Potential of UV and SWIR Hyperspectral Imaging for Determination of Levels of Phenolic Flavour Compounds in Peated Barley Malt

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Abstract

In this study, Ultra-violet (UV) and Short-wave infra-red (SWIR) Hyperspectral Imaging (HSI) was used to measure the concentration of phenolic flavour compounds on malted barley that are responsible for smoky aroma of Scotch whisky. UV HSI is a relatively unexplored technique that has the potential to detect specific absorptions of phenols. SWIR HSI has proven to detect phenols in previous applications. Support Vector Machine Classification and Regression was applied to classify malts with ten different concentration levels of the compounds of interest, and to estimate the concentration respectively. Results reveal that UV HSI is at its current development stage not suitable for this task whereas SWIR HSI is able to produce robust results with a classification accuracy of 99.8% and a squared correlation coefficient of 0.98 with a Root Mean Squared Error (RMSE) of 0.32ppm for regression. The results indicate that with further testing and development, HSI may potentially be exploited in an industrial production environment.

Keywords – Barley malt, hyperspectral imaging, Scotch whisky, short-wave infra-red, smokiness, ultra-violet

1. Introduction

Hyperspectral Imaging (HSI) is a technique that combines spectroscopy with spatial information. Regular multispectral systems, such as RGB cameras, collect information in a limited number of distinct wavebands spread out over a certain spectral range. HSI in contrast captures intensities over a continuous spectral range in very narrow wavebands. Each pixel does not only represent spatial information but also spectral information in form of a continuous spectrum. Depending on the system, this can entail hundreds of wavebands. The HSI data is stored in a three dimensional data-cube, often referred to as a hypercube where each pixel represents spatial information in form of x and y coordinates combined with high-resolution spectral information in the λ coordinate.

In the past, applications of HSI are in the field of remote sensing such as precision agriculture (Datt, McVicar, Van Niel, Jupp, & Pearlman, 2003), land cover analysis (Tong Qiao, Ren, Sun, Zheng, & Marshall, 2014) or military target detection (Manolakis & Shaw, 2002; Young, Marshall, & Gray, 2016). Due to recent advances in imaging technology in the last decades, HSI became more popular for lab-based applications such as food quality monitoring (Marshall, Kelman, Qiao, Murray, & Zabalza, 2015; T. Qiao et al., 2015; Sun, 2010), medical applications (Lu & Fei, 2014) and even artwork inspection (Polak et al., 2016). The popularity derives from the non-destructive nature of HSI, where samples can be analysed chemometrically without altering their physical integrity. A second advantage is the rapid data acquisition. Classical analysis techniques such as High Performance Liquid Chromatography (HPLC) typically require not only the destruction of the sample but also several days in a lab for analysis. HSI data can be acquired in real-time and the subsequent data analysis is subject to the efficiency of algorithms and the computational power of the host system. As a result, HSI poses the potential of a real-time chemometric analysis tool that can seamlessly be integrated into the processing chain of industrial production, notably food and drink production.

Scotch Whisky is central to the UK economy, accounting for around a quarter of the country's food and drink exports (Scotch Whisky Association, 2015). It is a high-quality spirit drink exclusively produced in Scotland in a manner strictly regulated by law. Maintaining high quality standards during production is therefore of major interest for the industry. Flavour character is central to this, with the flavour compounds present in Scotch coming naturally from the raw materials, and modified or generated through the production process. Certain Scotch Whiskies are characterised by smoky flavours, which are introduced through the exposure of the malted barley to peat smoke during kilning (drying of the malted grain). Volatile phenolic compounds in the peat smoke adhere to the surface of the barley and are carried through the production process giving the smoky character of the final product.

