API -other publishers have built on this and work out of the box: CrossRef, Copernicus Publishers, and the Public Knowledge Project (PKP)	CRAN
antiword	Jeroen Ooms	Extract Text from Microsoft Word Documents	CRAN

rOpenSci Software: some of the benefits

- reduce redundant small software efforts
- funnel effort into sustainable, well-maintained software (see lack of support for software MAINTANENCE in academia)
- bring maintainers into a community
- give otherwise isolated projects a louder voice
- hopefully we make each piece of software more sustainable

but, software sustainability is hard

each panel is a pakage, each dot a person



rOpenSci software used in

research
within companies
fun side projects
journalism
and more

here are some of the academic research uses

... usually found in methods section of papers

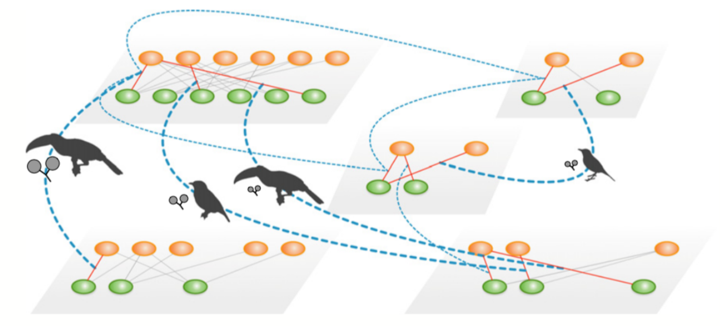
use case 1

Claypool, K., & Patel, C. J. (2018). A transcript-wide association study in physical activity intervention implicates molecular pathways in chronic disease. BioRxiv ↗

We used the ***rentrez*** *R package to execute the query on GEO [Gene Expression Omnibus] ...*

use case 2

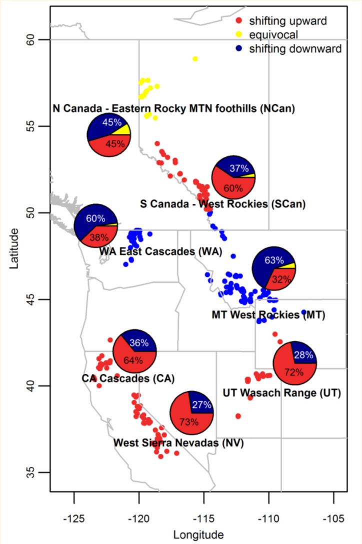
Emer, C., et al. (2018). Seed-dispersal interactions in fragmented landscapes - a metanetwork approach. Ecology Letters ↗



We compiled 16 studies of BSD [bird seed dispersal]-interactions in fragments of the SE Brazilian Atlantic Forest ... We updated

use case 3

Harsch, M. A., & HilleRisLambers, J. (2016). Climate Warming and Seasonal Precipitation Change Interact to Limit Species Distribution Shifts across Western North America. PLOS ONE. ↗



To fill in missing elevation records and correct elevation records ... we estimated altitude ... using

rOpenSci *omics Tools

Taxonomy

- taxa - Taxonomic classes and taxonomically aware data manipulation
- taxize - Taxonomic "toolbelt" - work w/ taxonomy web APIs
- taxizedb - taxize, but with local SQL databases
- rentrez - NCBI's Entrez services
- biomartr - Biomart R client
- genbankr - Parse GenBank files into useful objects
- rsnps - SNPs data retrieval

(although most omics R packages are in Bioconductor, rOpenSci is open to submissions!)

Taxonomic data from >20 sources - taxize

Taxonomic hierarchies from NCBI/ITIS/COL/etc

```r
library('taxize')
classification("Chironomus riparius", db = "gbif")
```

```
#> $`Chironomus riparius`
#>                    name    rank      id
#> 1            Animalia kingdom       1
#> 2          Arthropoda  phylum      54
#> 3             Insecta   class     216
#> 4             Diptera   order     811
#> 5        Chironomidae  family    3343
#> 6          Chironomus   genus 1448033
#> 7 Chironomus riparius species 1448237
```

Taxonomic IDs

always try to move from:

