Extended abstract of Keynote Presentation at 1st International sensorFINT Conference, Izola, Slovenia, 10-12 May 2022

The Road Less Travelled: NIR (hyper)spectral imaging in cereal quality and safety

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Near infrared (NIR) hyperspectral imaging has increasingly been investigated for the quantification of cereal grain composition and detection of quality and safety characteristics, since the first publication in the mid-2000s. It advanced on conventional NIR spectroscopy by offering, in addition to compositional, spatial information. This enables more detailed characterisation of heterogenous cereal samples. Although this presentation focusses on cereals, it can be applied in similar ways to confectionary.

Frederick William Herschel, an astronomer and musician, is acknowledged for having discovered radiation beyond the red in the early 1800s. The NIR region, however, was not considered significant at the time as analytical techniques that could provide more clear-cut results were favoured. About 150 years later Karl Norris, an Engineer at the USDA, USA performed work which led to the developed of the first commercial NIR spectrophotometer. Shortly after, Phil Williams purchased, what was probably the first NIR instrument for industry use and about four years later NIR spectroscopy was the main method used for protein analysis of wheat in Canada.

Since its first use in the cereal industry, NIR spectroscopy has become the quality control method of choice for many more applications due to the advancement in instrumentation, computing power and multivariate data analysis (Manley, 2014).

During the late 1990s, NIR hyperspectral imaging equipment became available for commercial use. With the staring imager, whole images are acquired consecutively, one wavelength at a time – substantial time is thus required to record the wavelengths one by one. With the linescan or pushbroom system, all spectral information is acquired simultaneously.

Early studies on whole grain cereals used the advantage of pixel-wise information. The PC scores images enable visualisation of similarity/differences, whether chemical composition or scattering properties, in samples by means of a heat map. The example in Figure 1 allowed us to distinguish between, in this case, hard (H) and soft (S) maize kernels (Manley et al, 2009). These clusters can be assigned dummy variables and can be shown as a classification plot and subsequently be projected onto the scores image to form a classification image. In this case, the clusters in the PCA scores plot obtained were due to differences in endosperm texture of whole maize kernels. Relevant information in imaging data is often only being observed in lower-order principal components and not in *e.g.* principal component one. It is thus important to evaluate these components also.

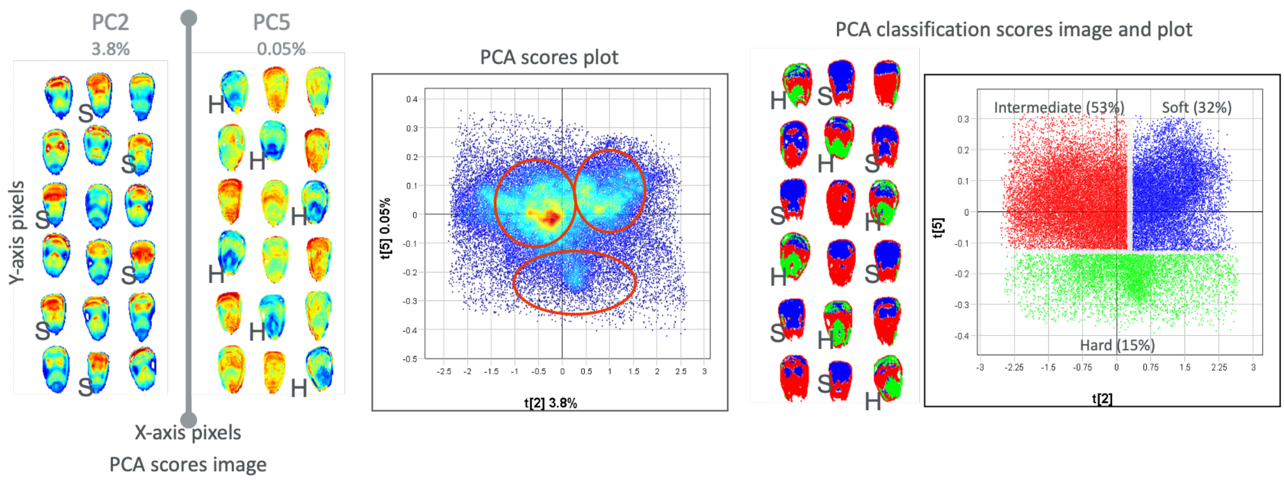

Figure 1 NIR hyperspectral PCA results of maize kernels differing in kernel hardness.