Different distilleries use malted barley that has been peated (smoked) to different degrees, depending on their flavour requirements. Distillers typically specify a set peating level in terms of ppm level of phenols, calculated as the total of the major phenolic flavour compounds present on the malt. The current methods to determine the levels of phenols, HPLC or spectrophotometric techniques (Bringhurst & Brosnan, 2014), cannot be carried out on the malt itself. They rely on a pre-distillation step to extract the phenols, with the analysis performed on the resulting distillate. This is not only time-consuming, but can result in a degree of inaccuracy if the distillation/extraction is not carried out efficiently. For the industry, it would be of significant benefit to be able to determine the phenol levels directly from the malt. Because of the non-destructive nature and the rapid data acquisition, we explore HSI as a potential real-time method.

In the past, phenols have successfully been detected in seeds, skins and stems of grapes (Jara-Palacios, Rodríguez-Pulido, Hernanz, Escudero-Gilete, & Heredia, 2016; Zhang et al., 2017) by near infra-red (NIR) HSI as well as the detection of phenols in wood that is used for wine barrels (Baca-Bocanegra, Nogales-Bueno, Hernández-Hierro, & Heredia, 2018). We have also presented groundwork for the detection of phenols in March 2017 (Tschannerl et al., 2017), where NIR to shortwave infra-red (SWIR) HSI covering a spectral range from 950 – 1700 nm was found to be able to differentiate three different levels of phenol concentrations in peated malt with support vector machine classification. However, due to the limited number of different concentrations studied, no effective regression model to estimate the exact concentration could be trained. The aim of this study is to extend the work done through the evaluation of samples with a wider range of phenol concentrations, scanning them in different spectral regions to further identify the potential of HSI for the estimation and generating more robust systems. To achieve this, 10 peated malts with different phenol levels were scanned with a SWIR camera[1] that covers a spectral range of 1000 – 2500 nm. Additional information is extracted from wavelengths above 1700 nm that have not been explored in the previous publication. Since phenols typically expose absorption in the

[1] Note that in literature, the nomenclature for visible light, NIR and SWIR systems vary. In this article, SWIR is used as an abbreviation for the spectral range of 1000 – 2500 nm.

ultra-violet (UV) range (Dearden & Forbes, 1959) with peaks between 260 – 300 nm, the UV spectrum poses another spectral range of interest. UV hyperspectral imaging is yet quite unexplored with limited applications (Li, Lyu, Liao, & Wu, 2016; Merkel, 2015) due to increased difficulties in the imaging process. Not only are UV HSI cameras hardly available and still a subject of research (Hsu et al., 2017; Zucco, Caricato, Egidi, & Pisani, 2015), broadband light sources in wavelengths under 400 nm with sufficient illuminance are very scarce. In this study, a UV system covering the range of 220 – 400 nm is evaluated for suitability as a novel technology for imaging barley malt and estimating the phenol content. This study focuses only on the use of UV and SWIR HSI, simply because SWIR has proven successful in the past and UV HSI is of interest as it is a yet quite unexplored technology that might show benefits for this particular application. VIS HSI is not considered here as phenolic flavour compounds will unlikely expose any significant absorption bands in this range. The novelty of this paper is to examine spectral regions of HSI that have previously not been explored to estimate phenolic flavour compound concentrations by conducting experiments on a larger variety of samples that were utilised in previous studies. UV and SWIR HSI can be used to clearly distinguish between and estimate phenol levels in barley malt.

The rest of the paper is structured as follows: Section 2 gives some details about the chemical background of the phenolic flavour compounds examined in this study. Section 3 gives details of the samples imaged and the data acquisition process. Section 4 provides information on the constitution of HSI data and necessary pre-processing steps as well as on the methodology of data analysis and performance evaluation. Section 5 provides the results along with discussions and Section 5 gives a conclusion with possible future outlook.

2. Chemical background

When purchasing malted barley, Scotch whisky distillers will specify the level of "total phenols" that they require. This is the sum of eight individual phenolic flavour compounds; phenol (PubChem CID: 996), guaiacol (PubChem CID: 460), p-cresol (PubChem CID: 2879), m-cresol (PubChem CID: 342), o-cresol (PubChem CID: 335), 4-methylguaiacol (PubChem CID: 7244), 4-

ethylguaiacol (PubChem CID: 62465) and 4-ethylphenol (PubChem CID: 31242). Although these may not be the only flavour compounds present in peat smoke, these marker phenols have been used for decades as a measure of smoky character (Swan & Howie, 1982; Thomson, 1982). In today's malt specifications the level of total phenols generally required is in the range of 0 – 50 ppm (Bringhurst & Brosnan, 2014).

