

1 **Potential of UV and SWIR Hyperspectral Imaging for Determination of**
2 **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.

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

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

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

80 In the past, phenols have successfully been detected in seeds, skins and stems of grapes (Jara-
81 Palacios, Rodríguez-Pulido, Hernanz, Escudero-Gilete, & Heredia, 2016; Zhang et al., 2017) by
82 near infra-red (NIR) HSI as well as the detection of phenols in wood that is used for wine barrels
83 (Baca-Bocanegra, Nogales-Bueno, Hernández-Hierro, & Heredia, 2018). We have also presented
84 groundwork for the detection of phenols in March 2017 (Tschannerl et al., 2017), where NIR to
85 shortwave infra-red (SWIR) HSI covering a spectral range from 950 – 1700 nm was found to be
86 able to differentiate three different levels of phenol concentrations in peated malt with support
87 vector machine classification. However, due to the limited number of different concentrations
88 studied, no effective regression model to estimate the exact concentration could be trained. The aim
89 of this study is to extend the work done through the evaluation of samples with a wider range of
90 phenol concentrations, scanning them in different spectral regions to further identify the potential
91 of HSI for the estimation and generating more robust systems. To achieve this, 10 peated malts
92 with different phenol levels were scanned with a SWIR camera¹ that covers a spectral range of
93 1000 – 2500 nm. Additional information is extracted from wavelengths above 1700 nm that have
94 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.

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

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

117 **2. Chemical background**

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

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

127 Peat can be sourced from various locations across Scotland, including both island and mainland
128 sites. The composition of the peat varies depending on its origin. This influences the relative levels
129 of phenolic compounds on the peated malt, which in turn influences flavour (Harrison & Priest,
130 2009). Each compound imparts a subtly different aroma. Phenol is for example tends to be
131 described as medicinal, while guaiacol is more smoky. The HPLC method, currently used, is both
132 applicable to barley malt steam distillates and new make spirits. The levels are measured in mg/kg
133 or ppm respectively and the total of all compounds combined is used as a marker to the degree of
134 peatiness of the malted barley. Therefore, in this study our aim was to estimate the total phenol
135 levels rather than the concentration of the individual compounds.

136 **3. Data acquisition**

137 *3.1 Sample preparation*

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

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

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

151 3.2 *Imaging process*

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

162 UV imaging was done with pco. Sensicam UV that covers a spectral range of 220 – 400 nm with a
163 spectral resolution of 3.8 nm. It requires a specialised illumination done with a Hamamatsu L6301-
164 50 Deuterium lamp that has a broadband UV coverage, but it is very low in light intensity. This
165 results in an increased exposure time of 300 ms. Additionally, a 3 x 3 spatial and 4-fold spectral
166 binning were applied. This means that 3 x 3 spatial pixels and 4 spectral bands are added up to not
167 only reduce noise but also to increase the camera's light sensitivity. However, the binning process
168 also degrades the spatial resolution and spectral resolution. This results in an image with 342 pixels
169 per scanned line and 248 active bands. As a result of the increased exposure time, the UV scanning
170 process requires several minutes, whereas the SWIR imaging can be done in under a minute. The
171 SWIR imaging was done with the Specim SWIR system covering a range from 1000 – 2500 nm
172 with a spectral resolution of 12 nm. Illumination is done with customary halogen lightbulbs
173 allowing for an exposure time of only 2.5 ms, Binning was not applied resulting in an image with
174 384 pixels per line and 288 active spectral bands.

