

## Feature extraction for hyperspectral mineral domain mapping: A test of conventional and innovative methods

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# 1 Feature extraction for hyperspectral mineral domain mapping: A 2 test of conventional and innovative methods

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8

9 **Abstract:** Hyperspectral (HS) imaging holds great potential for the mapping of geological targets.  
10 Innovative acquisition modes such as drone-borne or terrestrial remote sensing open up new scales  
11 and angles of observation, which allow to analyze small-scale, vertical, or difficult-to-access outcrops.  
12 A variety of available sensors operating in different spectral ranges can provide information about the  
13 abundance and spatial location of various geologic materials. However geological outcrops are  
14 inherently uneven and spectrally heterogeneous, may be covered by dust, lichen or weathering crusts,  
15 or contain spectrally indistinct objects, which is why classifications or domain mapping approaches are  
16 often used in geoscientific and mineral exploration applications as a means to discriminate mineral  
17 associations (e.g. ore or alteration zones) based on overall variations in HS data. Feature extraction  
18 (FE) algorithms are prominently used as a preparatory step to identify the first order variations within  
19 the data and, simultaneously, reduce noise and data dimensionality. The most established FE  
20 algorithms in geosciences are, by far, Principal Component Analysis (PCA) and Minimum Noise Fraction  
21 (MNF). Major progress has been conducted in the image processing community within the last decades,  
22 yielding innovative FE methods that incorporate spatial information for smoother and more accurate  
23 classification results. In this paper, we test the applicability of conventional (PCA, MNF) and innovative  
24 FE techniques (OTVCA: Orthogonal total variation component analysis and WSRRR: Wavelet-based  
25 sparse reduced-rank regression) on three case studies from geological HS mapping campaigns,  
26 including drone-borne mineral exploration, terrestrial paleoseismic outcrop scanning and thermal HS  
27 lithological mapping. This allows us to explore the performance of different FE approaches on complex  
28 geological data with sparse or partly inaccurate validation data. For all case studies, we demonstrate  
29 advantages of innovative FE algorithms in terms of classification accuracy and geological interpretability.

30 We promote the use of advanced image processing methods for applications in geoscience and mineral  
31 exploration as a tool to support geological mapping activities.

32

33 **Keywords:** feature extraction, domain mapping, mineral exploration, image processing, hyperspectral imaging,  
34 classification

## 35 **1. Introduction**

36 A main application of spectral imaging in geosciences and mineral exploration is the  
37 discrimination of mineralogical or lithological domains, i.e. mixed material classes that are  
38 defined based on their relevance for the respective objective, such as distinctive ore or  
39 alteration zones. Domain mapping may correspond to a classification of overall data  
40 characteristics in the spatial and spectral domain. This approach differs from traditional mineral  
41 mapping, which uses the abundance of single minerals or compounds based on specific  
42 spectral characteristics.

43 Domain or class mapping is a well-established remote sensing method and numerous  
44 approaches exist (Lu and Weng, 2007; Li et al., 2014; Benediktsson & Ghamisi, 2015), each  
45 tailored to the data type and objective of the study. The classification of spectral image data  
46 has a number of challenges such as high data dimensionality at a high redundancy, which  
47 leads to both memory and time intensive processing as well as the “curse of dimensionality”  
48 (Hughes, 1968). The latter describes the phenomenon of declining classification accuracies  
49 with rising data dimensionality at constant number of classes and training data (Hughes, 1968).

50 Feature extraction (FE) methods are a common approach to tackle these challenges (Jia et  
51 al., 2013; Benediktsson & Ghamisi, 2015). By projecting the data into a lower dimensional  
52 feature space and selecting the most meaningful data features, the data size, dimensionality  
53 and redundancy can be reduced dramatically, while most of the informative value is preserved.  
54 The extraction of appropriate features is key for a successful subsequent classification, as it  
55 determines the amount and relevance of information preserved and passed to the classifier.

56 The most traditional FE approaches such as principal component analysis (PCA) and minimum

57 noise fraction (MNF), first introduced by Pearson (1901) and Green et al. (1988), respectively,  
58 are based on the extraction of orthogonal features. These well-established approaches,  
59 however, only consider the input spectral information (e.g., reflectance information) and  
60 disregard the valuable spatial information of neighboring pixels, which, if included, can  
61 significantly improve the mapping abilities of machine learning algorithms (Ghamisi et al.,  
62 2018; Fauvel et al., 2013). Respective advanced algorithms that are able to model both  
63 spectral and spatial information simultaneously (“spatially constrained” methods) have been  
64 developed over time and have outperformed classical FE approaches in terms of resulting  
65 classification accuracy using standard test datasets (Rasti et al., 2014; Rasti et al., 2016; Rasti  
66 & Gudmundsson, 2016). Such datasets commonly represent well validated land cover or urban  
67 scenes with rather distinct and homogeneous classes; thus, contrasting typical geoscience  
68 scenery. These algorithms incorporate spatial information either via a penalty term augmented  
69 to the fidelity term of a cost function or solve the problem subject to a constrain. In Rasti et al.  
70 (2016) and Rasti et al. (2014), two spatially constrained FE approaches, orthogonal total  
71 variation component analysis (OTVCA) and wavelet-based sparse reduced-rank regression  
72 (WSRRR), were proposed and used, respectively, and their performances were evaluated for  
73 land cover classification. The former one incorporates the spatial information via total variation  
74 penalty and the latter one includes spatial information by applying  $\ell_1$  penalty on the wavelet  
75 coefficients. The obtained results in those previous studies also demonstrate that OTVCA and  
76 WSRRR improved the performance of conventional feature extraction approaches in terms of  
77 classification accuracies for land cover classification in both rural and urban areas.

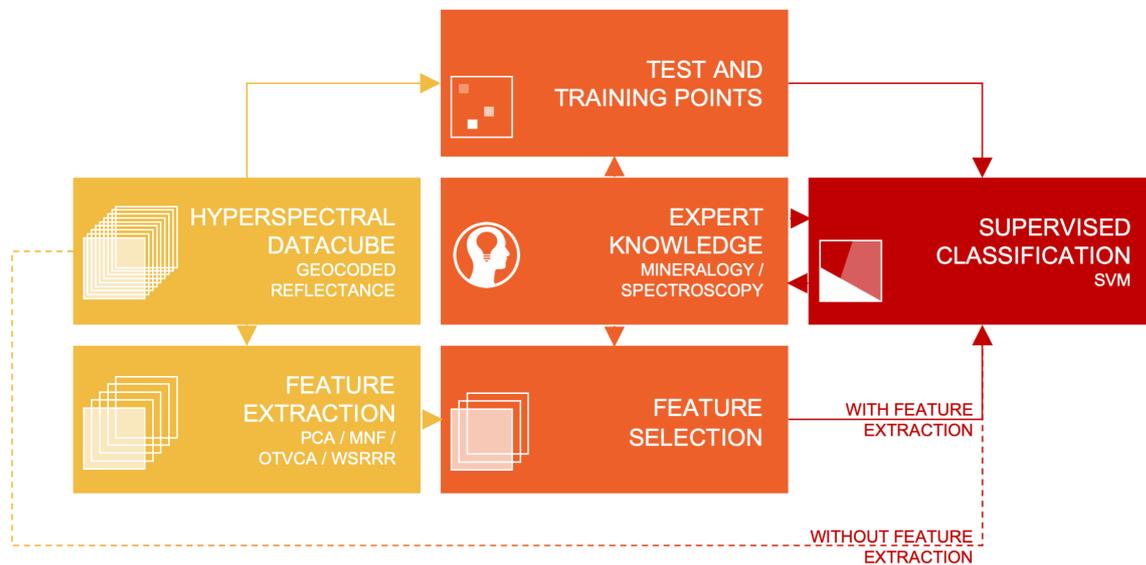
78 The presented study aims to showcase the potential of advanced FE for domain mapping in  
79 geoscientific and economic geology applications. Using three case studies, we compare the  
80 performance of two conventional (PCA, MNF) and two advanced spatially constrained FE  
81 algorithms (OTVCA, Rasti et al. (2016): Orthogonal total variation component analysis,  
82 WSRRR, Rasti et al. (2014): Wavelet-based sparse reduced-rank regression). A supervised  
83 support vector machine (SVM) classification is performed on each dataset to evaluate the  
84 quality and relevance of the extracted features in terms of classification accuracy and

85 geological meaningfulness. The case studies include real and representative applications of  
 86 remote sensing in geosciences that cover different challenges with regard to target  
 87 characteristics, platform and sensor, i.e. including (1) drone-borne data from a lightweight, low  
 88 signal-to-noise ratio (SNR) sensor in the visible and near infrared (VNIR) range, (2) terrestrial  
 89 small-angle (non-nadir) data from a sensor operating in the VNIR to short-wave infrared  
 90 (SWIR) range, (3) terrestrial small-angle data in the long-wave infrared (LWIR) range providing  
 91 spectrally highly mixed signatures. In all three examples, the provided training data is  
 92 extremely limited and the domains of interest are spectrally indistinct, which is typical for  
 93 geological targets.