Peat can be sourced from various locations across Scotland, including both island and mainland sites. The composition of the peat varies depending on its origin. This influences the relative levels of phenolic compounds on the peated malt, which in turn influences flavour (Harrison & Priest, 2009). Each compound imparts a subtly different aroma. Phenol is for example tends to be described as medicinal, while guaiacol is more smoky. The HPLC method, currently used, is both applicable to barley malt steam distillates and new make spirits. The levels are measured in mg/kg or ppm respectively and the total of all compounds combined is used as a marker to the degree of peatiness of the malted barley. Therefore, in this study our aim was to estimate the total phenol levels rather than the concentration of the individual compounds.

3. Data acquisition

3.1 Sample preparation

Some preliminary results of data classification from us, based on three categories of peating level using NIR HSI were reported in (Tschannerl et al., 2017). The objective here was to classify into finer granulated levels with the goal of estimating the actual concentration utilising different UV and SWIR HSI technologies. The peated malt samples selected for this study represented the range of total phenol concentrations typically used in Scotch whisky production, namely 0 ppm (unpeated) to 50ppm (heavily peated). A 124.5ppm (atypically highly smoked) sample was added to the set to further test the method. The sample set contained in total ten samples with the following total phenol concentrations: 0, 3.8, 8.2, 12.5, 15.5, 20.5, 30, 40, 50 and 124.5 ppm.

During kilning, peat smoke is passed through a bed of malted barley. Due to the nature of this process, each grain has a different amount of phenols adhering to its surface. So, the concentration

cannot be measured from a single spatial point. HPLC can measure the average concentration of a distillate extract, but for image data, this needs to be accounted for. Therefore, the grains were spread out on a flat surface to maximise the surfaces to be imaged using HSI.

3.2 Imaging process

The two hyperspectral systems both operate in the pushbroom mode, i.e. the camera measures a single line at a time through an entrance slit. The light is then dispersed into its spectral components by optical elements, most commonly a diffraction grating. Two dimensional images representing the spatial line in one dimension and the spectrum of each pixel in the other are recorded subsequently which forms a 2D slice of the 3D hypercube. Since only one line at a time is measured, either the object or the camera has to move to acquire all necessary spatial information. For remote sensing data, it is common to mount cameras on airborne devices. In industrial applications however, it is common to fix the camera and move the objects with linear translational stages or conveyor belts which are in turn synchronised with the frame rate of the camera to retain geometry. The functionality of pushbroom scanning is visualised in Figure 1.

UV imaging was done with pco. Sensicam UV that covers a spectral range of 220 – 400 nm with a spectral resolution of 3.8 nm. It requires a specialised illumination done with a Hamamatsu L6301-50 Deuterium lamp that has a broadband UV coverage, but it is very low in light intensity. This results in an increased exposure time of 300 ms. Additionally, a 3 x 3 spatial and 4-fold spectral binning were applied. This means that 3 x 3 spatial pixels and 4 spectral bands are added up to not only reduce noise but also to increase the camera's light sensitivity. However, the binning process also degrades the spatial resolution and spectral resolution. This results in an image with 342 pixels per scanned line and 248 active bands. As a result of the increased exposure time, the UV scanning process requires several minutes, whereas the SWIR imaging can be done in under a minute. The SWIR imaging was done with the Specim SWIR system covering a range from 1000 – 2500 nm with a spectral resolution of 12 nm. Illumination is done with customary halogen lightbulbs allowing for an exposure time of only 2.5 ms, Binning was not applied resulting in an image with 384 pixels per line and 288 active spectral bands.