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

181 **4. Data processing**

182 *4.1 Pre-processing*

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

$$187 \quad \mathbf{r} = \frac{\mathbf{s} - \mathbf{d}}{\mathbf{w} - \mathbf{d}} \times 100\%$$

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

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

200 additive effects, it is common to employ spectral derivatives, either 1st or 2nd order. These are most
 201 commonly realised with Savitzky-Golay smoothing to minimise noise interferences. A widely used
 202 technique to compensate for multiplicative scattering distortions is Multiplicative Scatter
 203 Correction (MSC) (Zhao, Zhang, & Chen, 2005), which estimates scattering coefficients from a
 204 supposedly ideal signal whilst minimising the scatter for each individual signal. One of the most
 205 commonly used techniques in HSI however is the conversion of the spectra to the Standard Normal
 206 Variate (SNV) (Rinnan et al., 2009). For a given set of n measured reflectance spectra $\mathbf{R} =$
 207 $\{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n\}$, the SNV for one spectrum \mathbf{r}_i is calculated by:

$$208 \quad \mathbf{r}_i(SNV) = \frac{\mathbf{r}_i - \boldsymbol{\mu}}{\boldsymbol{\sigma}}, \quad \boldsymbol{\mu} = \frac{1}{n} \sum_{i=1}^n \mathbf{r}_i, \quad \boldsymbol{\sigma} = \sqrt{\frac{1}{n} \sum_{i=1}^n (\mathbf{r}_i - \boldsymbol{\mu})^2}$$

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

214 4.2 Data analysis

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

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

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

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

$$245 \quad OA = \frac{\sum_{i=1}^c n_i}{N} \times 100\%$$

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

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

250
$$Kappa = \frac{p_0 - p_e}{1 - p_e} \times 100$$

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

254
$$p_e = \frac{1}{N^2} \sum_{i=1}^c n_{i1} n_{i2}$$

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

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

262
$$RMSE = \left(\frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2 \right)^{\frac{1}{2}}$$

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

267
$$r^2 = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$$

268 where \bar{y} represents the mean of all values. r^2 takes on values between 0 and 1, with 1 indicating
 269 100% prediction accuracy of the model.

5. Results and Discussion

270

271 5.1 Classification results under varying settings

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

285 As stated in Section 4, for a subset size of 50 pixels, we gain c.a. 46 000 samples for SWIR and 17
286 000 for UV. With a higher amount of testing samples, misclassifications are more likely, which
287 results in lower OA. This becomes evident particularly for the UV dataset, where a subset size of
288 50 pixels with 5% training ratio can only achieve a 65.4% OA. Increasing the size can however
289 achieve an OA of 96.9%. The SWIR dataset consistently outperforms the UV dataset with a
290 minimum OA of 98.9% for a subset size of 50 and reaches an OA of 99.8% with increased training
291 ratio or number of pixels. Varying the ratio of training and testing data has a similar effect where
292 only 1% of all samples for the UV dataset can achieve an OA of 76.2% and it reaches 97.5% for
293 the SWIR dataset.

294 To gain a more detailed insight, confusion matrices for the best and the worst combinations of
295 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

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

328 *5.3 Results of regression*

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

343 **6. Conclusion**

344 In this paper, we examined the potential of HSI for the estimation of the concentration of phenolic
345 flavour compounds on malted barley. For this purpose, barley samples with ten different
346 concentrations were generated and imaged with a UV HSI system covering a spectral range from
347 220 – 400 nm and a SWIR system covering a range of 1000 – 2500 nm. The samples were then
348 classified using a SVM with RBF kernel. Results show that especially the SWIR dataset is able to

349 discriminate very precisely between ten concentration levels with an OA of up to 99.8%. The UV
350 dataset in comparison performs worse in all cases. Similar results were observed for the SVR,
351 where the UV dataset can only achieve an r^2 value of 0.91 whereas the SWIR dataset can achieve
352 a value up to 0.99 with an RMSE 0.32 ppm. It was also established that UV HSI is a still
353 underdeveloped technology, where the availability of appropriate light sources is scarce which
354 results in aggravated imaging conditions and very low SNR images. In conclusion, it could be
355 shown that SWIR HSI has in its current stage of development very much the potential to be used in
356 industrial applications to quantify and classify the mean phenol concentration levels of an entire
357 barley batch. As this study focuses on UV and SWIR, future work might include looking at VIS to
358 NIR HSI to estimate phenol levels as the latter is more cost effective than UV and SWIR.
359 Additionally, we will concentrate on training classifiers or regression models that can be evaluated
360 in real life production conditions of peated malt as well as estimating the spatial distribution of the
361 phenolic flavour compounds across the batch. Furthermore, applying different feature extraction
362 techniques such as folded-PCA (Zabalza et al., 2014), singular spectrum analysis (Zabalza et al.,
363 2015), curvelet transform (Tong Qiao et al., 2017), sparse representation (Tong Qiao et al., 2018)
364 and multi-kernel classification (Fang, Li, Duan, Ren, & Benediktsson, 2015) might help in creating
365 datasets with an even higher predictive power.

