Microbiome data containers in R/Bioconductor

CSC course, Leo Lahti, Nov 28 – Dec 2, 2022



Overview

- Rationale for data containers
- Microbiome data containers

Data containers support collaborative development of analysis methods & workflows

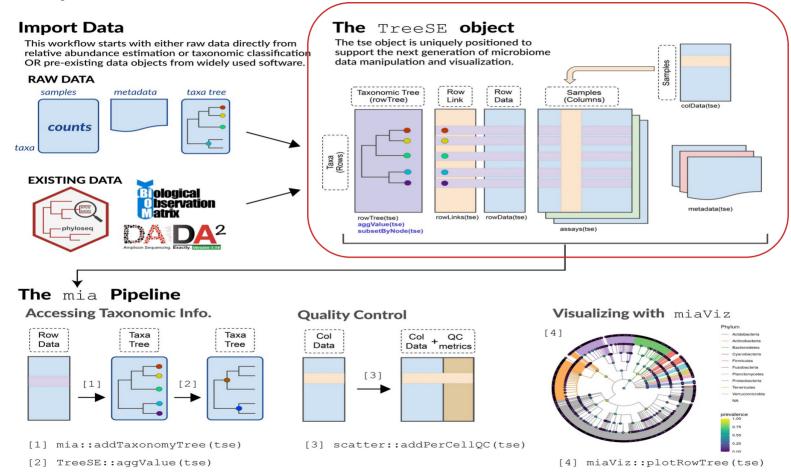
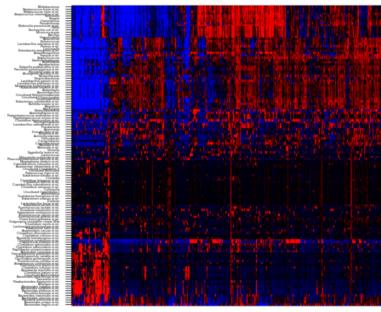


Fig: Domenick Braccia, EuroBioC 2020

microbiome.github.io

"Omics" data

taxonomic abundance table (features x samples)



Gut microbiota: 1000 western adults (Lahti *et al.* Nature Comm. 2014)

Each data type has its own special properties

- Genomics
- Epigenomics
- Microbiomics
- Lipidomics
- Proteomics
- Glycomics
- Foodomics
- Transcriptomics
- Metabolomics
- Culturomics

Software for the Integration of Multiomics Experiments in Bioconductor FREE

Marcel Ramos: Lucas Schiffer; Angela Re; Rimsha Azhar; Azfar Basunia; Carmen Rodriguez; Tiffany Chan; Phil Chapman; Sean R. Davis; David Gomez-Cabrero; Aedin C. Culhane; Benjamin Haibe-Kains; Kasper D. Hansen: Hanish Kodali: Marie S. Louis: Arvind S. Mer; Markus Riester; Martin Morgan; Vince Carev; Levi Waldron



+ Author & Article Information

Cancer Res (2017) 77 (21): e39-e42.

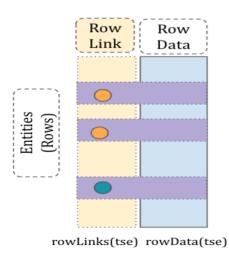
(Tree)SummarizedExperiment

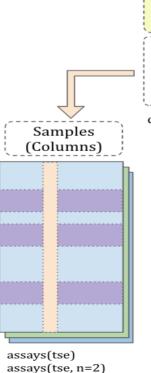
RangedSummarizedExperiment

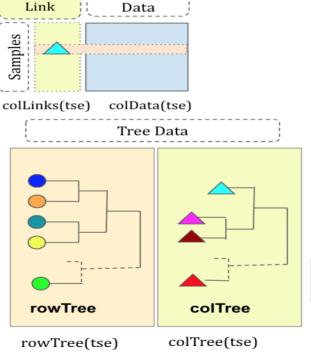
MultiAssayExperiment

SingleCellExperiment

SpatialExperiment







Column

Column

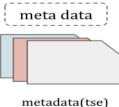


Fig: TreeSummarizedExperiment by Huang et al. (2021)

Optimal container for microbiome data?