Figure 2 depicts false colour representations of the same barley sample with the UV camera at wavelength 295 and the SWIR camera at wavelength 1483 along with a mean spectrum over the spectral range of each camera of each image region. Additionally, normalised histograms of both datasets at the same wavelengths are plotted. One can see that the UV measurements are in general of very low intensity and expose a much lower Signal-to-Noise Ratio (SNR). The SWIR range also seems to capture more spectral features of the barley itself from visual inspection.

4. Data processing

4.1 Pre-processing

When imaging different samples, lighting conditions may vary between the samples and even within the samples across the scan line. A common way of accounting for this effect is to convert the measured raw radiance spectra **s** to percent reflectance spectra **r** by the following formula (Yao & Lewis, 2010):

$$\mathbf{r} = \frac{\mathbf{s} - \mathbf{d}}{\mathbf{w} - \mathbf{d}} \times 100\%$$

where **d** and **w** represents the dark and white reference respectively. The dark reference is acquired by imaging without any light exposure to the sensor, which is to estimate the sensor's shot noise. The white reference is acquired by imaging an optimally reflective white surface, e.g. Spectralon, which has lambertian scattering. i.e. it reflects incident light equally diffuse in all direction over the desired spectral range. The white image can estimate the sensor's light sensitivity to the current illumination and normalises the signal based on that.

The spectra measured are not only dependent on the chemical absorption but also on physical light scattering due to the surface structure of the objects. As the barley grains have a very uneven surface, different portions are differently exposed to light. This results in shadow effects as well as varying light scattering attributes. These spectral variations typically manifest themselves in additive or multiplicative components on the base spectra. Various spectral pre-processing techniques are reviewed in (Rinnan, Berg, & Engelsen, 2009) to address these problems. For

additive effects, it is common to employ spectral derivatives, either 1st or 2nd order. These are most commonly realised with Savitzky-Golay smoothing to minimise noise interferences. A widely used technique to compensate for multiplicative scattering distortions is Multiplicative Scatter Correction (MSC) (Zhao, Zhang, & Chen, 2005), which estimates scattering coefficients from a supposedly ideal signal whilst minimising the scatter for each individual signal. One of the most commonly used techniques in HSI however is the conversion of the spectra to the Standard Normal Variate (SNV) (Rinnan et al., 2009). For a given set of n measured reflectance spectra $\boldsymbol{R} = \{\mathbf{r_1}, \mathbf{r_2}, \dots, \mathbf{r_n}\}$, the SNV for one spectrum $\mathbf{r_i}$ is calculated by:

$$\mathbf{r_i}(SNV) = \frac{\mathbf{r_i} - \boldsymbol{\mu}}{\boldsymbol{\sigma}}, \quad \boldsymbol{\mu} = \frac{\mathbf{1}}{\boldsymbol{n}}\sum_{\boldsymbol{i=1}}^{\boldsymbol{n}} \mathbf{r_i}, \quad \boldsymbol{\sigma} = \sqrt{\frac{\mathbf{1}}{\boldsymbol{n}}\sum_{\boldsymbol{i=1}}^{\boldsymbol{n}} (\mathbf{r_i} - \boldsymbol{\mu})^2}$$

where $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$ represents the mean and standard deviation of $\mathbf{R}$ respectively. This equals a statistical standardisation and has proven to be a very effective pre-processing technique for hyperspectral data (Amodio, Capotorto, Chaudhry, & Colelli, 2017; Yu et al., 2016). All signals here were pre-processed by converting to SNV and the UV signals were additionally smoothed using the Savitzky-Golay filter prior to conversion.

4.2 Data analysis

As the distribution of phenols adhering to the surface of the grains is expected to be very uneven, the pixels will therefore have varying spectral responses. In the final application, the mean concentration of an entire batch of barley malt is desired. To achieve this, rather than considering individual pixels as observed we take the average over a subset of pixels instead for analysis. To avoid detecting dense regions with locally high concentrations, these subsets are not formed by spatially connected regions but by selecting a subset of pixels randomly distributed over the entire image.

