Multi-output 1-dimensional convolutional neural networks for simultaneous prediction of different traits of fruit based on near-infrared spectroscopy

Puneet Mishra and Dário Passos

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Abstract

In spectral data predictive modelling of fresh fruit, often the models are calibrated to predict multiple responses. A common method to deal with such a multi-response predictive modelling is the partial least-squares (PLS2) regression. Recently, deep learning (DL) has shown to outperform partial least-squares (PLS) approaches for single fruit traits prediction. The DL can also be adapted to perform multi-response modelling. This study presents an implementation of DL modelling for multi-response prediction for spectral data of fresh fruit. To show this, a real NIR data set related to SSC and MC measurements in pear fruit was used. Since DL models perform better with larger data sets, a data augmentation procedure was performed prior to data modelling. Furthermore, a comparative study was also performed between two of the most used DL architectures for spectral analysis, their multi-output and single-output variants and a classic baseline model using PLS2. A key point to note that all the DL modelling presented in this study is performed using novel automated optimisation tools such as Bayesian optimisation and Hyperband. The results showed that DL models can be easily adapted by changing the output of the fully connected layers to perform multi-response modelling. In comparison to the PLS2, the multi-response DL model showed ~13 % lower root mean squared error (RMSE), showing the ease and superiority of handling multi-response by DL models for spectral calibration.