## 94 2. Methodology

### 95 2.1 General workflow

96 Figure 1 depicts a generalized overview on the used processing workflow.



97

98 *Figure 1. General workflow of hyperspectral data classification with and without prior application of*  
 99 *feature extraction methods.*

100

101 In preparation, each case dataset was fully corrected for spectral and spatial rightness  
 102 according to its sensor- and platform specific workflow (compare Jakob et al., 2017; Lorenz et

103 al., 2018a). Pixels unrelated to the geological target of the case study (e.g., calibration panels,  
104 sky, vegetation) were masked prior to further processing.

105 A set of established (PCA, MNF) and innovative (OTVCA, WSRRR) FE algorithms was applied  
106 separately on each dataset using the same number of output features within each case study.

107 The processing time was determined under equal computational prerequisites for each run. All  
108 the methods investigated in this paper are implemented in Matlab on a computer having

109 Intel(R) Core(TM) i7-6700 processor (3.40 GHz), 32 GB of memory and 64-bit Operating  
110 System. Within each case study, an equal number of features was selected from each FE

111 result. The feature subsets were defined by manually choosing image features with a  
112 geological meaning while rejecting features dominated by noise or illumination differences. For

113 each case study, the feature subsets were used as an input for an SVM classification to  
114 discriminate geological domains of interest and provide a basis for a comparison of the FE

115 approaches regarding their geoscientific value. The training data corresponds to regions of  
116 interest that were defined based on geological validation from field observations, samples and

117 spectral reference measurements. An additional classification on the full, original dataset was  
118 performed for each case study to compare the classification performance of features vs. full

119 data dimensionality. The accuracy of each classification result was estimated using three  
120 established accuracy measures: average accuracy (AA), overall accuracy (OA) and kappa

121 coefficient (k).

122 The tested FE algorithms as well as the used classifier are introduced in the following.

## 123 2.2 Algorithms used

124 **Principal component analysis (PCA)** aims at transforming the input hyperspectral data into  
125 a lower dimensional subspace using a linear transformation approach which maximizes the

126 signal variance (Jolliffe, 2002). PCA reduces the dimensionality of hyperspectral datasets with  
127 interrelated variables, while it retains most of the variation in the dataset. The output of PCA is

128 a set of features, also known as principal components (PCs), which are orthogonal to each  
129 other and are ordered in such a fashion that the first PC corresponds to the greatest variance,

130 the second component corresponds to the second greatest variance and so on. Therefore, the  
 131 first few principal components which capture the major variance of the data can be a  
 132 representative for the higher dimensional data.

133 **Minimum noise fraction (MNF)**, which was specifically proposed to analyze remotely-sensed  
 134 hyperspectral and multispectral images, computes the normalized linear combinations of the  
 135 original bands which maximize the SNR by minimizing the variance of the noise with respect  
 136 to the variance of the signal, and therefore, maximize the quality of the input hyperspectral  
 137 data (Green et al., 1988). In a similar manner to PCA, MNF produces orthogonal features  
 138 ordered by their information content in which the first few components contain very high SNR.  
 139 While PCA searches for an orthogonal subspace to capture the maximum variance of the data,  
 140 MNF seeks a subspace to maximize the signal to noise ratio, making it more suitable for data  
 141 restoration and data quality improvement.

142 **Orthogonal total variation component analysis (OTVCA)** was recently introduced in Rasti  
 143 et al. (2016) by developing a non-convex optimization technique and a low-rank (subspace)  
 144 model. It extracts the most informative features from the observed data ( $F$ ). OTVCA estimates  
 145 the reduced features by solving the following constraint cost function problem:

$$146 \quad (\hat{\mathbf{A}}, \hat{\mathbf{V}}) = \arg \min_{\mathbf{A}, \mathbf{V}} \frac{1}{2} \|\mathbf{F} - \mathbf{A}\mathbf{V}^T\|_{\mathbf{F}}^2 + \lambda \sum_{i=1}^r \left\| \sqrt{(\mathbf{D}_h \mathbf{a}_{(i)})^2 + (\mathbf{D}_v \mathbf{a}_{(i)})^2} \right\|_1 \text{ s. t. } \mathbf{V}^T \mathbf{V} = \mathbf{I}_r, \quad (1)$$

147 where  $\mathbf{V}$  contains the low-rank basis,  $\|\mathbf{A}\|_{TV}$  is the total variation norm applied spatially (Rasti  
 148 et al., 2016) and  $\lambda$  is known as the TV tuning parameter which balances the amount of  
 149 smoothness. We should note that the low-rank features,  $\mathbf{A}$ , and the basis matrix (for the  
 150 subspace),  $\mathbf{V}$ , are unknown. Therefore, they both need to be estimated. To solve the  
 151 aforementioned optimization problem, a cyclic descent (CD) was suggested in Rasti et al.  
 152 (2016). As can be seen in Eq. (1), the cost function is composed of two terms. The first term,  
 153 the fidelity term, tries to minimize the difference between  $\mathbf{F}$  and the estimated  $\mathbf{A}\mathbf{V}^T$ . The second  
 154 term is the regularization term, which models the spatial dependencies using the total variation  
 155 norm.

156 **Wavelet-based sparse reduced-rank regression (WSRRR)** was proposed in Rasti et al.  
157 (2014), to represent hyperspectral images using a few informative features automatically.  
158 WSRRR uses a sparse and low-rank model to represent the hyperspectral data. In Rasti et al.  
159 (2014), the following optimization model is used to estimate  $W$  and  $V$ , simultaneously:

$$160 \quad (\hat{W}, \hat{V}) = \arg \min_{W, V} \frac{1}{2} \|F - DWV^T\|_F^2 + \lambda \sum_{i=1}^r \|w_{(i)}\|_1 \text{ s.t. } V^T V = I_r, \quad (2)$$

161 where  $D$  contains the two-dimensional wavelet basis and  $W$  contains unknown 2D wavelet  
162 coefficients. In order to enforce sparsity into (2), an  $l_1$  penalty on the wavelet coefficients was  
163 considered. The promotion of sparsity on the extracted features improves the SNR, which  
164 leads to more accurate classification maps. As can be seen in Eq. (2), the cost function  
165 consists of two terms. The first term, the fidelity term, tries to minimize the difference between  
166  $F$  and the estimated  $DWV^T$ . The second term, the regularization term, tries to model spatial  
167 dependencies using an  $l_1$  norm applied on wavelet coefficients.

168 **Support vector machines (SVM) classifier** is a widely-used technique for the classification  
169 of hyperspectral images since it can effectively handle the high dimensionality of hyperspectral  
170 images when only a limited number of training samples is available. Based on the studies  
171 conducted in Ghamisi et al. (2017), SVM is found to be efficient, stable, and accurate compared  
172 to several other machine learning-based classification techniques. There is a large number of  
173 scientific papers (such as these two review papers Ghamisi et al. (2017) and Benediktsson &  
174 Ghamisi, (2015)) which clearly demonstrate that a joint use of a robust FE technique and the  
175 SVM classifier can shape a strong machine learning approach, particularly for the classification  
176 of hyperspectral images. SVM tries to define an optimal separating hyperplane, also known  
177 here as a classification boundary, within the multidimensional feature space to differentiate  
178 between the training samples of two classes of interest. The best hyperplane is the one that  
179 leaves the maximum margin from the closest training samples (also known as support vectors)  
180 of both classes. The hyperplane is placed in the multidimensional feature space by considering  
181 an optimization problem that is solved via structural risk minimization.

182 The SVM was initially introduced to tackle linear problems, although decision boundaries often  
183 need to be nonlinear to address classification problems due to the complex and nonlinear  
184 nature of hyperspectral image classification. In such cases, a nonlinear mapping using kernel  
185 methods is used to project the data into a high-dimensional feature space where the input  
186 nonlinear data are linearly separable. For the current study, we use the Gaussian radial basis  
187 function (RBF) kernel, which is the most widely-used kernel for hyperspectral image analysis  
188 (Scholkopf & Smola, 2002; Waske et al., 2009). The RBF kernel contains two important  
189 parameters, including  $C$  (the parameter that controls the amount of penalty during the SVM  
190 optimization) and  $\gamma$  (the spread of the RBF kernel), which are automatically traced using a  
191 parameter selection method based on cross-validation (Chapelle et al., 2002).

