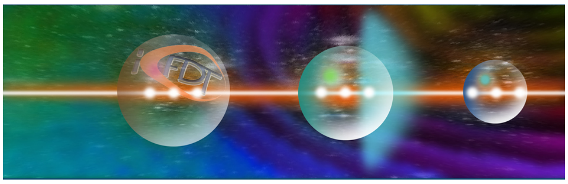

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A Physics-Informed Deep Learning Model for Data-Unsupervised Extraction of Information in the Spectroscopy Field

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Spectroscopic analyses are between the most used methodologies to investigate any state of matter. In fact, from the analysis of the electromagnetic spectra it is possible to extract several quantities that are characteristics of the analysed medium. Therefore, the spectrum must usually be analysed and computed by some specific algorithms, such as pre-processing and calibration tools, to extract the various pieces of information of interests. Such algorithms are usually developed by using a sort of supervised approach, where some ad hoc controlled experiments are performed to finely tune the algorithms to achieve the highest performances. However, such supervised approaches are sometimes prohibitive or not economical, limiting the diagnostic potentialities to only qualitative results or not accurate quantitative measurements. Therefore, new methodologies based on not supervised approaches, which do not require controlled experiments and labelled data, would help in improving the diagnostic potentialities and performances in these fields and applications.
This study introduces an innovative unsupervised physics-informed deep learning methodology for data pre-processing, calibration and information extraction directly from raw measurements. Unlike traditional supervised approaches, this methodology automates data processing without relying on controlled experiments, but processing the data according with physics theoretical models, a relevant aspect if we consider that controlled experiments are not always possible.
In this work, the potentialities of this new approach are investigated by a series of synthetic cases and some experimental tests. The analyses clearly demonstrate the huge potentialities of the physics-informed deep learning model, allowing for preprocessing and calibration performances comparable with supervised models.
Obtaining such great performances without the need of controlled experiments and labelled data opens to the possibility to improve pre and post processing of diagnostics even in applications where standard calibration approaches are not affordable. Moreover, even if the model has been particularized for spectroscopic applications, it is worth it to highlight that the methodology is fully general and can be easily transferred to any other field.

Keywords: Physics-Informed Neural Network, Deep Learning Model, PINN, Spectroscopy, Unsupervised Information Extraction

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