

# Black Box no more: How to use modern neural network QC tools to make better predictions.

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## Summary

Black Box - In science, computing, and engineering, a black box is a system which can be viewed in terms of its inputs and outputs without any knowledge of its internal workings. Its implementation is "opaque" (black). (Wikipedia, [https://en.wikipedia.org/wiki/Black\\_box](https://en.wikipedia.org/wiki/Black_box)).

New QC tools mean that neural networks (NN) are no longer black boxes. Today, Partial Dependence Analysis (Friedman, 2001), SHAP Analysis (Lundberg and Lee, 2017), and Importance values from modern neural network QC tools, in addition to conventional correlation and error analysis, mean that we are no longer flying blind when we use NNs. We can use these QC tools to determine what attributes we should and should not use in NNs and MLRs (multi-linear regression) and whether we should be using a non-linear NN or a linear MLR to make predictions. In fact, in our opinion, the traditional workflow should be abandoned, and these tools should be used first.

Traditionally, when working with NNs we have been flying blind. What I consider the traditional workflow when working with NNs was to use MLR to determine what variables were important in the MLR and then throw those variables blindly into a NN to see whether it produced results that had better correlations with the output and/or were more pleasing to the eye than the MLR results.

Now there is a better approach.

## Theory / Method / Workflow

Today there are numerous ways to see into a neural network.

- Correlation
- Error Plots
- Importance
- Partial Dependence Plots
- SHAP Plots

This talk will explore the workflow that we now use to assess which variables to use for prediction and how they are used. This new workflow delves into the NN first because with these new tools we can quickly assess what variables are important and whether or not non-linear relationships are required.

The new workflow consists of the following:

1. Assess the correlation between predictors and predictions.
2. Assess the inter-correlations between predictors.
3. Examine the importance of the predictors on the predictions using PD plots.

4. Re-examine the correlations in 1 & 2 to eliminate correlations that are adversely affecting the prediction and repeat 3 & 4.
5. Use PD plots and SHAP plots to pick the final predictor variables.

## Results

First known correlations of the input variables to the output are assessed to reduce the number of input variables to those that are uncorrelated. Figure 1 shows that we have reduced the number of input attributes from 22 to 11 just by accounting for these correlations. This is done because correlated input variables can wreak havoc, especially on our understanding of neural networks. Later, we will see how we can use PD plots to help us deal with these issues. For now, we want to limit the input variables to those that make the most sense for predicting the output. For example, there is a direct relationship between density and porosity, so if we were predicting porosity and had a quality density attribute but it was correlated to acoustic impedance, we would keep density and drop impedance. If the quality of the density was questionable, and there was a significant correlation with acoustic impedance, then we would keep impedance and drop density. However, when a highly correlated variable is dropped, sometimes it can be beneficial to try switching to the other variable if the neural network solution seems to be stuck in a local minimum.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	
	AI_RMS Amplitude	Density_RMS Amplitude	SI_RMS Amplitude	VP_RMS Amplitude	VS_RMS Amplitude	Mu_RMS Amplitude	MuRho_RMS Amplitude	MuRho_RMS Amplitude	VpVsRatio_RMS Amplitude	PoissonRatio_RMS Amplitude	Lambda_RMS Amplitude	K_RMS Amplitude	E_RMS Amplitude	LamdaRho_RMS Amplitude	Ie_RMS Amplitude	PostisicAmplitude_RMS Amplitude	Most Positive Curvature_RMS Amplitude	Most Negative Curvature_RMS Amplitude	Relative Acoustic Impedance_RMS Amplitude	Eigenstructure Coherence_RMS Amplitude	Event Density_RMS Amplitude	Distance to Well_RMS Amplitude	
1																							
2	0.662																						
3	0.952	0.615																					
4	0.993	0.584	0.955																				
5	0.93	0.518	0.992	0.947																			
6	0.965	0.569	0.913	0.965	0.899																		
7	0.912	0.526	0.972	0.924	0.973	0.926																	
8	0.886	0.546	0.936	0.89	0.929	0.915	0.977																
9	-0.093	-0.016	-0.267	-0.117	-0.299	-0.217	-0.398	-0.393															
10	0.001	-0.006	-0.006	0.001	-0.007	-0.002	-0.008	-0.003	0.044														
11	0.646	0.336	0.458	0.63	0.43	0.606	0.372	0.368	0.309	0.029													
12	0.953	0.557	0.85	0.948	0.83	0.97	0.835	0.8	-0.055	0.003	0.734												
13	0.001	-0.016	-0.002	0.003	-0	0.003	-0.004	-0.003	0.012	0	0.037	0.008											
14	0.477	0.255	0.31	0.456	0.279	0.393	0.197	0.225	0.722	0.026	0.889	0.506	0.02										
15	0.162	0.111	0.16	0.161	0.157	0.154	0.157	0.161	-0.023	0.019	0.134	0.145	0.969	0.074									
16	-0.303	-0.27	-0.292	-0.309	-0.289	-0.334	-0.35	-0.326	0.219	0.015	-0.022	-0.302	0	0.084	-0.037								
17	0.038	-0.021	0.064	0.058	0.066	0.095	0.095	0.111	-0.137	0.011	0.017	0.076	0.009	-0.034	0.045	0.048							
18	0.006	-0.075	0.049	0.019	0.065	0.006	0.038	0.027	-0.119	-0.01	-0.073	-0.015	-0.011	-0.099	0.007	0.148	-0.104						
19	-0.25	-0.208	-0.23	-0.255	-0.228	-0.265	-0.265	-0.244	0.132	0.011	-0.054	-0.25	-0.008	0.021	-0.011	0.849	0.05	0.174					
20	-0.162	-0.059	-0.19	-0.17	-0.196	-0.129	-0.148	-0.145	0.065	0.018	-0.054	-0.11	0.025	-0.017	-0.042	-0.237	-0.074	-0.229	-0.215				
21	0.114	0.185	0.113	0.093	0.09	0.098	0.095	0.123	0.03	-0.007	0.079	0.082	-0.008	0.107	0.025	-0.039	0	-0.134	-0.025	-0.006			
22	-0.004	-0.138	-0.025	0.016	-0.005	0.019	-0.007	-0.034	-0.013	0.01	0.02	0.041	0.013	-0.019	-0.016	-0.039	-0.008	0.118	0.045	0.015	-0.7		