PC scores incremental plots can visually show the effect of topography on the images (McGoverin at al. 20011) (Figure 2). Negative PC1 scores were associated with the high points of the kernels (the points closest to the detector). Positive PC1 scores were associated with the lowest points. Similarly, it can be shown how negative and positive score extremes of PC2 and PC3 were largely associated with the kernel edges. The shape and surface roughness, influences spectral data collection and subsequent analysis and interpretation. The complex topographies of grains required spectral preprocessing and more than a single PC to separate the various sources of spectral variation and to explain it efficiently.

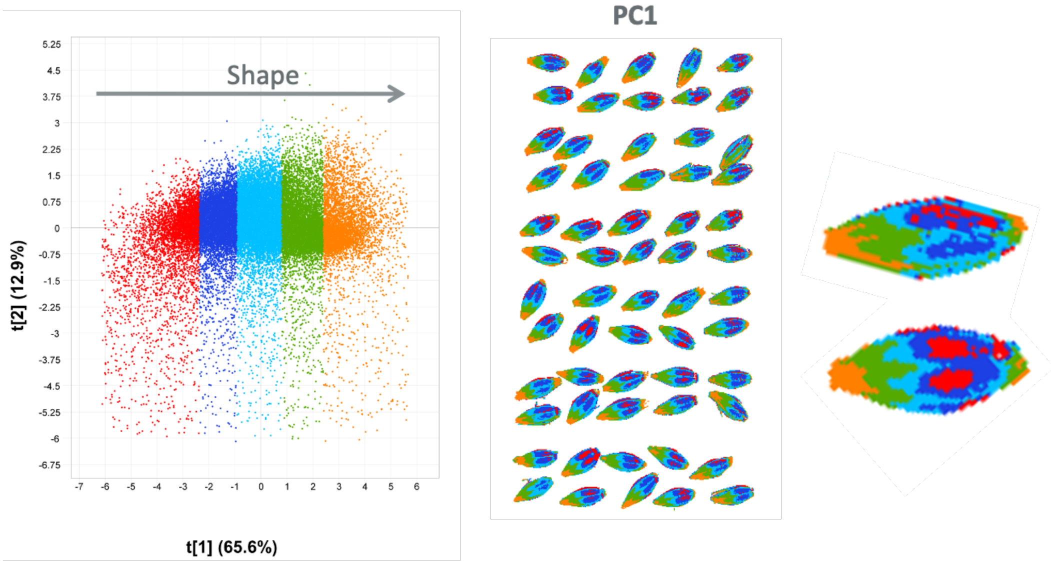

Figure 2 PC scores incremental plot (left) and incremental image (right) showing effect of topography on the images.

When objects from different classes have many similar pixels, the object-wise approach may provide more accurate predictions (Burger & Geladi, 2006). The object-wise approach is increasingly used in recent NIR hyperspectral imaging. Object-wise refers to the average or median spectrum of all pixels in an image (or part thereof) for development of prediction or classification models. Although there is merit in the use of the object-wise approach, the value of the information provided in the spatial dimension of a hyperspectral image with the pixel-wise approach should not be underestimated or neglected. In addition, due to computing power, data fusion is becoming more common – also with development in multiblock chemometric techniques such as sequential and orthogonalised partial least squares linear discriminant analysis (SO-PLS-LDA) Biancolillo et al., 2015) as well as multiblock waveband selection with sequential and orthogonalized covariance selection-linear discriminant analysis (SO-CovSel-LDA) (Biancolillo et al., 2015).

A final thought as conclusion. The increasing use of reduced number of variables, but still referring to hyperspectral imaging let to the letter by Polder and Gowen (2020) in which they suggest that the imaging community to rather use the term imaging spectroscopy or spectral imaging and not hyperspectral imaging. This is as hyperspectral imaging is both a special case of spectroscopy as well as a special case of imaging. It should always be made sure the correct adjective is used when naming the imaging technique.

Acknowledgements
This presentation has been part of the H2020 MSCA RISE Consortium 'SuChAQuality'. The project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement 101008228. COST Action CA19145 for the invitation and the South African Department of Science and Innovation for funding.

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