"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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8/21/2019

Overview

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

CRAN: The Comprehensive R Archive Network

- CRAN is a website dedicated to hosting the R language and R packages
  - packages are shared collections of R code
- There are currently 14,762 available packages
  - search via google
  - table (index) of available packages
  - CRAN Task Views

Available CRAN Packages By Name

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

A3	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	Tools for ABC Analyses
abd	The Analysis of Biological Data
abe	Augmented Backward Elimination
abf2	Load Gap-Free Axon ABF2 Files
ABHgenotypeR	Easy Visualization of ABH Genotypes
abind	Combine Multidimensional Arrays
abjutils	Useful Tools for Jurimetrical Analysis Used by the Brazilian Jurimetrics Association
abn	Modelling Multivariate Data with Additive Bayesian Networks
abnormality	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

Many 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
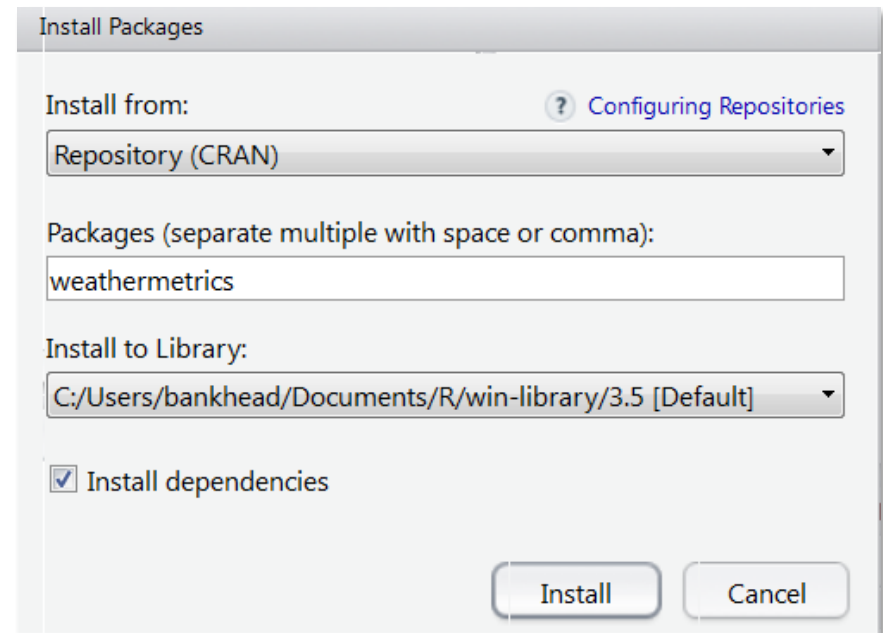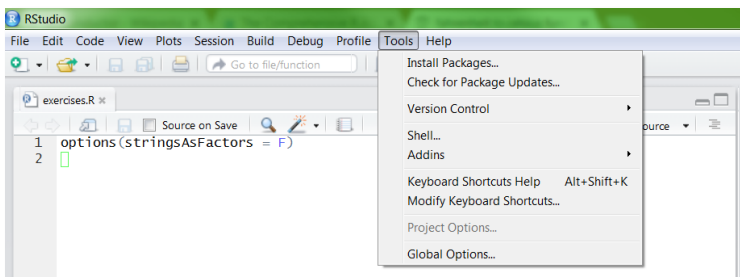
Useful Commands for Exploring R Packages

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

available.packages() – returns packages that are available from CRAN

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

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

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- R packages and datasets for working with high-throughput genomic data
  - http://bioconductor.org
  - Bioconductor was started in Fall 2001
  - Two releases each year
  - v3.9 has 1,741 packages
- Packages undergo formal initial review and continuous automated testing

nature methods

Perspective | Published: 29 January 2015

Orchestrating high-throughput genomic analysis with Bioconductor

Wolfgang Huber ✉, Vincent J Carey, Robert Gentleman, Simon Anders, Marc Carlson, Benilton S Carvalho, Hector Corrada Bravo, Sean Davis, Laurent Gatto, Thomas Girke, Raphael Gottardo, Florian Hahne, Kasper D Hansen, Rafael A Irizarry, Michael Lawrence, Michael I Love, James MacDonald, Valerie Obenchain, Andrzej K Oleś, Hervé Pagès, Alejandro Reyes, Paul Shannon, Gordon K Smyth, Dan Tenenbaum, Levi Waldron & Martin Morgan - Show fewer 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

Project Goals

1. Provide widespread access to a broad range of powerful statistical and graphical methods for the analysis of genomic data.

2. Facilitate the inclusion of biological metadata in the analysis of genomic data, e.g. literature data from PubMed, annotation data from LocusLink/Entrez.

3. Provide a common software platform that enables the rapid development and deployment of plug-able, scalable, and interoperable software.

4. Further scientific understanding by producing high-quality documentation and reproducible research.

5. Train researchers on computational and statistical methods for the analysis of genomic data.

How to Install Bioconductor Packages
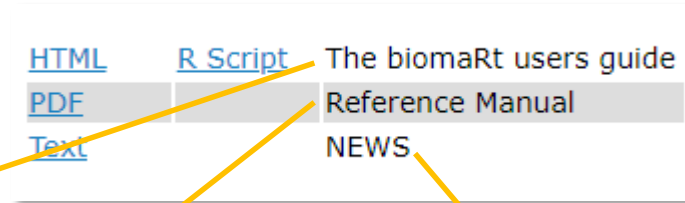
First install core packages:

```
> install.packages("BiocManager")
```

Next install specific packages of interest:

```
> BiocManager::install("biomaRt")
```

Exercise: Install Bioconductor. Install the biomaRt package. This may take time…

Package Reference Manuals, Vignettes, and News

HTML	R Script	The biomaRt users guide
PDF		Reference Manual
Text		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 idenfiers 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 1250000.
    4.6 Retrieve all entrezgene identifiers and HUGO gene symbols of genes which have a "MAP kinase activity" GO term associated with it.

