Classification of heavy metal contaminated samples based on micro-CT images using machine learning algorithms

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Being able to predict whether a sample is contaminated with any toxic substances or not is crucial, especially when it comes to health, and this is where machine learning algorithms are essential [1-2]. In our research the emphasis was put on the ability to classify samples contaminated with two types of heavy metals: zinc (Zn), cadmium (Cd), and the mixture of these two elements (Zn+Cd), based on the micro-computed tomography (micro-CT) images. Contaminated samples, which were operculum, were coming from the Carassius Gibelio fish. Prior to the micro-CT scan fish were bred in the environment containing a concentration of 4 mg/ml of water of each element. Additionally, a control group, with no exposure to any heavy metal was cultured.

After micro-CT scans, images were reconstructed in order to get information, which would help algorithms learn about the dataset, and finally, which would be able to classify samples into proper groups. The key features of the reconstructed images were: grayscale maximum value in a given group, masses of the samples, mean grayscale values, and area under the grayscale histograms.

Applied machine learning models included: logistic regression, SVM (Supporting Vector Machine), decision trees, and KNN (K-nearest neighbors, with different numbers of neighbors k = 1, 2, 3, ..., 10). Results left us no doubt that most of the applied machine learning models are very good when it comes to classification. The best results were achieved for the simplest logistic regression, where the overall accuracy was 90%, a second-best algorithm was KNN with an accuracy of 71% for k = 1 and 86% for k = 4, next were decision trees with an accuracy of 70% and SVM with an overall accuracy of 50%.

References

[1] Heavy metals in suspended matters during a tidal cycle in the turbidity maximum around the Yangtze Estuary, Huaijing Zhang et al., Acta Oceanologica Sinica 34, 36–45(2015).

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