National spectral data and learning algorithms for potentially toxic elements modelling in forest soil horizons

Asa Gholizadeh^a, Mohammadmehdi Saberioon^b, Eyal Ben-Dor^c, Raphael A. Viscarra Rossel^d, Lubos Boruvka^a

^a*Department of Soil Science and Soil Protection, Faculty of Agrobiolgy, Food and Natural Resources, Czech University of Life Sciences Prague, Kamýcka 129, Suchbát, Prague 16500, Czech Republic*

^b*Helmholtz Centre Potsdam GFZ German Research Centre for Geosciences, Section 1.4 Remote Sensing and Geoinformatics, Telegrafenberg, Potsdam 14473, Germany*

^c*Remote Sensing Laboratory, Department of Geography and Human Environment, Porter School of Environment and Earth Science, Tel Aviv University, Tel Aviv 69978, Israel*

^d*Soil and Landscape Science, School of Molecular and Life Sciences, Faculty of Science and Engineering, Bentley Campus, Curtin University, G.P.O. Box U1987, Perth WA 6845, Australia*

Abstract

Forest ecosystems are among the main parts of the biosphere; however, they have been endangered from the significant elevation and harmful effects of air and soil pollutants, including potentially toxic elements (PTEs). The concentration of PTEs in forest soils varies not only laterally but also vertically with depth. Forest surface organic horizons are of particular interest in forest ecosystem monitoring due to their role as stable adsorbents of the deposited atmospheric substances. Therefore, the main purpose of this study was to conduct rapid examinations of forest soils PTEs (Cr, Cu, Pb, Zn, and Al), testing the capability of VIS–NIR spectroscopy coupled with machine learn-

*Email address: gholizadeh@af.czu.cz (Asa Gholizadeh)

**Email address: saberioon@gfz-potsdam.de (Mohammadmehdi Saberioon)

ing (ML) techniques (partial least square regression (PLSR), support vector machine regression (SVMR), and random forest (RF)) and fully connected neural network (FNN), a deep learning (DL) approach, in forest organic horizons. One-thousand-and-eighty forested sites across the Czech Republic at two soil layers, defining the fragmented (F) and humus (H) organic horizons, were investigated (total 2160 samples). PTEs as well as total Fe and SOC, as auxiliary data, were conventionally and spectrally determined and modelled in the combined organic horizons (F + H) and in each individual horizon using the ML and DL algorithms. Results indicated that the concentration of all PTEs was higher in the horizon H compared to the F horizon. Although the spectral reflectance of samples tended to decrease with increased PTEs concentration. Strongly significant positive correlations between all PTEs and total Fe in all horizons were obtained, which were higher in the H and F + H horizons than the F horizon. The highest correlations of PTEs with the spectra were at 460–590 nm, which is mostly linked to the presence of Fe-oxide. These results show the importance of Fe for spectral prediction of PTEs. Cr and Al were the most accurately predicted elements, regardless of the applied learning technique. SVMR provided the best results in assessing the H horizon (e.g., $R^2 = 0.88$ and root mean square error (RMSE) = 3.01 mg/kg, and $R^2 = 0.82$ and RMSE = 1682.25 mg/kg for Cr and Al, respectively); however, FNN predicted the combined F + H horizons the best ($R^2 = 0.89$ and RMSE = 2.95 mg/kg, and $R^2 = 0.86$ and RMSE = 1593.64 mg/kg for Cr and Al, respectively) due to the larger number of samples. In the F horizon, almost no parameters were predicted adequately. This study shows that given the availability of a larger sample size, FNN can be

a more promising technique compared to ML methods for assessment of Cr and Al concentration based on national spectral data in the forests of the Czech Republic.

Keywords: Soil contamination, Organic horizon, Reflectance spectroscopy, Machine learning, Deep learning.

