App authorship

This app was created by Albert Xue in the Bagheri Lab at Northwestern University. Its original implementation was on an SNA dataset created in collaboration with the Mirkin and Mrksich labs. All code was developed by Albert Xue and is freely available for all to use. The github repo is intended to be published alongside our manuscript with the following authors: Gokay Yamankurt, Eric J. Berns, Albert Xue, Andrew Lee, Neda Bagheri, Milan Mrksich, Chad A. Mirkin.

App introduction

This app creates a dimensional stacking figure to visualize multiple dimensions of data. The app “stacks” the different dimensions on top of one another such that all datapoints can be visible simultaneously (See example\_output.pdf). This allows viewing of complicated relationships amongst many variables. However, there are limitations: the data needs to be discrete or categorical and continuous values will not work properly, datasets with more than ~10 variables and/or 1500 samples will not fit well, and the variable stacking order requires manual tuning.

This app is interactive meaning any change you make on the front should immediately update on the user interface. If you make a change that breaks the code/figure, you can either reload the app (losing all progress) or revert the change.

App startup

To start the app, you need both R and RStudio installed. Then, double click on ui.R and RStudio should pop up (if not, configure it so all .R files run with RStudio). Press Ctrl-Shift-Enter to run the app and a user interface should pop up. To exit or restart the app, simply close the pop-up app window.

File Inputs and Outputs

File input is on the left. “Choose data file” loads in the

In the first method, look at the example\_bubble\_colors.csv file. There are 19 columns and 19 rows, each representing the X- and Z-positions in the GRKXZC array, respectively. The example\_bubble\_sizes.csv file has the same format but defines the bubble sizes. Both bubble size and bubble color should be normalized between 0 and 1, but the interface allows some tweaking of values for aesthetic reason. This app can support any number of amino acids. For both the size and color files, the app requires a row and column to define the amino acid letters.

The second method merges both bubble colors and sizes. This style can be found in example\_data\_file.csv. The first two columns must be color and size, followed by the amino acid letter for the two positions. The first row will be ignored by the app, but is useful to input information for your reference.

\*\*To be revised\*\*

Currently, the csv file must be located in the same folder as server.R and ui.R. This is due to differences in how computers handle file directories. Similarly, the output file name should also print out to the same folder as server.R, and you will have to manually move them from there.

The “Choose output file name” will specify the names of the table/figure, should you choose to make them. It is set to “example\_output” by default.

Plotting Parameters

This app supports basic visual changes such as colors, amino acid ordering, and tweaking the size/color of bubbles to fit an aesthetic.

In the default example, the 19 columns represent the 19 amino acids in the X-position while the rows correspond to the Z-position. Color corresponds to enzymatic activity of a deacetylation experiment and size corresponds to the signal to noise ratio (S/N) of the peptide. You can see that incorporating the S/N information prioritizes certain peptides for analysis. The default color uses red and has amino acids sorted by their mean circle size, but this can be sorted by bubble color or alphabetical instead under “Amino acid order”. Sorting can also be reversed under “Order of amino acids.”

Under “Tinkering parameters”, the size scaling factor allows a user to tweak all of the bubble sizes for aesthetic reason. For example, you may wish to decrease all bubble sizes slightly if many bubbles are overlapping. Amino acid label resizing also scales the column and row amino acid labels. Both resizing numbers are multiplicative, meaning a 2 doubles the sizes while a 0.5 halves the sizes, etc. There are a few default color schemes under “Select color scale,” but there is no way right now to specify custom colors.

Author information

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