	1	2	3	4	5	6	7	8	9	10
	SI_RMS Amplitude	VpVsRatio_RMS Amplitude	PoissonRatio_RMS Amplitude	E_RMS Amplitude	LamdaRho_RMS Amplitude	Most Positive Curvature_RMS	Most Negative Curvature_RMS	Relative Acoustic Impedance_RMS	Eigenstructure Coherence_RMS	Event Density_RMS
1 SI_RMS Amplitude										
2 VpVsRatio_RMS Amplitude	-0.267									
3 PoissonRatio_RMS Amplitude	-0.006	0.044								
4 E_RMS Amplitude	-0.002	0.012	0							
5 LamdaRho_RMS Amplitude	0.31	0.722	0.026	0.02						
6 Most Positive Curvature_RMS Amplitude	0.064	-0.137	0.011	0.009	-0.034					
7 Most Negative Curvature_RMS Amplitude	0.049	-0.119	-0.01	-0.011	-0.099	-0.104				
8 Relative Acoustic Impedance_RMS Amplitude	-0.23	0.132	0.011	-0.008	0.021	0.05	0.174			
9 Eigenstructure Coherence_RMS Amplitude	-0.19	0.065	0.018	0.025	-0.017	-0.074	-0.229	-0.215		
10 Event Density_RMS Amplitude	0.113	0.03	-0.007	-0.008	0.107	0	-0.134	-0.025	-0.006	
11 Distance to Well_RMS Amplitude	-0.025	-0.013	0.01	0.013	-0.019	-0.008	0.118	0.045	0.015	-0.7

Figure 1: Correlation tables are used to winnow down the predictors. Note the predicted value, Event Density\_RMS, is highly correlated with the Distance to Well\_RMS Amplitude predictor (bottom right). Cross correlations between predictors are shown in the other cells. Cells highlighted with bright colours are highly correlated. The upper plot shows the correlations between all the available attributes. The lower plot shows the correlations between attributes after winnowing. (After Gray et al., 2023b).

Comparing Figure 2 and Figure 3 we can see the most notable change from the traditional prediction workflow. We now start with the NN and use it to decide whether or not to move to multi-linear regression (MLR) instead of starting with the MLR and using it to determine the input variables for the NN. The reason is that in the NN QC's, particularly the PD and SHAP plots, we can see the non-linear effects of predictor variables (Friedman, 2001). For example, in Figure 2, we can see that the input attribute "Distance to Well" has a strong non-linear effect on the output, [Microseismic] Event Density. From our microseismic expert's domain knowledge, we know that this relationship makes sense, and so we continue with a NN because it can account for this non-linear relationship. Alternatively, we can transform the "Distance to Well" attribute with some transform that we think should linearize it, e.g. an exponential or a square root, and then test that linearization by running another NN with the transformed attribute replacing the non-linear one.