- taxonomic name -- to
- taxonomic ID -- to
- whatever other data

ENTREZ in R - rentrez

Retrieve datasets from a particular organism

```r
library(rentrez)
x <- entrez_search(db = "popset", term = "Latrodectus katipo[Organism]")
x_summs <- entrez_summary(db = "popset", id = x$ids)

titles <- extract_from_esummary(x_summs, "title")
COI_ids <- x$ids[c(2,6)]
COI <- entrez_fetch(db = "popset", id = COI_ids, rettype = "fasta")
substr(COI, 1, 500)
#> [1] ">AY383604.1 Latrodectus katipo isolate 1 tRNA-Leu (trnL) gene,
#> partial sequence; and NADH dehydrogenase subunit 1 (ND1) gene,
#> partial cds; mitochondrial
#> ATTACCTAAATTATATCAATAATTATTAATTCAGTTATCCCTATAATCTCTCTCCTAATCAGAGTCTCGT
#> TTTACACTATCTTAGAACGAAAAATTTTAAGTTATATCCAAATTCGTAAAGGGCCTAATAAAGTGGGTTT
#> CCTTGGTATTCTCCAACCCTTTAGAGACGCAATTAAACTTTTCAACAAAAATCTTATTAAACCTTTCTCT
#> TCTAATTTTTTAATTTTCTACATCTCCCCCGCCTTATCTTTAACTCTTGCTCTCCTTATTTCTTCAATCA
#> TTCCTTTCTTTTACTTTTCTCCTTATGATAACAAACATAATATCTTGATATTCTTAATCTTAT"
```

Genomic Data Retrieval - biomartr
Interfaces to:

- NCBI
- ENSEMBL
- ENSEMBLGENOMES
- Ensembl Biomart
- Gene Ontology

Parsing GenBank files into semantically useful objects - genbankr

```
library(genbankr)
x <- system.file("sample.gbk", package="genbankr")
gb <- readGenBank(x)
#> GenBank Annotations
#> Human herpesvirus 5 strain VR1814, complete genome.

#> Accession: GU179289
#> 1 Sequence(s) with total length length: 235233
#> 174 genes
#> 170 transcripts
#> 191 exons/cds elements
#> 61 variations
#> 24 other features
genes(gb)
cds(gb)
exons(gb)
transcripts(gb)
```

Spatial tools

Spatial

- geojson - GeoJSON classes
- geojsonio - GeoJSON/TopoJSON input/output
- geojsonlint - lint GeoJSON
- geoops - fast C++ based GeoJSON operations
- geonames - Geonames API client
- lawn - Turf.js javascript GeoJSON operations
- wicket - Well-Known Text tools
- wellknown - WKT <-> R objects
- rnaturalearth - NaturalEarth data
- osmplotr - Open Street Maps plots
- osmdata - Open Street Maps data
- opencage - OpenCage geocoding API

Geospatial: Geonames data - geonames

http://www.geonames.org/

```
library(geonames)
```

Find a contry code

```
GNcountryCode(lat = 47.03, lng = 10.2)
```

Search for nearby streets

```
GNfindNearbyStreets(lat = 37.45, lng = -122.18)
```

Search by place name

```
GNsearch(q = "london", maxRows = 10)
```

Postal code search

```
GNpostalCodeSearch(postalcode = 90210, country = "FI")
```