Two different machine learning approaches were applied for data modelling. As we consider 10 different levels of phenol concentration, a classification problem is implied. Support Vector Machines (SVM) were in the past successfully used for HSI data classification and regression and

are still a very popular tool (Crichton et al., 2017; Kang, Xiang, Li, & Benediktsson, 2017; Tong Qiao et al., 2015). The general idea is to find a hyperplane that separates two classes by selecting a small number of observations, the support vectors, of each class that are closest to the hyperplane. By maximising the margin of each support vector to the plane, the model achieves optimal generalisation characteristics. Training several SVMs in a one-against-all approach enables the extension to a multi class case. SVMs have the advantage of easily integrating non-linearity in the data by employing kernel functions, most commonly a Gaussian kernel. Two parameters C and γ control the complexity and the width of Gaussian kernel respectively. These parameters are tuned using a grid search algorithm with five-fold cross-validation. SVMs are very popular because they pose a very robust mathematical model with a convex optimisation function that can be optimised with a relatively low amount of training samples (Zhao et al., 2005). Deep learning methods such as neural networks that have recently gained much attention in research (Lee & Kwon, 2017; Mou, Ghamisi, & Zhu, 2017) produce very good results but require a large amount of training data and generally rely on non-convex optimisation, which makes them less robust as a globally optimal solution is not guaranteed.

A common way of measuring the quality of the classification is by examining the confusion matrix, which lists the number of correctly classified observations, false positives and false negatives for each class individually. Based on that, the Overall Accuracy (OA) of all correctly classified observations in relation to all observations can be obtained. For a dataset with N observations and c classes, the OA is defined as:

$$OA = \frac{\sum_{i=1}^{c} n_i}{N} \times 100\%$$

where n_i represents the number of correctly classified pixels in class i. The OA therefore relates the number of correctly classified pixels to all pixels.

Additionally, Cohen's kappa coefficient is also calculated to assess the classification performance. It quantifies the agreement between the ground truth and the classification results as follows:

$$Kappa = \frac{p_0 - p_e}{1 - p_e} \times 100$$

where p_0 is the observed level of agreement, identical to the OA, and p_e represents the value expected if the two groups of results, ground truth and classification results, were completely independent, defined by:

$$p_e = \frac{1}{N^2} \sum_{i=1}^{c} n_{i1} n_{i2}$$

where n_{i1} and n_{i2} refer to the ground truth and the classification results respectively.

SVMs have been extended to Support Vector Regression (SVR) in (Drucker, Burges, Kaufman, Smola, & Vapnik, 1997) maintaining its major characteristics of maximum-margin separation and low sample number training. SVR was used to train a prediction model for the actual concentration of phenols. The same algorithm used for SVM was applied for SVR parameter tuning. Two popular measures are typically applied to evaluate the quality of the regression results. For *N* observations, the Root Mean Squared Error (RMSE) is calculated by

$$\text{RMSE} = \left(\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2\right)^{\frac{1}{2}}$$

where y_i represents the actual value of the observation and $\hat{y}_i$ the estimated value. It has the same unit as the estimated value and can be interpreted as the average error made when estimating. As this is scaled to the range of values possible, the coefficient of correlation value r^2 is often employed as an absolute measure for the quality of the model. It is calculated as follows

$$r^2 = \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2}$$

where $\bar{y}_i$ represents the mean of all values. r^2 takes on values between 0 and 1, with 1 indicating 100% prediction accuracy of the model.

5. Results and Discussion

5.1 Classification results under varying settings

To observe the effect of different sizes of pixel subsets, the average over 50, 200 and 500 pixels was taken to generate the samples for classification. Due to different spatial resolutions, this results in a total of 46 702, 11 675 and 4 669 observations for SWIR and 17 174, 4 292 and 1 719 observations for UV in sum for all classes respectively. Out of these, 1%, 5% and 10% have randomly been selected for training and the rest for testing the predictive models. Results for both UV and SWIR with varying sizes of subsets and varying ratios of training and testing pixels are shown in Table 1**Error! Reference source not found.**. For both datasets, a lower size of pixel subsets also results in a lower classification accuracy. The peat smoking process results in a variable distribution of phenols across the grains. By taking the mean over a certain region, it is attempted to introduce a sufficient statistic that can represent the mean concentration of the whole barley batch. The smaller these subsets are, the less likely it is that these subsets represent a sufficient statistic. Larger subsets are therefore more likely to represent a more precise spectrum for the overall concentration and lead to better classification results.