In Figure 3, we see a different situation where the input attributes "Most Positive Curvature" and Vp, used to predict High Gas (gas production), have enough scatter that a straight line is going to be optimal fit. In this case, we use the NN QC tools to make the decision to move to an MLR. This is a complete flip from the traditional workflow where attributes that generate the best MLR are used in the NN. The difference today is that we can see into the NN using newly available NN QCs discussed in this paper.

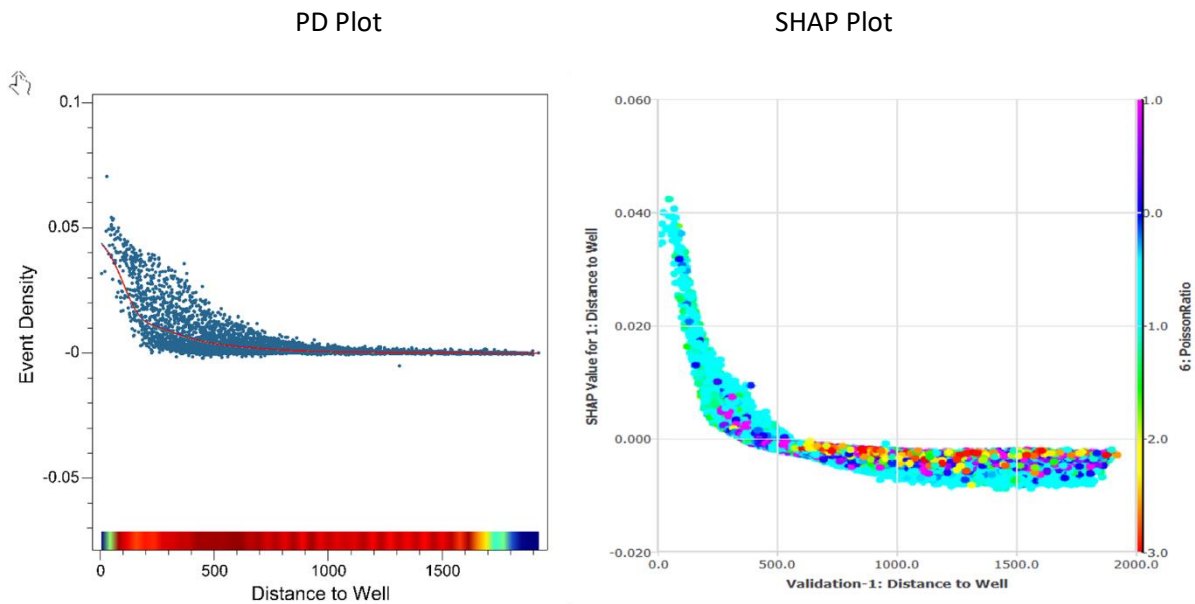


Figure 2: Partial Dependence (PD) Plot (left) and SHAP Plot (right) showing the impact of the Distance to Well attribute on the prediction of microseismic Event Density. Note the non-linear shape of the data and curves. Note the Y-Axis of the PD plot shows the impact on the attribute being predicted and the SHAP plot shows the “SHAP Values”. The SHAP plot is also coloured by Poisson’s ratio values. The colours at the base of the PD plot indicate the density of input points with reds being high density. (After Gray et al., 2023b).

Once we have determined the input attributes and the prediction method (NN or MLR) we are using, then it is time to further assess the inputs. The objective here is to follow Occam’s razor. “In philosophy, Occam’s razor is the problem-solving principle that recommends searching for explanations constructed with the smallest possible set of elements.” (Wikipedia, [https://en.wikipedia.org/wiki/Occam%27s\\_razor](https://en.wikipedia.org/wiki/Occam%27s_razor)). In addition, “the probability of observing one or more spurious correlation increases as the number of independent seismic attributes considered as potential predictors increases” (Kalkomey, 1997). Therefore, we want to make our prediction with the smallest number of inputs possible to explain the changes observed in the output. In our experience, far too many inputs are typically used, and this tends to lead to overprediction and an inability to repeat the result on the next project. Using as few inputs as possible significantly reduces the risk of overprediction and simplifies the understanding of the relationships. It is also best if the input attributes, or a combination of them, have a known physical relationship with the output (Kalkomey, 1997). In addition, we have often used this QC process to identify previously unsuspected relationships that we subsequently determined had a physical basis. Convolutional NNs (CNN) or the use of an operator, incorporating neighboring points to improve the relationship (Ratcliffe and Alder, 2000), means that even more predictors are being used. For example, a 3-point operator will triple the number of input attributes and can quickly lead to spurious correlations. At the same time, we have seen the use of operators and CNNs significantly improve the prediction. This is because the wavelet and the Fresnel zone spread information about particular points in the subsurface to neighboring points in the seismic

data. How to reconcile these issues is best left to the domain experts for whom these QCs will be extremely beneficial.