Geospatial: conversion between data/spatial data formats - geojsonio

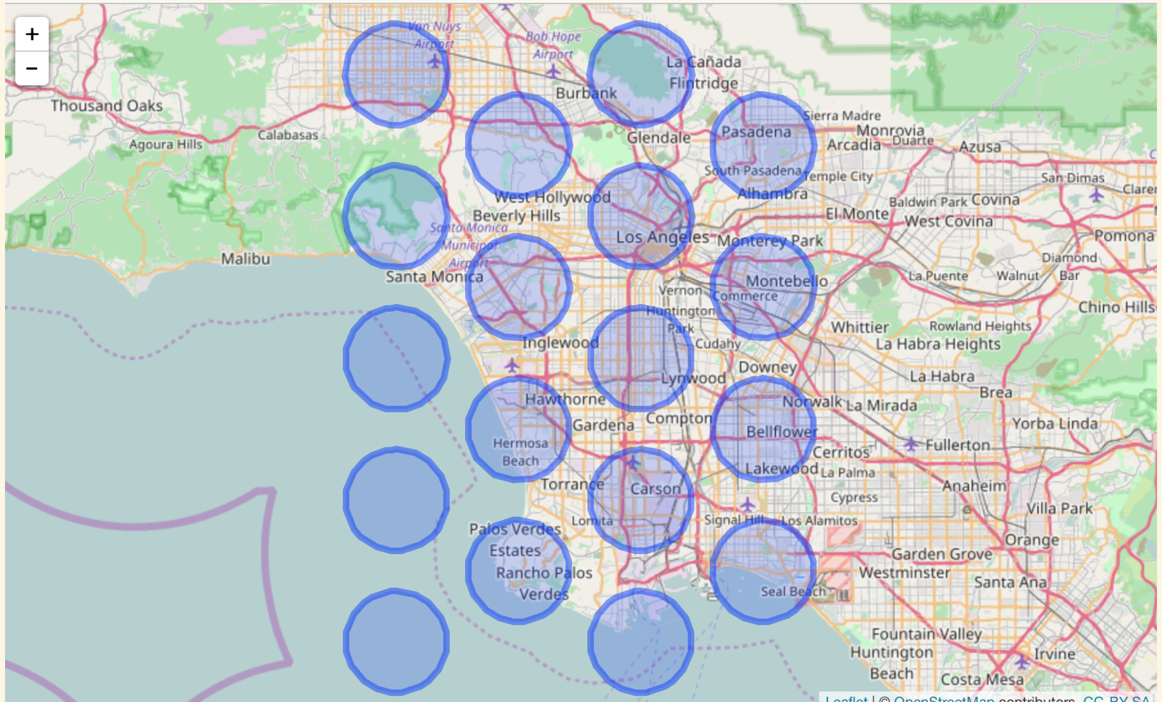
- geojson_list - convert to GeoJSON as R list
- geojson_json - convert to GeoJSON as JSON
- geojson_read/geojson_write - read/write GeoJSON

from most R object types + many spatial data formats

Geospatial: Spatial ops. w/ GeoJSON & w/o heavy dependencies - lawn

```r
library(lawn)
bbox <- c(-118.521, 33.715, -118.145, 34.179)
lawn_hex_grid(bbox, 10, 'miles') %>%
  as_feature(hex_grid) %>%
  purrr::map(lawn_centroid) %>%

  purrr::map(lawn_circle, radius = 5) %>%
  view
```



Climate data tools

Climate data

- rnoaa - NOAA climate data
- isdparser - parse NOAA Integrated Surface Data Files
- FedData - various US federal datasets (DEM's, hydrography, soil survey, climate, etc.)
- weathercan - Environment and Climate Canada data
- getCRUCLdata - CRU CL v. 2.0 Climatology Elements
- GSODR - Global Summary Daily Weather Data

NOAA climate data - rnoaa

- NCDC API
- Severe weather data
- Sea ice data
- NOAA buoy data
- Tornadoes
- HOMR - Historical Observing Metadata Repository
- Storm data
- GHCND FTP data

rnoaa - example

NCDC API

```r
library(rnoaa)
ncdc(datasetid = 'PRECIP_HLY', locationid = 'ZIP:28801',
    datatypeid = 'HPCP', limit = 5, token =  "<YOUR_TOKEN>")
```

GHCND FTP data

```r
ids <- c("ASN00003003", "ASM00094299", "ASM00094995", "ASM00094998")
meteo_pull_monitors(ids)
```

Tides and Currents data from COOPS

```r
ops_search(station_name = 9063053, begin_date = 20150927, end_date = 20150928,
    product = "daily_mean", datum = "stnd", time_zone = "lst")
```