1. Introduction

Soil is considered the most dynamic, complex, and biodiverse habitat that exists, providing many benefits for humans (Wall et al., 2015). It provides fundamental natural resources for the survival of most terrestrial life (Du & Zhou, 2011) and, as an open system exchanges matter and energy with its surrounding atmosphere, lithosphere, biosphere, and hydrosphere (Shi et al., 2018). However, it is subjected to severe human disturbance by industrial activities, which represent the main global change driver (Smith et al., 2015) leading to serious soil degradation, including soil contamination (Gholizadeh & Kopackova, 2019).

Potentially toxic elements (PTEs), as a main group of soil contaminants, can be found in soluble and adsorbed fractions. Their accumulation in soil harms the environment and endangers ecosystems and human health (Srivastava et al., 2017; Sihag et al., 2019) via energy and material cycling (Sun et al., 2009). Soil receives PTEs in various ways, including mineral dust and gas dust emissions from industrial enterprises and vehicles, liquid and solid household waste, sewage from agricultural enterprises, pesticides, and impurities of organic and mineral fertilizers (Su et al., 2014; Plyatsuk et al., 2019). PTEs also fall from the atmosphere into the soil, principally in the

20 form of oxides that gradually dissolve, passing into hydroxides or carbonates
21 or in the form of exchanged cations (Panchenko et al., 2018).

22 Soils of forested regions contain a large proportion of the world’s carbon
23 (C), minerals, and energy resources. They influence the composition and
24 quality of the atmosphere and shape climate conditions on both a regional
25 and global scale (Percy & Ferretti, 2004; Baciak et al., 2015). Forest soil
26 organic horizons and their individual layers (fragmented (F) and humus (H))
27 as topsoil horizons are the most dynamic parts of the forest environment
28 (Chodak et al., 2007; Pavlu et al., 2016), and are significantly affected by the
29 airborne supply of PTEs (Boska et al., 2016; Tzvetkova et al., 2016) or by
30 their uptake from deeper soil horizons (Sucharova et al., 2011). Moreover, the
31 forest floor is well known for its ability to bind and retain PTEs (Stevenson,
32 1994). Metals derived from atmospheric deposition are trapped and held
33 in forest organic horizons (Sucharova et al., 2011), especially the H horizon
34 (Reimann & Caritat, 2000), for a long time. Hence, assessment of PTE
35 concentration and spatial variability in forest surface soil is of particular
36 interest for the prediction of dynamics within a forest ecosystem and further
37 remediation (Fujii et al., 2014; Tzvetkova et al., 2016).

38 Determining PTE concentration in soil requires large-scale sampling (Ren
39 et al., 2009; Gholizadeh et al., 2015). In addition, due to the high spatial
40 variability in forest topsoil, a large number of samples must be analyzed to
41 characterize the soil adequately at a large scale (Chodak et al., 2004). Tra-
42 ditionally, the assessment of PTE concentration in soil has been carried out
43 through conventional soil testing and long-term trials in sequential steps,
44 with increasing complexity and cost (Hang et al., 2009; Liu et al., 2018a).

Therefore, an efficient and rapid analytical approach to measuring and monitoring soil PTEs in the forest at a suitable spatial scale is desirable (Arellano et al., 2015). A fast, simple, and cost-effective method such as visible–near infrared (VIS–NIR) can potentially be used to detect PTEs in the organic horizons of forest soil (Chodak et al., 2007; Liu et al., 2018a).

Soil VIS–NIR spectra include weak, wide, and overlapping absorption bands with fundamentals in the mid-infrared (MIR) region (Gholizadeh et al., 2016). The hidden information, therefore, needs to be extracted from the spectra to establish a proxy approach to detect soil parameters (Viscarra Rossel & Behrens, 2010). Machine learning (ML) techniques including partial least square regression (PLSR), support vector machine regression (SVMR), random forest (RF), artificial neural networks (ANN), and cubist have frequently been used to calibrate soil contamination prediction models (Kemper & Sommer, 2002; Ferreira et al., 2008; Gholizadeh et al., 2015; Liu et al., 2018b). However, with the development of large soil spectral libraries, we need to seize the opportunity to utilize big data analytics to process the spectral data, which goes beyond using commercial software or packaged ML algorithms (Padarian et al., 2018).

