

"No doubt about it, Ellington—we've mathematically expressed the purpose of the universe. God, how I love the thrill of scientific discovery!"

DCMB BioComputing BootCamp Day 3, Session IV: Working with Packages from CRAN and Bioconductor

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Overview

- 1. CRAN
- 2. Bioconductor
- 3. Package Installation
- 4. Package Documentation
- 5. Package Source Code
- 6. Example: BioMart bioconductor package

CRAN: The <u>C</u>omprehensive <u>R</u> <u>Archive Network</u>

- CRAN is a website dedicated to hosting the R language and R packages
 - packages are shared collections of R code
- There are currently
 12,884 available packages
 - search via google
 - table (index) of available packages
 - CRAN Task Views

Available CRAN Packages By Name

<u>ABCDEFGHIJKLMNOPQRSTUVWXYZ</u>

3 Accurate, Adaptable, and Accessible Error Metrics for Predictive Models

 abbyyR
 Access to Abbyy Optical Character Recognition (OCR) API

 abc
 Tools for Approximate Bayesian Computation (ABC)

 abc.data
 Data Only: Tools for Approximate Bayesian Computation (ABC)

ABC.RAP Array Based CpG Region Analysis Pipeline

ABCanalysis Computed ABC Analysis

abcdeFBA ABCDE_FBA: A-Biologist-Can-Do-Everything of Flux Balance Analysis with this package

ABCoptim Implementation of Artificial Bee Colony (ABC) Optimization
ABCp2 Approximate Bayesian Computational Model for Estimating P2
abcrf Approximate Bayesian Computation via Random Forests

abctools
abd
Tools for ABC Analyses
abd
The Analysis of Biological Data
abe
Augmented Backward Elimination
abf2
Load Gap-Free Axon ABF2 Files
ABHgenotypeR
abind
Combine Multidimensional Arrays

abjutils Useful Tools for Jurimetrical Analysis Used by the Brazilian Jurimetrics Association

Modelling Multivariate Data with Additive Bayesian Networks

<u>abnormality</u> Measure a Subject's Abnormality with Respect to a Reference Population

abodOutlier Angle-Based Outlier Detection

ABPS The Abnormal Blood Profile Score to Detect Blood Doping

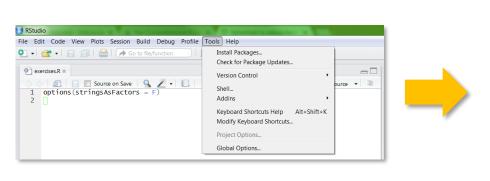
CRAN Package Table

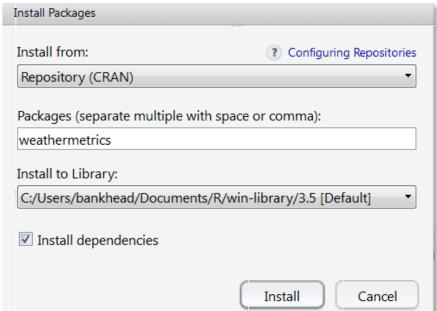
What do R Packages Contain?

- R code
- Help pages
- Data: example data sets included for demonstration purposes
- Other documentation
 - vignettes: documents that integrate code and how to perform a specific task
 - tutorials
- Code written in other languages (e.g. C, FORTRAN)
- Directives used to help install the package

Ways to Install a Package

- 1. On the command prompt type:
- > install.packages('weathermetrics')
- 2. In RStudio select Tools -> Install Packages from the top of the main screen





Useful Commands for Exploring R Packages

from CRAN

```
search() – lists packages currently loaded sessionInfo() – lists packages with version #'s packageDescription() – prints brief description install.packages() - install an R package from CRAN update.packages() – checks for package updates and installs updates if necessary
```

installed.packages() – returns packages that are installed on the user's system

available.packages() – returns packages that are available

Exercise: What packages are currently loaded? What packages are installed on your computer?



