Data and text mining

**MatrixQCvis: shiny-based interactive data quality exploration for omics data**

Thomas Naake* and Wolfgang Huber

Genome Biology Unit, European Molecular Biology Laboratory, Heidelberg 69117, Germany

*To whom correspondence should be addressed.

Associate Editor: Jonathan Wren

Received on June 23, 2021; revised on October 6, 2021; editorial decision on October 25, 2021

**Abstract**

**Motivation:** First-line data quality assessment and exploratory data analysis are integral parts of any data analysis workflow. In high-throughput quantitative omics experiments (e.g. transcriptomics, proteomics and metabolomics), after initial processing, the data are typically presented as a matrix of numbers (feature IDs × samples). Efficient and standardized data quality metrics calculation and visualization are key to track the within-experiment quality of these rectangular data types and to guarantee for high-quality datasets and subsequent biological question-driven inference.

**Results:** We present MatrixQCvis, which provides interactive visualization of data quality metrics at the per-sample and per-feature level using R’s shiny framework. It provides efficient and standardized ways to analyze data quality of quantitative omics data types that come in a matrix-like format (features IDs × samples). MatrixQCvis builds upon the Bioconductor SummarizedExperiment S4 class and thus facilitates the integration into existing workflows.

**Availability and implementation:** MatrixQCvis is implemented in R. It is available via Bioconductor and released under the GPL v3.0 license.

**Contact:** thomas.naake@embl.de

**Supplementary information:** Supplementary data are available at Bioinformatics online.

1 Introduction

Initial first-line data quality assessment is an integral part of data analysis for subsequent biological question-driven inference. To ensure facile exploration of data quality, we developed MatrixQCvis, implemented in the R programming language. MatrixQCvis provides shiny-based interactive visualization and quantification of data quality metrics at the per-sample and per-feature level. It is broadly applicable to quantitative omics data types that come in a matrix-like format (features × samples). It enables the detection of low-quality samples, outliers, drifts and batch effects in datasets. Visualizations include boxplots and violin plots of the (count or intensity) values, mean versus standard deviation plots, MA plots (see Fig. 1a) and Hoeffding’s D statistic (non-parametric measure of independence between M and A), empirical cumulative distribution function plots, visualizations of the distances between samples and multiple types of dimension reduction plots. Furthermore, MatrixQCvis facilitates differential expression analysis based on the limma (moderated t-tests, Ritchie et al., 2015) and proDA (Wald tests, Ahlmann-Eltze and Anders, 2019) packages.

Similarly to the iSEE package (Rue-Albrecht et al., 2018), MatrixQCvis builds upon the widely used Bioconductor SummarizedExperiment S4 class (see Fig. 1b) and thus facilitates the integration into existing workflows. Compared to iSEE, which provides a general interface for exploring data in a SummarizedExperiment object, MatrixQCvis focuses on the upstream, initial first-line, data quality control steps and incorporates dedicated visualization capabilities for assessing data quality, although overlaps exist (e.g. dimension reduction plots). Several software packages exist that center around the assessment of data quality: among others, arrayQualityMetrics (Kauffmann et al., 2009), initially developed more than 10 years ago for the quality assessment of microarrays, that creates automatic reports of the data quality. Contrary to arrayQualityMetrics, which is built upon outdated visualization libraries, MatrixQCvis uses the shiny (Chang et al., 2021) framework and provides a high number of interactive visualizations to explore the data. MeTaQuaC (Kühring et al., 2020), a recently published R package, is dedicated to metabolomics data analysis, accepts either the Biocrates data output or a generic file format and creates a static quality control report. On the other hand, MatrixQCvis is not restricted to a specific technology and centers around interactive exploration of data quality.

We highlight the usability and functionality of the MatrixQCvis package in applications of clinical proteomics and transcriptomics studies in the Supplementary Material, using the datasets of Jiang et al. (2019) and Brueffer et al. (2018).

2 Usage scenario and user interface

Many tools and software packages exist that directly process raw data and translate these to biological discovery, but offer limited
Fig. 1. Examples of MatrixQCvis functionality and user interface. (a) MA plot of human plasma proteomics samples identifying a dependence between M and A values for Sample 6 indicating problems with its data. More visualizations using the clinical datasets of Jiang et al. (2019) and Brueffer et al. (2018) are shown in the Supplementary Material. (b) MatrixQCvis builds upon the SummarizedExperiment S4 class, a container for assay data (e.g. proteomics intensity values) and associated metadata on the features and samples. The figure is adjusted from the vignette of the SummarizedExperiment package. (c) Sidebar panel. MatrixQCvis enables to interactively normalize, transform, perform batch correction and impute the dataset. Furthermore, samples can be excluded or selected. In the shown example, phosphate-buffered saline samples are excluded. (d) Main panel. Navigation within MatrixQCvis is realized by browsing through tabs. Each visualization is embedded within a dedicated tab.

3 Conclusion

The shiny application MatrixQCvis generates interactive data quality workflows and facilitates to monitor data quality along the major data processing steps via several commonly applied data quality metrics and visualizations. It enables users to create a dynamic, easy-to-share and easy-to-store report using user-specified settings. MatrixQCvis can be integrated into existing workflows and provides a means to scrutinize the data quality of rectangular datasets in a fast, efficient and standardized manner.

Acknowledgements

We acknowledge feedback from the SMART-CARE consortium on usability of MatrixQCvis and all developers and maintainers of the R/Bioconductor packages MatrixQCvis is built upon.

Funding

This work was supported by the Bundesministerium für Bildung und Forschung [grant agreement no. 161L0212E].

Conflict of Interest: none declared.

References

Ahlmann-Eltze, C. and Anders, S. (2019) proDA: probabilistic dropout analysis for identifying differentially abundant proteins in label-free mass spectrometry, bioRxiv.

Brueffer, C. et al. (2018) Clinical value of RNA sequencing-based classifiers for prediction of the five conventional breast cancer biomarkers: a report from the population-based multicenter Sweden cancerome analysis network-brest initiative. JCO Precis. Oncol., 2, 1.

Chang, W. et al. (2021) shiny: Web Application Framework for R, R Package Version 1.6.0. https://cran.r-project.org/web/packages/shiny/ (22 September 2021, date last accessed).

Jiang, J. et al.; Chinese Human Proteome Project (CNHPP) Consortium. (2019) Proteomics identifies new therapeutic targets of early-stage hepatocellular carcinoma. Nature, 567, 257–261.

Kauffmann, A. et al. (2009) arrayQualityMetrics—a bioconductor package for quality assessment of microarray data. Bioinformatics, 25, 415–416.

Kuhring, M. et al. (2020) Concepts and software package for efficient quality control in targeted metabolomics studies: mTeQuaC. Anal. Chem., 92, 10241–10245.

Richer, M.-E. et al. (2015) limma powers differential expression analyses for RNA-sequencing and microarray studies. Nucleic Acids Res., 43, e77.

Rue-Albrecht, K. et al. (2018) iSEE: Interactive SummarizedExperiment Explorer. F1000Res., 7, 741.