Abstract

Visualisation of physical variation in grain near infrared images using principal compoment score gradients

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Introduction

In contrast to bulk NIR spectroscopic analysis, imaging provides localised information. When analysing the spectral results, e.g. by PCA, early components often describe the physical status of the sample (particle size, surface properties) while the chemical information of cereal grains shows up in higher components that explain a very small percentage of the total sum of squares. Classical pre-processing methods were not able to completely remove these physical effects. The chemical information may be localised and form clear clusters in the score space. The physical effects observed in early components rarely form well-delineated clusters in the score space. Therefore a gradient classification method was tested in order to explore the cause and position of the variation in relation to the grain morphology and topography. This was shown for barley, wheat and sorghum.

Materials and Methods

NIR hyperspectral images of whole grain barley, wheat and sorghum were acquired using a SisuCHEMA SWIR (short wave infrared) hyperspectral imaging system with spatial resolution of 150 x 150 μm^2. Images were obtained from 1000 to 2498 nm with 6.65 nm spectral steps. Raw images were corrected to pseudo-absorbance using Evince version 2.4.0 multivariate image analysis software. PCA with mean centering was applied and score images and score plots used interactively by brushing for image cleaning. Standard normal variate (SNV) and Savitzky-Golay smoothing were applied. Principal component score gradients (almost equal segments of the score axis) were made in the score space in the direction of the respective PCs.

Results and Discussion

Studying defects in cereal grains, chemical information was only explained in PCs 4 or 5. Principal component score gradients applied to earlier PCs were efficient in explaining variation in topography of the grains. The number of PCs necessary to explain variation in physical effects confirms the sensitivity of imaging to difference in depth and shape of samples. However, with image analysis it is possible to separate difference in penetration depth, i.e. scattering and chemical information.

Conclusion

Principal component score gradients allow illustration of topography of cereal grains in lower PCs of NIR images. The ideal would be a pre-processing technique that could remove these physical effects observed during image analyses.

Reference paper as:
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