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.