Local Climatalogical Data

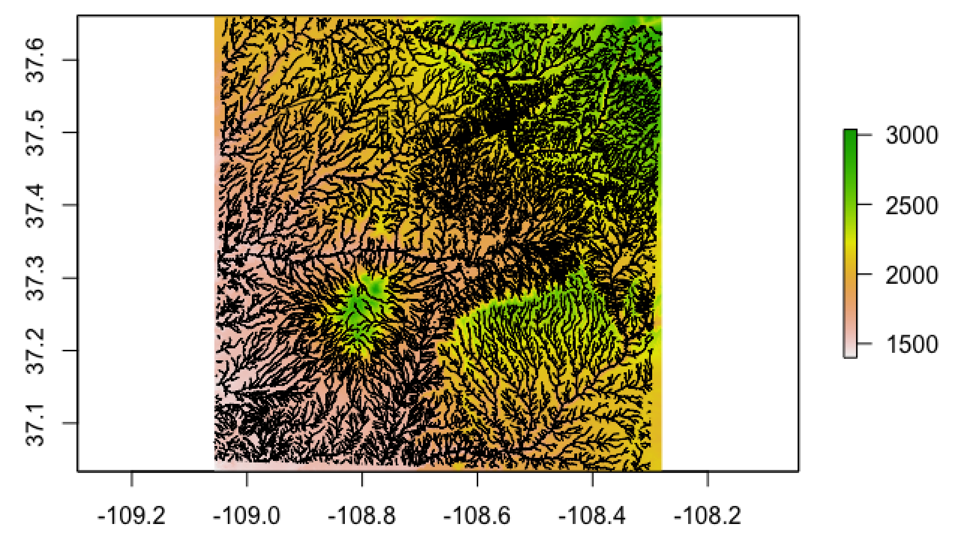
```r
lcd(station = "01338099999", year = "2017")
```

various federal datasets - FedData

plot the National Hydrography Dataset for a study area

```r
library(FedData)
vepPolygon <- polygon_from_extent(
    raster::extent(672800, 740000, 4102000, 4170000),
        proj4string = "+proj=utm +datum=NAD83 +zone=12")
NED <- get_ned(template = vepPolygon, label = "VEPIIN")

NHD <- get_nhd(template = vepPolygon, label = "VEPIIN")
raster::plot(NED)
NHD %>% lapply(sp::plot, col = 'black', add = TRUE)
```



Wrapping web APIs

Wrapping web APIs:
High level concepts

- Each pkg is a snowflake: every web API is different
- Try to cater to both beginners and power users
- Fail fast and fail well: APIs may not do it for you
- Pass on curl options! empower your users to:
    - investigate http request problems
    - set proxy options (IT often blocks certain sites/ports)
    - and more

Defensive programming

- Fail fast
- Defend against many things
- Give users good errors

Check out my defensive programming chapter

Basic structure of functions

DRY - don't repeat yourself

```r
get_foo <- function(query, ...) {
   cli <- crul::HttpClient$new(url = "https://foobar.com", opts = list(...))
   res <- cli$get("/hello-world", query = list(query = query))
   res$raise_for_status()
   if (res$response_headers$`content-type` != "application/json") stop("message")

   jsonlite::fromJSON(res$parse("UTF-8"))
}
```

```r
#' @export
#' @param query (character) Query terms
#' @param ... curl options, see `curl::curl_options` for help
#' @examples
#' foo_bar("cellular")
foo_bar <- function(query, ...) get_foo(query = query, ...)
```

Example pkg wrapping web API

ritis: client for ITIS taxonomic data

ritis: notes/thoughts

- imports: solrium, crul, jsonlite, data.table, tibble
- package API: fxns for REST API and Solr API
- a downside of this package possibly: a lot of functions
- return tibbles from all functions
- but `raw` JSON/XML output for those that want it
- Solr queries handled by solrium package

Combining many sources into one package

Many into one considerations

- Is it really a good idea?
- Inputs:
  - What parameters can be unified across sources?
  - Allow users to fiddle with sources specific options
  - Fail consistently across sources if possible
- Outputs:
  - What if any outputs can be combined

Many into one e.g.: spocc

Many into one e.g.: spocc

- All 10 sources share common input: taxonomic names
- Pagination is similar-ish across sources (requires some source specific variable mapping)
- Geospatial search: WKT and bounding boxes then map to what source requires
- Most can toggle whether to return records that have coordinates or not
- Outputs: combine the minimum set of similar fields

