Subject: Asses Prediction Quality bug
Posted by Christophe on Fri, 19 Apr 2024 15:00:56 GMT
View Forum Message <> Reply to Message

Hello everyone,

When I run Chemistry/Machine Learning/Assess Prediction Quality onto my data, I get the expected results but then if I save the file, when I try to re-open this file with DW only the Main table remains. All my previous graphs and all my filters are gone !!!!
Any clues ???

Thanks

Christophe

Subject: Re: Asses Prediction Quality bug
Posted by nbehrnd on Sun, 21 Apr 2024 18:06:48 GMT
View Forum Message <> Reply to Message

Hello Christophe,

one possible cause could be that the display of the data only was minimized. As depicted in the silent .mp4 attached, there are little chevrons to act either in horizontal, or vertical direction. Else, to ease a replication of your observation, create a test set of data (free of any PI relevant information), and attach it in a reply.

Norwid

File Attachments
1) chevrons.mp4, downloaded 404 times

Subject: Re: Asses Prediction Quality bug
Posted by Christophe on Mon, 22 Apr 2024 07:53:41 GMT
View Forum Message <> Reply to Message

Hello Norwid,

I still have the problem. You will find attached a sample of my data. Open it, you will find the Table, some UMAP analyses and on the right part my filters. Now run Chemistry/Machine Learning/Assess Prediction Quality. Select "Skelspheres" for the descriptor and tick "Use random fractions instead of time based ones" and then OK. Save the file and try to open it again. You will see that everything but the table are now gone.
Thank you for your help
All the best
Christophe

Subject: Re: Asses Prediction Quality bug
Posted by nbehrnd on Tue, 23 Apr 2024 20:40:39 GMT
View Forum Message <> Reply to Message

Hello Christophe,

affirmative, I can replicate the observation: though the file is saved (as .dwar file), the plots are gone if the file is then closed and opened again.

Because a .dwar file is plain text (though DW's structure IDs are not not necessarily human readable, in comparison to a SMILES strings), I started all over: a pristine copy of test.dwar was monitored by git version control. After the analysis, but prior to closing, the saved file is different: a good amount of lines are «reorganized» (old swapped for new ones, and a few truly new ones). Then, once opened again (and for the sake of git saved again), there are again differences in this .dwar file (in comparison to the state just after the analysis). Now git's notes about lines deleted are much larger in number, than about lines updated/swapped.

I think these observations indeed would support your line of thought the results of the Machine Learning analysis are not fully saved. A pattern different from panels (reversibly) hidden by click on the chevrons and possibly a bug.

Norwid

Subject: Re: Asses Prediction Quality bug
Posted by thomas on Tue, 23 Apr 2024 21:22:30 GMT
View Forum Message <> Reply to Message

Hi Christophe and Norvid,

thank you for investing time in this. I have finally fixed it. The issue was caused by a faulty column order entry in the saved file where one column was referred to twice. The fix will be in the next auto-update. Now the loader tolerates multiple column entries and in addition the faulty entry won't be generated in the first place.

Thomas

Subject: Re: Asses Prediction Quality bug
Posted by Christophe on Wed, 24 Apr 2024 10:52:58 GMT
View Forum Message <> Reply to Message

Hi Norwid and Thomas,

Thank you very much for your time.
I'll be waiting for the next update, no big deal.

All the best
Christophe