366

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371

Conflict of Interest

372 The authors declare no conflict of interest.

373

References

374

375 Amodio, M. L., Capotorto, I., Chaudhry, M. M. A., & Colelli, G. (2017). The use of hyperspectral imaging to
376 predict the distribution of internal constituents and to classify edible fennel heads based on the harvest
377 time. *Computers and Electronics in Agriculture*, *134*, 1–10.

378 Baca-Bocanegra, B., Nogales-Bueno, J., Hernández-Hierro, J. M., & Heredia, F. J. (2018). Evaluation of
379 extractable polyphenols released to wine from cooperage byproduct by near infrared hyperspectral
380 imaging. *Food Chemistry*, *244*, 206–212.

381 Bringhurst, T., & Brosnan, J. (2014). Scotch whisky: raw material selection and processing. In *Whisky* (pp.
382 49–122). Elsevier.

383 Crichton, S. O. J., Kirchner, S. M., Porley, V., Retz, S., von Gersdorff, G., Hensel, O., & Sturm, B. (2017).
384 High pH thresholding of beef with VNIR hyperspectral imaging. *Meat Science*, *134*, 14–17.

385 Datt, B., McVicar, T. R., Van Niel, T. G., Jupp, D. L. B., & Pearlman, J. S. (2003). Preprocessing EO-1
386 Hyperion hyperspectral data to support the application of agricultural indexes. *IEEE Transactions on*
387 *Geoscience and Remote Sensing*, *41*(6), 1246–1259.

388 Dearden, J. C., & Forbes, W. F. (1959). Light Absorption Studies: Part Xiv. the Ultraviolet Absorption
389 Spectra of Phenols. *Canadian Journal of Chemistry*, *37*(8), 1294–1304.

390 Drucker, H., Burges, C. J. C., Kaufman, L., Smola, A., & Vapnik, V. (1997). Support vector regression
391 machines. *Advances in Neural Information Processing Systems*, *1*, 155–161.

392 Fang, L., Li, S., Duan, W., Ren, J., & Benediktsson, J. A. (2015). Classification of Hyperspectral Images by
393 Exploiting Spectral-Spatial Information of Superpixel via Multiple Kernels. *IEEE Transactions on*
394 *Geoscience and Remote Sensing*, *53*(12), 6663–6674.

- 395 Harrison, B. M., & Priest, F. G. (2009). Composition of peats used in the preparation of malt for Scotch
396 whisky production - influence of geographical source and extraction depth. *Journal of Agricultural and*
397 *Food Chemistry*, 57(6), 2385–2391.
- 398 Hsu, P. S., Lauriola, D., Jiang, N., Miller, J. D., Gord, J. R., & Roy, S. (2017). Fiber-coupled, UV–SWIR
399 hyperspectral imaging sensor for combustion diagnostics. *Applied Optics*, 56(21), 6029.
- 400 Jara-Palacios, M. J., Rodríguez-Pulido, F. J., Hernanz, D., Escudero-Gilete, M. L., & Heredia, F. J. (2016).
401 Determination of phenolic substances of seeds, skins and stems from white grape marc by near-infrared
402 hyperspectral imaging. *Australian Journal of Grape and Wine Research*, 22(1), 11–15.
- 403 Kang, X., Xiang, X., Li, S., & Benediktsson, J. A. (2017). PCA-Based Edge-Preserving Features for
404 Hyperspectral Image Classification. *IEEE Transactions on Geoscience and Remote Sensing*, 55(12), 1–
405 12.
- 406 Lee, H., & Kwon, H. (2017). Going Deeper with Contextual CNN for Hyperspectral Image Classification.
407 *IEEE Transactions on Image Processing*, 26(10), 4843–4855.
- 408 Li, H., Lyu, H., Liao, N., & Wu, W. (2016). Measuring spatially varying, multispectral, ultraviolet
409 bidirectional reflectance distribution function with an imaging spectrometer. *Optical Engineering*,
410 55(12), 124106.
- 411 Lu, G., & Fei, B. (2014). Medical hyperspectral imaging: a review. *Journal of Biomedical Optics*, 19(1),
412 010901.
- 413 Manolakis, D., & Shaw, G. (2002). Detection algorithms for hyperspectral imaging applications. *IEEE Signal*
414 *Processing Magazine*, 19(1), 29–43.
- 415 Marshall, S., Kelman, T., Qiao, T., Murray, P., & Zabalza, J. (2015). Hyperspectral imaging for food
416 applications. In *Proceedings - 23rd European Signal Processing Conference (EUSIPCO 2015)* (pp.