Multiple assays seamless interlinking

Hierarchical data supporting samples & features

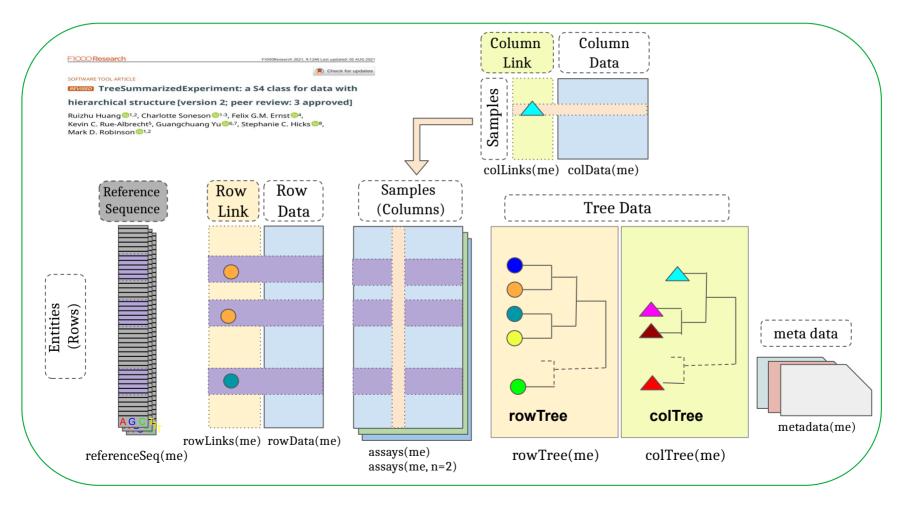
Side information extended capabilities & data types

Optimized for speed & memory

Integrated with other applications & frameworks

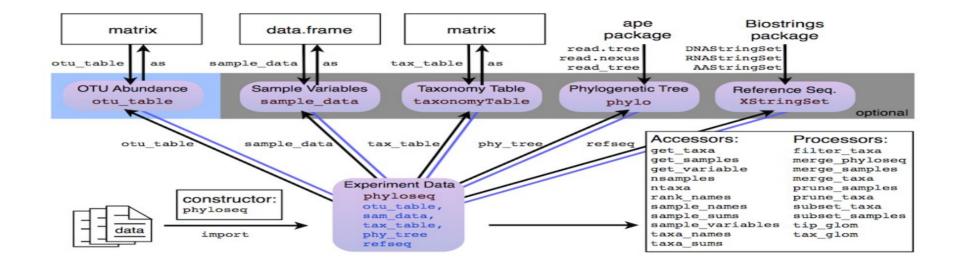
Reduce overlapping efforts, improve interoperability, ensure sustainability.

(Tree)SummarizedExperiment



Alternative data container: phyloseq

Standard for (16S) microbiome bioinformatics in R (J McMurdie, S Holmes et al.)



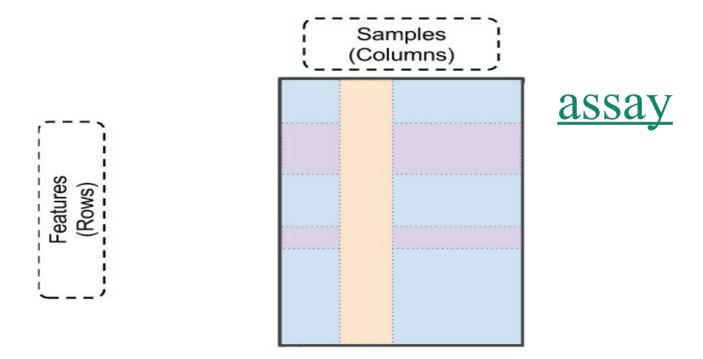
REVISED Bioconductor Workflow for Microbiome Data Analysis: from raw reads to community analyses [version 2; peer review: 3 approved]





