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1 **Sedimentary structure discrimination with hyperspectral imaging in**
2 **sediment cores**

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17

18 **Abstract**

19 Hyperspectral imaging (HSI) is a non-destructive, high-resolution imaging technique that is currently
20 under significant development for analyzing geological areas with remote devices or natural samples
21 in a laboratory. In both cases, the hyperspectral image provides several sedimentary structures that
22 must be separated to temporally and spatially describe the sample. Sediment sequences are composed
23 of successive deposits (strata, homogenite, flood) that are visible depending on sample properties. The
24 classical methods to identify them are time-consuming, have a low spatial resolution (millimeters) and
25 are generally based on naked-eye counting. In this study, we compare several supervised classification
26 algorithms to discriminate sedimentological structures in lake sediments. Instantaneous events in lake
27 sediments are generally linked to extreme geodynamical events (e.g., floods, earthquakes), so their
28 identification and counting are essential to understand long-term fluctuations and improve hazard
29 assessments. Identification and counting are done by reconstructing a chronicle of event layer
30 occurrence, including estimation of deposit thicknesses. Here, we applied two hyperspectral imaging
31 sensors (Visible Near-Infrared, VNIR, 60 μm , 400-1 000 nm; Short Wave Infrared, SWIR, 200 μm , 1 000-
32 2 500 nm) on three sediment cores from different lake systems. We highlight that the SWIR sensor is
33 the optimal one for creating robust classification models with discriminant analyses (prediction
34 accuracies of 0.87-0.98). Indeed, the VNIR sensor is impacted by the surface reliefs and structures that
35 are not in the learning set, which causes mis-classification. These observations are also valid for the
36 combined sensor (VNIR-SWIR) and the RGB images. Several spatial and spectral pre-processing were
37 also compared and enabled one to highlight discriminant information specific to a sample and a sensor.
38 These works show that the combined use of hyperspectral imaging and machine learning improves the
39 characterization of sedimentary structures compared to conventional methods.

40

41 **Keywords:** Hyperspectral Imaging, Machine Learning, Discrimination methods, Visible and Near-
42 Infrared Spectroscopy, Automatic Detection, Sedimentary Deposits

43 **1 Introduction**

44 Natural archives, such as sediment cores, are composed of a succession of deposits, so they record
45 past climate and environment biological-physical-chemical variations. There are two main processes:
46 continuous sedimentation and event layers, and the former can be interrupted by the latter. The
47 continuous sedimentation enables one to create an age-depth model and infer the environment and
48 climate conditions. Event layers, e.g., related to floods (Gaume et al., 2009; Glur et al., 2013), storms
49 (Sabatier et al., 2012), landslides, earthquakes (Wilhelm et al., 2016), tsunamis (Chagué-Goff, 2010),
50 and eruptions, are linked to some of the most damaging disasters in terms of economic and societal
51 losses. Currently, in an overwhelming majority of laboratory studies on natural archives, sedimentary
52 structures are first visually described; subsequently, numerous physical (X-ray imaging, computed
53 tomography scan, grain-size) and chemical (X-ray fluorescence or diffraction, scanning electron
54 microscopy) analyses are undertaken. From those results, the event layers are identified and
55 described. Then, layers with identical characteristics (e.g., color and texture) are usually counted by
56 naked-eye observation. This approach is time-consuming, characterized by a low spatial resolution and
57 subject to high uncertainties due to human interpretation (Lotter and Lemcke, 1999). To overcome
58 these limits, several semi-automatic methods were developed to discriminate these sedimentary
59 deposits from RGB images. The main approaches study the strata from annually laminated sediment
60 to create an age-depth model with their discretization, but they only use a line or a combination of
61 segments, and a deposit is characterized by the detection of the maxima (Meyer et al., 2006; Weber
62 et al., 2010). Similarly, for the automatic detection of event layers, Vanni re et al. (2013) proposed to
63 use a 1/Red signal and threshold. Some studies also used discrimination methods based on labeled
64 pixels to create classification maps, e.g., an adaptive neuro-fuzzy inference system (Ebert and Trauth,
65 2015) or K-nearest neighbor (Ndiaye et al., 2012). Thereby, only the color signal has been investigated,
66 while many other parameters are potentially useful to distinguish event layers, such as the texture,
67 grain size, and chemical composition (Fouinat et al., 2017; Gilli et al., 2013; Wilhelm et al., 2018). A
68 more relevant approach will automatically detect event layers considering all of these parameters.

69 In the current literature, a great number of works focus on the use of hyperspectral imaging (HSI) data
70 for resource management. For instance, in agriculture applications (Teke et al., 2013) several works
71 are focusing on the analysis of (i) environmental stress in crops and associated diseases (Feng et al.,
72 2017), (ii) crops variability (Rubwurm and Korner, 2017), and (iii) soil erosion stages (Chabrilat et al.,
73 2014) among many others. In forestry and environmental management, relevant works care about
74 analyzing the status and health of forests (Shang and Chisholm, 2014), and infestations in plantation
75 forestry (Peerbhay et al., 2015). In geological exploration and mineralogy, HSI data have been used for
76 detection and mapping of mineral deposits (Contreras Acosta et al., 2019; Dumke et al., 2018) or soil
77 composition analysis (Shi and Wang, 2014). HSI is a non-destructive high-resolution laboratory analysis
78 that enables a semi-automatic description of the natural deposits based on their physical-chemical
79 characterization. HSI can improve chemical knowledge by analyzing the sample surface. It has been
80 used to characterize mineralogical fingerprints (Feng et al., 2018; Lorenz et al., 2019; Tusa et al.,
81 2020b), organic matter (Jacq et al., 2019c; Van Exem, 2018), pigments (Butz et al., 2017; Makri et al.,
82 2020; Schneider et al., 2018), and particle size distribution (Jacq et al., 2019b). Some of these studies
83 highlight sedimentary structures with proxy estimation but without spatially characterizing them. To
84 describe these deposits, image or classification approaches were used with hyperspectral remote
85 sensing imaging (Ghamisi et al., 2017; Li et al., 2019). These approaches have been used in the
86 laboratory for mineralogical characterization of rock cores or for the detection of veins from other
87 sensor data that require destructive sampling (Contreras Acosta et al., 2020, 2019; Tusa et al., 2020a,
88 2019). These works employ methods such as random forest (RF) or support vector machine (SVM) to
89 classify each hyperspectral pixel into a dominant mineral class or for a mixture of minerals, they used
90 visible and near-infrared (VNIR), short and long wave infrared (SWIR, LWIR) hyperspectral cameras.
91 These approaches are therefore interesting for the problem of detecting sedimentary deposits, but
92 sediments from aquatic environments are moreover more complex than those from rocks because of
93 the presence of moisture and particles that will interfere in the hyperspectral signal (Verpoorter et al.,
94 2014). To this day, only one study based on lake or marine sediments employs HSI to characterize

95 spatial variations in volcanic tephra layers with a VNIR camera using a supervised classification method
96 based on an artificial neural network and manual non-destructive labeling (Aymerich et al., 2016).

97 As we have just seen, in the literature many hyperspectral image classification methods have been
98 applied on remote sensing, but few to sedimentary images. Therefore, to classify sediments from cores
99 to know their composition, we want to study three supervised classification methods (decision tree
100 DT, random forest RF, and artificial neural network ANN) and three parametric methods (linear and
101 quadratic discriminant analysis LDA/QDA, partial least-square discriminant analysis PLS-DA). These six
102 methods are problematically specific (Khaledian and Miller, 2020). The hyperspectral images used in
103 this study come from a visible and near-infrared camera (VNIR, pixel size: 60 μm) and a shortwave
104 infrared sensor (SWIR, pixel size: 200 μm). The two sensors can also be combined to estimate a VNIR-
105 SWIR composite sensor (pixel size: 200 μm) or reduced to create composite RGB images. Several
106 spectral and spatial pre-processing and compression algorithms were compared. Thus this study
107 proposes to compare numerous approaches (the type of image, pre-processing, and discrimination) to
108 separate and characterize the sedimentary structures of three different samples and provide a
109 simplified methodology for its application to other sites.

110 2 Materials and methods

111 2.1 Sample site descriptions

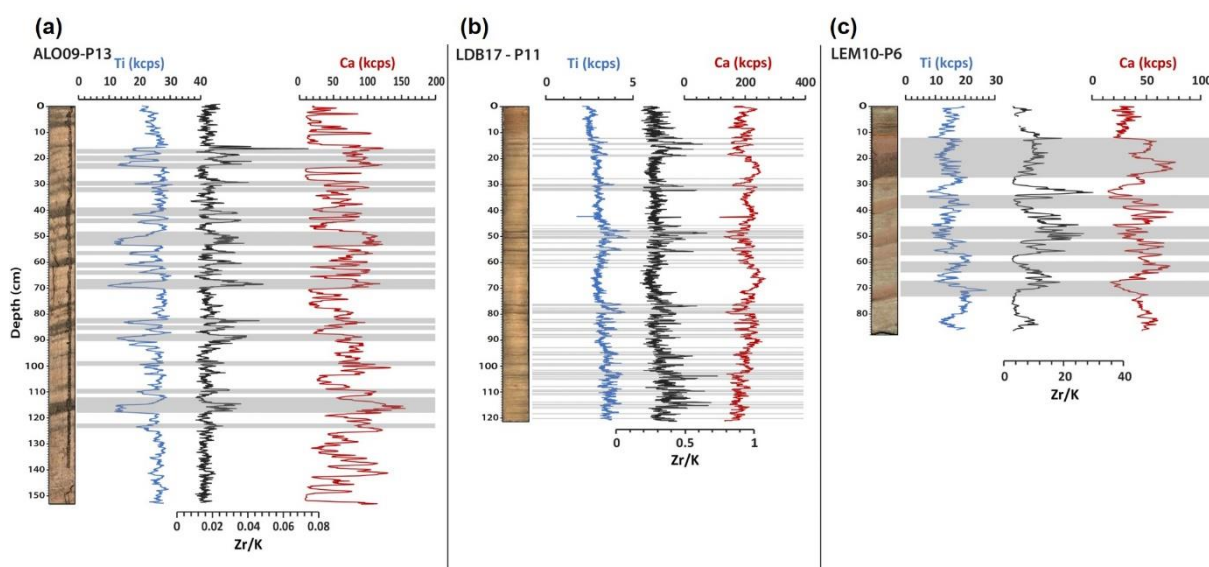


112

113

Figure 1: Locations, tributaries, and effluents of the lakes: (a) Bourget and Geneva, (b) Allos

114 Three sediment cores were selected from three lakes located in the western French Alps (Figure 1) in
115 different watersheds, representing different geological contexts and surface areas that present event
116 layers with different geochemical compositions. The studied cores were retrieved from Lake Allos
117 (ALO09_P13, IGSN: IEFRA08JN, coring year: 2009) (Wilhelm et al., 2015, 2012), the deep basin of Lake
118 Le Bourget (LDB17_P11, coring year: 2017, water inflow: 10.65 m.an⁻¹) (Jenny, 2013; Jenny et al., 2014),
119 and Lake Geneva (LEM10_P6, IGSN: IEFRA008N, coring year: 2010, water inflow: 13.07 m.an⁻¹) (Jenny,
120 2013; Rapuc et al., 2020).