1.1. Deep learning (DL)

Deep learning (DL), a deep architecture of ANN with the capability of processing large-scale data (LeCun et al., 2015), can be a solution for the shortage of ML methods in big data analysis. Its advantages over common ML algorithms are that it supports more sophisticated modelling and permits the easy use of large amounts of computational resources for training such models (Behrens et al., 2018). DL is a model made of multiple pro-

70 cessing layers to learn data representation in big datasets (LeCun et al.,
 71 2015). It contains more layers and deeper architectures than traditional neu-
 72 ral networks (Padarian et al., 2018) and tries to hierarchically learn in-depth
 73 features of input data with very deep neural networks (Chen et al., 2014).
 74 The network is first layer-wise initialized via unsupervised training and then
 75 tuned in a supervised manner, permits the use of raw or unprocessed data
 76 (e.g., images or spectra), and automatically discovers the required represen-
 77 tations or predictions.

78 Currently, DL is widely used in image analysis including soil image recog-
 79 nition thanks to its ability to learn multiple (hierarchical) levels of data rep-
 80 resentation (LeCun et al., 2015; Li et al., 2018; Tziolas et al., 2020). However,
 81 it has only been used in reflectance spectroscopy of some basic soil properties
 82 (Padarian et al., 2018) and soil microplastic contamination (Ng et al., 2019).
 83 In spite of the key role of the soil organic horizon in the forest ecosystem
 84 and its active and firm binding of PTEs, the technique has not yet been used
 85 for VIS–NIR spectroscopy of soil PTEs, either directly or indirectly via their
 86 intercorrelation with spectrally active attributes such as soil organic carbon
 87 (SOC) and iron (Fe). VIS–NIR spectroscopy applied to high organic C soils
 88 is likely to yield different responses compared to soils with high mineral con-
 89 tent.

90 One such DL model, used in this study, is fully connected neural network
 91 (FNN), which is a deep neural network architecture (Figure 1), formed by
 92 repeatedly stacking the fully connected layer and activation function after the
 93 input layer. Each node in a particular layer is connected to all nodes in the
 94 next layer. The fully connected layer provides a linear transformation and the

95 activation function adds nonlinearity to extract nonlinear features from the
 96 input data. The large number of parameters in the FNN model means that
 97 it can fit arbitrary patterns theoretically, which allows new insight that can
 98 be applied to data directly. The parameters of the FNN model are optimized
 99 throughout backpropagation and the gradient descent algorithm (Qian, 1999;
 100 Yang et al., 2019).

Figure 1: General structure of FNN used in this study.

101 About one-third of the landscape of the Czech Republic is covered by
 102 forests, and over the last few decades, the country has been heavily affected
 103 by industrial activity. Consequently, this study aims to construct soil PTE
 104 (Cr, Cu, Pb, Zn, and Al) prediction models through testing the capability
 105 of VIS–NIR spectroscopy coupled with DL in the organic horizon of forests
 106 of the Czech Republic. Our specific objectives are (i) to model forest soil
 107 PTEs in combined (F + H) and individual (F and H) organic horizons with
 108 spectra and the DL approach (FNN), (ii) to compare the results with the
 109 results obtained from ML techniques (PLSR, SVMR, and RF), and (iii) to

110 assess the predictability of the models.

111 2. Materials and methods

112 2.1. Experimental sites, soil sampling, and laboratory analyses

113 The total land area of the Czech Republic is 78,865 km², of which one-
114 third (34%) is covered by forests (Czech Statistical Office, 2019). In this
115 study, in order to proportionally represent various forest stands (forest com-
116 position, soil classes, and altitudes), sampling sites were distributed over all
117 the country's forested areas. The samples originate from the Forest Soil Sur-
118 vey (Fiala et al., 2013) and were obtained from forested sites of the whole
119 Czech Republic from 2000 to 2008 (Figure 2). Soil samples were collected
120 from 1080 points separately from two individual organic horizons, F and H
121 (total 2160 samples).

Figure 2: Location of Czech forests and soil sampling sites.