Software Review

☑

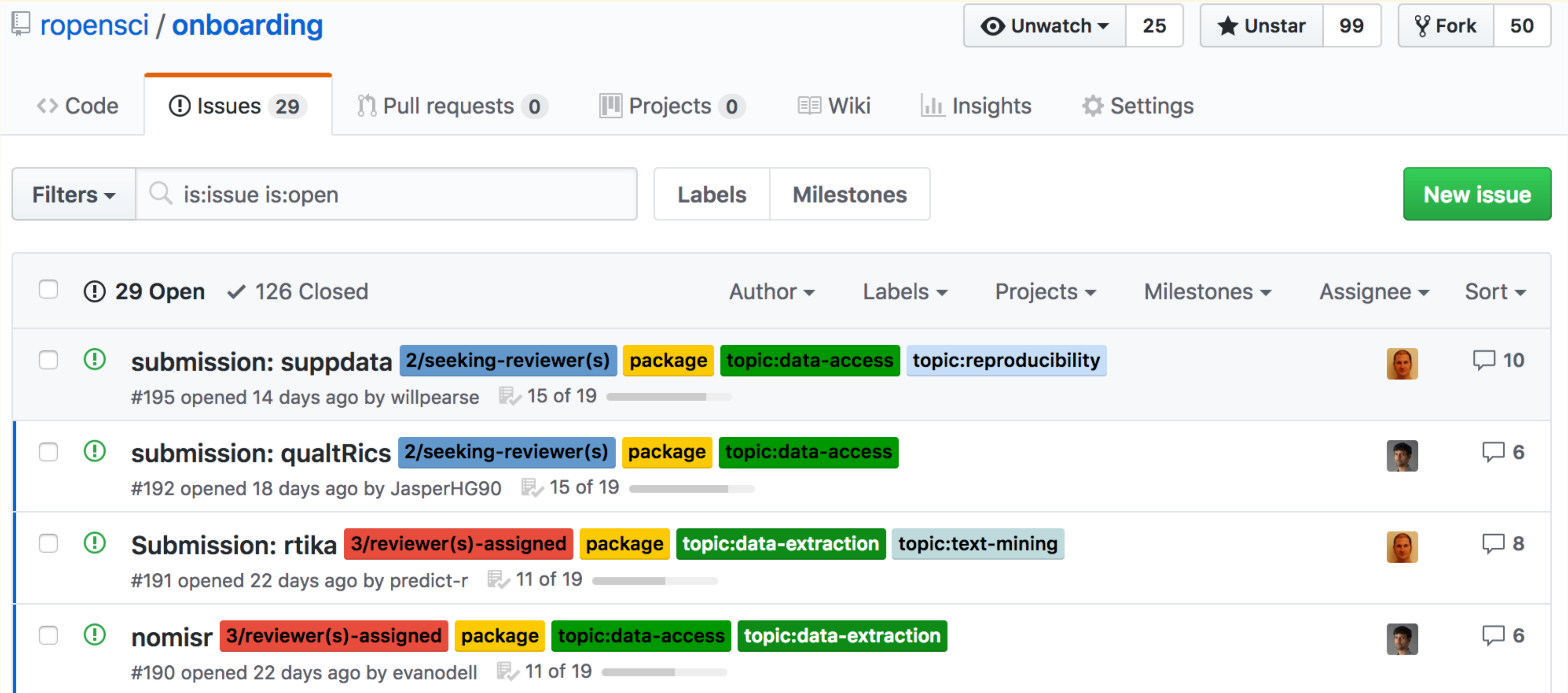
rOpenSci Software Review

- R package maintainer submits to ropensci/onboarding
- Editors determine fit or not a fit
- Editors assign reviewers
- Reviewers have ~ 3 weeks
- Reviewers and maintainer go back and forth refining pkg
- After approval, pkg moved to rOpenSci
- A number of e.g.'s of pkgs from government agencies

rOpenSci Software Review

- Completely open source tools
- Free to run
- All reviews/conversations in the open
- Reviews are/can be linked to code changes
- Paired with journal submission: JOSS and MEE