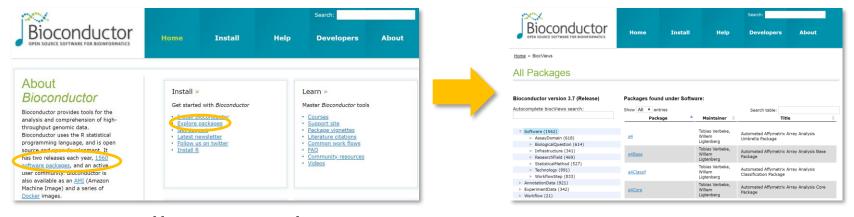
- R packages and datasets for working with high-throughput genomic data
 - http://bioconductor.org
 - Bioconductor was started in Fall 2001
 - Two releases each year
 - v3.7 has 1,560 packages
- Packages undergo formal initial review and continuous automated testing

Perspective | Published: 29 January 2015 Orchestrating high-throughput genomic analysis with Bioconductor Wolfgang Huber ®, Vincent J Carey, Robert Gentleman, Simon Anders, Marc Carlson, Benilton 5 Carvalho, Netcor Corrada Bravo, Sean Davis, Laurent Gatto, Thomas Girke, Raphael Gottardo, Floriar Hahne, Kasper D Hansen, Rafael A Irizarry, Michael Lawrence, Michael I Love, James MacDonald, Valeire Obenchain, Andreg K Oles, Hervé Pagès, Aléjandro Reyes, Paul S hannon, Gordon K Smyth, Dan Teenebaum, Levi Waldron & Martin Morgan - Show Yewer authors

Nature Methods 12, 115-121 (2015) | Download Citation ±

Version	Release Date	Package Count	Dependency
1.0	1 May 2002	15	R 1.5
1.1	19 Nov 2002	20	R 1.6
1.2	29 May 2003	30	R 1.7
1.3	30 Oct 2003	49	R 1.8
1.4	17 May 2004	81	R 1.9
1.5	25 Oct 2004	100	R 2.0
1.6	18 May 2005	123	R 2.1
1.7	14 Oct 2005	141	R 2.2
1.8	27 Apr 2006	172	R 2.3
1.9	4 Oct 2006	188	R 2.4
2.0	26 Apr 2007	214	R 2.5
2.1	8 Oct 2007	233	R 2.6
2.2	1 May 2008	260	R 2.7
2.3	22 Oct 2008	294	R 2.8
2.4	21 Apr 2009	320	R 2.9
2.5	28 Oct 2009	352	R 2.10
2.6	23 Apr 2010	389	R 2.11
2.7	18 Oct 2010	418	R 2.12
2.8	14 Apr 2011	466	R 2.13
2.9	1 Nov 2011	517	R 2.14
2.10	2 Apr 2012	554	R 2.15
2.11	3 Oct 2012	610	R 2.15
2.12	4 Apr 2013	671	R 3.0
2.13	15 Oct 2013	749	R 3.0
2.14	14 Apr 2014	824	R 3.1
3.0	14 Oct 2014	934	R 3.1
3.1	17 Apr 2015	1024	R 3.2
3.2	14 Oct 2015	1104	R 3.2
3.3	4 May 2016	1211	R 3.3
3.4	18 Oct 2016	1296	R 3.3
3.5	25 Apr 2017	1383	R 3.4
3.6	31 Oct 2017	1473	R 3.4
3.7	1 May 2018	1560	R 3.5

How to Install Bioconductor Packages



First install core packages:

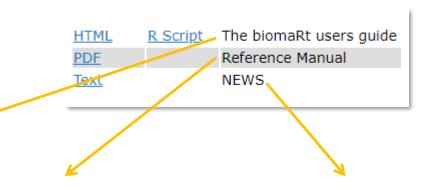
- > source("https://bioconductor.org/biocLite.R")
- > biocLite()

Next install specific packages of interest:

> biocLite("biomaRt")

Exercise: Install Bioconductor. Install the biomaRt package.

Package Reference Manuals, Vignettes, and News



The biomaRt users guide

Steffen Durinck, Wolfgang Huber, Mike Smith

23 May 2018

Package

biomaRt 2.36.1

Contents

- 1 Introduction
- 2 Selecting a BioMart database and dataset
- 3 How to build a biomaRt query
- 4 Examples of biomaRt queries
 - 4.1 Annotate a set of Affymetrix identifiers with HUGO symbol and chromosomal locations of corresponding genes
 - 4.2 Annotate a set of EntrezGene identifiers with GO annotation
 - 4.3 Retrieve all HUGO gene symbols of genes that are located on chromosomes
 - 17,20 or Y, and are associated with specific GO terms
 4.4 Annotate set of identifiers with INTERPRO protein domain identifiers
 - 4.5 Select all Affymetrix identifiers on the hgu133plus2 chip and Ensembl gene identifiers for genes located on chromosome 16 between basepair 1100000 and
 - 4.6 Retrieve all entrezgene identifiers and HUGO gene symbols of genes which have a "MAP kinase activity" GO term associated with it.