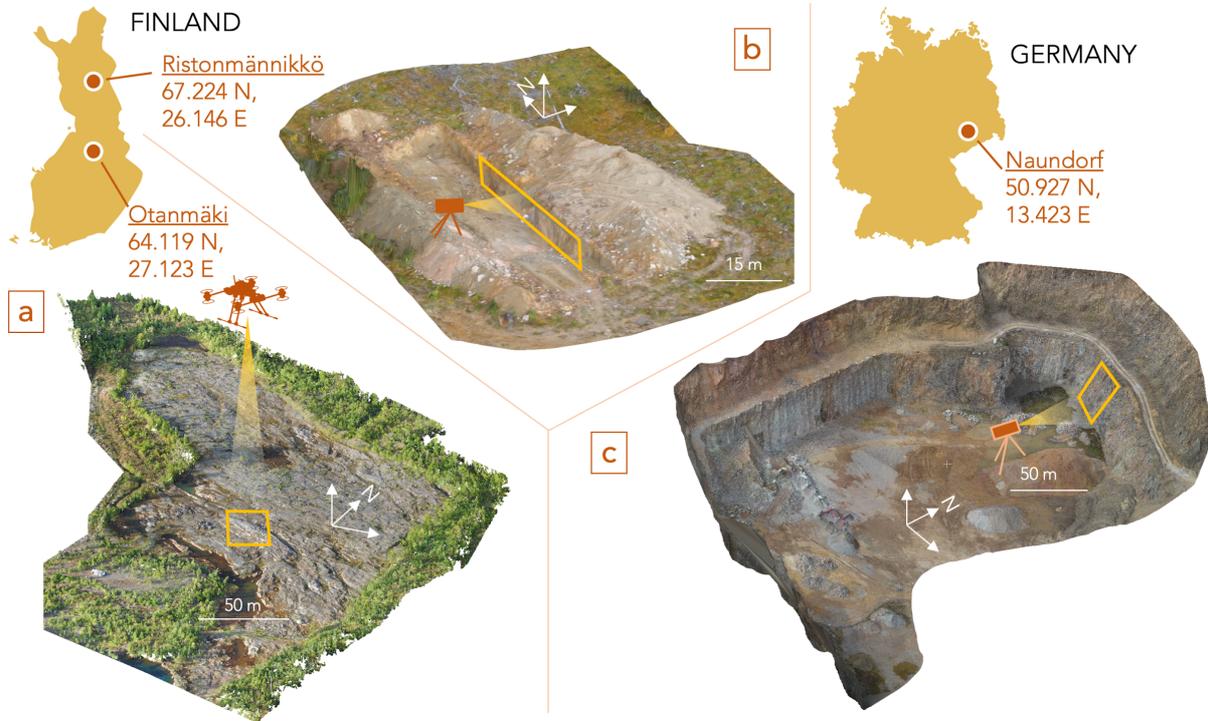
### 192 **3. Introduction of case studies**

#### 193 3.1 Case study 1: UAS-borne VNIR

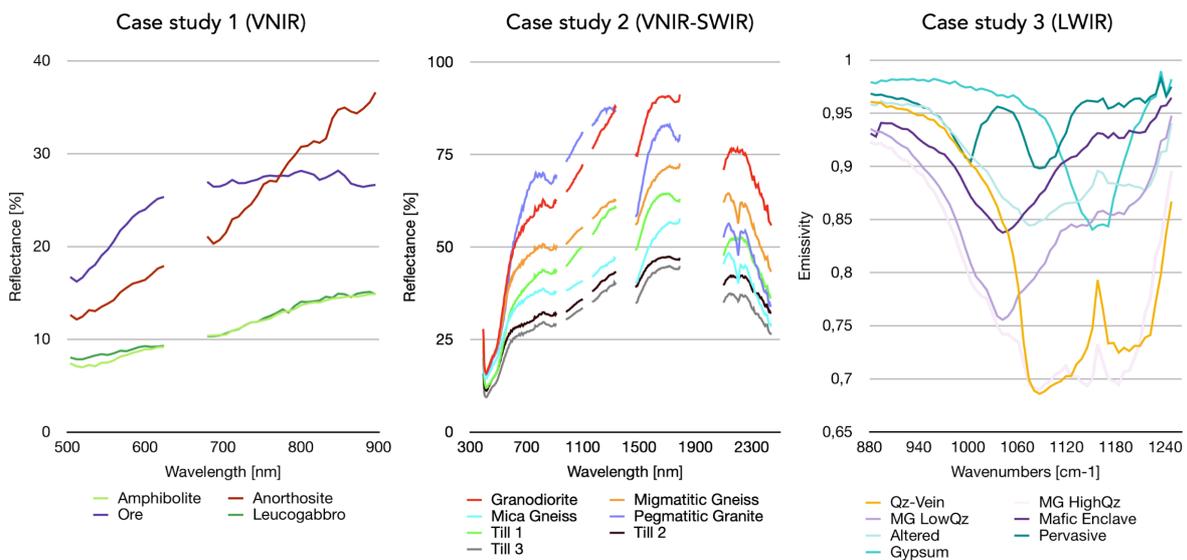
194 The first case study is a drone-borne hyperspectral survey over the Otanmäki mine, located  
195 200 kilometers southeast of Oulu in the center of Finland. The analyzed scene covers parts of  
196 the Metsämalmi outcrop, located at the eastern margin of the Otanmäki deposit (Fig. 2a). The  
197 site is characterized by Paleoproterozoic gabbro-anorthosites that intruded the Archean  
198 granitic gneiss basement. The gabbros host Fe-Ti-V oxide ore bodies, linked to a magnetite-  
199 ilmenite mineralization of economic interest (Pääkkönen, 1956; Lindholm et al., 1980; Huhma  
200 et al., 2018). Recent geochemical studies attest to the high complexity of the Otanmäki suite  
201 in terms of lithology and geometry (Kärenlampi et al., 2019). The ore bodies occur as hundreds  
202 of lenses and veins with widths of 3–50 m and lengths up to 200 m (Maier et al., 2015),  
203 containing up to 40 wt.% magnetite.

204 All abundant lithologies, including the ore, lack distinctive absorption features in the examined  
205 spectral range. The irregular shape of the ore bodies, their heterogeneous composition and  
206 locally dense lichen cover further contribute to create a challenging target for supervised  
207 classification methods. For this example, we defined four distinct classes: ore, amphibolite,

208 anorthosite and leucogabbro (Fig. 3). This distinction is based on a detailed, hand-drawn and  
 209 subsequently geolocated geologic map made by *Rautaruukki Oy*, which was kindly provided  
 210 by the *Otanmäki Mine Oy* company.



211  
 212 *Figure 2. Location of the three study areas as well as coverage of the discussed data sets (indicated by*  
 213 *yellow polygons): a) UAS-based VNIR (case study 1), b) terrestrial VNIR-SWIR (case study 2), c)*  
 214 *terrestrial LWIR (case study 3)*



216 *Figure 3. Spectral characteristics of the classes defined for each case study area. The displayed*  
 217 *spectra are averages of all pixels used for training of each respective class. Spectral artifacts due to*  
 218 *sensor gaps and strong atmosphere-related noise are whitened out for better visibility.*

219

220 The ore zone extents were mapped based on field observations, drillings, and magnetic  
 221 susceptibility measurements. Due to potential local positioning inaccuracies, the geological  
 222 map could not be used directly for the extraction of test and training pixels, but served as a  
 223 general guideline for class discrimination and visual verification of classification results. The  
 224 final selection of validation points was supported by geological as well as spectral field  
 225 observations, and refined based on spectral homogeneity in the hyperspectral image to avoid  
 226 accidental mislabeling due to shaded or highly inhomogeneous areas. The selected validation  
 227 points were divided into 60–400 training pixels (average of 200 px) and 90–400 test pixels  
 228 (average of 200 px) per class. The data set was acquired using a light-weight VNIR  
 229 hyperspectral imager deployed from a hexacopter drone (for details see Table 1). The detailed  
 230 acquisition and processing workflow can be found in Jakob et al. (2017) and Jackisch et al.  
 231 (2019), respectively.

