Subject: Displaying change in r value from a selected sample of a dataset
Posted by Jo W on Tue, 17 Jan 2023 13:57:55 GMT
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In DW it's possible to obtain a fitted line on a sample from a larger dataset. This I find really helpful for example, in looking for sub sets of compounds that may have some possible correlation but may be overlooked when you just look at the dataset as a whole.

However, when doing this in DW, the r values does not correspondingly change to the new fitted line (see attached image for clarification).

- i.e., in the attached image you can take a sample and see the change in the fitted line but the r value stays the same, in this case at 0.49.

It would be good to also see not only the new fitted line on the selected sample, but also the change in the r value as well.

Is it possible to add this as a (minor?) feature change?

File Attachments
1) Displaying change in r value from selected sample of a dataset.docx, downloaded 403 times

Subject: Re: Displaying change in r value from a selected sample of a dataset
Posted by thomas on Fri, 20 Jan 2023 11:44:24 GMT
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Many thanks for suggesting. I just have implemented the change and deployed as dev update.

Subject: Re: Displaying change in r value from a selected sample of a dataset
Posted by Jo W on Fri, 20 Jan 2023 12:34:19 GMT
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Many thanks

Subject: Re: Displaying change in r value from a selected sample of a dataset
Posted by Jo W on Sat, 21 Jan 2023 13:53:41 GMT
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Thomas

Is it also possible to add this to "Assess Prediction Quality" feature- i.e., a selected portion of the 2D graph is assessed rather then the existing choice which at the moment is the "structure" column in the table?

Subject: Re: Displaying change in r value from a selected sample of a dataset
Posted by thomas on Sun, 22 Jan 2023 17:07:51 GMT
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I am not sure, whether I understand correctly: Couldn't you achieve the same thing by just calling "File->New From Selection" and then run the "Assess Prediction Quality"?

Subject: Re: Displaying change in r value from a selected sample of a dataset
Posted by Jo W on Fri, 03 Feb 2023 22:08:52 GMT
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I tried this and it works - so many thanks for the suggestion. I didn't realise you could do that.

It would also be convenient sometimes, to keep the various predictions in the same DW file rather than generate a new one and ideally have all the predictions on the same graph - and if possible to colour code each of the generated fitted lines (e.g predicted vs experimental generated from KNN, PLS etc) to easily visually compare the predictions and also have the r values listed. Is that possible?

Subject: Re: Displaying change in r value from a selected sample of a dataset
Posted by Jo W on Thu, 09 Feb 2023 01:46:39 GMT
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Dear Thomas
When selected data points are highlighted on the 2D graph, the r-value is now adjusted due to the recent update.

However, the correlation matrix is not temporarily updated - is it possible to also see the correlation table updated - ie it shows the correlations of just the selected data points (until they are deselected)? At the moment that is not the case.

Subject: Re: Displaying change in r value from a selected sample of a dataset
Posted by thomas on Tue, 21 Feb 2023 13:59:22 GMT
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The correlation dialog is implemented as modal dialog, which prevents the change of data, view settings, row selection, etc as long as the dialog is open. Thus, with the current architecture changing the selection and immediately see the correlation matrix change, is not possible.

However, I have added a combo box to the dialog, which allows switching between all, selected, visible, and row list members. Changes here cause an immediate recalculation of the matrix. I hope this is a reasonable compromise...

Thomas