Subject: Forcing column headers on import, using regression
Posted by skarrila on Tue, 26 Jul 2016 01:13:03 GMT
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I use this package for exploratory data visualization, not for cheminformatics.

To de-pivot I need to have the first row of my cut/paste Excel data as headers. I managed to force this by making an extra column with string in first row and numbers after that; otherwise I got generic column names. Is there some built-in feature for the purpose of forcing a row to become column headers? If not, how can I effectively cut/paste a row to become headers?

The package is excellent in what it does, but I can't access the least squares regression with my data. If you simply have a column "y" as targeted output, and columns "x1",..., "xn" as model inputs, how is linear regression executed to fit a predictive model? It seems that the regression function is currently "hidden" so it can only be used with computed chemical characteristics...

Thank you and best regards.

Subject: Re: Forcing column headers on import, using regression
Posted by thomas on Tue, 09 Aug 2016 11:36:22 GMT
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Sorry for the delay. I see the point and added two menu options to enforce pasting with and without a header row. The 'Paste' macro task now also has these options.

To your second point: I had built in a PLS regression only temporarily and just for the purpose of calculating atom type based contributions for polar and non-polar surface prediction, but I didn't invest the time to build an UI, test, and document it to open it for general model building. If there is sufficient interest, I may add it after the upcoming DataWarrior update.

Kind regards,

Thomas