232

233

234

235 *Table 1. Overview on important sensor, target and acquisition parameters for the three case studies.*

Case Study	1	2	3
Location	Otanmäki, Finland	Ristonmäntikkö, Finland	Naundorf, Germany
Geological target	Fe-Ti-V deposit (scraped outcrop)	Tectonic structures in crystalline basement and sedimentary cover rocks (artificial trench wall)	Hydrothermal alteration zones (quarry face)

Deployed Sensor	Senop Rikola Hyperspectral Imager (504–900 nm, frame based)	Specim AisaFENIX (380–2500 nm, push-broom)	Telops Hyper-Cam LW (7700-11800 nm, frame-based)
Sensor Setup	Drone-based (hexacopter)	Ground-based (tripod)	Ground-based (tripod)
Sensor Orientation	Nadir	Horizontal	Near-horizontal (varying)
Sensor-Target Distance	50 m	13 m	55 m
Data size (columns/rows/bands)	960/890/50	1389/326/450	667/746/58
Image footprint	ca. 30 m x 27 m	ca. 20 m x 4 m	ca. 15 m x 16 m
Extracted features/ selected features	15/6	20/10	20/12

### 236 3.2 Case study 2: terrestrial VNIR-SWIR

237 The VNIR-SWIR dataset from the Ristonmännikkö site was acquired during a ground-based  
238 hyperspectral imaging campaign at a paleoseismic trench dug across a post-glacial fault in the  
239 northern Finnish part of the Fennoscandian Shield (Kirsch et al., 2019; Fig. 2b). At this site,  
240 neotectonic deformation has produced discrete reverse fault scarps with small offsets within  
241 an Archean basement and glacial-cover sediment sequence. Seven lithologic classes were  
242 considered for classification, comprising basement units (granodiorite, migmatitic gneiss, mica  
243 gneiss, pegmatitic granite) and cover sequences (till 1, 2 and 3). The training data for the  
244 supervised classification is based on image spectra at 30 sample locations, labelled according  
245 to generalized lithologic descriptions provided by the geologists on site. Laboratory (X-ray  
246 diffraction analysis) and in-situ (handheld X-ray fluorescence (XRF) analyzer and VNIR-SWIR

247 spectrometer) analytical data were used for the validation of the spectral features and to  
248 establish a link between lithologic classes and spectral, mineralogical, and chemical  
249 composition (Kirsch et al., 2019). In order to increase the number of training pixels per class  
250 and to compensate for any georeferencing, registration and sample-localization errors, 24  
251 pixels surrounding each of the original validation points were also included in the training  
252 dataset. The selected validation points were divided into 50–175 training pixels (average of  
253 100 px) and 20–35 test pixels (average of 25 px) per class. A non-orthorectified geological  
254 map of the outcrop (Ojala et al., 2019) served as a guideline for a visual evaluation of  
255 classification results.

256 Damp, cold and cloudy conditions during image acquisition had a clearly negative effect on the  
257 SNR of the hyperspectral data, which is manifested by low reflectance values, strong water  
258 absorptions and noisy spectra, particularly in the SWIR range (Fig. 3). This may lead to  
259 spectrally indistinctive classes but illustrates an acquisition during operational conditions.

260 Details on the acquisition and processing workflow can be found in Table 1, as well as in  
261 Lorenz et al. (2018a), Kirsch et al. (2018) and Kirsch et al. (2019), respectively.

### 262 3.3 Case study 3: terrestrial LWIR

263 The third case study was performed at the Naundorf quarry in the state of Saxony, Germany  
264 (Fig. 2c). It showcases parts of the As-Zn-Cu-In-Ag-bearing polymetallic sulfide vein network  
265 characteristic for the Freiberg mining district. In the Naundorf quarry, the faults are associated  
266 with phyllic hydrothermal alteration of the late Variscan biotite granite host.

267 The site has already been investigated using different HS sensors in Kirsch et al. (2018). The  
268 long-wave infrared data set was acquired as a mosaic of data frames using a Telops Hyper-  
269 Cam LW HS imager (for details see Table 1). The detailed acquisition and processing workflow  
270 can be found in Lorenz et al. (2018b) and Kirsch et al. (2018), respectively. According to the  
271 mineralogical discrimination of Kirsch et al. (2018), the main lithological classes of the  
272 Naundorf quarry are monzogranite, moderately altered and pervasively altered monzogranite,  
273 mafic enclaves of quartz-monzonitic composition and quartz veins. For this study, the analyzed

274 scene was further subdivided, yielding a total of spectrally distinct 7 classes (Fig. 3): Qz-rich  
275 zones/veins, monzogranite (high and low quartz), mafic enclaves, moderately altered  
276 monzogranite, pervasive alteration, and gypsum. A schematic geological map of the outcrop  
277 was used for a general visual evaluation of the classification results. The map is based on field  
278 observations in the accessible portion of the outcrop and visual interpretation of an RGB  
279 textured digital outcrop model in the inaccessible part of the outcrop. However, due to the  
280 inaccessibility of most of the outcrop (in particular the middle and upper part) and the visual  
281 similarity of some classes, the map only outlines general expected lithological variations. A  
282 detailed discrimination of the hydrothermal alteration zone into gypsum-rich parts and  
283 pervasive alteration, the discrimination of monzogranite with differing quartz content or the  
284 exact location of all mafic enclaves for the full extent of the study area was not feasible. For  
285 this reason, the validation map does only include generalized lithological classes. Validation  
286 points for training and test data were therefore selected manually based on the available  
287 accurately geolocated geological as well as spectral field observations, and refined according  
288 to spectral homogeneity in the hyperspectral image to avoid mislabeling in shaded or  
289 inhomogeneous areas. The selected validation points were divided into 20–80 training pixels  
290 (average of 37 px) and 60–300 test pixels (average of 155 px) per class.

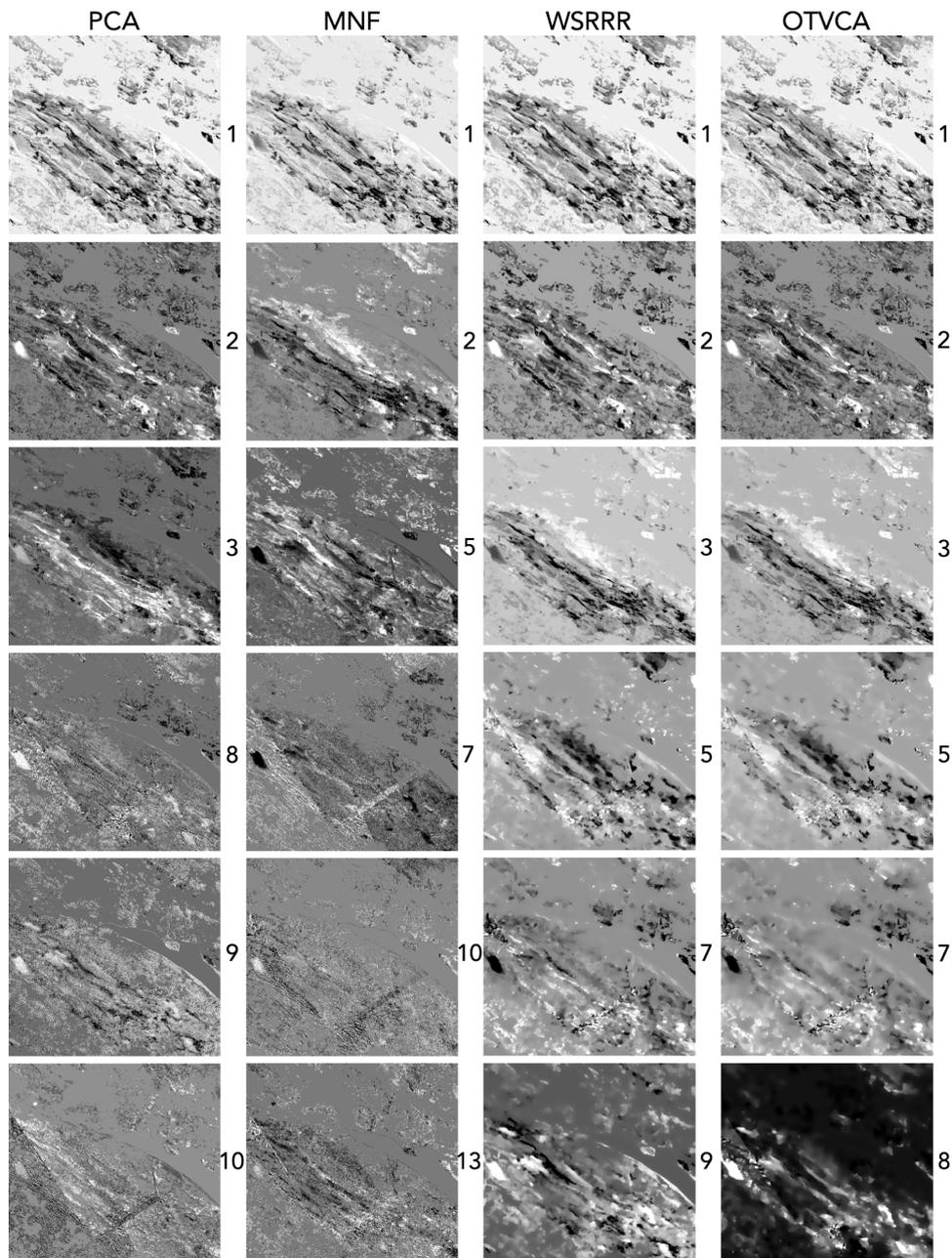
## 291 4. Results

### 292 4.1 General performance of the tested FE methods

293 A comparison of the geologically most relevant feature bands per tested FE algorithm (shown  
294 exemplary for the first case study in Fig. 4) reveals similar content and quality in the first two  
295 or three bands for all tested FE methods. In successive bands, major differences arise.

296 The most obvious trend is the overall more smooth and coherent appearance of the feature  
297 bands extracted by the spatially constrained methods OTVCA and WSRRR, with an apparent  
298 increase in spatial smoothing towards higher feature numbers. This effect is stronger for  
299 OTVCA and leads to the manifestation of large-scale blurry structures in feature bands of

300 higher index. In contrast, the traditional methods PCA and MNF yield much noisier, but also  
301 more detailed feature bands with consistent spatial resolution/scale throughout all feature  
302 bands. However, apart from the very first feature bands, extracted geology-relevant features  
303 additionally highlight noise and image artifacts that overprint the relevant information. In the  
304 depicted UAV-borne case study 1, these artifacts comprise mostly illumination differences  
305 between individual images of the processed mosaic as well as remaining topography-related  
306 artifacts. OTVCA and WSRRR seem to suppress this effect and show an overall much better  
307 separation of geology-related features and image artifacts, which allows for a much easier  
308 manual selection of relevant feature bands with parallel rejection of artifact- or noise-only  
309 feature bands.



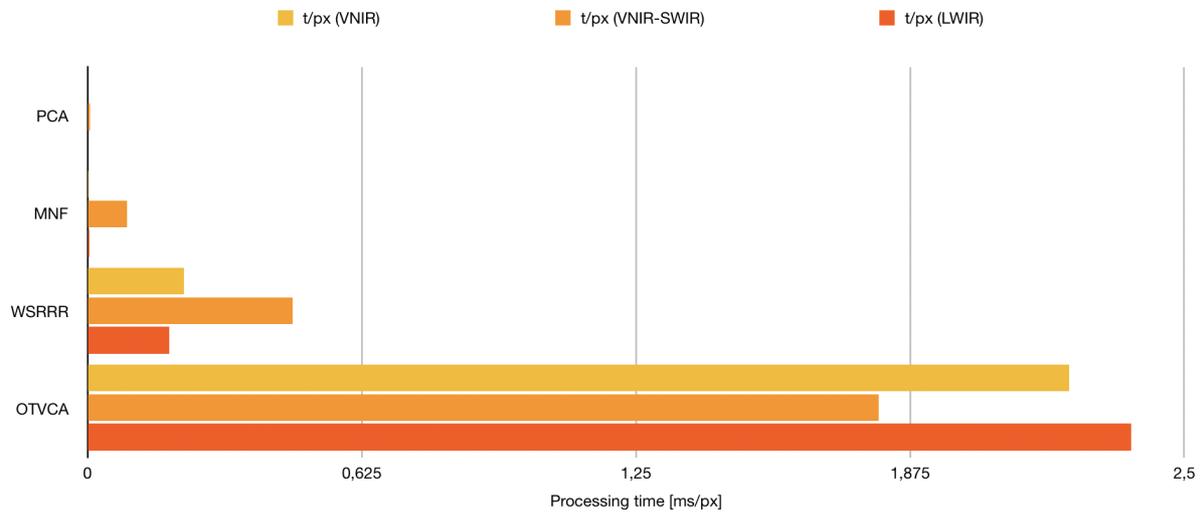
310

311 *Figure 4. Comparison of the six geologically most relevant feature bands per tested FE algorithm*  
 312 *(index indicated by number label), which were selected for subsequent classification (case study:*  
 313 *UAS-VNIR).*

314

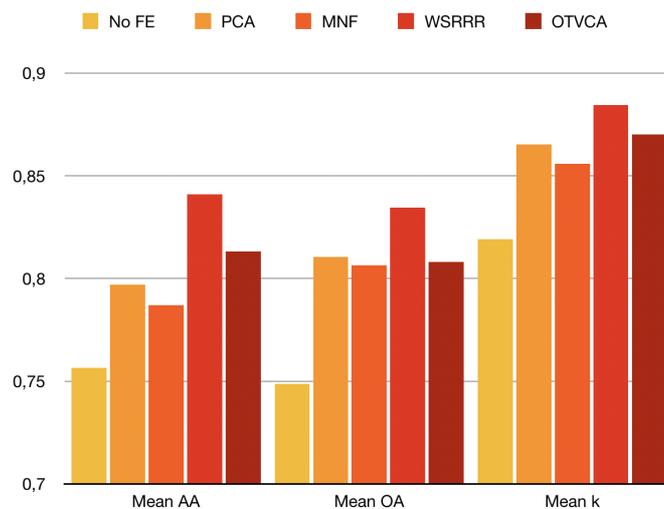
315 The analysis of the processing time for feature extraction from each of the dataset shows clear  
 316 differences in dependence of the algorithm (Fig. 5). The traditional FE methods, PCA and MNF,  
 317 exhibit extremely short processing times (in average ~2 microseconds/pixel for PCA and ~30  
 318 microseconds/pixel for MNF), while the innovative FE methods require longer processing times

319 (in average ~0.3 milliseconds/pixel for WSRRR and ~2.1 milliseconds/pixel for OTVCA). In  
 320 particular OTVCA is very computing-intensive (about 1000 times slower than PCA). The trend  
 321 is consistent for all three case studies.



322  
 323 *Figure 5. Performance of the tested FE algorithms in regards of processing time (in milliseconds per*  
 324 *data pixel) for the extraction of 20 image features per dataset.*

325  
 326 In terms of accuracy performance of SVM, the usage of FE prior to SVM is clearly  
 327 advantageous, as it increases all analyzed accuracy measures (OA, AA, k) by several percent  
 328 compared to no prior FE (Fig. 6).



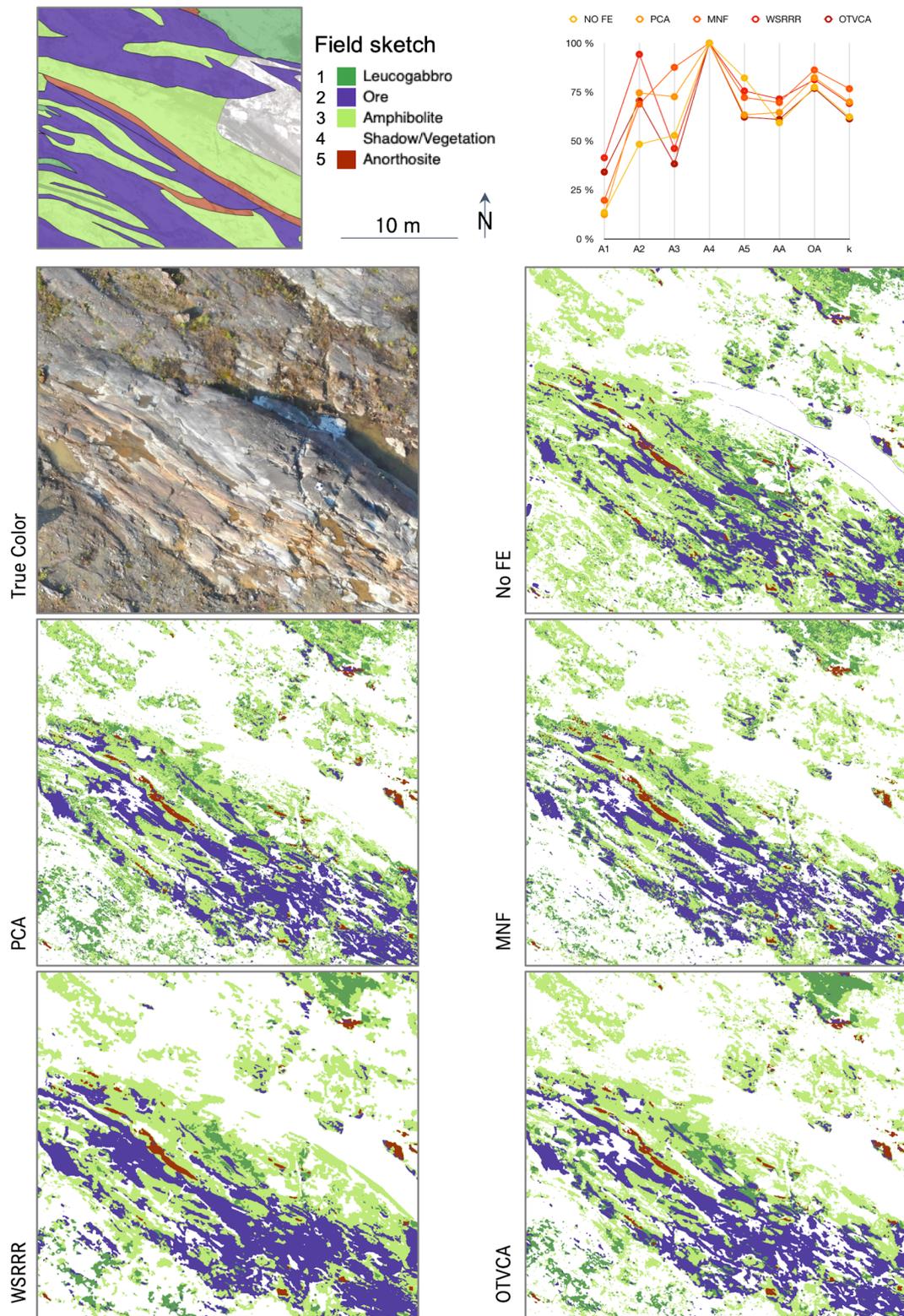
329  
 330 *Figure 6. Average performance of SVM classification in terms of accuracy using the tested FE*  
 331 *algorithms as well as using no prior FE.*