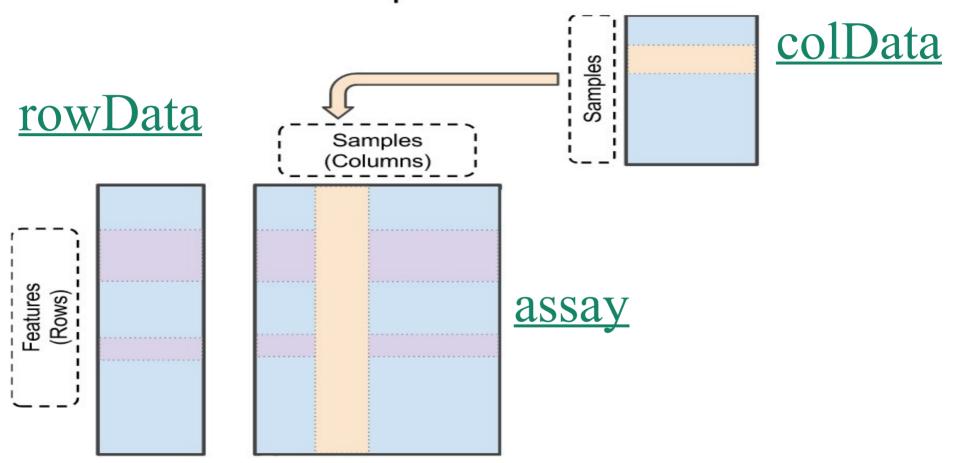


SummarizedExperiment

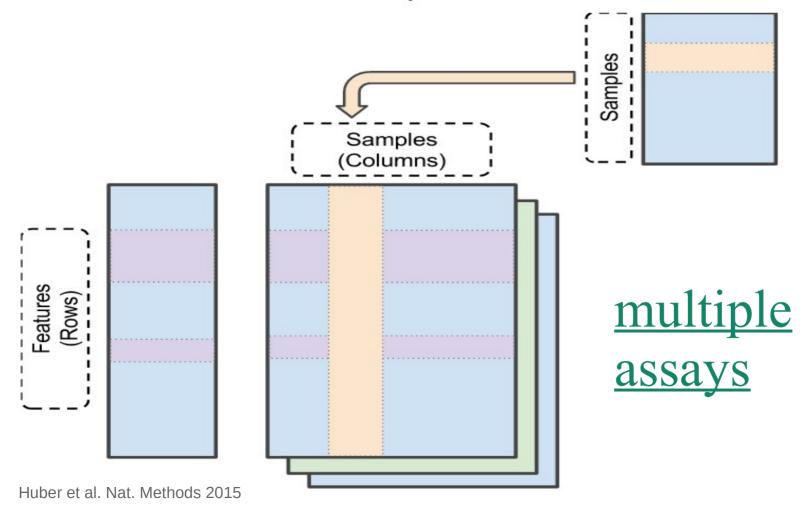


Huber et al. Nat. Methods 2015

SummarizedExperiment



SummarizedExperiment



Integrating parallel data sources

Recommended	Cols (samples)	Rows (features)	Option
Data transformations	match	match	assays
Alternative experiments	match	free	altExp
Multi-omic experiments	free (mapping)	free	MultiAssay

Data operations

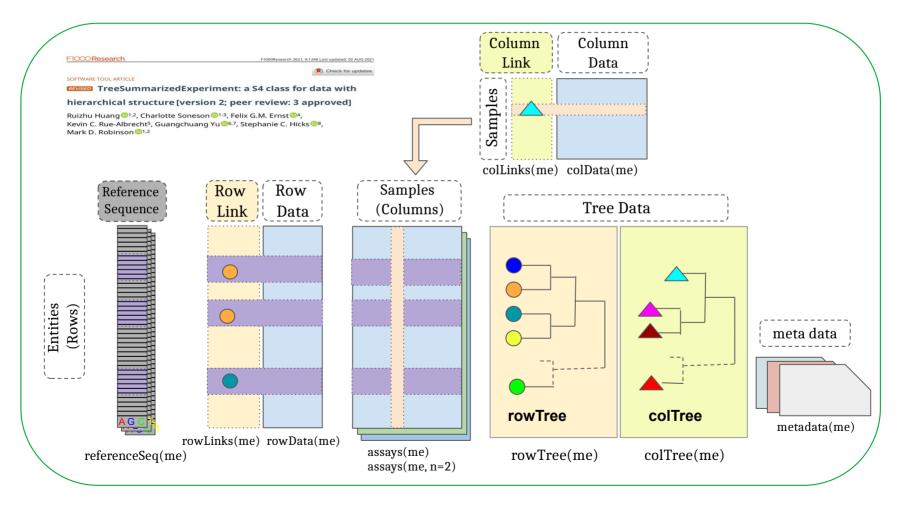
Abundance data: assay(tse, "counts")

Feature information: rowData(tse)

Sample information: colData(tse)

Alternative experiments: altExp(tse, "Genus")

TreeSummarizedExperiment



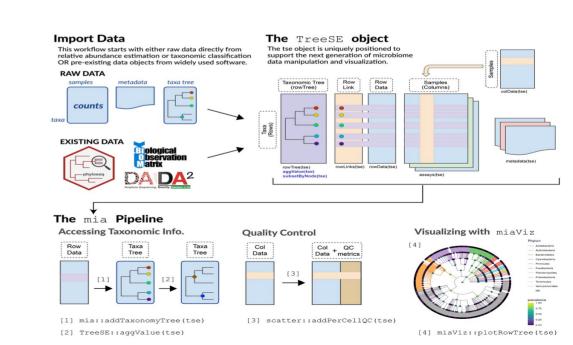
Summary

Data containers:

- Standardized data presentations
- Optimized techniques
- Key part of the data science workflow

They facilitate:

- Transparent analysis
- Reproducible research
- Interoperability of tools
- Usability & documentation
- Collaboration



Acknowledgments

Course organizers:

- Finnish IT Center for Science (CSC)
- Department of Computing, University of Turku, Finland

Material preparation supported by:















