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Taking into Account Mutual Correlations during Selection of Significant Input Features in Neural Network Solution of Inverse Problems of Spectroscopy

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In neural network solutions to many physical problems, there is a need to reduce the dimension of the input data in order to achieve a more accurate and stable solution while reducing computational complexity. When solving an inverse problem in spectroscopy, multicollinearity is often observed between the input features, making it necessary to use a selection method that takes into account the correlation between the input features.

The method used in this study is based on the iterative selection of features with the highest correlation with respect to the target variable and on the elimination of features with high mutual correlation.

The paper compares the quality of a neural network solution to the problem of determining the concentrations of heavy metal ions in water by Raman spectra on the complete set of input features and on its subsets compiled using the selection method under consideration, as well as using traditional methods of selecting significant input features.

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