332 The highest accuracy throughout all categories is accomplished by WSRRR (AA = 84%,  
333 OA=83%, k=88%, average of all case studies). Interesting is also the consistently better  
334 accuracy performance of PCA in comparison to MNF in all case studies (difference of 0.4-1%  
335 for all accuracy measures).

#### 336 4.2 Classification results VNIR (Otanmäki)

337 The main host rock types of the Otanmäki site are leucogabbro, amphibolite and anorthosite.  
338 In theory, those lithologies are not discriminable in the analyzed part of the electromagnetic  
339 spectrum, as their main mineral components, plagioclase and amphibole, are spectrally  
340 indistinct in the VNIR. Leucogabbro and amphibolite accordingly show nearly equal spectral  
341 signatures in our data (Fig. 3). However, differences in the overall spectral shape of anorthosite  
342 and leucogabbro/amphibolite do exist (Fig. 3), which might correspond to alteration of the  
343 protolith or minor abundances of spectrally active minerals. The ore zones can be distinguished  
344 from non-ore zones based on locally abundant iron oxide absorption features of weathering  
345 products of the magnetite/ilmenite mineralization.

346 In all performed classifications, anorthosite is clearly delineated as linear features following a  
347 NW-SE trend (Fig. 7). In contrast, leucogabbro and amphibolite are only separated clearly  
348 when using advanced spatially constrained FE methods. Despite their spectral similarity, slight  
349 differences in texture and brightness might allow a discrimination based on spatial features.  
350 Traditional FE attempts are not able to separate the two classes and show an intermingled and  
351 noisy result. The leucogabbro is mapped as a coherent unit in the NE part of the area, which  
352 corresponds to the spatial distribution of the unit in the reference geological map. The  
353 distribution pattern of the detected ore zones does not completely match those of the  
354 geological reference map, but agree largely with the general location and orientation of the  
355 mapped units and are coherent in all classification results.



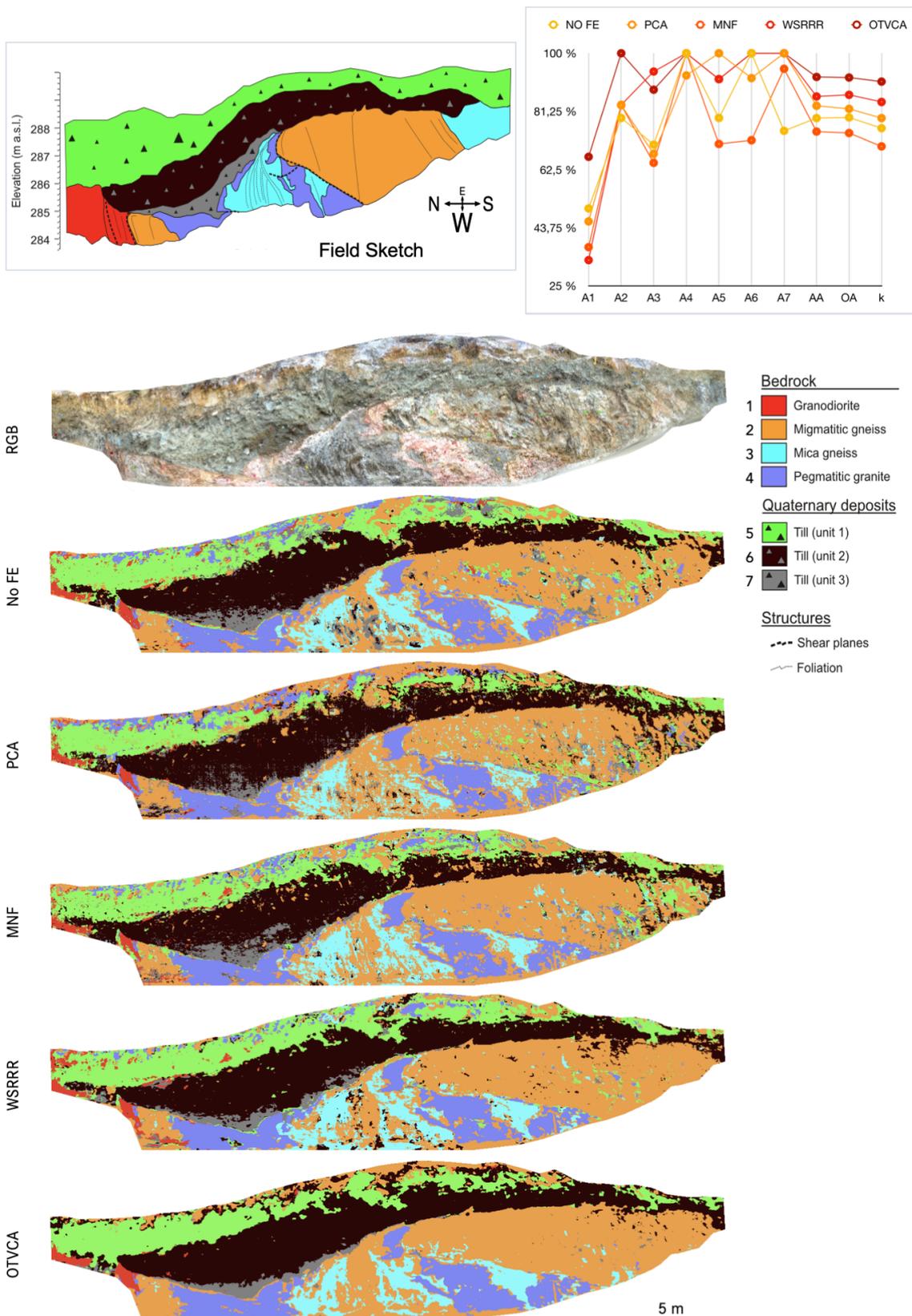
356

357 *Figure 7. Performance of SVM classification based on different FE approaches for the drone-borne*  
 358 *VNIR survey over the Otanmäki ore deposit (Finland). A1-A5 refer to the respective class specific*  
 359 *accuracies.*

360 Not only do variable rock compositions inhibit a clearer classification, but the reference  
361 geologic map itself is prone to slight shifts in x-y directions. This might be due to inaccurate  
362 georeferencing of this map, but also the time difference between the geological mapping and  
363 our data acquisition might contribute to inaccuracies in regards of alteration, vegetation and  
364 soil coverage. Also, this geologic map was part of a much larger regional geologic mapping,  
365 meaning a larger scale was applied to distinguish target rocks at the time. It is unclear how  
366 well the drawn boundaries superimpose on the actual rock zones, but a shift of 1-2 m in each  
367 direction is likely.

#### 368 4.3 Classification results VNIR-SWIR (Ristonmännikkö)

369 In the Ristonmännikkö case study, all methods deliver geologically sensible and interpretable  
370 results that to a large extent match the reference geological map (Fig. 8). Discrepancies to the  
371 geologic map and the validation data set that result in low classification accuracies (Fig. 8)  
372 include (i) the occurrence of migmatitic gneiss within the mica gneiss unit in the center of the  
373 outcrop in the classification image, which is mapped as either mica gneiss or pegmatitic granite  
374 in the reference map, (ii) the missing occurrence of mica gneiss in the right side of the reference  
375 image, (iii) the granodiorite mapped in the far left side of the classification image, which has a  
376 smaller spatial extent than the one in the reference map. These differences can be mostly  
377 explained by the missing geolocation of the field sketch, which challenges to locate the extent  
378 of the mapped lithological boundaries within the classification image. Such, the units on either  
379 end of the reference map are possibly only partly covered by the hyperspectral scan.  
380 Furthermore, misinterpretation during geological mapping cannot be excluded.  
381 There are only subtle differences between the classification results. For instance, the areal  
382 extent of till unit 3 differs slightly between the images.



