tidyHeatmap: an R package for modular heatmap production based on tidy principles

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Background

The heatmap is a powerful tool for visualising multi-dimensional data, where individual values can be organised in a two-dimensional matrix and their values expressed as colours. Rows and columns can be ordered according to their reciprocal similarity using hierarchical clustering; and dendrograms can be added to the plot to facilitate the interpretation. Row- and column-wise visual annotations, such as coloured tiles, can also be included. Within the R environment, several packages have been developed to produce heatmaps. The simplest and most readily available tool, `heatmap`, is provided within the `stats` package (R Core Team 2013) and offers basic heatmaps with simple tile annotations. The versatile package `ggplot2` can be also used to produce basic heatmaps (Wickham 2016). More powerful software exists for producing fully annotated, multi-panel heatmaps, such as `Pheatmap` (Kolde 2012) and `ComplexHeatmap` (Gu, Eils, and Schlesner 2016). The versatility of these packages comes at the cost of adding complexity in the user interface, characterised by many parameters and annotation functions that introduce a steep learning curve to produce complex, clear, and good-looking graphics.

Recently, efforts have been made toward the harmonisation of data frame structures and data analysis workflows using the concept of tidiness. Tidy data frames are characterised by having a specific structure where each variable is a column and each observation is a row. They provide ease of manipulation, modelling, and visualisation. The `tidyverse` is a suite of R libraries that defined the standard for tidy data and APIs (Wickham et al. 2019). The unique correspondence between quantities and annotations, characteristic of tidy data frames, allows complex operations to be performed from simple user inputs, such as a list of column names.

Tidy paradigm for visualisation

`tidyHeatmap` is a graphical R package that introduces tidy principles to the creation of information-rich heatmaps. It is available in the CRAN R repository. This package currently uses `ComplexHeatmap` as its graphical engine; however, due to its modular design it can be readily expanded to interface other engines. The command-line user interface is organised into (i) a main plotting utility; (ii) annotation layer utilities; and (iii) file output utilities. The input data frame streams along the utility path using the pipe operator from `magrittr`, allowing a high-level of modularity. The main utility allows the user to plot a base heatmap with dendrograms. The annotation utilities allow the user to serially add tile, point, bar and/or line annotation boxes to the side of the heatmap. The orientation of the annotations (row- or column-wise) is inferred by the `tidyHeatmap` algorithms, based on the input data frame. The file output utility allows the user to write vector or bitmap images directly from the R object, in the style of `ggplot2`. User defined row- or column-wise clusters can be defined effortlessly by applying the `group_by` function from `dplyr` (Wickham et al. 2020) to the input data frame. Data transformation, row and column scaling is done internally. Together, this leads to a decrease of coding burden of 3 and 5 folds for lines and characters respectively compared to `ComplexHeatmap` (e.g., for Figure 1). Besides offering a modular and user-friendly interface, `tidyHeatmap`