121

122 Figure 2: XRF analysis for Ti, Zr/K, and Ca of the three cores: (a) Allos, (b) Bourget, and (c) Geneva

123 The sediment from the three selected cores was first described and logged after naked-eye
124 observations. When they were present, the event layers were distinguished from the continuous
125 sedimentation by using sedimentological and geochemical results; for these three cores X-ray
126 fluorescence, particle size distribution, and total organic carbon were made.

127 Lake Allos sediment sequence (ALO09_P13) presents two different sedimentary units. The upper part
128 is enriched in organic matter and presents Total Organic Carbon (TOC) values > 1.5% (Wilhelm et al.,
129 2012). The rest of the sequence is composed of light-gray homogeneous silty clay (median = 10 μm),

130 corresponding to the continuous sedimentation, which is interrupted by coarser (median = 40 μm)
131 normally graded beds (Wilhelm et al., 2012). These beds present higher values of dry bulk density,
132 lower TOC values (< 1%), and are enriched in calcium contents (Figure 2). XRF signals also show peaks
133 of Zr/K and low Ti values due to an increase of the grain size at the base of the layers and a depletion
134 in silicate particles, respectively. The graded beds were interpreted as linked to turbidity currents
135 triggered by gravity reworking or flood events (Wilhelm et al., 2012).

136 Lake Bourget sediment sequence (LDB17_P11) presents two main units. The first one (0-10 cm) is
137 laminated with an alternation of white/light-gray and dark-gray/brown laminae. These laminae are
138 mainly composed of diatoms, micrite, organic matter (TOC > 2.5%), and autochthonous calcite with a
139 mean grain size comprise between 15 and 30 μm (Giguet-Covex et al., 2010). The second unit is non-
140 laminated and corresponds to homogeneous light-gray sediment composed of carbonate particles,
141 silts, clays, and a few diatoms. The mean grain size of this unit is almost constant and is comprised
142 between 4 and 9 μm . The organic matter content is under 5% (Giguet-Covex et al., 2010), and
143 carbonate particles represent at least half of the total sediment (Arnaud, 2005). Several darker
144 deposits, enriched in detrital silicate and carbonate particles, interrupted the continuous
145 sedimentation and were interpreted as underflow deposits linked to flood events (Giguet-Covex et al.,
146 2010; Jenny et al., 2014). These deposits present peaks of Ti and Zr/K signals at their base (Figure 2),
147 which support the higher detrital content and the increase of grain size within these layers.

148 Like the two other sediment sequences, the Lake Geneva sequence (LEM10_P6) presents two principal
149 sedimentary units. The upper laminated unit corresponds to an alternation of light and dark-gray
150 laminae, enriched in organic matter (TOC values > 5%; (Jenny, 2013)). This unit is followed by
151 homogeneous light-gray silty clay identified as a non-laminated unit (Jenny, 2013), which presents
152 lower organic content (TOC values < 2%) and higher values of calcium (Figure 2). The mean grain size
153 of these two units is higher (> 25 μm) than Lake Bourget sediment sequence values. The lower unit is
154 interrupted by thick and coarse graded beds that show peaks of Zr/K, and higher values of Ti (Figure 2)

155 are linked to increased detrital silicates compared to the continuous sedimentation. These deposits
156 present similarities with those observed in the two other sequences and were interpreted as flood
157 layers.

158 Once clearly identified, those layers were visually counted. The data sets will be referred to using the
159 name of the lake, but it must be understood that there may be differences (color, chemical, physical)
160 among different sequences from the same lake.

161 2.2 VNIR and SWIR hyperspectral image acquisition

162 Two hyperspectral reflectance cameras were used to analyze these cores at the UMR CNRS M2C lab
163 facilities, University of Normandie-Rouen (France). They cover two consecutive spectral ranges: 400-1
164 000 nm (visible and near-infrared, Specim VNIR PFD OLE23) and 968-2 574 nm (shortwave infrared,
165 Specim SWIR OLES22.5). They have a theoretical spatial pixel size of 60 μm and 200 μm , respectively.
166 The real resolution may vary due to surface roughness. Relevant data were obtained with a flattening
167 and a cleaning of the core to have a plane surface that revealed sediment structures (Butz et al., 2015;
168 Jacq et al., 2020). Then, the camera was calibrated with a spectral acquisition on a reference, as the
169 image of a known object has squared pixels (true shape) and relevant reflectance intensities (color and
170 signal-to-noise ratio).

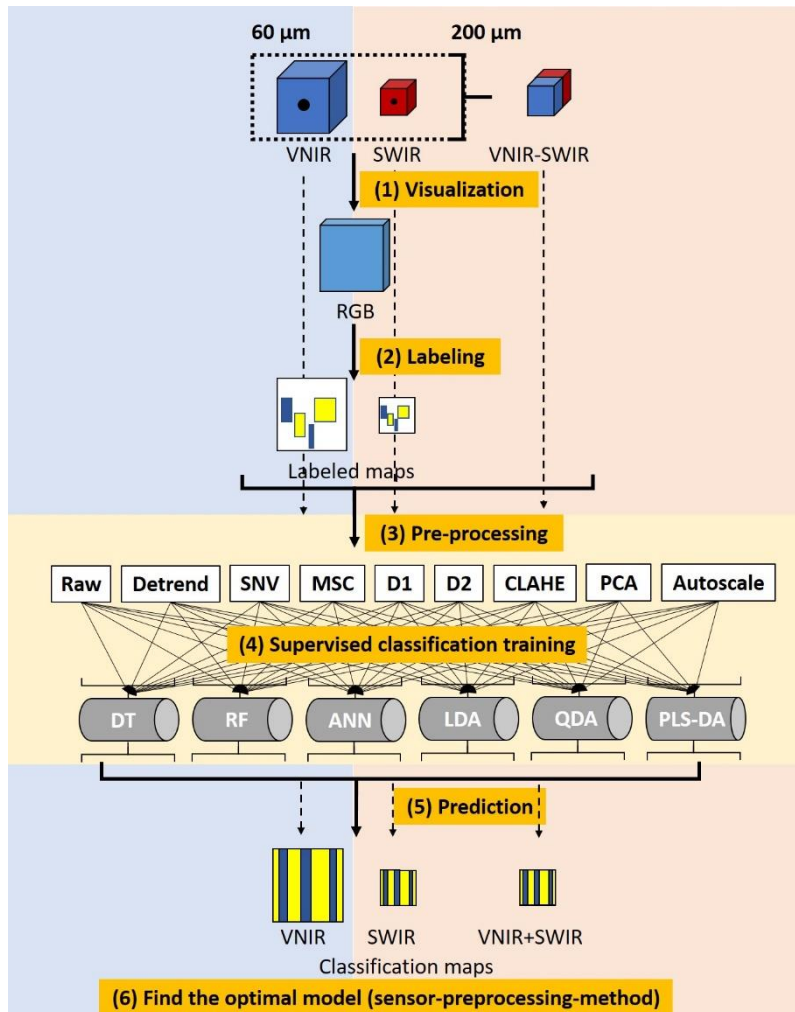
171 The resolution of the two datasets (VNIR and SWIR) was also homogenized at a common spatial
172 resolution of 200 μm to obtain a VNIR-SWIR composite sensor. The two hyperspectral images were
173 combined into a unique one (i.e., VNIR-SWIR) with image registration (Liu et al., 2011) adapted to HSI
174 on a wavelength plane characteristic of a similar chemical compound. In previous work, we found that
175 the 970 nm (VNIR) and 1 200 nm (SWIR) wavelengths were optimal for combining (Jacq et al., 2019a).
176 They are related to hydroxyl chemical bonds mostly associated with moisture in sediment cores (Bull,
177 1991; Viscarra Rossel and Behrens, 2010). Therefore, a composite sensor was created to merge the
178 VNIR and SWIR datasets to cover the range of 400-2 500 nm. No reflectance adjustment was used to
179 correct for shifts in the spectral overlap range between the two sensors. In this study, we compare the

180 classification performances of three datasets: VNIR at a spatial resolution of 60 μm , SWIR at a
181 resolution of 200 μm , and VNIR-SWIR at a resolution of 200 μm .

182 Pre-processing can be used to correct the data from noise or aberrant values and highlight discriminant
183 wavelengths. The three dimensions of the HSI, spectral, and spatial pre-processing procedures can be
184 used (Rinnan et al., 2009; Vidal and Amigo, 2012). The spectral pre-processing procedures compared
185 in this study are normalization (autoscale), linear baseline correction (detrrend), scattering effect
186 correction (Standard Normal Variate (SNV) and Multiplicative Scatter Correction (MSC)) (Barnes et al.,
187 1989), and Savitzky-Golay first and second derivatives (D1 and D2) (Savitzky and Golay, 1964). The
188 derivatives use second-order polynomial fitting and a window of 7 and 13 wavelengths for the first and
189 second derivatives respectively. Principal component analysis (PCA) was also used as a compression
190 of the spectral dimension (Pearson, 1901). Contrast limited adaptive histogram equalization (CLAHE)
191 was used on the spatial dimensions with an estimation based on the grayscale image levels and applied
192 to each image wavelength (Zuiderveld, 1994). Thus, nine datasets per sensor were used for training in
193 an independent way.

194 2.3 Data Analysis

195 Six commonly used machine learning algorithms were used to create classification models with three
196 types of spectral data (VNIR, SWIR, and VNIR-SWIR) (Figure 3). First, an RGB image was made from the
197 VNIR HSI to visually and manually label continuous sedimentation and event layer pixels by an expert.
198 Then, machine learning methods were used to construct discrimination models. In addition, nine pre-
199 processing procedures (spatial and spectral) were used and compared with raw data. Consequently,
200 162 discriminations models were created for each sample to find the optimal sensor (of three), method
201 (of six), and pre-processing procedure (of nine) as presented in Figure 3.