383

384 *Figure 8. Performance of SVM classification based on different FE approaches for the terrestrial VNIR-*

385 *SWIR survey at Ristonmännikö paleoseismic trenches (Finland). A1-A7 refer to the respective class*

386 *specific accuracies.*

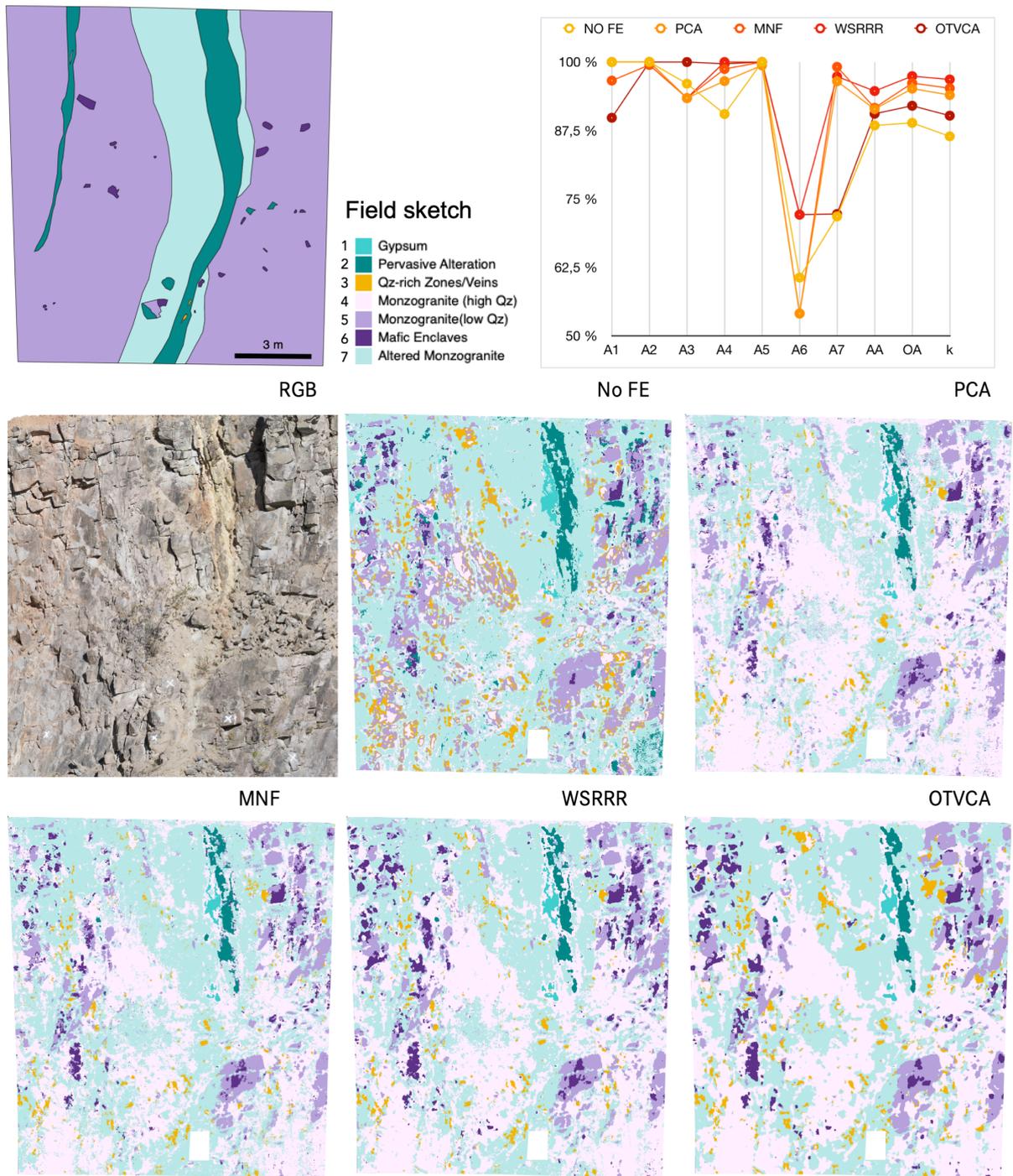
387 The noise level is greatest in the PCA image, followed by the classification image without prior  
388 FE, but some of the noise may actually correspond to real features, such as (i) pixels in the till  
389 units mapped as either one of the basement units, which may correspond to basement-derived  
390 pebbles in the till, and (ii) the pixels mapped as till 3 in any of the basement units (e.g., evident  
391 in the WSRRR image) which may be explained by the draping of these units with the friable till  
392 material from above.

393 OTVCA provides the smoothest/cleanest result amongst all trialed classification approaches,  
394 the highest accuracy measures for all AA (92%), OA (92 %) and k (91%), and most closely  
395 resembles the appearance of a geologic map. However, locally, the uniformity displayed by  
396 the OTVCA image may hinder the delineation of faults, which manifest themselves as small-  
397 scale, non-continuous, lithologically variable layers (e.g., shear plane in the lower left part of  
398 the scene easily identified in the PCA and MNF images).

399 The suppression of noise may also result in the sharp appearance of transitions between units  
400 which may be gradual in reality (e.g. boundary between till units 2 and 3), and the obliteration  
401 of textural features, such as interlayering or foliation (compare smoothness of OTVCA with  
402 “striped” appearance of MNF in the central portion of the image).

#### 403 4.4 Classification results LWIR (Naundorf)

404 All classification results for the Naundorf scene yield geologically plausible results that align  
405 well with field observations documented in the geological reference map (Fig. 9). The  
406 classification maps show a ubiquitous distribution of low- and high-quartz monzogranite host  
407 rocks and clearly defined zones of gypsum and pervasively altered monzogranite spatially  
408 limited to the core of the hydrothermal zone. The altered monzogranite is correctly mapped  
409 around pervasively altered hydrothermal zones, the mapped mafic enclaves correspond to  
410 their true size, shape and (random) distribution in the unaltered host rock.



411

412 *Figure 9. Performance of SVM classification based on different FE approaches for the terrestrial LWIR*  
 413 *survey at Naundorf quarry (Germany). A1-A7 refer to the respective class specific accuracies.*

414

415 The classification with no prior FE has the poorest performance in terms of overall classification  
 416 accuracy (Fig. 9, AA=88%, OA=89%, k=86% for no FE vs. AA=95%, OA=97%, k=97% for  
 417 WSRRR). In comparison with the other classification maps, the classification with no prior FE

418 generally has a noisy appearance showing areas of mixed lithologies and units with highly  
419 serrated boundaries. From a geological perspective, the areal extents of mafic enclaves and  
420 high-Qz monzogranite appear underestimated, the quartz-rich veins are overestimated, and  
421 pervasively altered monzogranite is locally misclassified in areas outside of the hydrothermal  
422 zone. Whereas PCA, MNF and WSRRR deliver almost identical results, the OTVCA image is  
423 less noisy and generally exhibits pixel groups of larger size. This aggregation leads to a slight  
424 overestimation of areal extent of enclaves and other units as well as some geometric distortion  
425 and loss of textural details (e.g. the vein-like shape of gypsum in the upper part of the  
426 hydrothermal zone).

427 Particularly low classification accuracies are obtained for the mafic enclave class, which is  
428 spectrally very similar to the low-quartz monzogranite. Due to the spectral non-distinctiveness  
429 of this class, classifications based on PCA and MNF lead to speckled results that lower the  
430 accuracy ( $A_6=54\%$ ), whereas spatially constrained FE methods are able to discriminate this  
431 class as small but coherent regions ( $A_6=72\%$ ).

## 432 **5. Discussion**

433 The results of the study showed a clear trend on the advantageous usage of feature extraction  
434 and selection for enhanced lithological classification. Data classification without prior FE  
435 showed to return the lowest accuracy of all classification attempts, which supports the theory  
436 on the “curse of dimensionality”. Variations of illumination due to shadow and changing  
437 weather conditions during data acquisition are particularly problematic when applying  
438 classification on datasets without prior FE. Within the classification result these illumination  
439 differences can become visible e.g. as sharp and straight class borders, affecting class  
440 discrimination. This effect can be substantially reduced by prior FE and the rejection of affected  
441 feature bands for classification.

442 The importance of masking spectrally distinct but geologically irrelevant interfering image  
443 parts, such as vegetation or reference targets, prior to FE is apparent. Particularly in cases

444 where spectral differences between lithologies are subtle, those spectrally highly variant  
445 objects would otherwise dominate over geological information in extracted features.