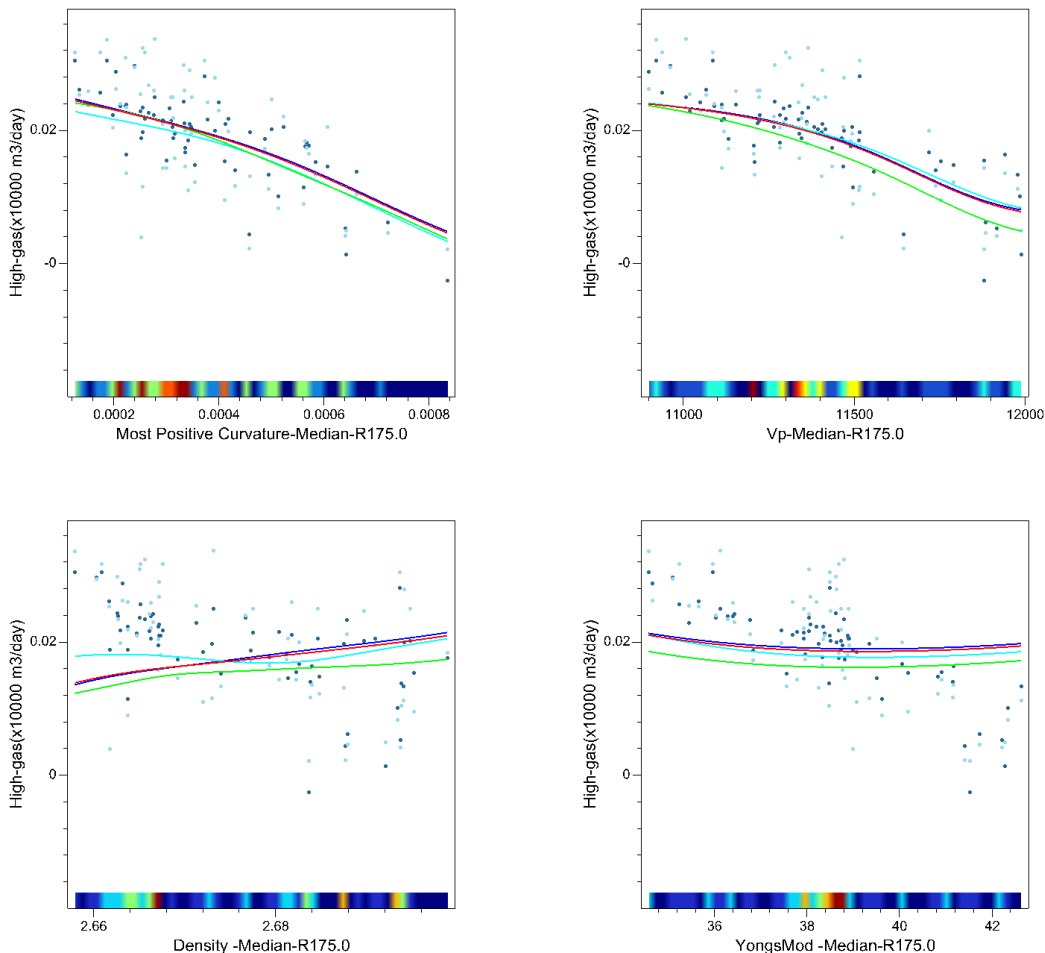


Figure 3: Partial Dependence (PD) Plots show the impact of individual variables on the output. Light blue dots are individual data points. Dark blue dots are this neural network's prediction of those points. The lines indicate how different sets of variables predict the result, gas production in this case. The blue line shows the influence on the solution using training data. The green line shows the influence on the solution using validation data. The light blue line shows the influence on the solution using blind data. The pink line shows the influence on the solution using all data. (After Gray et al., 2023a).