As stated in Section 4, for a subset size of 50 pixels, we gain c.a. 46 000 samples for SWIR and 17 000 for UV. With a higher amount of testing samples, misclassifications are more likely, which results in lower OA. This becomes evident particularly for the UV dataset, where a subset size of 50 pixels with 5% training ratio can only achieve a 65.4% OA. Increasing the size can however achieve an OA of 96.9%. The SWIR dataset consistently outperforms the UV dataset with a minimum OA of 98.9% for a subset size of 50 and reaches an OA of 99.8% with increased training ratio or number of pixels. Varying the ratio of training and testing data has a similar effect where only 1% of all samples for the UV dataset can achieve an OA of 76.2% and it reaches 97.5% for the SWIR dataset.

To gain a more detailed insight, confusion matrices for the best and the worst combinations of Table 1 are visualised in Figure 3. On the diagonal, the correct numbers of classified pixels are

296 listed and all other elements indicate misclassified samples. In the UV dataset, one can see that
297 with both fixed subset size and training ratio Class 1 and 10 seem to be the easiest to discriminate
298 as almost no samples are misclassified. This is likely due to the fact that they represent the extreme
299 cases of 0 and 124.5 ppm phenol concentration. Classes 2 and 5 – 9 seem to have the most
300 misclassified samples as can be observed in both Figure 3 (a – b) and (e – f). For the SWIR dataset,
301 classes 1 – 5 seem to have the most misclassifications, whereas classes 6 and 7 are consistently
302 well classified.

303 *5.2 Results from mean spectra of spatially coherent regions*

304 In addition to the classification results obtained under various training ratios and randomly
305 generated subsets, the classification was also tested on mean spectra of spatially coherent regions.
306 For this, classifiers were trained for both datasets utilising 20% of the samples generated by taking
307 the average over 50 random pixels. 50 pixels were chosen as this generates a larger number of
308 training samples and will likely capture more statistical variations. Validation sets were produced
309 by calculating the average of 50 × 50 windows for all samples of both datasets. This results in 300
310 samples for the UV dataset and 840 samples for the SWIR dataset respectively over all classes.
311 Greyscale representations of wavelength 1483nm and 284nm for the SWIR and UV datasets
312 respectively are illustrated alongside a ground truth and the classification results in Figure 4. For
313 the UV data, classes 1 and 10 are the best qualified classes, which is consistent with the results
314 from Figure 3. Likewise, classes 6 and 7 are visually classified the best in the SWIR dataset, which
315 again confirms the previous results. The OAs achieved are in both cases however much lower than
316 in Table 1, particularly for the UV dataset which is only 47.7%.

317 As previously stated, the phenol concentrations are very likely to vary drastically for each barley
318 grain. This also results in spatial agglomerations of very high phenol concentration or a total
319 absence of phenols. By taking the mean of spatially coherent regions, we are likely generating
320 samples that represent exactly these variations. The ground truth is not necessarily valid anymore
321 as a result. The low classification accuracy is therefore not a reliable statistic. In fact, misclassified
322 pixels can even be interpreted positively as our classifier is able to pick up spatial variations of

concentrations. Generating a ground truth to evaluate the correctness is impossible which is why different methods of validation are needed here. The high accuracies on the randomly generated samples lead us to believe that this classification is quite accurate. With this, it might be able to estimate the spatial distribution of phenol concentration within a barley batch, providing useful additional information for the industry.

