ON THE IMPACT OF MACHINE LEARNING APPLIED ON RESEARCH CHARACTERISATION DATA; A NANOINDENTATION CASE STUDY

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ABSTRACT

Data science and machine learning ease the efficient mining and potential for further processing of large materials data sets, resulting in the extraction and identification of high-value materials knowledge, towards design, quality and manufacturing. The growing generation of data in the characterization field brings up new opportunities and challenges. Materials scientists turn their focus on the computational applications that can deal with the complexity of these data and deliver important results [1]. Data-driven approaches can provide valuable information regarding the underlying structure and behavior of materials. To name a few, opportunities fall within the areas of material's property prediction, structure prediction, automated determination of phase diagrams using high-throughput combinatorial experiments, advanced and smart materials modelling and discovery, artificial intelligence in characterization field. Supervised regression algorithms can be used for the prediction of mechanical properties of constructive materials and for the inverse design of materials, in which used algorithms help identify materials that satisfy desired properties [2].

In the case study, data generated from the nanoindentation were used in order to reconstruct the surface constituent phases of mortar grids through machine learning algorithms. Specifically, K-Means algorithm (unsupervised learning) was applied to two 49-measurements (7x7) datasets with information about the modulus (E) and hardness (H) in order to discover the underlying structure of the data. The resulted clusters from K-Means were then evaluated and values range assigned so as to signify the various constituent phases of the mortar. Furthermore, another dataset from nanoindentation containing information about E, H and the surface colour of the measured area (obtained from optical microscope) was used as training set in order to develop a random forests model (supervised learning) which predicts the surface colour from the E and H values.

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