The final inputs, Vp and “Most Positive Curvature” used for the prediction of production (Gray et al, 2023a) are shown in Figure 4. Also shown are the linear fits through these data estimated by the MLR. The MLR was chosen over the NN because with the scatter in the data there is no clear non-linear relationship that we can observe between these attributes and the “High Gas” output. However, an NN was used for the prediction of “Event Density” because of the clear non-linear relationship between it and the input “Distance to Well”. In addition, domain experts, us in this case, determined that there are reasonable physical justifications for the selection of these attributes. For example, for our final MLR for

“High Gas”, lower values of Vp are indicators of where gas saturations are high and higher values of “Most Positive Curvature” indicate faults that may affect completions. By simplifying from 20+ attributes down to 2, we can now also focus on these features to improve future completions and production.

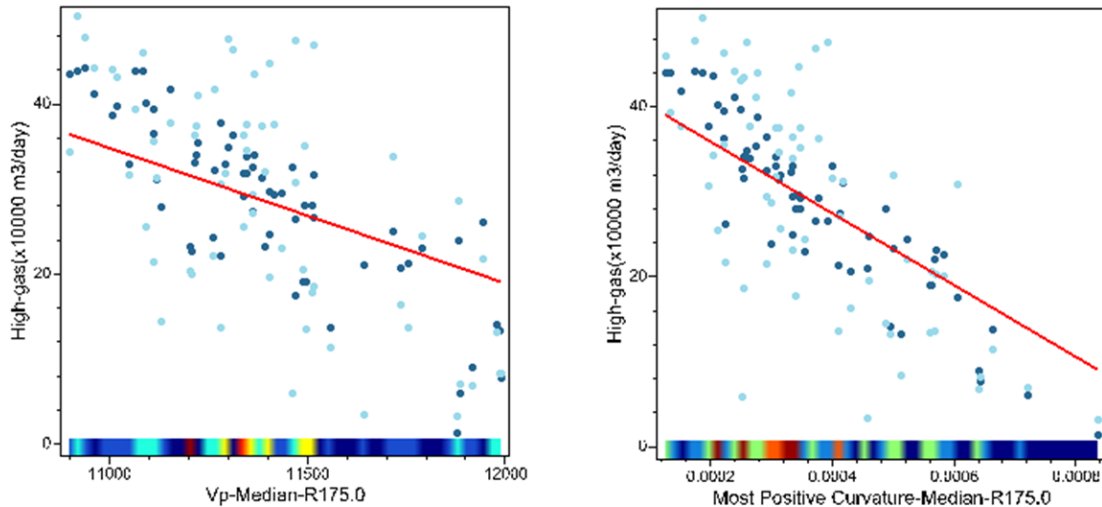


Figure 4: PD plots showing the Input attributes, Vp and “Most Positive Curvature” used in the final MLR prediction iteration for High Gas (production).

The QC tool Importance (Greenwell et al., 2018) is shown in Figure 5 for the same NN as used in Figure 3. Importance is an indication that the partial dependence is not flat (Greenwell et al., 2018). The assumption is that if the relationship between the input and output is not flat, then that input is important. In Figure 5, the input YongsMod (Young’s modulus) is not important. Examining the graph in the right lower corner of Figure 3, we can see that the lines drawn on that graph are nearly flat. This is why Young’s modulus is not considered to be important in this iteration of the NN. However, if we examine the dots on the plot, it appears that the YongsMod attribute is important. In our experience, this misalignment of the lines on the PD plot with the data points indicates a probable correlation between YongsMod and another of the input attributes. Another indication that there are correlations between attributes is if expected relationships between input attributes and the output are not observed in the lines in the PD plot or in the SHAP plot. At this point, we examine the correlations between the misaligned input attribute and other attributes, especially concentrating on other misaligned attributes. For example, in Figure 3, Density is also misaligned. In this case, we would consider the correlation between density and Young’s modulus more closely and try dropping each one while keeping the other and perhaps dropping both. In these iterations of the NN, these attributes

should show greater importance. This also stresses the importance of not looking at only one of these QCs. It is preferable to take them as a whole. If we had only looked at the Importance QC, we would have dropped the YongsMod attribute, but by looking at the individual data points in the PD plot, we can see that YongsMod is likely important.

