maplet: An extensible R toolbox for modular and reproducible omics pipelines

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Abstract

This paper presents maplet, an open-source R package for the creation of highly customizable, fully reproducible statistical pipelines for omics data analysis, with a special focus on metabolomics-based methods. It builds on the SummarizedExperiment data structure to create a centralized pipeline framework for storing data, analysis steps, results, and visualizations. maplet’s key design feature is its modularity, which offers several advantages, such as ensuring code quality through the individual maintenance of functions and promoting collaborative development by removing technical barriers to code contribution. With over 90 functions, the package includes a wide range of functionalities, covering many widely used statistical approaches and data visualization techniques.

Availability and implementation

The maplet package is implemented in R and freely available at https://github.com/krumsieklab/maplet.
1 Introduction

A major shift within the biomedical community in recent years has been a push to promote reproducibility in research\textsuperscript{1-3}. This has led to substantial changes in scientific publishing, including new rules for the mandatory sharing of source code and accompanying data for publication in peer-reviewed journals\textsuperscript{4}. Adapting data analysis workflows to these new prerequisites often requires significant time and effort to develop code that is easily readable, robust, and sharable.

The most effective way to facilitate reproducibility in everyday data analysis workflows is through modular toolboxes that automate large parts of a typical omics data processing pipeline while also allowing for high customizability. A modular toolbox is designed such that specific tasks are encapsulated as individual functions. This design offers several advantages, such as ensuring robust code through the individual development, testing, and maintenance of functions and promoting collaborative development by removing technical barriers to code contribution.

Here we present maplet, an open-source R package that provides a modular pipeline framework for flexible and reproducible omics data analysis, with a special focus on metabolomics data. maplet contains a diverse collection of functions, covering preprocessing, statistical analysis, pathway analysis, visualization, and various other functionalities. The toolbox is under active development by an international team. While there are other toolboxes for creating analytical pipelines, such as MetaboAnalyst\textsuperscript{R6} or structToolbox\textsuperscript{7}, none provide the same degree of reproducibility and extensibility offered by maplet.

2 Toolbox

2.1 Pipeline Design

The maplet package allows for the creation of fully reproducible analytical pipelines. This is achieved by using a centralized pipeline object that is passed between each function and records all data, results, plots, analysis steps and their parameters. The pipeline object builds on SummarizedExperiment\textsuperscript{6}, a container class provided by Bioconductor\textsuperscript{7} which stores datasets and all corresponding annotations in a single object.

maplet is designed to be used with a pipe operator – either the popular %>% operator from the magrittr package\textsuperscript{8} or the recently introduced |> operator from base R. Pipe operators enable the smooth connection of processing steps in a maplet pipeline - seamlessly passing the container object from function to function. This makes code more readable and eliminates the need for intermediate result variables. Figure 1 presents a subsection of a pipeline and a diagram representing how each step in the pipeline is stored in the container object.

2.2 Modularity

maplet follows a modular ‘one function, one operation’ design. Each task is encapsulated in a single function, which enables the rapid development of pipelines where any step can be flexibly inserted, removed, or rearranged. Another key advantage of this modular design is the ability to maintain high-quality code. Since functions have no interdependencies, they can be rigorously evaluated and maintained separately. Finally, the modular structure promotes a culture of open-source development by
removing the technical barriers to code contribution for unfamiliar developers. Any interested user can add a desired functionality based on a simple function template and only minimal knowledge of the inner workings of the package.

2.3 Functionality

Currently, maplet contains a growing set of over 90 functions organized into various groups, such as data loading, annotation, data modification, preprocessing, statistical analysis, visualization, reporting results, exporting data, and pipeline maintenance. This covers many commonly used analytical methods necessary for standard data analysis encountered in everyday research projects. There are specialized loading functions for working with data from various popular omics platforms and a wide variety of functionalities commonly used by bioinformatics researchers, including linear models, missing-value imputation, PCA, heatmaps, as well as more advanced functionalities such as pathway analysis and network inference. The maplet package comes with several extensive example pipelines and documentation to aid new users in the design of new workflows.

2.4 Report Generation and Result Access

Once a maplet pipeline has been executed, results can be visualized through comprehensive reports automatically assembled by maplet using R markdown/knitr. These reports lay out all functions in the pipeline in the order they were executed, including the name of the function, arguments, and any plots or statistics tables produced by the function. The report is compiled into a single HTML, PDF, or Word document, which stores all results in a single location and can be easily shared. Moreover, maplet comes with a series of accessor functions, which allow the user to extract processed data, statistical results or plots from the pipeline object and further analyze them using their own R code.

3 Conclusion

The maplet R package facilitates the fast development of reproducible analysis pipelines for omics data. Its modular design allows for highly customizable, fully reproducible omics pipelines, while also improving readability, ensuring code quality, and promoting open-source development.
**Figure 1.** maplet pipeline. All data and annotations are stored in a central SummarizedExperiment object, which is passed between functions. Each function generates a result entry, containing all function-specific information as well as the results the function generated (such as statistics tables and plots).

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References

1. Baker, M. 1,500 scientists lift the lid on reproducibility. *Nature News* **533**, 452 (2016).
2. Brito, J. J. *et al.* Recommendations to enhance rigor and reproducibility in biomedical research. *GigaScience* **9**, (2020).
3. Winchester, C. Give every paper a read for reproducibility. *Nature* **557**, 281–281 (2018).
4. Baker, M. Why scientists must share their research code. *Nature News* doi:10.1038/nature.2016.20504.
5. Morgan, M., Obenchain, V., Hester, J. & Pagès, H. *SummarizedExperiment: SummarizedExperiment container.* (Bioconductor version: Release (3.12), 2021). doi:10.18129/B9.bioc.SummarizedExperiment.
6. Chong, J. & Xia, J. MetaboAnalystR: an R package for flexible and reproducible analysis of metabolomics data. *Bioinformatics* **34**, 4313–4314 (2018).
7. Lloyd, G. R., Jankevics, A. & Weber, R. J. M. struct: an R/Bioconductor-based framework for standardized metabolomics data analysis and beyond. *Bioinformatics* **36**, 5551–5552 (2020).
8. Huber, W. *et al.* Orchestrating high-throughput genomic analysis with Bioconductor. *Nature Methods* **12**, 115–121 (2015).
9. Stefan Milton Bache & Hadley Wickham. *magrittr: A Forward-Pipe Operator for R.* (2020).