rOpenSci Onboarding

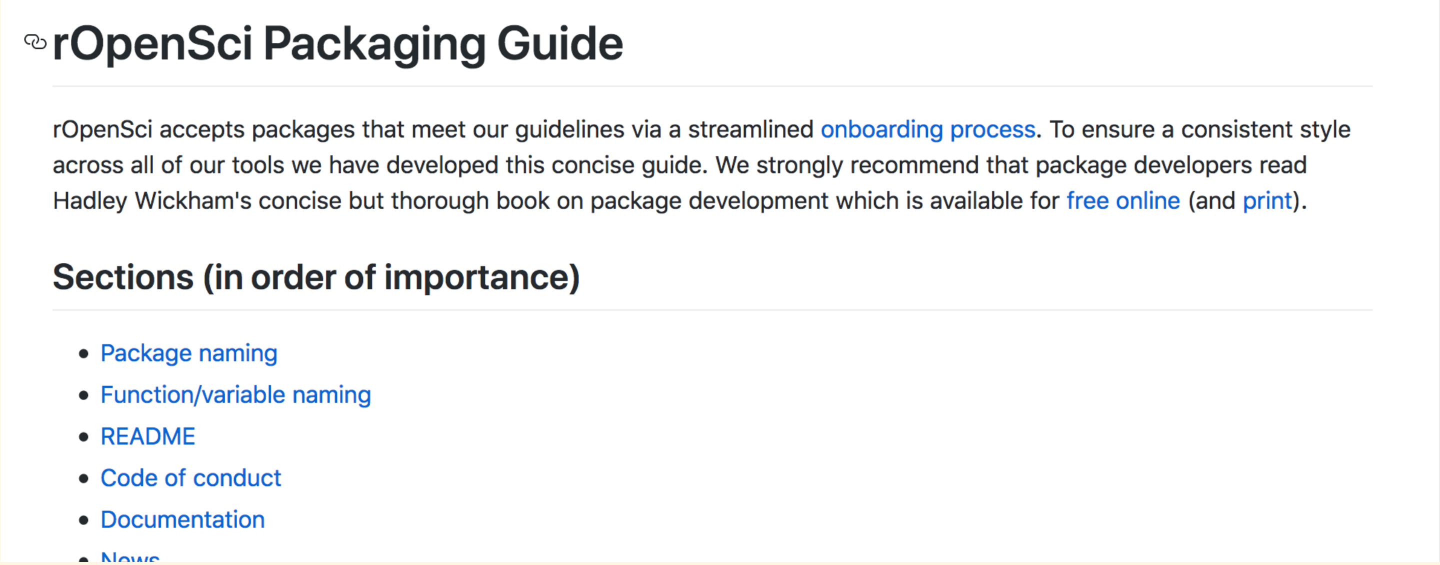


submission: suppdata 2/seeking-reviewer(s) package topic:data-access topic:reproducibility
#195 opened 14 days ago by willpearse 15 of 19 — 10

submission: qualtRics 2/seeking-reviewer(s) package topic:data-access
#192 opened 18 days ago by JasperHG90 15 of 19 — 6

Submission: rtika 3/reviewer(s)-assigned package topic:data-extraction topic:text-mining
#191 opened 22 days ago by predict-r 11 of 19 — 8

nomisr 3/reviewer(s)-assigned package topic:data-access topic:data-extraction
#190 opened 22 days ago by evanodell 11 of 19 — 6



rOpenSci Packaging Guide

rOpenSci accepts packages that meet our guidelines via a streamlined onboarding process. To ensure a consistent style across all of our tools we have developed this concise guide. We strongly recommend that package developers read Hadley Wickham's concise but thorough book on package development which is available for free online (and print).