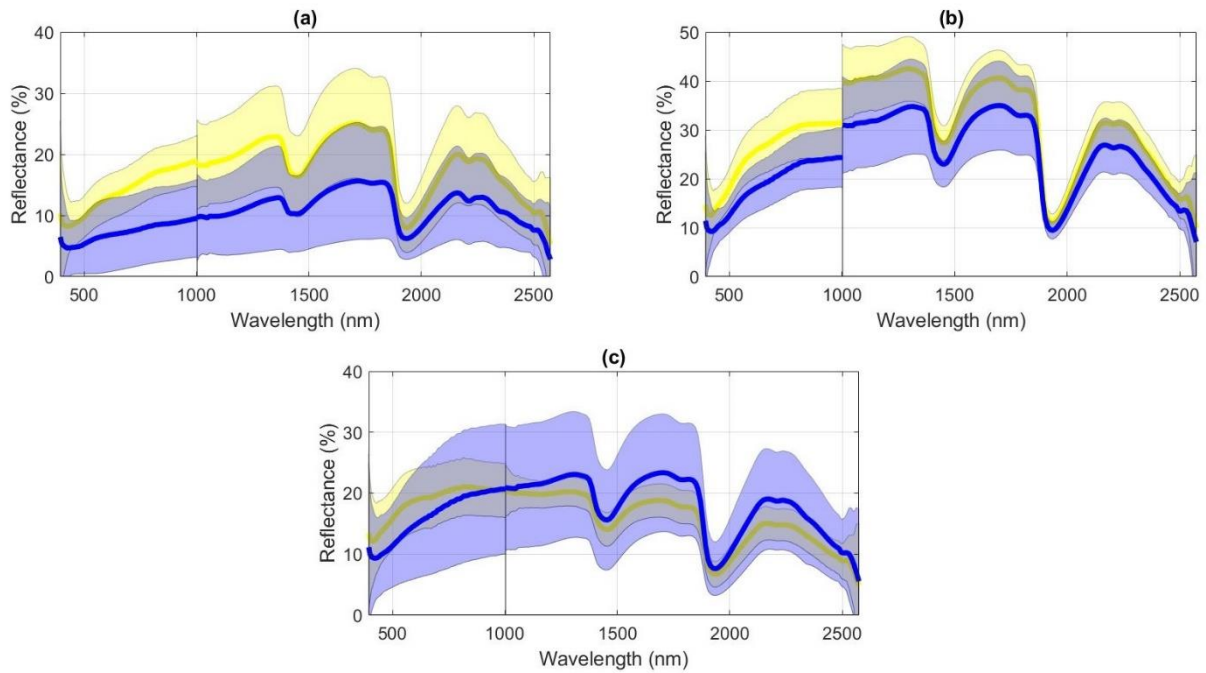
202

203 Figure 3: Data processing to create a classification model to predict each pixel: (1) Visualization with RGB images at both
 204 resolutions; (2) Manual labeling of the image; (3) Data pre-processing and (4) Creation of supervised classification models
 205 for each dataset (DT: Decision Tree, RF: Random Forest, ANN: Artificial Neural Network, LDA: Linear Discriminant Analysis,
 206 QDA: Quadratic Discriminant Analysis, PLS-DA: Partial Least Squares Discriminant Analysis); (5) Prediction for each image;
 207 (6) Estimation of the optimal model depending on the sensor, pre-processing procedure, and discrimination model

208 **2.3.1 Data labeling**

209 Hyperspectral VNIR data can be reduced to three planes that correspond to a Red-Green-Blue image
 210 from the VNIR sensor (611-549-464 nm, according to the RGB standard) (CIE, 1999). The RGB images
 211 are representation modes adapted for naked-eye assessment and were used to visualize the sample
 212 to label the sedimentary structures. Thus, the user must manually select rectangular areas that
 213 correspond to the different studied classes based on the known deposits characterized by

214 geochemical, textural, and mineralogical analysis. The resulting maps were used as a mask with 0
215 values for non-labeled pixels and other values for labeled pixels (1: event layer, 2: continuous
216 sedimentation). It was also used to extract the labeled pixels and their corresponding spectrum (Figure
217 4). For the SWIR dataset, these maps were also made with VNIR data at 60 μm and resized at 200 μm .



218
219 Figure 4: Spectral variations of labelled pixels for each class (blue = event layers; yellow = continuous sedimentation) and for
220 the three cores: (a) Allos, (b) Bourget and (c) Geneva. The reflectance of the sediments depends on the specific sedimentary
221 properties of the sites studied. It seems difficult to visually estimate specific discriminating spectral areas of the two classes
222 studied, therefore statistical approaches will allow to find the discriminating variations

223 2.3.2 Classification modeling

224 Several methods commonly used in the literature were chosen for comparison because there is no
225 universal method (Khaledian and Miller, 2020). Six methods were used to create a supervised
226 classification model to discriminate the two sedimentary processes (Figure 5, Supplementary table 1).
227 Decision trees are a rule-based approach to classification and regression problems (Breiman et al.,
228 1984). They use the values in each feature to split the dataset to a point where all data points that

229 have the same class are grouped together. A tall tree with multiple splits generates better
230 classifications.

231 The random forest is a classification algorithm consisting of many decisions trees (Ho, 1995). It uses
232 bagging and features randomness when building each individual tree to try to create an uncorrelated
233 forest of tree whose prediction by committee is more accurate than that of any individual tree.

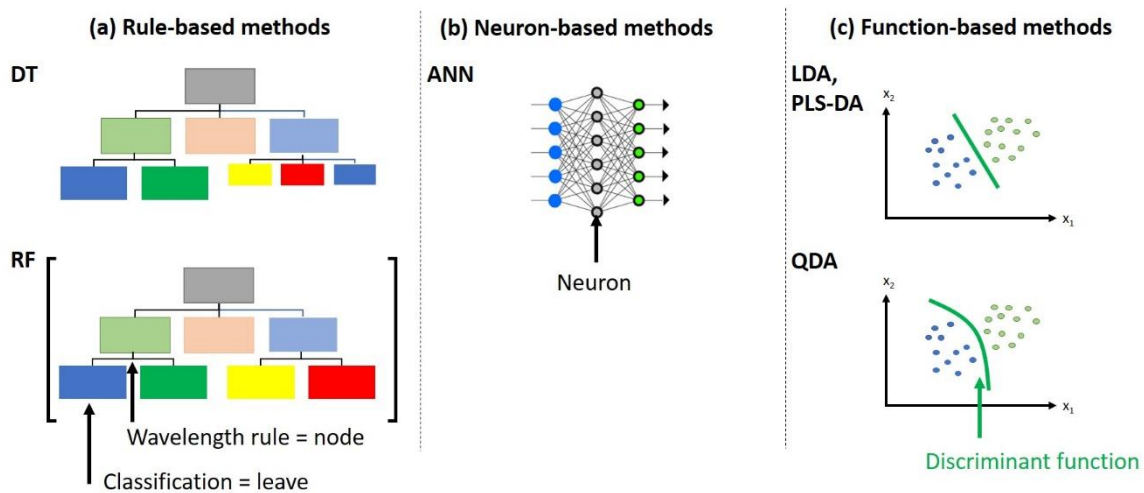
234 ANN is a set of connected input-output network in which weight is associated with each connection
235 (Ivakhnenko and Lapa, 1965; McCulloch and Pitts, 1943; Rosenblatt, 1958). It consists of one input
236 layer, one or more intermediate layers, and one output layer. Learning of neural network is
237 performed by adjusting the weight of connection. By updating the weight iteratively performance of
238 the network is improved. During training, the interconnection weights are optimized until the
239 network reaches the specified level of accuracy. It has many advantages like parallelism, less affected
240 with noise, good learning ability

241 Linear discriminant analysis (LDA) is a straightforward method applying the generative approach for
242 classification (Fisher, 1936). It is based on the assumption that each class can be modeled by a
243 Gaussian distribution and that all the classes share the same covariance matrix. In practice, LDA
244 requires few computations to estimate the classifier parameters that amount to computing
245 percentages and means, plus a matrix inversion.

246 Quadratic discriminant analysis (QDA) is similar to LDA but without the assumption that the classes
247 share the same covariance matrix, i.e., each class has its own covariance matrix (Fisher, 1936). In this
248 case, the boundary between classes is a quadratic surface instead of a hyperplane.

249 Partial least squares-discriminant analysis (PLS-DA) is a versatile algorithm that is used for predictive
250 and descriptive modeling as well as for discriminative variable selection (Wold et al., 1984). However,
251 versatility needs to optimize a wealth of parameters before reaching reliable and valid outcomes.

252 Khaledian and Miller (2020) propose to consider different properties to define the optimal approach
 253 to answer the problem. These methods are based on common or specific assumptions as presented
 254 briefly above. Some require a large amount of data, such as ANN, while others are less sensitive to
 255 sample size. The computation time is also related to the amount of data, as well as to the complexity
 256 of the problem, the number of iterations, and the adjustments. Some are easily interpretable (DT, LDA,
 257 QDA, PLS-DA), or complex (RF, ANN with few neurons), and some are "black boxes" (ANN with many
 258 neurons). Here we use the ANN with few neurons to prioritize the spectral interpretability. Some
 259 require the user to define hyperparameters that are presented in Supplementary table 1. Thus, these
 260 different methods were chosen to see the effect of these properties on the different datasets (sensors,
 261 pre-processing) in predicting the two sedimentary deposit types for the three different sites.



262

263 Figure 5: Schematic representation of the machine learning methods used in this study depending on their basis: (a) rules;
 264 (b) neurons; and (c) functions

265 The models were fitted with a randomly selected 70% of the data during calibration, and the remaining
 266 data were used in the test set (Supplementary table 2). This ratio was applied to the class with fewer
 267 labeled pixels to have a consistent number in each group in the calibration step. The same calibration
 268 and test sets were used for each classification method, but they were different for each pre-processing
 269 procedure. The labeled pixel number depends on the ability of the user to precisely see the deposits;
 270 then, only pixels that certainly belong to these classes are labeled to avoid introducing uncertainty by

271 uncertain labeling. Due to the compression of the labeled high-resolution map, the pixels of the
272 contours may have been removed as being uncertain, which slightly changes the labeling percentages
273 between the two resolutions. That change explains the difference between the cores with labeled
274 pixels of between 0.45% and 15.71% for one class. It also allows visualization of the learning capacity
275 depending on the number of calibration pixels. 5% of the Allos lake image was labeled, against 1.1%
276 for the Bourget lake or 16% for the Geneva lake.

277 2.3.3 Quantitative and qualitative assessments of model classification

278 The quantitative performances of the classification models were estimated by the overall accuracy,
279 precision and recall in calibration and prediction:

$$280 \text{ Accuracy} = \frac{\text{True positive} + \text{True negative}}{\text{True positive} + \text{True negative} + \text{False positive} + \text{False negative}} \quad (1)$$

$$281 \text{ Precision} = \frac{\text{True positive}}{\text{False positive} + \text{True positive}} \quad (2)$$

$$282 \text{ Recall} = \frac{\text{True positive}}{\text{False negative} + \text{True positive}} \quad (3)$$

283 Given a classifier and an instance, there are four possible outcomes. If the instance is positive and it is
284 classified as positive, it is counted as a “true positive”; if it is classified as negative, it is counted as a
285 “false negative”. If the instance is negative and it is classified as negative, it is counted as a “true
286 negative”; if it is classified as positive, it is counted as a “false positive”.

287 The overall accuracy is the proportion of correct predictions (both “true positives” and “true
288 negatives”) among the total number of cases examined. The precision corresponds to the fraction of
289 first class correct predictions (only “true positives”) among the retrieved first class. The recall is the
290 fraction of relevant first-class predictions that were retrieved. Thus, a value closer to 1 indicates
291 better predictive ability.

