Subject: PCA
Posted by khom on Tue, 19 Jun 2018 20:09:01 GMT
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Could you please tell me how I could get access to the loading plot of a PCA analysis? Thank you.

Subject: Re: PCA
Posted by thomas on Sun, 08 Jul 2018 16:33:15 GMT
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I am not sure, whether I understand your question correctly. If you intend to make a PCA from multidimensional data and then plot the 2 or 3 most significant dimensions, then you need to do these steps:

- Data-> Calculate Principal Components...
- select the columns that contain your input data (or a descriptor column of chemical structures)
- click OK

Does this answer your question?

Thomas

Subject: Re: PCA
Posted by khom on Tue, 10 Jul 2018 18:43:51 GMT
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Thomas,
I am sorry that I did not pose my question clearly. The PCA plots (PC1 vs PC2, for example) generated as per your instructions are the scores, describing the relations among the observations (samples, rows); I am trying to see if the corresponding loadings plots describing the relationships among the variables (columns) can be displayed as well. Thank you.
Kellie

Subject: Re: PCA
Posted by thomas on Wed, 11 Jul 2018 10:57:08 GMT
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Kellie,
thank you for clarifying. Currently the linear contribution factors (loadings) of the original dimensions are just used internally. One could think of adding a button that allows to copy them as a new table into the clipboard. A paste operation would then create a new DataWarrior file allowing to depict the contributions.
Thomas

Subject: Re: PCA
Posted by thomas on Wed, 11 Jul 2018 13:30:13 GMT
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A small update: I just added a checkbox in the PCA dialog that allows to open an additional window after PCA calculation showing a table with the originally selected variables in rows and their Eigen values in columns. Plots of scores and loadings are equivalent to this example: https://learnche.org/pid/latent-variable-modelling/principal -component-analysis/interpreting-score-plots-and-loading-plo ts

Thus, the next version will have it.

Thomas

Subject: Re: PCA
Posted by khom on Wed, 11 Jul 2018 17:49:58 GMT
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Thomas,
Thank you very much indeed!! The info from the link are very useful also.
Kellie