417 2854–2858). Nice, France.

418 Merkel, R. (2015). Latent Fingerprint Aging from a Hyperspectral Perspective: First Qualitative Degradation
419 Studies Using UV/VIS Spectroscopy. In *Proceedings - 9th International Conference on IT Security*
420 *Incident Management and IT Forensics (IMF 2015)* (pp. 121–135). Magdeburg, Germany.

421 Mou, L., Ghamisi, P., & Zhu, X. X. (2017). Unsupervised Spectral–Spatial Feature Learning via Deep
422 Residual Conv–Deconv Network for Hyperspectral Image Classification. *IEEE Transactions on*
423 *Geoscience and Remote Sensing*, 56(1), 1–16.

424 Polak, A., Kelman, T., Murray, P., Marshall, S., Stothard, D. J. M., Eastaugh, N., & Eastaugh, F. (2016). Use
425 of infrared hyperspectral imaging as an aid for paint identification. *Journal of Spectral Imaging*, 5(1),
426 1–10.

427 Qiao, T., Ren, J., Craigie, C., Zabalza, J., Maltin, C., & Marshall, S. (2015). Quantitative Prediction of Beef
428 Quality Using Visible and NIR Spectroscopy with Large Data Samples Under Industry Conditions.
429 *Journal of Applied Spectroscopy*, 82(1), 137–144.

430 Qiao, T., Ren, J., Craigie, C., Zabalza, J., Maltin, C., & Marshall, S. (2015). Singular spectrum analysis for
431 improving hyperspectral imaging based beef eating quality evaluation. *Computers and Electronics in*
432 *Agriculture*, 115, 21–25.

433 Qiao, T., Ren, J., Sun, M., Zheng, J., & Marshall, S. (2014). Effective compression of hyperspectral imagery
434 using an improved 3D DCT approach for land-cover analysis in remote-sensing applications.
435 *International Journal of Remote Sensing*, 35(20), 7316–7337.

436 Qiao, T., Ren, J., Wang, Z., Zabalza, J., Sun, M., Zhao, H., ... Marshall, S. (2017). Effective Denoising and
437 Classification of Hyperspectral Images Using Curvelet Transform and Singular Spectrum Analysis.
438 *IEEE Transactions on Geoscience and Remote Sensing*, 55(1), 119–133.

439 Qiao, T., Yang, Z., Ren, J., Yuen, P., Zhao, H., Sun, G., ... Benediktsson, J. A. (2018). Joint bilateral
440 filtering and spectral similarity-based sparse representation: A generic framework for effective feature
441 extraction and data classification in hyperspectral imaging. *Pattern Recognition*, 77, 316–328.

442 Rinnan, Å., Berg, F. van den, & Engelsen, S. B. (2009). Review of the most common pre-processing
443 techniques for near-infrared spectra. *TrAC - Trends in Analytical Chemistry*, 28(10), 1201–1222.