292 Once a model is considered relevant, it is used on each pixel of the hyperspectral image to classify
293 them and estimate a classification map. An expert must then visually and qualitatively evaluate its

294 spatial coherence, using the different successive deposits and its noise level. Hence, a qualitative index
295 with values between 0 and 5 (arbitrary) is used. A value of 0 corresponds to an irrelevant classification
296 map induced by a model that cannot generalize (under or over-fitting); a value of 5 shows globally
297 relevant classifications on the whole image; whereas a value in this interval indicates more or less
298 relevant predictions but with defects (noise, mispredicted deposits). Moreover, it is important to
299 understand the models on the importance they give to different wavelengths. Complex models like RF
300 and neural networks with a large number of neurons are not easily interpretable.

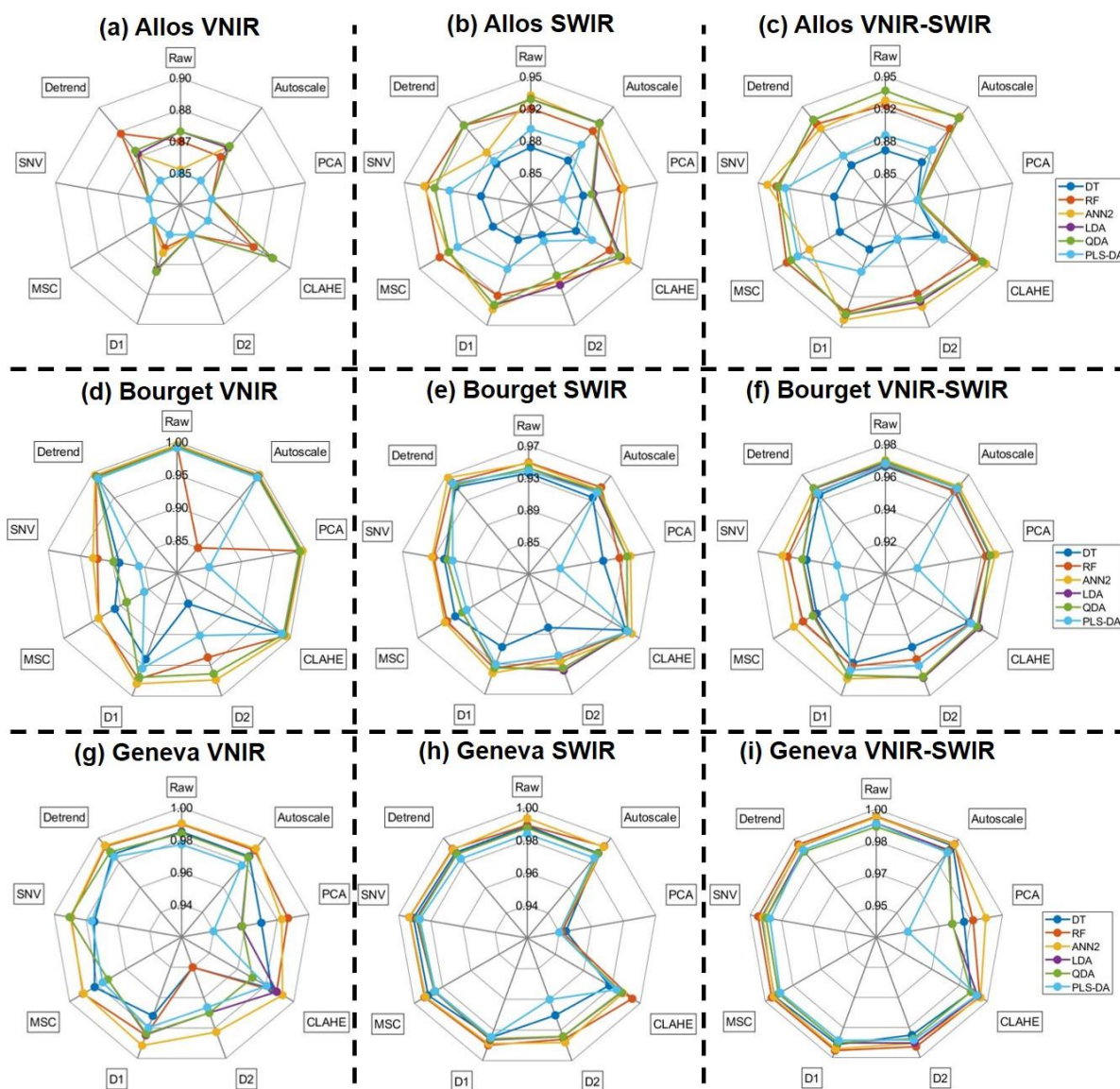
301 **3 Results and interpretations**

302 **3.1 Comparison of the classification methods and pre-processing procedures**

303 Nine pre-processing procedures were tested on each sample, each sensor, and each discrimination
304 method to find the optimal combination (Figure 6). As shown in Figure 4, the spectra of the two classes
305 overlap partially or totally, so the pre-processing step must highlight the wavelengths with
306 discriminating variations to create performant and robust models. PCA and second derivatives (D2)
307 had the lowest prediction accuracies for each sensor and sample (Figure 6). The PCA reduction may
308 not maintain the discriminant information in the main PCs and D2. Raw, CLAHE, autoscaled, and
309 detrended data had the highest discriminant properties in all cases (Figure 6). Some pre-processing
310 procedures are sensor-dependent, such as SNV and MSC, which presented low accuracy for the VNIR
311 sensor and high accuracy for the SWIR sensor. The first derivative (D1) had intermediate accuracy for
312 all cases except for the SWIR sensor and Allos sample, for which good performances were obtained.

313 Among the discriminant methods, DT had the lowest prediction accuracy in most cases, whereas ANN,
314 QDA, and RF had the highest accuracy. For the ANN, few neurons (2-3) appeared to be better than
315 more neurons. The latter has many more parameters and may overfit the small amount of training
316 data, which limits its generalization capability on the test set. The accuracies of the optimal methods
317 are close and must be discussed with all quantitative values and interpretations of their discriminant

318 spectral properties. It is important to consider that the results are sample- and site-specific.



319
 320 Figure 6: Radar charts of the impact of pre-processing on the overall prediction accuracy of each classification method and
 321 lake core hyperspectral image (a-c: Lake Allos; d-f: Lake Bourget; g-i: Lake Geneva; a, d, g: VNIR sensor; b, e, h:
 322 c, f, i: VNIR-SWIR sensor)

323 3.2 Optimal models for each image type

324 The calibration and prediction accuracies, precisions and recalls of the optimal models were higher
 325 than 0.8 and mainly 0.9, which highlights the presence of spectral discriminant information in both
 326 sensors (Table 1, Supplementary table 3Supplementary table 5). Nevertheless, it also highlights that
 327 the best discriminant capacity derived from the SWIR sensor and therefore the VNIR sensor does not

328 contain as much discriminating information. The combination of the two sensors, which should present
 329 a better discriminant capacity through the greater amount of spectral information, presents an
 330 intermediate discriminant ability. Thus, the predictions are certainly biased by some VNIR data
 331 variations.

332 Among all the models developed, some observations have been made (Supplementary table 3-
 333 Supplementary table 5). ANNs with two neurons are often the optimal discriminant method based on
 334 the prediction accuracy and parsimonious because adding neurons does not improve the accuracy.
 335 However, for the qualitative index, discriminant analysis methods (LDA, QDA, PLS-DA) generally had
 336 the best performance levels. The computation time is lower for the LDA, PLS-DA, and DT methods, and
 337 all of these methods are fast to compute, so the computation time was not used to select the optimal
 338 model. It is also more important when there is more data to learn which is the case for the Allos section
 339 compared to the others. Based on a compromise between these two first properties (quantitative and
 340 qualitative index), the optimal methods in most cases were LDA or PLS-DA. Table 1 highlights an
 341 optimal pre-processing procedure that mainly depends on the sample. The discrimination methods
 342 appear to have had a low impact on it, which suggests that an optimal pre-processing procedure can
 343 highlight the discriminant wavelengths.

344 Table 1: Optimal models for each sample and based on the parameters indicating their performance and robustness

345

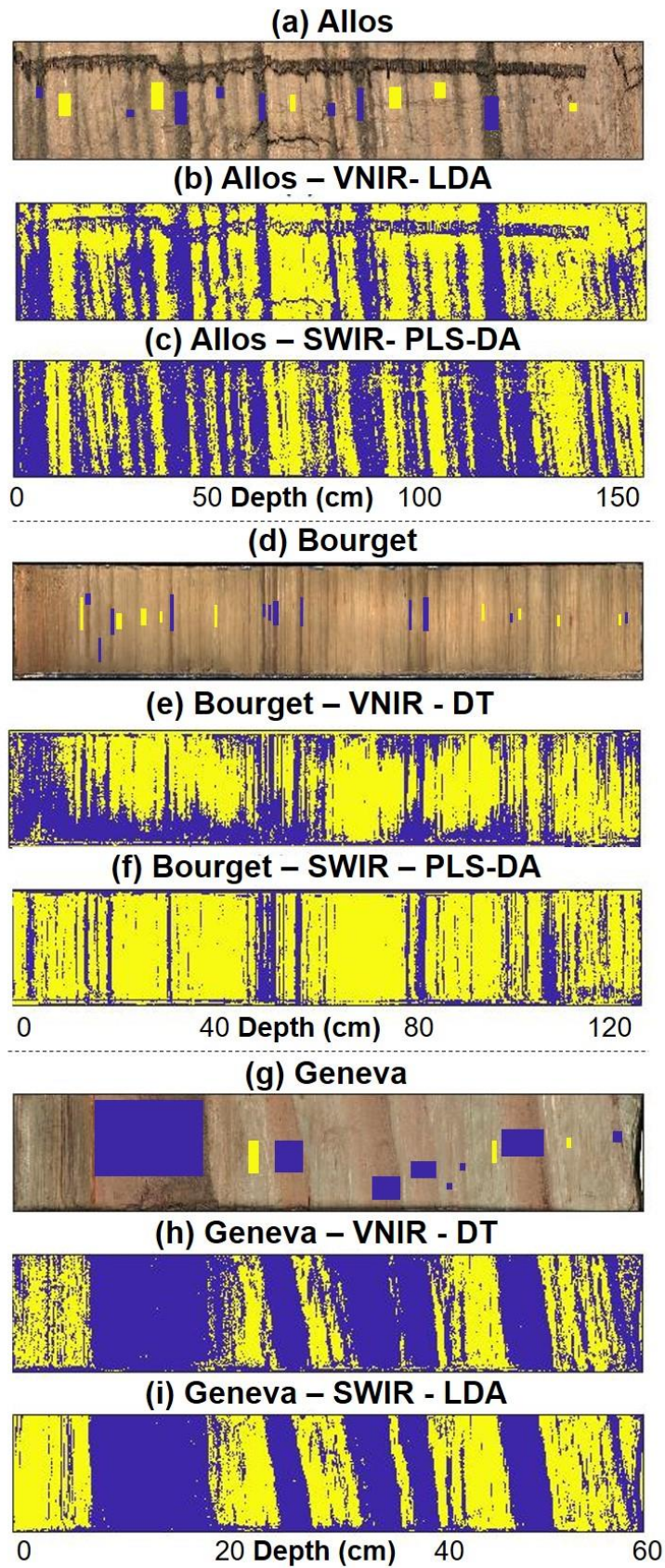
Site	Allos	Bourget	Geneva
Sensor	SWIR	SWIR	SWIR
Method	PLS-DA	PLS-DA	LDA
Processing	SNV	Detrend	SNV
Accuracy _{cal}	0.900	0.969	0.992
Precision _{cal}	0.908	0.988	0.996