122 The soil samples were air-dried, ground, sieved (≤ 2 mm), and thoroughly
123 mixed before soil analysis. Potentially toxic elements (Cr, Cu, Pb, Zn, and

Al) were extracted using aqua regia (ISO 11466:1995), followed by atomic absorption spectroscopy to determine their pseudo-total content. Samples and standards were matrix matched and all analyses were performed in triplicate (Gholizadeh et al., 2015). SOC and total Fe were also determined as auxiliary data for further use (since they are spectrally active parameters (Gholizadeh et al., 2018a) and have strong adsorption with PTEs) by rapid dichromate oxidation (Sparks, 1996) and aqua regia (ISO 11466:1995).

More information about the proportions of various tree species, soil classes, and altitudes can be seen in Table 1. Two-thirds of the sampling locations (65.6%) were formed by sites with prevailing coniferous trees; the most frequent species was Norway spruce (*Picea abies* L. Krast., 51.5%), followed by Scots pine (*Pinus sylvestris* L., 13.8%). Among sites with prevailing broad-leaved trees (34.4%), oak (*Quercus sp.*, 17.9%), and European beech (*Fagus sylvatica* L., 16.6%) dominated. Regarding soil classes, the dominant soil class was Cambisols (70.1%); mostly Dystric (36.7%), Hyperdystric (28.9%), and Eutric (22.6%). Podzols (15.4%) and Stagnosols (5.2%) were also rather ample; however, other soil classes (e.g., Arenosols, Leptosols, Retisols, Luvisols, and Fluvisols) were less frequent. Table 1 also indicates that most of the sampling sites (47.1%) were located between 400 m and 600 m a.s.l., with fewer sites outside this range.

Table 1: Proportion of sites with different prevailing tree species, soil classes and altitudes in the set of sampling sites.

Prevailing tree species	Number of sites	%	Soil classes	Number of sites	%	Altitudes (m a.s.l.)	Number of sites	%
Coniferous	709	65.5	Cambisols	758	70.1	<200	28	2.6
Spruce	557	51.5	Podzols	166	15.4	200-300	61	5.6
Broadleaved	372	34.4	Stagnosols	56	5.2	300-400	170	15.7
Oak	193	17.9	Leptosols	23	2.1	400-500	266	24.6
Beech	179	16.6	Arenosols	21	1.9	500-600	243	22.5
Pine	149	13.8	Retisols	19	1.8	600-700	111	10.3
Fir	2	0.2	Luvisols	17	1.6	700-800	65	6.0
Larch	1	0.1	Fluvisols	17	1.6	800-900	65	6.0
			Histosols	2	0.2	900-1000	43	4.0
			Gleysols	1	0.1	>1000	29	2.7
			Phaeozems	1	0.1			

144 2.2. Spectroscopic measurements and preprocessing

145 Diffuse reflectance spectra were measured using an ASD FieldSpec Pro FR
146 VIS–NIR spectrometer (ASD Inc., Denver, CO, USA) using a high-intensity
147 contact probe in the spectral range of 350–2500 nm. The samples were placed
148 in 9 cm diameter petri dishes and formed 2 cm layers of soil and were scanned
149 in the center (3 replications each) in a dark room. A SpectralonTM (Lab-
150 sphere, North Sutton, NH, USA) was used for white referencing before the
151 first scan and once every 6 measurements (Shi et al., 2016). For each soil
152 measurement, 30 spectra were averaged to improve the signal-to-noise ratio
153 (SNR).

154 Noisy portions between 350 nm and 400 nm as well as 2451 nm and
155 2500 nm were removed, leaving spectra in the range from 400–2450 nm
156 for further processing. The resulting spectra were then smoothed using the
157 Savitzky-Golay approach with a second-order polynomial fit, a window size
158 of 11 wavelengths in order to remove the artificial noise within the working
159 spectral range (Savitzky & Golay, 1964), and first derivatives were used to
160 remove baseline offset (Gholizadeh et al., 2018c). In this study, in order to
161 recognize influential outliers in a set of predictor variables, ensemble sparse
162 partial least squares was applied (Aggarwal, 2013).