5.3 Results of regression

Even though the differentiation between ten concentration levels implies a classification problem, from a scientific point of view it would also be interesting to estimate the actual concentration level. For this purpose, we applied regression on the same datasets. Likewise, 3 regression runs with 3 selections of random subsets were performed for comparison. Results for varying number of pixel subsets and varying ratio of training and testing samples are summarised in Table 2. Similar to the classification, it can be seen that the UV data produces significantly worse results especially for small sizes of pixel subsets and resulting higher number of samples and for a low training sample ratio. On the other hand, the SWIR dataset is able to achieve an r^2 value of 0.92 in the worst case, or 0.99 in the best case in comparison to 0.91 from the UV dataset. With an RMSE between 0.75 and 0.32 ppm, the SWIR dataset is able to estimate the phenol concentration in an acceptable precision. For more accurate levels of the individual compounds, HPLC and other chemometric analysis tools are still a better choice. But, it is important to bear in mind that these compounds are only markers of flavour. So, the SWIR HSI may in fact be giving a better measure of all compounds that are of sensory importance.

6. Conclusion

In this paper, we examined the potential of HSI for the estimation of the concentration of phenolic flavour compounds on malted barley. For this purpose, barley samples with ten different concentrations were generated and imaged with a UV HSI system covering a spectral range from 220 – 400 nm and a SWIR system covering a range of 1000 – 2500 nm. The samples were then classified using a SVM with RBF kernel. Results show that especially the SWIR dataset is able to

discriminate very precisely between ten concentration levels with an OA of up to 99.8%. The UV dataset in comparison performs worse in all cases. Similar results were observed for the SVR, where the UV dataset can only achieve an r^2 value of 0.91 whereas the SWIR dataset can achieve a value up to 0.99 with an RMSE 0.32 ppm. It was also established that UV HSI is a still underdeveloped technology, where the availability of appropriate light sources is scarce which results in aggravated imaging conditions and very low SNR images. In conclusion, it could be shown that SWIR HSI has in its current stage of development very much the potential to be used in industrial applications to quantify and classify the mean phenol concentration levels of an entire barley batch. As this study focuses on UV and SWIR, future work might include looking at VIS to NIR HSI to estimate phenol levels as the latter is more cost effective than UV and SWIR. Additionally, we will concentrate on training classifiers or regression models that can be evaluated in real life production conditions of peated malt as well as estimating the spatial distribution of the phenolic flavour compounds across the batch. Furthermore, applying different feature extraction techniques such as folded-PCA (Zabalza et al., 2014), singular spectrum analysis (Zabalza et al., 2015), curvelet transform (Tong Qiao et al., 2017), sparse representation (Tong Qiao et al., 2018) and multi-kernel classification (Fang, Li, Duan, Ren, & Benediktsson, 2015) might help in creating datasets with an even higher predictive power.

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Conflict of Interest

The authors declare no conflict of interest.

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Table 1 SVM Classification OA in % for varying number of pixel subset sizes and a training ratio of 5% and varying training ratio with subset size 200.

# Pixels	UV		SWIR		Ratio(%)	UV		SWIR	
	OA	Kappa	OA	Kappa		OA	Kappa	OA	Kappa
50	65.4	61.6	98.9	98.8	**1**	76.2	73.6	97.5	97.3
200	90.3	89.2	99.7	99.7	**5**	90.3	89.3	99.5	99.5
500	96.9	96.7	99.8	99.9	**10**	93.7	93.0	99.8	99.8

Table 2 Correlation coefficient and Root Mean Squared Error of SVR with varying numbers of subset sizes and a training ratio of 5% and varying training ratios with subset size 200

# Pixels	UV		SWIR		Ratio(%)	UV		SWIR	
	r^2	*RMSE*	r^2	*RMSE*		r^2	*RMSE*	r^2	*RMSE*
50	0.56	1.55	0.92	0.75	**1**	0.74	1.23	0.95	0.63
200	0.82	1.04	0.98	0.42	**5**	0.83	1.05	0.98	0.43
500	0.91	0.77	0.99	0.32	**10**	0.85	1.00	0.98	0.36