Vignette

---

exportFASTA   *Exports getSequence results to FASTA format*

Description

Exports getSequence results to FASTA format

Usage

exportFASTA(sequences, file)

Arguments

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

martDisconnect(mart = mart)
}
```

User's Manual

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

    o 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.

Package News

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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

V6 Engine — Exploded View
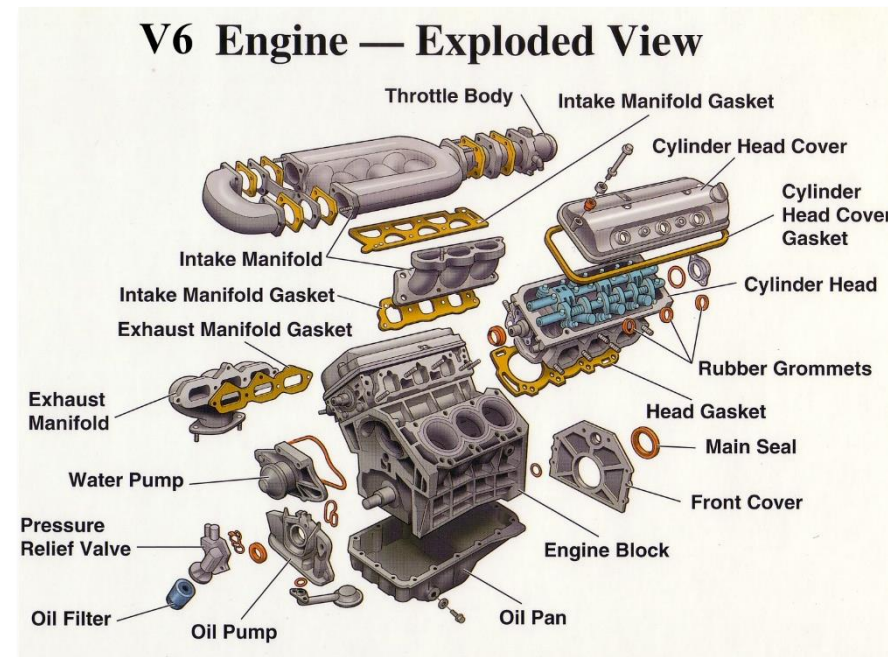
Exercise: Download the source code package for weathermetrics and view the code for the function fahrenheit.to.celsius()

- 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"
   2. `download.packages(pkgs = "weathermetrics", destdir = ".", type = "source")`
- Use gunzip or winzip to decompress the package
- Use grep to find the file with fahrenheit.to.celsius
    - HINT: R/temperature_conversions.R
- Open the file and find the function

HADLEY · WICKHAM · HADLEYVERSE

The Hitchhiker's Guide to the Hadleyverse

- Developed popular ggplot2, dplyr, reshape packages

- Chief data scientist at Rstudio

- Hadleyverse are 55 packages (2015) developed by Hadley Wicham

Hadley Wicham
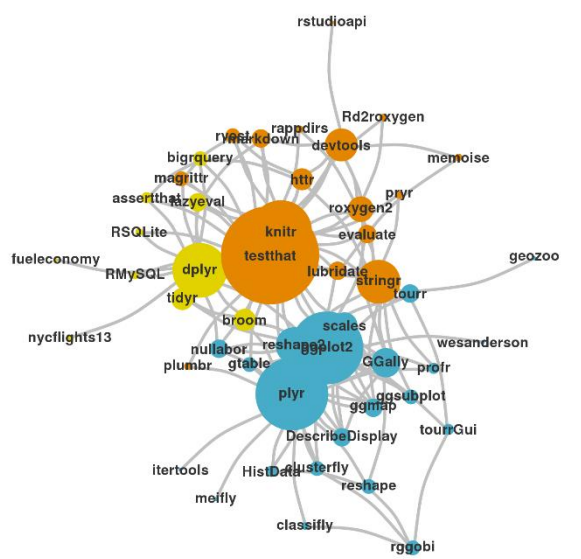
Tidyverse

packages
- ggplot2: data graphics and visualization
- dplyr: data frame manipulation
- tidyr: data wrangling (reshape replacement)
- readr: methods to read rectangular data formats
- purr: supports piping data to replace loops
- tibble: updated data.frames
- stringr: string manipulation methods
- forcats: updated factors

Note: R programming styles vary, tidyverse is something you should be aware of but not all R programmers use it.

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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

Durinck *et al.*, Nature Protocols (2009)

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" (Section 3) to construct a query

HINT: filters = c('hgnc_symbol')

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

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

HINT: mart = ensembl

Closing Remarks/Advice

- Comment your code

- Short programs are better

- Plan!

- Be prepared to iterate
  - Make a change
  - Run
  - Make another change
  - Run
  - …

References

- Gentleman, Robert. R Programming for Bioinformatics. CRC Press, 2009.

- Slides sourced in part from Barry Grant