exportFASTA

Exports getSequence results to FASTA format

Description

Exports getSequence results to FASTA format

Usage

exportFASTA(sequences, file)

.

sequences A data-frame that was the output of the getSequence function file File to which you want to write the data

Author(s)

Steffen Durinck

Examples

if(interactive())(
mart <- useMart("ensembl", dataset="hsapiens_gene_ensembl")
#seq<-getSequence(chromosome=c(2,2),start=c(100000,30000),end=c(100300,30500),mart=mart)</pre>

martDisconnect(mart = mart)

#exportFASTA(seq,file="test.fasta")

CHANGES IN VERSION 2.36.0

BUG FIXES

o Patched problem returning the list of available datasets, if the description of one or more datasets included an apostrophe (introduced with new primate species in Ensembl).

o Caught scenario where ensemblRedirect=FALSE was still being ignored.
o Changed query submission when redirection is detected to cope with
apparently new behaviour of the Ensembl mirrors.

MINOR CHANGES

o Increase query timeout limit to 5 minutes.

CHANGES IN VERSION 2.34.0

NEW FEATURES

 added the listEnsemblArchives() function. This returns a table of the available Ensembl archives, and replaces the archive = TRUE argument to several functions, which was no longer working.

BUG FIXES

o The Ensembl BioMart server doesn't always respond well if queries with more than 500 filter values are submitted. If a query that exceed this is detect biomaRt will now submit the query in batches and concatonate the result when completed.

MINOR CHANGES

o You can now provide a host with 'http://' at the start, or a trailing '/' (typically copy/pasted from a browser) and useMarts() etc will cope.

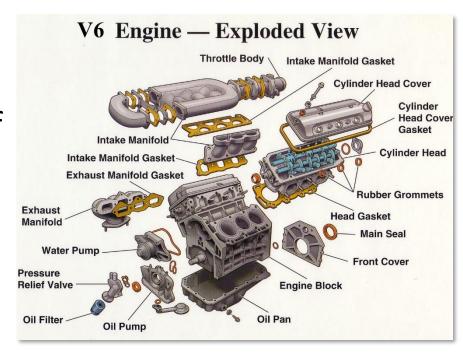
Vignette

User's Manual

Package News

Package Source Code

- What if you wanted to find out more about how a package is implemented?
- By default the binary form of a package is downloaded and installed
- Download the "source" version of the package to view the code



Exercise: Download the source code package for weathermetrics and view the code for the function fahrenheit.to.celsius()

- Here are two ways you can download the source code for the weathermetrics package:
 - 1. Go to https://cran.r-project.org/web/packages/weathermetrics/index.html and download "Package source"
- Use gunzip or winzip to decompress the package
- Use grep to find the file with fahrenheit.to.celsius
- Open the file and find the function

biomaRt Allows Users to Search Across Genomic Annotation Databases

- biomaRt is an R interface to the BioMart software suite (http://biomart.org) that is a repository of inter-connected genome annotation databases
- Challenges in genome annotation are a widespread in the field of bioinformatics for several reasons:
 - 1. Our understanding the genome continues to evolve
 - 2. Many researchers investigating the genome across the globe may use slightly different conventions
 - 3. Genome annotation is biased by historical nomenclature
- Example: AKT1 also has an Entrez gene ID of 207 and Refseq transcripts called NM_005163.2, NM_001014432.1, NM_001014431.1
- Example: AKT1 also has Ensembl transcripts called ENST00000555528.5, ENST00000349310.7, ENST00000407796.6

Exercise: Retrieve Entrez and Ensembl IDs for AKT1, TP53, EGFR, PIK3CA using biomaRt

- 1. Load the package (biomaRt should already be installed from earlier in this session)
- > library(biomaRt)
- 2. Select a mart and a dataset to query
- > ensembl = useMart("ensembl", dataset = "hsapiens_gene_ensembl")
- 3. Use the biomaRt vignette "How to build a biomaRt query" (Section3) to construct a query

HINT: filters = c('hgnc_symbol')

HINT: attributes = c('hgnc_symbol','entrezgene','ensembl_gene_id')

HINT: inputValues = c('AKT1','TP53','EGFR','PIK3CA')

HINT: mart = ensembl

References

- Gentleman, Robert. R Programming for Bioinformatics. CRC Press, 2009.
- Slides Partially Sourced from Barry Grant