Title:

Wavelength optimization in MIR spectra for discrimination of ghee

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Abstract:

For qualitative or quantitative analysis using Infra red (IR) spectra coped with chemometrics, selection of informative & faithful wavelengths is a crucial step in online spectral measurement. For wavelength optimization there are many techniques reported in the literature such as genetic algorithms (GA), simulated annealing (SA) etc. However all these techniques are time consuming and require excessive computations to achieve the proper operational parameters. In this paper a simple approach using golden section line search algorithm in conjunction with loading vector of singular vector decomposition (SVD) of the spectra was used to select effective wavelength for discrimination of ten different ghee samples within 1818-909 cm^{-1}. Each of the wavelength variables was considered as an independent classifier for discrimination. The final wavelength points were reduced from 128 to 22 variables only. The performance of the wavelengths selected in this work was measured by comparing the predicted classification accuracy of optimized variables against all the spectral variables with the models prepared by PCA and SIMCA. The results showed that the predictive ability of the model with optimized variables has improved than the model using complete variables.

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