446 The study further showed clear differences in the performance of conventional and spatially  
447 constrained FE approaches. The use of traditional FE algorithms often leads to the  
448 discrimination of smaller objects within larger geological domains. The resulting speckled  
449 appearance mostly originates in spectrally indistinct classes, low SNR or small-scale  
450 illumination variations. Lithological domains, however, aim to be spatially homogeneous, even  
451 if of inhomogeneous mineralogical composition. Spatially constrained FE methods (OTVCA  
452 and WSRRR) yielded geologically more accurate classification results. The ability for spatial  
453 constraining allows to achieve a particularly smooth classification result, while still allowing the  
454 detection of small objects. This is especially advantageous for the detection of spatially small  
455 objects (e.g. mafic enclaves in the LWIR/Naundorf case study), which otherwise are easily  
456 missed due to this “class noise”. On the other hand, smooth classification results by spatially  
457 constrained FE methods can also lead to an overestimation in the size of small objects and  
458 loss of textural detail, in particular within non-continuous, lithologically variable zones.

459 Classifications based on spatially constrained feature extraction methods, however, are not  
460 comparable to a subsequent smoothing of a noisy classification image. Post-processing of the  
461 classification result by filtering, smoothing or segmenting often helps to increase the  
462 classification accuracy, as separated misclassified pixels are replaced by the surrounding true  
463 positives. However, this approach is not able to reconstruct initially false classified areas and  
464 can even cause the extrapolation of errors to larger pixel groups. Secondly, very small objects,  
465 even if correctly classified, might be removed by the smoothing. Spatially constrained feature  
466 extraction methods, in contrast, determine spatially related pixel groups before the  
467 classification is performed. The achieved smoothing is therefore solely data-driven. Small  
468 classified objects have a much higher probability to be of true nature than in spatially non-  
469 constrained FE. This makes spatially constrained feature extraction methods particularly suited  
470 for the classification of scenes with high spatial scale variability, for example for the mapping  
471 of veins, enclaves or clasts in a larger matrix. Similar to this study, where the performance of

472 different feature extraction approaches has been evaluated and compared against each other,  
473 in Rasti et al. (2016) and Rasti et al. (2014), OTVCA and WSRRR were proposed and used,  
474 respectively, and their performances were evaluated for land cover classification. The obtained  
475 results in those previous studies also demonstrate that OTVCA and WSRRR improved the  
476 performance of conventional feature extraction approaches in terms of classification  
477 accuracies for land cover classification in both rural and urban areas.

478 The consistently better accuracy performance of PCA in comparison to MNF in all case studies  
479 can be explained by their respective underlying approach. MNF seeks a projection to minimize  
480 the Gaussian noise and cannot take into account other noise types such as stripping, sparse  
481 noise, and shot noise. PCA, on the other hand, captures the variance of the dataset regardless  
482 of the type of the existing noise. In this context, if the dataset has high SNR, as this is the case  
483 for our datasets, PCA can represent the data into a few informative PCs. In the experiments,  
484 after performing PCA, we selected only the PCs with high SNR and, therefore, the PCs with  
485 lower SNRs which often degrade the classification results have been neglected. This could be  
486 the reason why PCA could outperform MNF in our experiments.

487 In terms of computation time, major differences were observed. The conventional methods,  
488 i.e., PCA and MNF, are non-iterative algorithms and therefore are much faster than the  
489 advanced approaches i.e., WSRRR and OTVCA which are both iterative algorithms. OTVCA  
490 performs slower than WSRRR due to the additional iteration step of the inner TV-optimization.  
491 We should note that the processing time of the advanced method could be improved using  
492 parallel programming which is out of the scope of this paper.

493 Applying FE and classification workflows in geological applications of spectral imaging showed  
494 to pose specific challenges which inhibit standard benchmarking approaches for accuracy  
495 assessment. Major challenges arise from partly inaccurate geological maps and limited  
496 amounts of reliable sample data. Geological maps or field sketches are often not directly  
497 transferable as validation input due to both qualitative and geolocational inaccuracies and  
498 differences in resolution. The latter are a direct consequence of the discrepancy between  
499 objective, centimeter-precise HSI data and subjectively generalized geological observations

500 on a decimeter to regional scale. Validation data with pixel-precision is limited to small  
501 accessible regions. These circumstances lead to either sparse or unconfident definitions of  
502 training and test pixels. We thus recommend the selection of training points based on a mixture  
503 of existing maps, geological experience and spectroscopic knowledge. We could show that by  
504 such careful selection of few, but confident training pixels, geologically sound classification  
505 results can be achieved. The returned classification accuracy figures, however, should be  
506 treated with caution, as they are often spatially unrepresentative and not an appropriate  
507 measure for the evaluation of the geological accuracy of a classified result. The challenges of  
508 the current study further show the need for well-labeled benchmark datasets for geological  
509 targets that would allow to evaluate the performance of innovative methods on a standardized,  
510 comparable basis. It also demonstrates that the rapid acquisition and processing of HS data  
511 can tremendously improve the accuracy of mapping and at the same time improve safety and  
512 decrease the time of field activities.

## 513 **6. Conclusion**

514 We applied a selection of feature extraction methods on three different data sets representing  
515 characteristic scenarios of spectral imaging in geosciences and mineral exploration. The data  
516 sets are real life case studies acquired using innovative spectral imaging approaches such as  
517 UAS-borne or small-angle terrestrial mapping and using sensors operating at different spectral  
518 ranges in the VNIR, SWIR and LWIR. To evaluate the performance of the extracted features  
519 for geoscientific applications, we subsequently applied an SVM classification using sparse  
520 training sets.

521 Our most important findings are:

- 522 1) In all three case studies, the use of machine learning algorithms allowed the  
523 discrimination of mineral domains by overall spatial and spectral differences, which is  
524 particularly advantageous for spectrally similar materials or datasets with low signal-to-  
525 noise.

- 526 2) Geological maps or field sketches are often not directly transferable as validation input  
527 due to generalization, local and qualitative inaccuracies, and a lack of reliable sample  
528 data. Besides the analysis of accuracy figures, additional evaluation of the classification  
529 result by geological expert knowledge is key to ensure scientifically meaningful results.
- 530 3) Applying FE prior to classification improved the classification accuracy and speed  
531 compared to direct classification on the whole dataset.
- 532 4) Innovative FE methods that promote spatial smoothness such as WSRRR and OTVCA  
533 outperformed more traditional FE methods such as PCA or MNF in all case studies.  
534 Beside the higher classification accuracy, the spatially constrained FE classification  
535 results are more accurate from a geological perspective.
- 536 5) While OTVCA was comparably slow, WSRRR showed the best compromise between  
537 classification accuracy and computation time of all methods. Further development and  
538 optimization of the method might allow to further speed up the processing and will be an  
539 important step towards (near-)real-time data processing.
- 540 6) The used methods could be successfully applied to diverse datasets in regards of  
541 spectral range, acquisition mode and data quality. The domain mapping approach using  
542 FE allowed us to extract valuable geological information even from spectrally indistinct  
543 lithologies or from data disturbed by atmospheric interference, low signal or illumination  
544 variations.

545 Our study promotes the use of innovative, spatially constrained FE algorithms for mineral  
546 domain mapping in geoscience and mineral exploration. The algorithms are robust against the  
547 physical content of the input dataset and can therefore be used beyond a specific type of  
548 reflectance data, for example supporting a multi-sensor classification approach.

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643

644 **List of Figure Captions:**

645 *Figure 1. General workflow of hyperspectral data classification with and without prior application of*  
646 *feature extraction methods*

647 *Figure 2. Location of the three study areas as well as coverage of the discussed data sets (indicated by*  
648 *yellow polygons): a) UAS-based VNIR (case study 1), b) terrestrial VNIR-SWIR (case study 2), c)*  
649 *terrestrial LWIR (case study 3)*

650 *Figure 3. Spectral characteristics of the classes defined for each case study area. The displayed*  
651 *spectra are averages of all pixels used for training of each respective class. Spectral artefacts due to*  
652 *sensor gaps and strong atmosphere-related noise are whitened out for better visibility.*

653 *Figure 4. Comparison of the six geologically most relevant feature bands per tested FE algorithm*  
654 *(index indicated by number label), which were selected for subsequent classification (case study:*  
655 *UAS-VNIR).*

656 *Figure 5. Performance of the tested FE algorithms in regards of processing time (in seconds per data*  
657 *pixel) for the extraction of 20 image features per dataset.*

658 *Figure 6. Average performance of SVM classification in terms of accuracy using the tested FE algorithms*  
659 *as well as using no prior FE*

660 *Figure 7. Performance of SVM classification based on different FE approaches for the drone-borne*  
661 *VNIR survey over the Otanmäki ore deposit (Finland). A1-A5 refer to the respective class specific*  
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668