Sections (in order of importance)

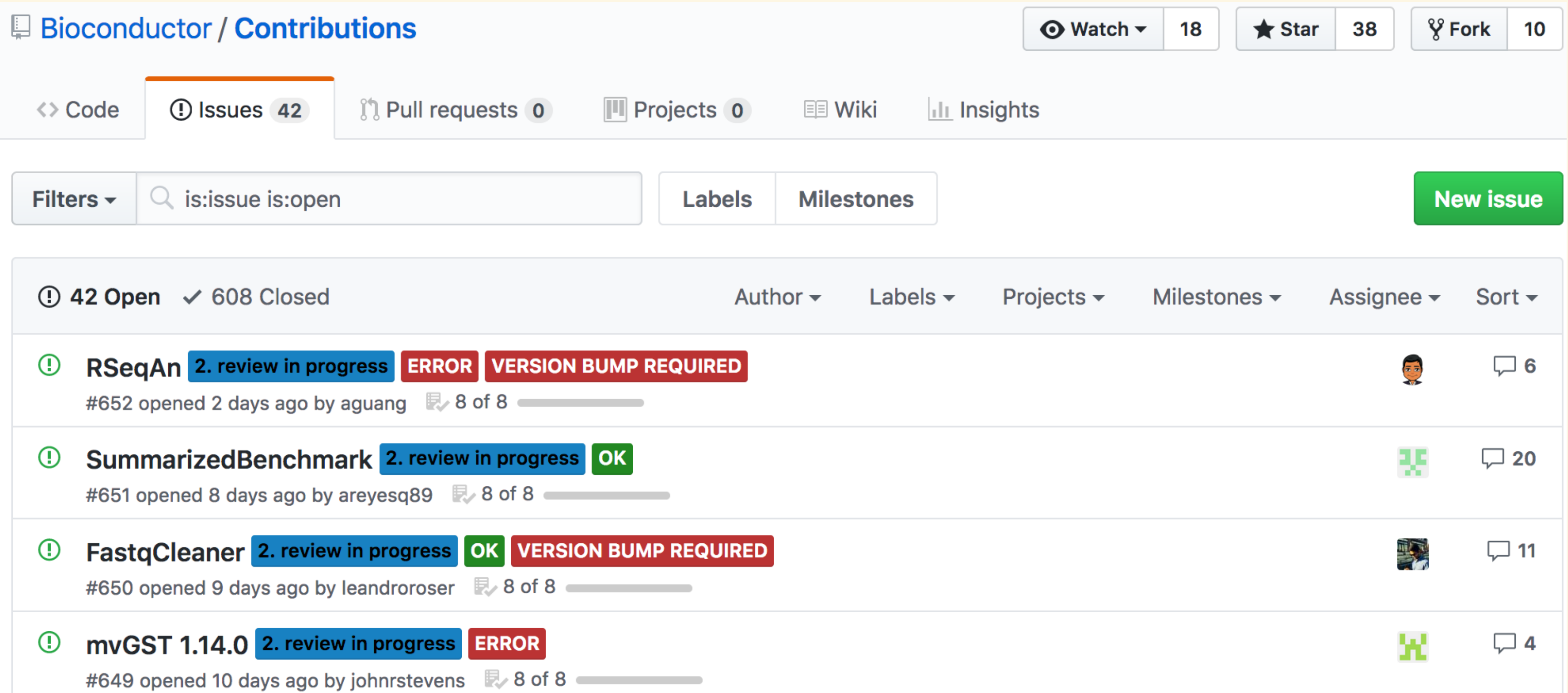
- Package naming
- Function/variable naming
- README
- Code of conduct
- Documentation
- News

not sure?

pre-submission inquiry!

checkout prior presub inquiries

Bioconductor Does Open Review too!



42 Open ✓ 608 Closed

RSeqAn 2. review in progress ERROR VERSION BUMP REQUIRED
#652 opened 2 days ago by aguang 8 of 8 — 6

SummarizedBenchmark 2. review in progress OK
#651 opened 8 days ago by areyesq89 8 of 8 — 20

FastqCleaner 2. review in progress OK VERSION BUMP REQUIRED
#650 opened 9 days ago by leandroroser 8 of 8 — 11

mvGST 1.14.0 2. review in progress ERROR
#649 opened 10 days ago by johnrstevens 8 of 8 — 4

talk to us 📢

what would you like to see?
what open data is too hard to get?
discussion forum: discuss.ropensci.org
submit a package/review a package: github.com/ropensci/onboarding

scotttalks.info/cdc18

Made w/: reveal.js v3.2.0

Some Styling: Bootstrap v3.3.5

Icons by: FontAwesome v4.4.0