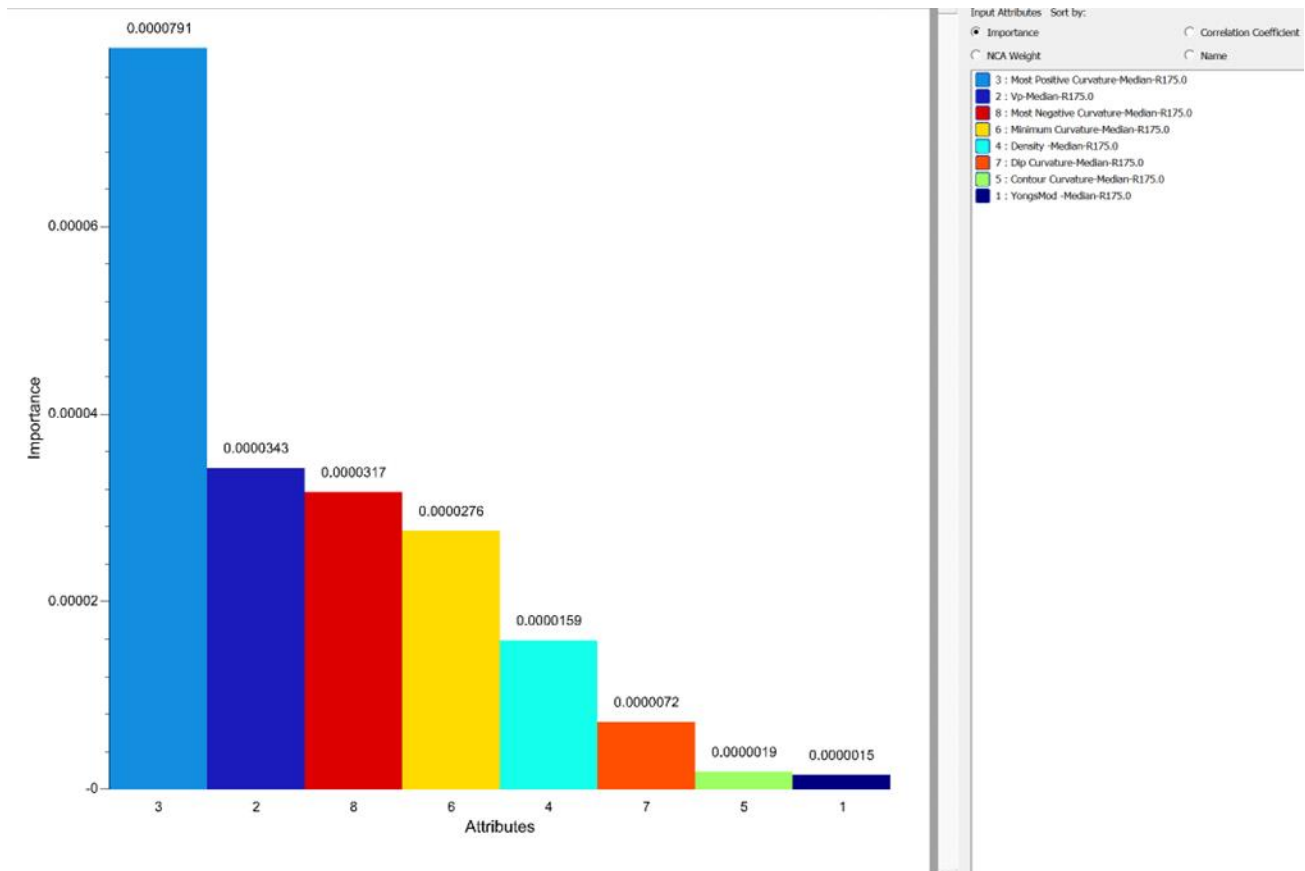


Figure 5: Importance plot showing the relative non-flatness of various inputs in predicting the output. For this NN, the “Most Positive Curvature” input attribute is most important and YongsMod (Young’s modulus) is least important in predicting the Microseismic Event Density. Read the text to see why these might not be accurate representations of the true importance of YongsMod in this case. (After Gray et al., 2023a).

## Conclusions

Our prediction workflow has improved substantially because of the value of new NN QC tools, particularly PD plots and SHAP plots. We now use these NN QC tools first to determine whether or not there are non-linearities in the relationships between the inputs and outputs of a neural network and if it is possible and how to linearize them. In addition, these plots give important clues about remaining correlations between the input attributes that allow us to understand how input attributes are

interacting with each other and thereby allow us to improve our predictions and understand why they are better.

## Novel/Additive Information

Incorporating the use of Partial Dependence plots and SHAP plots have fundamentally improved our ability to assess non-linearities when making predictions using both Neural Networks and Multi-Linear Regressions.

## Acknowledgements

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