Recall _{cal}	0.890	0.951	0.989
Accuracy _{pred}	0.902	0.958	0.989
Precision _{pred}	0.785	0.996	1.000
Recall _{pred}	0.885	0.949	0.989
Qualitative	5	5	5
Computation time (s)	0.800	0.219	0.113

346

347 The classification map comparison of the optimal and worst models highlights that the VNIR sensor is
348 more sensitive to surface reliefs, as observed in Figure 7.a-b with fissures and holes due to sampling
349 or Figure 7.d-e with shadows. Darker laminated areas are noticeable on the Bourget and Geneva
350 sediment sections (on the left of the picture), which were not initially labeled because of the non-
351 possibility of precisely labeling the two classes. In these areas, the VNIR sensor predicted that most of
352 the pixels in the event layer class might be due to the similar color with this class. In contrast, the SWIR
353 data correctly predicted the two groups due to the additional spectral discriminant information. For
354 the Allos sediment section (Figure 7.a-c), the event layers are easily distinguishable from the
355 continuous sedimentation due to their darker colors. However, there is also a color gradient linked to
356 a grain size gradient that is spectrally registered in the SWIR range (Jacq et al., 2019b), which explains
357 the wider layers estimated from the SWIR data than from the VNIR data, and the lightest layers are
358 not visible with the VNIR data.

359 All of these observations and the quantitative validation are consistent with the greatest discriminant
360 capacities being associated with the SWIR sensor for separating event layers from continuous
361 sedimentation. Thus, the combination of the two sensors is not better, as we expected due to the VNIR
362 data sensitivity to surface roughness, and the combination will not be used further.



363

364

Figure 7: Optimal (c, f, i) and worst (b, e, h) models for each sediment core sample (a, b, c: Allos; d, e, f: Bourget; h, i, j:

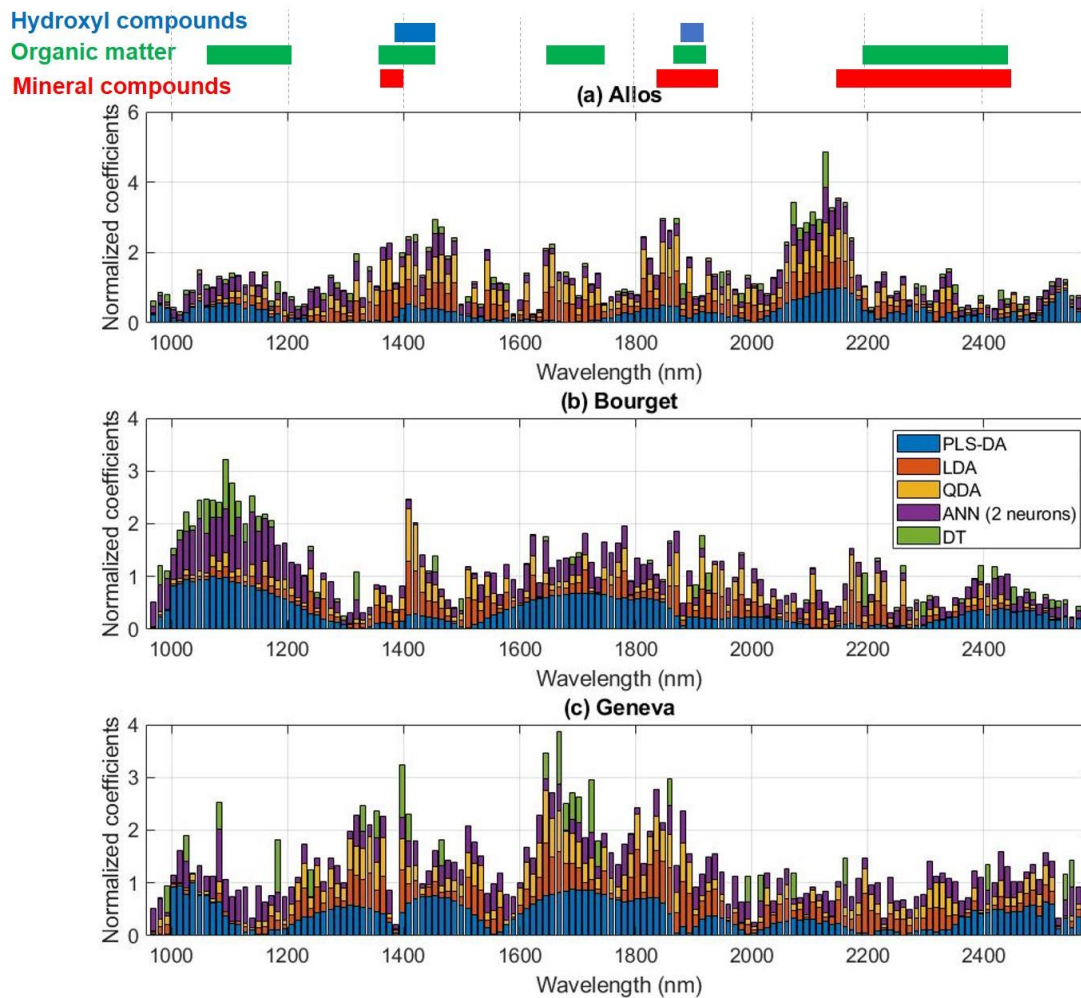
365

Geneva) and labeled areas (blue = event layers; yellow = continuous sedimentation)

366 3.3 Spectral signatures

367 Figure 4 shows the spectra corresponding to the two classes. For lakes Allos and Bourget, both classes
368 partially overlap, and the event layers show a lower reflectance that can be due to a darker color of
369 the layers. The overlap is more important for Lake Geneva. The color of the sediment is obviously
370 dependent on the sedimentary properties that are specific to the study sites. It is therefore difficult to
371 visually estimate discriminating spectral areas.

372 The different statistical approaches used will allow to estimate automatically the spectral areas
373 allowing to separate the two classes. The estimation of SWIR wavelength cumulative occurrence allows
374 to identify the discriminant wavelengths and to characterize them (Figure 8). It is interesting to observe
375 that the five approaches discussed in this figure show similar discriminating spectral areas, which
376 indicates that despite their differences they can adapt to the problematic. Five main discriminant
377 spectral areas present high cumulative values and can be associated with chemical properties. Organic
378 components can be related to spectral wavelengths between (1) 1 050-1 200 nm and (2) 1 650-1 750
379 nm (Cloutis, 1989; Viscarra Rossel and Behrens, 2010). The three others correspond to spectral ranges
380 with possible overlaps: (3-4) organic compounds and hydroxyl bonds (moisture, organic matter or
381 mineral) between 1 350-1 500 nm and 1 800-1 950 nm, and (5) mineral (clay) and organic compounds
382 between 2 150-2 300 nm (Krupnik and Khan, 2019; Verpoorter et al., 2014; Viscarra Rossel and
383 Behrens, 2010).



384

385 Figure 8: Comparison of the normalized coefficients (coefficient weights normalized to one for each method) used by the
 386 optimal SWIR models to highlight the discriminant wavelengths: (a) Allos, (b) Bourget, and (c) Geneva samples

387 The three optimal core models use similar discriminant wavelengths but have different importance
 388 depending on the sediment properties. The two hydroxyl bond spectral areas have important
 389 implications in the three models and could be due to interstitial moisture that may be associated with
 390 coarser particles present in the event layers. The model estimated for Lake Allos highlights another
 391 spectral area characteristic of clays (2 150-2 200 nm) associated with continuous sedimentation.
 392 Whereas Lake Bourget and Lake Geneva models use specific areas of organic matter (1 050-1 150 nm,
 393 1 350-1 400 nm, 1 650-1 750 nm) due to higher organic matter concentration in both sediment
 394 sequences. Thus we can see that the SWIR sensor allows to highlight several sedimentary properties

395 that can differentiate the two types of deposits. It should be noted that the sedimentary properties
 396 highlighted differ and are dependent on the studied site.

397 4 Discussion

398 4.1 Generalization of the model on the other sites

399 Optimal SWIR models developed on each core were used to produce the classification maps of the
 400 other cores and to observe the model generalization capability. Table 2 and Supplementary figure 1
 401 show the results of these classifications with the test accuracies and qualitative indicators. Most of the
 402 models agree on the difficulty of generalizing the model to other cores, which is explained by the
 403 differences in reflectance and thus in sediment composition of the sediment sequences as shown in
 404 Figure 4. As the continuous sedimentation of Lake Bourget and Lake Geneva is more organic than the
 405 one of Lake Allos, or the granulometry and interstitial humidity allowing to trace textural changes in
 406 the event deposits that are more significant for Lake Allos than the other. Unfortunately, mineralogical
 407 changes (silicates and carbonates) do not show marked absorptions in the spectral domains studied.
 408 Only the model developed with the Bourget data could estimate the classification maps for the other
 409 cores, possibly since it has less spectrally localized discriminant wavelengths than the other two models
 410 (Allos: 2 100-2 200 nm; Geneva: 1 650-1 700 nm).

411 Table 2: Comparison of site-specific models for the generalization to the other cores

		Samples			
		Allos	Bourget	Geneva	
Models	Allos	Accuracy _{pred}		0.367	0.043
		Qualitative		0	0
	Bourget	Accuracy _{pred}	0.973		0.365

		Qualitative	3		1
	Geneva	Accuracy _{pred}	0.433	0.644	
		Qualitative	0	0	

412 Based on these results, the estimation of a classification model is sample-specific. It can be made with
413 a linear discriminant method such as LDA or PLS-DA with the raw SWIR dataset, even if some
414 pretreatment slightly improves the performance.

415 4.2 Event layer classification with classical images

416 The true RGB image can also be converted into HSV (Hue, Saturation, Lightness) or L*a*b* (lightness,
417 color) color spaces and reduced to a grayscale level. The HSV and L*a*b* transformations have been
418 proven to be more adaptable for classification purposes (Bora et al., 2015; Hernández-Hernández et
419 al., 2016). The grayscale levels are the most straightforward color space.

