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An explainability study (XAI) of Deep CNN for near-infrared spectroscopy : IPA under the light

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Inception for Petroleum Analysis (IPA) [1] is a deep convolutional network inspired from state-of-the-art computer vision architectures. IPA showed improved performance, compared to PLS, without depending on complex pre-processing operations thanks to its several computational blocks. The network begins with three stacked convolutions, followed by a multi-branch module consisting of four different paths that are concatenated. The model learns complementary but complex, internal representations. eXplainable Artificial Intelligence (XAI), a hot topic in DL can bring understanding on such complex models and help to envisage deep networks as robust and performant alternatives to traditional PLS. Two studies using gradient-weighted class activation mapping (Grad-CAM) [2,3], already have been applied to shallow CNNs, extending these methods seems fundamental for DL to earn the confidence of the chemometrics community. The application of XAI [4,5] for NIR analysis can be greatly improved and is crucial for many practical applications such as agriculture, environmental monitoring and oil characterization.

The new framework we proposed is built on a two-step analysis. Explainability has been positioned at several points within the architecture to demonstrate the complementarity of each computational blocks. First, it was crucial to understand the features globally influential for the model, considering the chemical aspect necessary for the property of interest to impartially judge the quality of the deep CNN. Finally, layer-wise explanations was carried out to determine the contribution of each layer to the overall model performance.

Feature importance showed that both models put importance on the same spectral regions, while the PLS's interest is restricted and diffuse, IPA's interest is smoother and more moderate. The layer-wise explanations demonstrated that the performance of IPA comes from its complementary multi-branch layers inspired by the Inception model. It has been demonstrated, without any prior knowledge or pre-processing, that the network focus on relevant spectral region in terms of physico-chemical in relation to the full range of cetane number. In addition, this XAI methodology illustrated that these types of models are not only performant but also more robust than shallower CNNs and PLS. Specifically, IPA better identifies the important spectral regions in relation to the molecular composition of the product that influence the cetane number, such as aromatic content as well as the length of the hydrocarbons molecules.

References:
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Contributed Talk

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