444 Scotch Whisky Association. (2015). Facts & Figures about Scotch Whisky. Retrieved November 20, 2017,
445 from <http://www.scotch-whisky.org.uk/what-we-do/facts-figures/>

446 Sun, D.-W. (2010). *Hyperspectral imaging for food quality analysis and control*. London: Academic Press.

447 Swan, J. S., & Howie, D. (1982). Sensory and analytical studies on the regional composition of Scotch malt
448 whiskies. In F. G. Priest & I. Campbell (Eds.), *Current Developments in Mating, Brewing and*
449 *Distilling* (pp. 129–142). London: The Institute of Brewing.

450 Thomson, F. J. (1982). The estimation of total phenol on malt as a guide to degree of peating of peated
451 distilling malts. In F. G. Priest & I. Campbell (Eds.), *Current Developments in Mating, Brewing and*
452 *Distilling* (pp. 273–278). London: The Institute of Brewing.

453 Tschannerl, J., Ren, J., Jack, F., Marshall, S., Zhao, H., Tschannerl, J., ... Zhao, H. (2017). Employing NIR-
454 SWIR hyperspectral imaging to predict the smokiness of scotch whisky. In *Proceedings - Optical*
455 *Characterization of Materials (OCM 2017)* (pp. 1–12). Karlsruhe, Germany.

456 Yao, H., & Lewis, D. (2010). Spectral Preprocessing and Calibration Techniques. In D.-W. Sun (Ed.),
457 *Hyperspectral Imaging for Food Quality Analysis and Control* (pp. 45–78). London: Academic Press.

458 Young, A., Marshall, S., & Gray, A. (2016). Outlier and target detection in aerial hyperspectral imagery: a
459 comparison of traditional and percentage occupancy hit or miss transform techniques. In F. A. Sadjadi
460 & A. Mahalanobis (Eds.), *Prococeedings - Automatic Target Recognition XXVI* (p. 98440S).

461 Baltimore, Maryland, United States.

462 Yu, H., Liu, H., Wang, N., Yang, Y., Shi, A., Liu, L., ... Wang, Q. (2016). Rapid and visual measurement of
463 fat content in peanuts by using the hyperspectral imaging technique with chemometrics. *Analytical*
464 *Methods*, 8(41), 7482–7492.

465 Zabalza, J., Ren, J., Yang, M., Zhang, Y., Wang, J., Marshall, S., & Han, J. (2014). Novel Folded-PCA for
466 improved feature extraction and data reduction with hyperspectral imaging and SAR in remote sensing.
467 *ISPRS Journal of Photogrammetry and Remote Sensing*, 93, 112–122.

468 Zabalza, J., Ren, J., Zheng, J., Han, J., Zhao, H., Li, S., & Marshall, S. (2015). Novel two-dimensional
469 singular spectrum analysis for effective feature extraction and data classification in hyperspectral
470 imaging. *IEEE Transactions on Geoscience and Remote Sensing*, 53(8), 4418–4433.

471 Zhang, N., Liu, X., Jin, X., Li, C., Wu, X., Yang, S., ... Yanne, P. (2017). Determination of total iron-
472 reactive phenolics, anthocyanins and tannins in wine grapes of skins and seeds based on near-infrared
473 hyperspectral imaging. *Food Chemistry*, 237, 811–817.

474 Zhao, Q., Zhang, G. L., & Chen, X. D. (2005). Effects of multiplicative scatter correction on a calibration
475 model of near infrared spectral analysis. *Guangxue Jingmi Gongcheng/Optics and Precision*
476 *Engineering*, 13(1), 53–58.

477 Zucco, M., Caricato, V., Egidi, A., & Pisani, M. (2015). A Hyperspectral Camera in the UVA Band. *IEEE*
478 *Transactions on Instrumentation and Measurement*, 64(6), 1425–1430.

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482 *Table 1 SVM Classification OA in % for varying number of pixel subset sizes and a training ratio of 5% and varying*
 483 *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

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485 *Table 2 Correlation coefficient and Root Mean Squared Error of SVR with varying numbers of subset sizes and a training*
 486 *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

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