The Bioconductor Project: Current Status

Martin Morgan

Roswell Park Cancer Institute Buffalo, NY, USA martin.morgan@roswellpark.org

4 November 2016

Bioconductor











https://bioconductor.org https://support.bioconductor.org Analysis and comprehension of high-throughput genomic data.

- Started 2002
- 1296 R packages developed by 'us' and user-contributed.

Well-used and respected.

- 43k unique IP downloads / month.
- 17,000 PubMedCentral citations.

State of the project

- Packages
- Users
- Web & support sites
- Training & meetings
- Release & devel builders
- Funding
- Governance: (annual) Scientific Advisory Board; (monthly) Technical Advisory Board

Recent developments

- New package reviews
- ExperimentHub and AnnotationHub
- Large data representation: HDF5Array
- (Sneak peak) Organism.dplyr

HDF5Array

```
library(HDF5Array) # available in release & devel
n = 10000; m = 1000; # very large size
h5 = HDF5Array(matrix(rnorm(n * m), n))
h5 + h5 # 'delayed' computation
library(SummarizedExperiment)
SummarizedExperiment(h5) # rich context
```

Sneak peak: Organism.dplyr

```
> library(Organism.dplyr) # not yet publicly available
> src = src_ucsc("Homo sapiens") # any org.* + TxDb.*
using org. Hs.eg.db, TxDb. Hsapiens. UCSC.hg38.knownGene
> src
src: sqlite 3.8.6 [/home/mtmorgan/organism_dplry.sqlite]
tbls: id, id_accession, id_go, id_go_all, id_omim_pm,
  id_protein, id_transcript, ranges_cds, ranges_exon,
 ranges_gene, ranges_tx
> tbl(src, 'id') %>% filter(symbol == 'BRCA1') %>%
    select(ensembl, symbol, genename)
> exons(src, filter=list(symobl='BRCA1'))
                                               # GRanges
> exons_tbl(src, filter=list(symbol='BRCA1'))
                                               # tibble
```

Programming best practices

- Reuse & interoperability
- Correct, robust, efficient (vectorized) code; BiocParallel
- Documentation: classic or roxygen2
- Testing: *RUnit* or *testthat*
- Classic, tidy, and semantically rich data

Correct, robust, efficient...

```
f = function(n) {
                                f2 = function(n)
                                   vapply(1:n, c, integer(1))
  x = integer(0)
  for (i in 1:n)
      x = c(x, i)
                                f3 = function(n)
                                   seq_len(n)
  X
microbenchmark(f(1000),
                                 ## correct
  f(10000), f(100000))
                                 identical(f(100), f3(100))
f1 = function(n)  {
                                 ## robust!
                                f(0): f3(0)
  x = integer(n)
  for (i in 1:n)
    x[i] = i
                                 ## efficient
                                 system.time(f3(1e9)
  X
```

Classic, tidy, rich: RNA-seq count data

Classic

• Sample x (phenotype + expression) Feature data.frame

Tidy

 'Melt' expression values to two long columns, replicated phenotype columns. End result: long data frame.

Rich, e.g., SummarizedExperiment

 Phenotype and expression data manipulated in a coordinated fashion but stored separately.

Classic, tidy, rich: RNA-seq count data

```
df0 <- as.data.frame(list(mean=colMeans(classic[, -(1:22)])))
df1 <- tidy %>% group_by(probeset) %>%
    summarize(mean=mean(exprs))
df2 <- as.data.frame(list(mean=rowMeans(assay(rich))))
ggplot(df1, aes(mean)) + geom_density()</pre>
```

Classic, tidy, rich: RNA-seq count data

Vocabulary

- Classic: extensive
- Tidy: restricted endomorphisms
- Rich: extensive, meaningful

Constraints (e.g., probes & samples)

- Tidy: implicit
- Classic, Rich: explicit

Flexibility

- Classic, tidy: general-purpose
- Rich: specialized

Programming contract

- Classic, tidy: limited
- Rich: strict

Lessons learned / best practices

- Considerable value in semantically rich structures
- Current implementations trade-off user and developer convenience
- Endomorphism, simple vocabulary, consistent paradigm aid use

Future challenges

- Git
- Cloud. Possible visions:
 - As now, but 'in the cloud'
 - Integrated with 'third party' compute efforts, e.g., NCI, NIH in the United States

Acknowledgments

Core team (current & recent): Yubo Cheng, Valerie Obenchain, Hervé Pagès, Marcel Ramos, Lori Shepherd, Dan Tenenbaum, Greg Wargula.

Technical advisory board: Vincent Carey, Kasper Hansen, Wolfgang Huber, Robert Gentleman, Rafael Irizzary, Levi Waldron, Michael Lawrence, Sean Davis, Aedin Culhane

Scientific advisory board: Simon Tavare (CRUK), Paul Flicek (EMBL/EBI), Simon Urbanek (AT&T), Vincent Carey (Brigham & Women's), Wolfgang Huber (EBI), Rafael Irizzary (Dana Farber), Robert Gentleman (23andMe)

Research reported in this presentation was supported by the National Human Genome Research Institute and the National Cancer Institute of the National Institutes of Health under award numbers U41HG004059 and U24CA180996. The content is solely the responsibility of the authors and does not necessarily represent the official views of the National Institutes of Health.