420 Table 3 and Supplementary figure 2 show that the conventional image presents slightly lower
421 performances with the VNIR data and has the same mispredictions in terms of surface variations,
422 shadows, and laminated areas (Supplementary table 3). All of these observations highlight that these
423 methods learn the color of the deposits too well with VNIR data and do not learn enough from the
424 chemical composition. Then, machine learning and a conventional image can be used in the case of a
425 clean image and sample with only color differences between the classes and learning of all types of
426 sample events and defects.

427 Table 3: Comparison of the conventional image discriminant models with the optimal predictions being estimated by the
428 hyperspectral images

Sample	Performance	Grayscale	RGB	HSV	L*a*b*	VNIR HSI	SWIR HSI	
Allos	Method	ANN – 2 neurons					PLS-DA	

	Accuracy _{cal}	0.966	0.821	0.817	0.821	0.889	0.900
	Accuracy _{pred}	0.963	0.824	0.808	0.823	0.890	0.902
	Qualitative	4	4	4	4	3	5
Bourget	Method	ANN – 2 neurons				RF	PLS-DA
	Accuracy _{cal}	0.995	0.903	0.904	0.906	0.996	0.969
	Accuracy _{pred}	0.994	0.898	0.899	0.903	0.995	0.958
	Qualitative	2	2	2	2	3	5
Geneva	Method	ANN – 2 neurons				LDA	LDA
	Accuracy _{cal}	0.911	0.976	0.976	0.975	0.987	0.992
	Accuracy _{pred}	0.884	0.979	0.983	0.982	0.989	0.989
	Qualitative	1	2	2	2	4	5

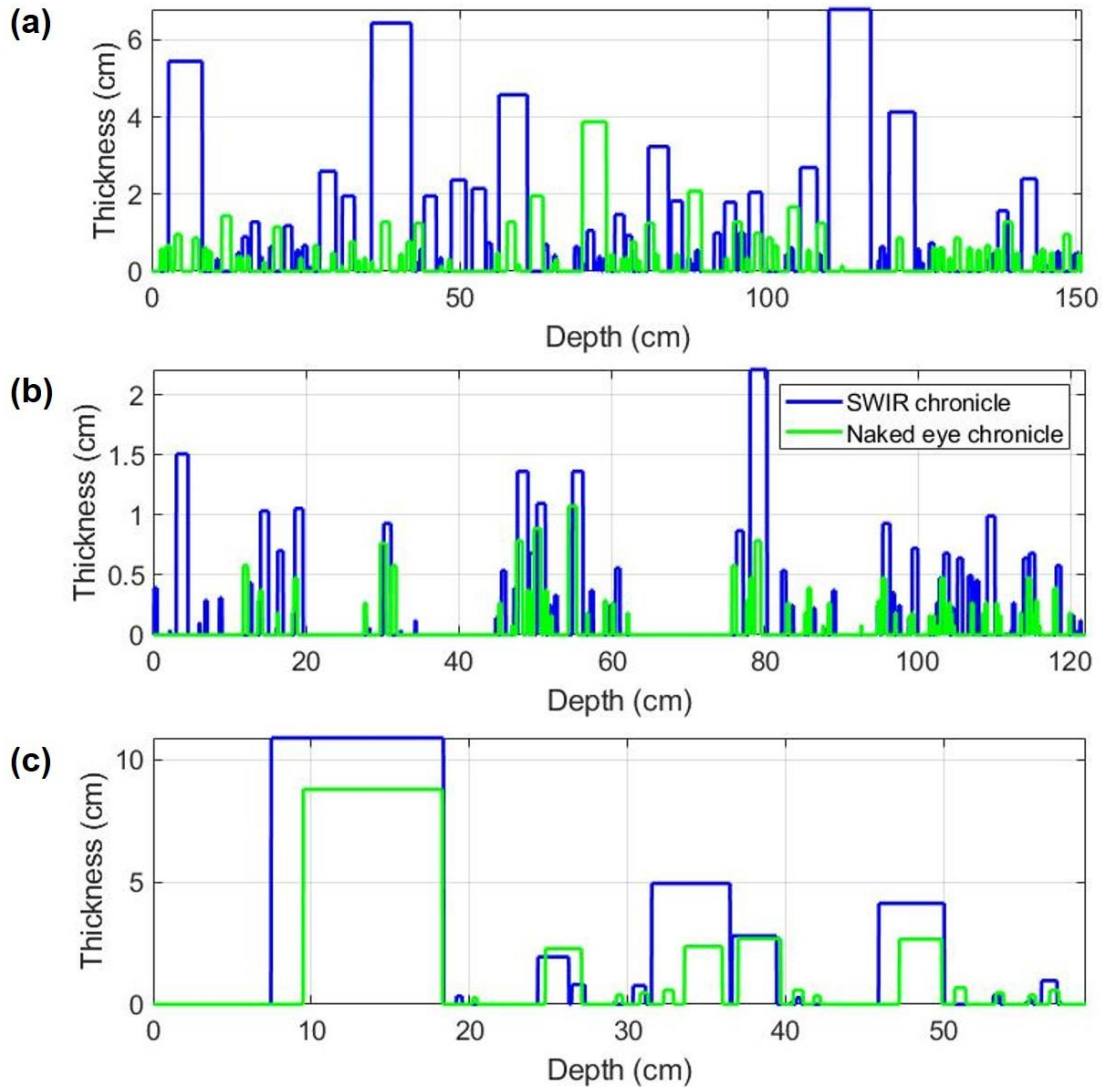
429 4.3 Comparison between HSI and naked-eye chronicles

430 The discretization of the event layers allows for estimation of event layer occurrence along the
431 sediment section and comparison of the event layers with naked-eye event chronicle. The classification
432 map was reduced to a summed profile, with pixels equal to 0 for continuous sedimentation and 1 for
433 an event layer. We assume that the deposits are parallel; if this is not the case, image processing must
434 be used to correct the deformation when possible. This profile can also be used as an event occurrence
435 probability with normalization by the image width in pixels. It was smoothed with a second-order
436 polynomial Savitzky-Golay filter to reduce misclassifications (Savitzky and Golay, 1964). A low
437 threshold (below 20%) allows the separation of all deposits but also the discovery of some artifacts,
438 and the boundaries can be overestimated due to curvatures. Conversely, a high threshold (above 70%)
439 only finds the large deposits, but close ones can be fused. Thus, a double threshold was used. First,

440 using the half-width of the image to classify each column to one class allowed discovery of the most
441 relevant deposits, but close layers could be observed as a large one. The second threshold of 15% of
442 the image width was used for event layers thicker than 5 mm to potentially divide them. Finally, the
443 chronicle can be reconstructed with the depth and thickness of each event layer. Naked-eye chronicles
444 of the three cores were estimated and can be compared with the hyperspectral ones (Jenny et al.,
445 2014; Rapuc et al., 2020; Wilhelm et al., 2012).

446 Figure 9 compares the identification of event layers in terms of depth and thickness between the HSI
447 and naked-eye approaches. In general, HSI results in thicker event layers than naked-eye observations.
448 This result can be explained by the limited ability of the eyes to characterize the event limits (resolution
449 grain) or its curvature (misidentification). Machine learning also enables one to identify new deposits
450 that were not visually detected (due to their small thickness or texture or color differences). They must
451 be assessed by other high-resolution techniques such as microscopy to verify their relevance. The
452 number of detected event layers was high (Table 4) due to the detection of supplementary thinner
453 layers.

454 Initially, this work was developed to study only flood events that were manually labeled. Nonetheless,
455 HSI does not appear to have sufficient discriminant spectral information to distinguish different
456 triggering mechanisms for the event layers (e.g., flood, slumps induced by seismic-shaking, etc.).
457 However, the HSI model is the first fast and non-destructive method to semi-automatically detect
458 event layers in different sedimentary contexts and represents a clear improvement in sedimentology.



459

460 Figure 9: Comparison of the naked-eye and HSI estimated chronicles for the three samples: (a) Allos; (b) Bourget; (c) Geneva

461 Table 4: Statistics from the naked-eye and HIS event layer detections. N is the number of event layers identified in each lake

462 core, and the other variables are statistics about the layer thickness

	N	$N_{<1}$ mm	Average (mm)	Standard deviation (mm)	Minimum (mm)	Maximum (mm)	
Allos	Naked eye	69	0	7.44	5.73	1.00	39.00
	HSI	88	12	9.64	13.51	0.32	68.19

Bourget	Naked eye	56	0	3.41	2.17	1.00	11.00
	HSI	72	19	4.24	4.28	0.20	22.31
Geneva	Naked eye	15	0	15.93	21.97	3.00	88.00
	his	26	11	11.37	23.81	0.22	109.01

463 4.4 Perspectives

464 It is worth noting that we only focused on event layers, and the models are site-specific. Some
465 strategies can be tested in future works. The first strategy would be to create a multi-site database to
466 learn several event types and include continuous sedimentation cases (strata or homogeneous). A
467 second strategy could be to use complementary information estimated by other sensors, such as XRF
468 spectroscopy, which is also a non-destructive high-resolution (up to 200 μm) analysis, for elemental
469 composition (Rapuc et al., 2020).

470 It would also be interesting to use a spatial-spectral approach to add information contained in both
471 dimensions, such as the color and grain size gradient, along a flood event. Deep learning with a
472 convolutional neural network (CNN) uses this type of approach and could be interesting for a large
473 multi-site database. This method introduces multi-scale local feature learning and some translation
474 and rotation invariance, which are of interest for image classification (Schmidhuber, 2015). We have
475 tested a CNN1D that uses only the spectral dimension, but it has poor performance that may be due
476 to too small of a database and a too simple of a problem that an ANN with few neurons could model.
477 In future work, we will use a CNN3D that uses a spatial-spectral approach (Ben Hamida et al., 2018).

478 We have shown that the combination of VNIR and SWIR does not increase the discriminating capacity.
479 Improvements can be made with surface defect correction before data acquisition or with pre-
480 processing after data acquisition, or the defects can be detected and removed from the classification
481 map. Another method could be to make two separate classifications with both sensors and

482 subsequently combine them with different weights using, for example, fuzzy or belief function
483 methods to improve the certainty of the predictions (Lian et al., 2019; Tehrani et al., 2019).

484 This study has shown that event layers can be estimated at high resolution with hyperspectral imaging
485 in the cores used in the calibration. A first discriminant model based on LDA or PLS-DA, which is
486 estimated with raw hyperspectral data, will enable one to determine the possibility of discrimination
487 among different classes. A similar method has already been used to detect tephra layers (Aymerich et
488 al., 2016). Then, our proposed method may be applied to case studies to detect any type of events
489 such as tsunamis, earthquakes, landslides, storms, and any other laminae. Thus, thanks to a precise
490 manual labeling that includes as much visual and spectral variability as possible, it will be possible to
491 build an automatic log-stratigraphy. This method will be very useful for paleoenvironmental and
492 paleoclimate studies to define the strategy to subsample cores for further analysis to validate
493 predictions or for any other purposes, and it will allow to create event chronicles or to correct the
494 observations from specific events.