163 2.3. Machine learning spectral modelling

164 Each horizon’s data were divided into a training (75%) and a testing
165 (25%) set using random stratified sampling (Gholizadeh et al., 2018c). The
166 training set was used to develop the regression model and the test set to val-
167 idate the developed model’s generalization capability (Kooistra et al., 2003).
168 Spectral modelling of the selected soil attributes was performed using three

169 ML techniques: PLSR, SVMR, and RF. The authors have previously de-
170 scribed the implementation of techniques for spectroscopic modelling in de-
171 tail (Gholizadeh et al., 2016, 2018b). All spectroscopic models were validated
172 using 10-repeated 10-fold cross-validation (Hastie et al., 2009; Viscarra Rossel
173 et al., 2019) and the validation statistics reported are the means of the 10
174 repeats.

175 *2.4. FNN spectral modelling*

176 In this experiment, the number of features of the input data was used as
177 the number of input layer nodes. In addition to the input layer, two hidden
178 layers, composed of neurons and rectified linear unit (leaky-ReLU) as the
179 activation function (Zhang et al., 2017), were utilized for each soil attribute.
180 The output layer had only one node. Additionally, Dropout regularization
181 was employed, which randomly selects some neurons of the network and
182 ignores them during training, while the other neurons can step in and handle
183 the representation required to predict missing neurons. Dropout forces the
184 network to be less sensitive to the specific weight of neurons. According to
185 Ahmed et al. (2019), Dropout has promising generalization and using it, the
186 network is less likely to become overfitted.

187 The network was trained with a batch size (i.e., a smaller sample dataset
188 from the whole training set) of 20. The maximum number of epochs (i.e., one
189 cycle through the entire training dataset) of the network was set at 400. The
190 network was trained with early stopping on the validation set with patience
191 of 25 epochs. The model was then trained with the Adam optimizer with an
192 initial learning rate of 0.001 to solve the optimization problem for minimizing
193 the mean square error (MSE) function.

194 *2.5. Assessment of techniques*

195 The final accuracy prediction was determined using standard model eval-
196 uation statistics: coefficient of determination (R^2) and the root mean squared
197 error (RMSE). R^2 is the proportion of variation in the response and is de-
198 scribed by the regression model, and the RMSE defines the prediction ability
199 of a model and the ME or bias is the error of means (Bellon-Maurel et al.,
200 2010; Gomez et al., 2016).

201 **3. Results**

202 *3.1. Statistical summary and PTEs, SOC, and total Fe*

203 General statistical results of soil PTEs, SOC, and total Fe including mean,
204 median, minimum (Min), maximum (Max), standard deviation (SD), coeffi-
205 cient of variation (CV), and skewness from all sampling locations for the F
206 + H, F, and H horizons are shown in Table 2.

Table 2: Statistics description of soil attributes for each horizon.

	Cr	Cu	Pb	Zn	Al	Fe	SOC
	(mg/kg)						(%)
Horizons F + H (n = 2160)							
Mean	20.65	20.96	98.96	135.98	6096.28	8671.02	33.68
Median	17.10	18.25	85.75	111	5048.50	6640	34.83
Min	3.20	4.79	14.40	27.20	315	527	11.79
Max	121	160	531	515	29300	92000	48.79
SD	13.55	11.47	57.59	80.26	4602.94	7618.19	7.35
CV (%)	66	55	58	59	76	88	22
Skewness	1.83	3.44	2.16	1.10	1.66	3.77	-0.29
Horizon F (n = 1080)							
Mean	14.16	18.10	71.11	95.11	3659.46	5132.69	38.61
Median	11.30	16.60	65.80	81.20	2820	4000	39
Min	3.20	6.18	14.40	27.20	315	527	11.79
Max	78.90	70.40	225.70	293	22730	28510	48.79
SD	9.64	7.51	31.78	48.79	2832.41	3996.90	5.36
CV (%)	68	42	44	51	77	78	13
Skewness	2.36	1.76	1.31	1.44	2.30	2.61	-1.53
Horizon H (n = 1080)							
Mean	27.15	23.83	126.14	176.86	8533.11	12209.35	28.75
Median	25.4	21	118	177	7600	10600	28.48
Min	6.15	4.79	27.30	31.40	1100	1720	14.60
Max	121	160	531	515	29300	92000	45.98
SD	13.78	13.79	64.40	84.65	4742.34	8666.60	5.54
CV (%)	51	58	51	48	56	71	19
Skewness	1.95	3.22	1.98	0.63	1.55	3.90	0.18

