liftr: an R Package for Persistent Reproducible Research

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The Reproducibility Crisis

- Always a concern in both academia & industry.
- R Markdown + knitr pretty much saved the day.

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| 1,500 scientists lift Survey sheds light on the 'crisis' ro | the lid on reproducibility | | | |
| IS THERE A R | REPRODUCIBILITY CRIS 7% 52% Don't know Yes, a significant crisis 1,576 researchers surveyed | IS? | | |

The New Challenge

Even higher reproducibility for statistical computing: regardless of *time* or *environment*.

Docker to the Rescue



- Docker allows applications and their dependencies to be packaged into discrete runtime environments, called **containers**.
- Apps packaged in this way can run from diverse infrastructures.

Our Solution: liftr

Persistent, OS-level reproducibility for R Markdown documents.



Containerize R Markdown Documents as Easy as 1-2-3



Introduce additional R Markdown metadata for containerizing reports.

Parse metadata in the document, and generate Dockerfile.

Build Docker image, run the container, and render the RMD document.



IDE integration: RStudio addins (emojified): 📦 🎉 🎌 🔟

Philosophies

- Continuous reproducibility. Reproducible research should be a continuous process, instead of simply archiving code/data.
- **Document first.** R Markdown documents should be the center. Everything should be driven by documents, not packages.
- Minimal footprint. Connect R Markdown and Docker wisely, achieve more flexibility by doing less.

Applications

- Individuals: off-the-shelf solution for achieving persistent, environment-irrelevant reproducibility for data analysis.
- Institutions: key backend component for automated, large-scale report compilation/orchestration services.

dockflow.org

| a dock | flow.org | |
|---|---|--|
| DockFlow | Home About GitHub | |
| Basic Workflows | | |
| Sequence Analysis R Markdown liftr config Import fasta, fastq, BAM, gff, bed, wig, and other sequence formats. Trim, transform, align, and manipulate sequences. Perform quality assessment, ChIP-seq, differential expression, RNA-seq, and other workflows. Access the Sequence Read Archive. | Oligonucleotide Arrays R Markdown liftr config Import Affymetrix, Illumina, Nimblegen, Agilent, and other platforms. Perform quality assessment, normalization, differential expression, clustering, classification, gene set enrichment, genetical genomics and other workflows for expression, exon, copy number, SNP, methylation and other assays. Access GEO, ArrayExpress, Biomart, UCSC, and other community resources. | |
| Annotation Resources R Markdown liftr config Introduction to using gene, pathway, gene ontology, homology annotations and the AnnotationHub. Access GO, KEGG, NCBI, Biomart, UCSC, vendor, and other sources. | Annotating Genomic Ranges R Markdown liftr config Represent common sequence data types (e.g., from BAM, gff, bed, and wig files) as genomic ranges for simple and advanced range-based queries. | |
| Annotating Genomic Variants R Markdown liftr config Read and write VCF files. Identify structural location of | Changing Genomic Coordinate Systems with rtracklayer::liftOver R Markdown liftr config | |

variants and compute amino acid coding changes for nonsynonymous variants. Use SIFT and PolyPhen database packages to predict consequence of amino acid coding The liftOver facilities developed in conjunction with the UCSC browser track infrastructure are available for transforming data in GRanges formats. This is illustrated

Easily containerized ~20 complex R Markdown workflows from Bioconductor.

Feature Roadmap

- Automatic inference of document dependencies (packrat)
- New renderers for bookdown, xaringan, and blogdown
- Improve CLI message interface (cli + crayon)
- Better Docker integration (reticulate + Docker API)

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