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applies publication-ready aesthetics such as `viridis` (Garnier 2018) and `brewer` (Neuwirth 2014) colour palettes and automatic sizing of row and column labels to avoid overlapping (Figure 1).
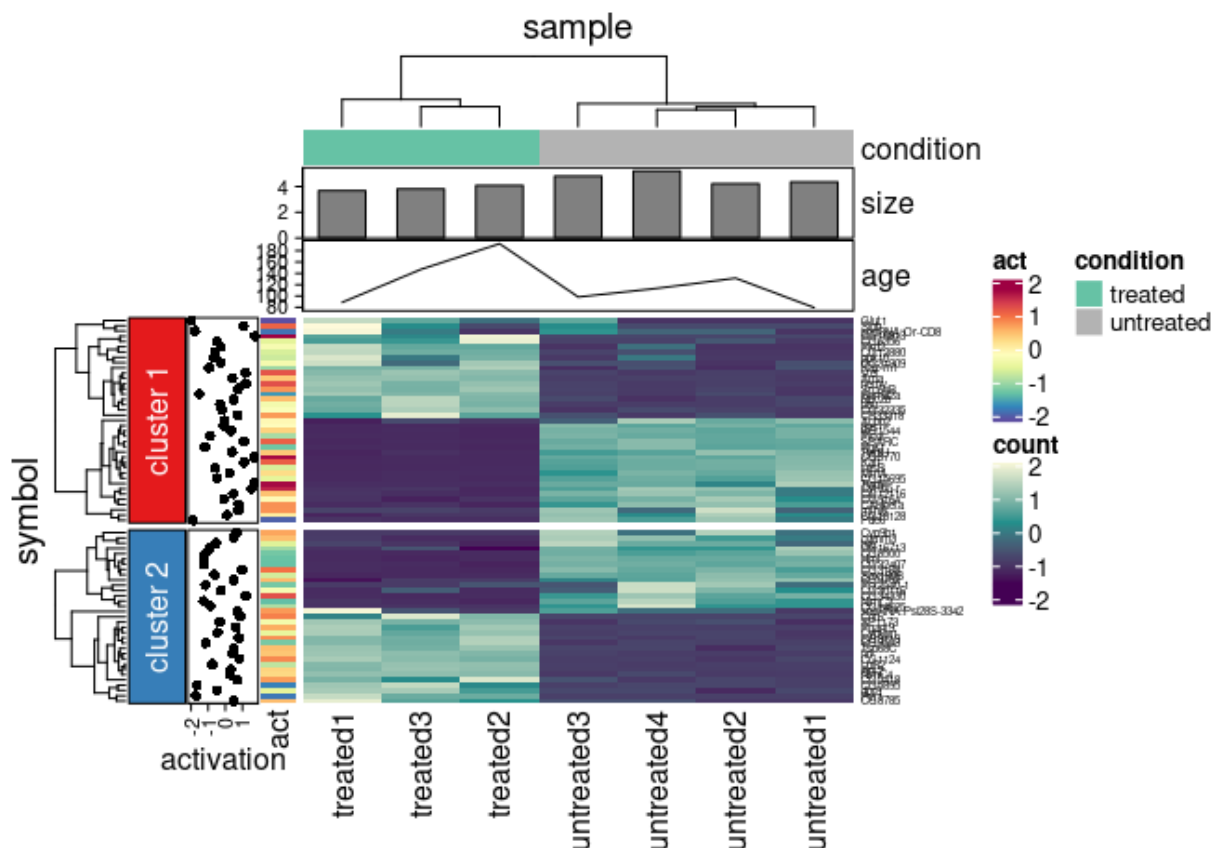

Figure 1: Heatmap of the pasilla dataset including grouping and multiple annotations. Some annotation data was simulated for visualisation purposes.

The input to `tidyHeatmap` is a tidy data frame with three basic columns including row and column element identifiers, and values that will be converted into colours. Additionally, further columns can include information about element grouping and annotation.

element	feature	value	annotation	group
chr or fctr	chr or fctr	numeric	...	...

The code interface consists of modular functions linked through the pipe operator. Custom colour palettes can be used by passing an array of colours or a colour function (e.g., circlize (Gu et al. 2014)) to the palette argument of the annotation utilities.

```
my_heatmap =

    # Grouping
    input_df %>%
    group_by(pathway) %>%

    # Plotting
```

```
    heatmap(feature, element, value) %>%

    # Annotation
    add_tile(condition) %>%
    add_tile(act) %>%
    add_point(activation) %>%
    add_bar(size) %>%
    add_line(age)

# Saving
my_heatmap %>% save_pdf("my_file.pdf")
```

Conclusions

In order to perform complex tasks, the use of disjointed data structures demands time consuming and bug-prone information matching. Joint, tidy data frames decrease the cost/benefit ratio for the user, automating a large part on the data manipulation. `tidyHeatmap` introduces a modular paradigm for specifying information-rich heatmaps, just requiring column names as input. Due to its intuitive user interface and its advanced default aesthetic features, `tidyHeatmap` is ideal for the quick production of publication-ready heatmaps. This software is designed for modular expandability. Future directions include the incorporation of more static and interactive heatmap visualisation engines.

Acknowledgements

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