495 **5 Conclusions**

496 We studied the potential of three hyperspectral sensors (VNIR, SWIR, VNIR-SWIR) to image three
497 sediment cores and created machine learning models. This study aimed to automatically discriminate
498 different types of sedimentation (continuous versus event layer) with non-destructive, high-resolution,
499 time-saving methods. Six discrimination methods coupled with raw data or eight pre-processing
500 procedures were used to find an optimal model. We found that the SWIR sensor enabled one to create
501 the most robust models with discriminant analysis (LDA, PLS-DA). Raw data presented relevant
502 predictions (0.87-0.95 but qualitative index 2-3), but the use of a pre-processing procedure can slightly
503 improve the performance (0.90—0.98) and robustness (4-5) of the model. The models were
504 quantitatively assessed with prediction accuracies for the three cores of 0.90, 0.95, and 0.98 and
505 qualitative index of 4-5. For the qualitative model, event layers presented colors and textures that
506 differed from those of continuous sedimentation and could be identified with naked-eye observation

507 to check the relevance of the prediction maps. The discriminant wavelengths are associated with
508 organic matter, some mineral bands, and moisture. This information is not recorded by the VNIR sensor
509 or RGB images, which explains their lower performance, its models seem to rely mainly on the color
510 which is not sufficiently discriminating information. Finally, event chronicles could be estimated from
511 the classification maps by calculating the depth and thickness of each deposit and seem relevant with
512 naked eye chronicles. Unfortunately, the hyperspectral sensors used in this study do not have sufficient
513 spectral discriminant information to characterize the trigger of the event layer and whether different
514 types of events were present in the same sediment core. Future work will enable the characterization
515 of the triggers by combining hyperspectral imaging with other sensors or using spatial-spectral
516 machine learning methods. This study highlights the sediment lithology discrimination capacity of
517 hyperspectral imaging with manual labeling. Future application of this method on sediment sections
518 will allow the creation of robust chronicles of events with characteristic wavelengths and enhance the
519 knowledge about the evolution of the frequency of extreme geodynamic events.

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525 **7 Computer Code Availability**

526 The Matlab codes used in this study to perform all these processing (machine learning and pre-
527 processing) can be accessed in the following repository:

528 https://github.com/JacqKevin/HSI_SupervisedClassification.

529 **8 Description of author's responsibilities.**

- 530 Kévin Jacq: Data acquisition and processing; Algorithm development; Writing original draft
- 531 William Rapuc: Data processing; Sedimentology interpretation; Writing original draft
- 532 Alexandre Benoit: Machine learning methods; Review and editing the draft
- 533 Didier Coquin: Machine learning methods; Review and editing the draft
- 534 Bernard Fanget: Spectroscopy and chemometrics methods; Review and editing the draft
- 535 Yves Perrette: Spectroscopy and chemometrics methods; Review and editing the draft
- 536 Pierre Sabatier: Sedimentology interpretation; Review and editing the draft
- 537 Bruno Wilhelm: Flood event interpretation; Data processing; Review and editing the draft
- 538 Maxime Debret: Data acquisition; Review and editing the draft
- 539 Fabien Arnaud: Data processing; Review and editing the draft

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771

772 9 List of captions

773 9.1 Figures

774 Figure 1: Locations, tributaries and effluents of the lakes: (a) Bourget and Geneva, (b) Allos.

775 Figure 2: XRF analysis for Ti, Zr/K, and Ca of the three cores: (a) Allos, (b) Bourget, and (c) Geneva

776 Figure 3: Data processing to create a classification model to predict each pixel: (1) Visualization with
777 RGB images at both resolutions; (2) Manual labeling of the image; (3) Data pre-processing and (4)
778 Creation of supervised classification models for each dataset (DT: Decision Tree, RF: Random Forest,
779 ANN: Artificial Neural Network, LDA: Linear Discriminant Analysis, QDA: Quadratic Discriminant
780 Analysis, PLS-DA: Partial Least Squares Discriminant Analysis); (5) Prediction for each image; (6)
781 Estimation of the optimal model depending on the sensor, pre-processing procedure and
782 discrimination model

783 Figure 4: Spectral variations of labelled pixels for each class (blue = event layers; yellow = continuous
784 sedimentation) and for the three cores: (a) Allos, (b) Bourget and (c) Geneva. The reflectance of the
785 sediments depends on the specific sedimentary properties of the sites studied. It seems difficult to
786 visually estimate specific discriminating spectral areas of the two classes studied

787 Figure 5: Schematic representation of the machine learning methods used in this study depending on
788 their basis: (a) rules; (b) neurons; and (c) functions

789 Figure 6: Radar charts of the impact of pre-processing on the overall prediction accuracy of each
790 classification method and lake core hyperspectral image (a-c: Lake Allos; d-f: Lake Bourget; g-i: Lake
791 Geneva; a, d, g: VNIR sensor; b, e, h: SWIR sensor; c, f, i: VNIR-SWIR sensor)

792 Figure 7: Optimal (c, f, i) and worst (b, e, h) models for each sediment core sample (a, b, c: Allos; d, e,
793 f: Bourget; h, i, j: Geneva) and labeled areas (blue = event layers; yellow = continuous sedimentation)

794 Figure 8: Comparison of the normalized coefficients (coefficient weights normalized to one for each
795 method) used by the optimal SWIR models to highlight the discriminant wavelengths: (a) Allos, (b)
796 Bourget, and (c) Geneva samples

797 Figure 9: Comparison of the naked-eye and HSI estimated chronicles for the three samples: (a) Allos;
798 (b) Bourget; (c) Geneva

799 9.2 Tables

800 Table 1: Optimal models for each sensor depending on the sample and discrimination method and
801 based on the parameters indicating their performance and robustness

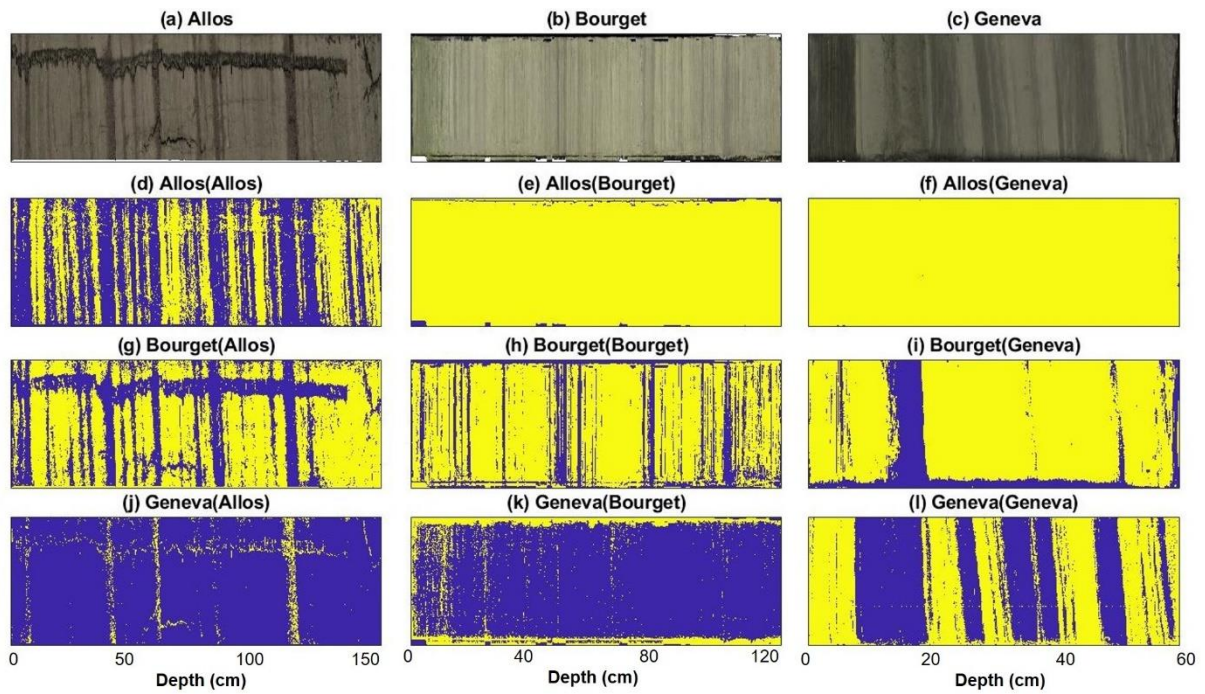
802 Table 2: Comparison of site-specific models for the generalization to the other cores

803 Table 3: Comparison of the conventional image discriminant models with the optimal predictions
804 being estimated by the hyperspectral images

805 Table 4: Statistics from the naked-eye and HSI event layer detections. N is the number of event layers
806 identified in each lake core, and the other variables are statistics about the layer thickness

807 **10 Supplementary Material**

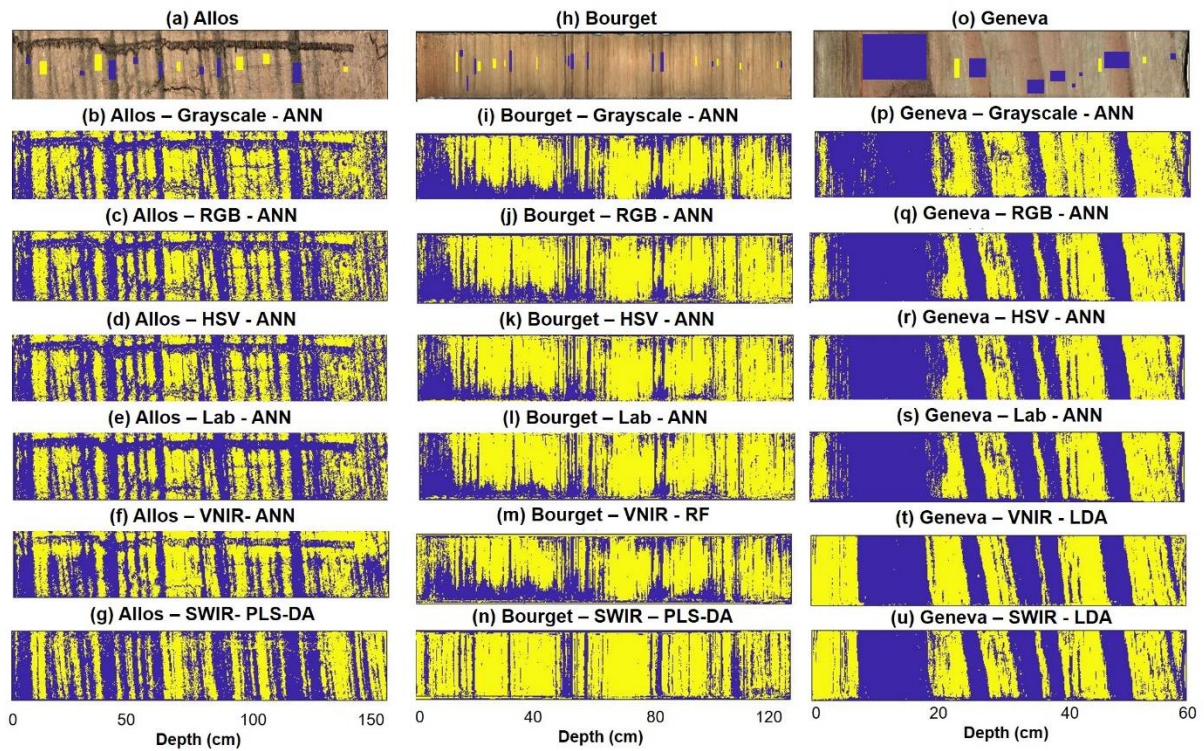
808 **10.1 Figures**



809

810 Supplementary figure 1: Classification maps estimated by model re-using: (d-e-f): Allos model; (g-h-i): Bourget model; (j-k-l):

811 Geneva model; (d-g-j): Allos data; (e-h-k): Bourget data; (f-i-l): Geneva data.



812

813 Supplementary figure 2: Comparison of the classification maps estimated by the learning of the conventional images and

814 HSI

815 10.2 Tables

816 Supplementary table 1: Parameters of each machine learning method

Method	Parameters
DT	Split predictor: Standard CART Split criterion: Gini's diversity index Decision tree pruning based on error criterion
RF	Ensemble-aggregation method: Adaptive logistic regression Number of ensemble learning cycles: 100
ANN	Number of neurons: 2-10 Training function: Scaled conjugate gradient backpropagation Performance function: Cross-Entropy

LDA	Discriminant type: Linear
QDA	Discriminant type: Quadratic
PLS-DA	Latent variable estimation method: NIPALS Maximum number of latent variables: 15 Selection of the number of latent variables: R ² differences between two consecutive latent variables are less than 2%

817

818 Supplementary table 2: The number of pixels for each sediment core image and the number of labeled pixels for the

819 calibration and validation sets for each class (1=event layer; 2=continuous sedimentation)

Sample	Sensors	Total pixels	Class	Number of areas labeled and pixels	Calibration pixels	Validation pixels
Allos	VNIR	30 433 152	1	8 areas, 598 722 (1.97%)	419 105 (1.38%)	179 617 (0.59%)
			2	6 areas, 961 079 (3.16%)	419 105 (1.38%)	541 974 (1.78%)
	SWIR, VNIR-SWIR	1 702 476	1	8 areas, 35 364 (2.08%)	24 755 (1.45%)	10 609 (0.62%)
			2	8 areas, 56 261 (3.30%)	24 755 (1.45%)	31 506 (1.85%)
Bourget	VNIR	21 096 723	1	12 areas, 155 876 (0.74%)	68 636 (0.33%)	87 240 (0.41%)
			2	9 areas, 98 051 (0.46%)	68 636 (0.33%)	29 415 (0.14%)
	SWIR, VNIR-SWIR	1 806 624	1	12 areas, 12 975 (0.72%)	5 709 (0.32%)	7 266 (0.40%)

			2	9 areas, 8 156 (0.45%)	5 709 (0.32%)	2 447 (0.14%)
Geneva	VNIR	13 711 712	1	8 areas, 2 034 596 (14.84%)	65 769 (0.48%)	1 968 827 (14.36%)
			2	3 areas, 93 956 (0.69%)	65 769 (0.48%)	28 187 (0.21%)
	SWIR, VNIR-SWIR	865 234	1	8 areas, 135 933 (15.71%)	4 078 (0.47%)	131 855 (15.24%)
			2	3 areas, 5 826 (0.67%)	4 078 (0.47%)	1 748 (0.20%)

820

Supplementary table 3: Optimal models for the VNIR data depending on the sample and discrimination method

Sample	Performances	DT	RF	ANN	LDA	QDA	PLS-DA
Allos	Processing	CLAHE	Detrend	CLAHE	CLAHE	CLAHE	CLAHE
	Neurons			2			
	Accuracy _{cal}	0.978	0.886	0.889	0.863	0.860	0.840
	Precision _{cal}	0.977	0.883	0.889	0.904	0.906	0.902
	Recall _{cal}	0.980	0.890	0.888	0.811	0.803	0.762
	Accuracy _{pred}	0.828	0.882	0.890	0.889	0.889	0.879
	Precision _{pred}	0.614	0.710	0.728	0.759	0.764	0.755
	Recall _{pred}	0.834	0.888	0.889	0.812	0.804	0.763
	Qualitative	3	3	3	2	2	2

	Computation time (s)	42.544	1272.513	263.840	8.086	251.592	12.975
Bourget	Processing	Raw	Raw	Raw	Raw	Raw	Raw
	Neurons			2			
	Accuracy _{cal}	0.999	0.996	0.996	0.994	0.994	0.993
	Precision _{cal}	0.999	0.996	0.996	0.998	0.997	0.997
	Recall _{cal}	0.999	0.996	0.996	0.990	0.991	0.988
	Accuracy _{pred}	0.994	0.995	0.996	0.993	0.992	0.991
	Precision _{pred}	0.998	0.998	0.998	0.999	0.999	0.999
	Recall _{pred}	0.993	0.995	0.996	0.991	0.991	0.988
	Qualitative	2	3	2	2	2	2
	Computation time (s)	1.817	139.542	5.174	1.216	54.210	2.057
Geneva	Processing	Detrend	Detrend	Detrend	Detrend	Detrend	Detrend
	Neurons			2			
	Accuracy _{cal}	0.998	0.990	0.992	0.987	0.987	0.985
	Precision _{cal}	0.998	0.985	0.989	0.985	0.985	0.984
	Recall _{cal}	0.999	0.995	0.994	0.988	0.988	0.985
	Accuracy _{pred}	0.987	0.993	0.994	0.989	0.989	0.985
	Precision _{pred}	1.000	1.000	1.000	1.000	1.000	1.000
	Recall _{pred}	0.987	0.993	0.994	0.989	0.989	0.986

821

	Qualitative	2	2	2	3	3	3
	Computation time (s)	2.615	200.019	16.167	1.142	52.417	2.814

Supplementary table 4: Optimal models for the SWIR data depending on the sample and discrimination method

Sample	Performances	DT	RF	ANN	LDA	QDA	PLS-DA
Allos	Processing	Raw	SNV	Autoscale	Raw	Raw	SNV
	Neurons			3			
	Accuracy _{cal}	0.982	0.925	0.922	0.920	0.920	0.900
	Precision _{cal}	0.982	0.949	0.944	0.933	0.933	0.908
	Recall _{cal}	0.982	0.898	0.896	0.905	0.904	0.890
	Accuracy _{pred}	0.876	0.928	0.935	0.927	0.926	0.902
	Precision _{pred}	0.725	0.853	0.869	0.840	0.840	0.785
	Recall _{pred}	0.882	0.888	0.895	0.904	0.903	0.885
	Qualitative	3	5	5	5	5	5
	Computation time (s)	1.214	95.740	6.989	0.664	39.287	0.800
Bourget	Processing	Detrend	Detrend	Detrend	Detrend	Detrend	Detrend
	Neurons			2			
	Accuracy _{cal}	0.994	1.000	0.976	0.971	0.972	0.969
	Precision _{cal}	0.995	1.000	0.994	0.993	0.994	0.988
	Recall _{cal}	0.993	1.000	0.958	0.949	0.949	0.951

	Accuracy _{pred}	0.952	0.959	0.967	0.954	0.955	0.958
	Precision _{pred}	0.984	0.986	0.997	0.997	0.997	0.996
	Recall _{pred}	0.953	0.961	0.960	0.944	0.944	0.949
	Qualitative	2	3	4	5	5	5
	Computation time (s)	0.266	10.402	0.402	0.167	24.268	0.219
Geneva	Processing	SNV	SNV	SNV	SNV	SNV	SNV
	Neurons			2			
	Accuracy _{cal}	0.998	1.000	0.996	0.992	0.992	0.991
	Precision _{cal}	0.998	1.000	0.998	0.996	0.996	0.996
	Recall _{cal}	0.999	1.000	0.994	0.989	0.988	0.985
	Accuracy _{pred}	0.991	0.993	0.993	0.989	0.988	0.987
	Precision _{pred}	1.000	1.000	1.000	1.000	1.000	1.000
	Recall _{pred}	0.991	0.993	0.993	0.989	0.988	0.987
	Qualitative	3	4	4	5	5	5
	Computation time (s)	0.155	5.436	0.255	0.113	21.478	0.163

822

Supplementary table 5: Optimal models for the VNIR-SWIR data depending on the sample and discrimination method

Sample	Performances	DT	RF	ANN	LDA	QDA	PLS-DA
Allos	Processing	CLAHE	SNV	SNV	Raw	Raw	SNV
	Neurons			2			

	Accuracy _{cal}	0.984	0.943	0.933	0.931	0.931	0.901
	Precision _{cal}	0.983	0.961	0.952	0.940	0.940	0.943
	Recall _{cal}	0.984	0.924	0.912	0.921	0.921	0.855
	Accuracy _{pred}	0.877	0.931	0.940	0.935	0.935	0.921
	Precision _{pred}	0.726	0.854	0.875	0.856	0.856	0.857
	Recall _{pred}	0.886	0.899	0.911	0.918	0.918	0.855
	Qualitative	3	5	4	5	5	5
	Computation time (s)	2.726	86.900	15.562	1.097	49.604	1.206
Bourget	Processing	Raw	Raw	Raw	Detrend	Detrend	Raw
	Neurons			2			
	Accuracy _{cal}	0.993	1.000	0.981	0.979	0.979	0.979
	Precision _{cal}	0.995	0.999	0.998	0.997	0.997	0.997
	Recall _{cal}	0.992	1.000	0.963	0.960	0.960	0.960
	Accuracy _{pred}	0.966	0.967	0.970	0.969	0.969	0.968
	Precision _{pred}	0.990	0.995	1.000	0.999	0.999	0.999
	Recall _{pred}	0.965	0.963	0.962	0.960	0.961	0.959
	Qualitative	1	2	2	3	4	4
	Computation time (s)	0.372	15.082	0.672	0.265	26.742	0.276
Geneva	Processing	Raw	Raw	Raw	Raw	Raw	Raw

	Neurons			2			
	Accuracy _{cal}	0.999	1.000	0.998	0.997	0.993	0.991
	Precision _{cal}	1.000	1.000	1.000	1.000	0.995	0.990
	Recall _{cal}	0.999	1.000	0.996	0.994	0.992	0.992
	Accuracy _{pred}	0.996	0.996	0.996	0.993	0.991	0.993
	Precision _{pred}	1.000	1.000	1.000	1.000	1.000	1.000
	Recall _{pred}	0.996	0.996	0.996	0.993	0.991	0.993
	Qualitative	2	2	4	4	4	4
	Computation time (s)	0.223	17.307	0.758	0.437	52.612	0.404

823