207 There were large variations in soil PTE content in forest soil of the F +
 208 H, F, and H horizons that reflect the different depths from which the samples
 209 originate. According to the pollution level defined in Czech soil quality and
 210 pollutant control standards (ČSN EN ISO 11267, 2014), Boruvka et al. (2015)
 211 and Pavlu et al. (2016), the F horizon is very close to threshold values, and
 212 the H horizon is classified as polluted. The average PTE content in the H

213 horizon was very high compared with the F and F + H horizons, presenting
 214 high mean values. For instance, on average, there was more than twice as
 215 much soluble Al in the H horizon (mean = 8533.11 mg/kg) compared to the F
 216 horizon (mean = 3659.46 mg/kg). The data distribution features were found
 217 in the SD values, which were higher in the H and F + H horizons than the
 218 F horizon. The data for PTEs of all horizons had strong positively skewed
 219 distribution, with the highest skewness of 3.44 for Cu in the F + H horizon
 220 and the lowest skewness of 0.63 for Zn in the H horizon. Table 2 also shows
 221 that the PTE content varied widely, presenting large CV values ($\geq 55\%$, 42% ,
 222 and 48% in the F + H, F, and H horizons, respectively), considered as high
 223 variability according to Wilding (1985), who categorized the datasets with
 224 $CV > 35\%$, $15\% < CV < 35\%$, and $CV < 15\%$ as high, moderate, and low
 225 variability, respectively. In general, soluble Al was the most heterogeneous
 226 PTE in Czech forest soils. The total Fe statistics corresponded with the
 227 outputs obtained from PTEs, providing the highest mean of 12209.35 mg/kg
 228 and the strongest skewness of 3.90 in the H horizon. In terms of SOC, the
 229 F horizon indicated higher average than the H and F + H horizons with
 230 $38.61\% \pm 5.36\%$ (SD), distribution showing low variability ($CV = 13\%$), and
 231 a negatively skewed distribution (skewness < -1).

232 3.2. Horizons spectral data patterns

233 Figure 3 highlights the average reflectance of the whole dataset per soil
 234 horizon with their variance. Visual inspection of the spectra shows that the
 235 overall reflectance patterns and waveforms of the spectral curves of different
 236 horizons were roughly the same; that is, the waveforms shaped an upward
 237 parabolic shape with two distinct absorption features around wavelengths

1400 nm and 1900 nm originated by the hygroscopic moisture. Some weak
 features can also be seen between 2000 nm and 2500 nm wavelengths. Fur-
 thermore, the reflectance spectra of the H horizon were lower across the entire
 spectra. On this basis, the F horizon had higher reflectance values compared
 to the H and F + H horizons. Overall, the spectral reflectance tended to
 decrease with increased PTE content (Figure 3).

Figure 3: Representative VIS–NIR average spectra (bold line) and their variance (shaded area) of soil samples collected from different horizons.

3.3. Correlation among PTEs, SOC, and total Fe

Correlation matrices were constructed to find the correlating soil at-
 tributes for the F + H, F, and H horizons (Figure 4). Strong positive signif-
 icant correlations among all PTEs in all horizons are obvious at $p < 0.001$,
 implying their robust mutual dependence, although the correlations were
 higher for the H and F + H horizons than the F horizon. In all horizons,
 the highest correlation among contaminants was observed between Cr and
 other PTEs. In contrast, the least correlation with others was with Pb (r
 ≤ 0.42) in the F horizon. As highlighted in Figure 4, Fe was significantly
 and positively correlated with all PTEs ($r \geq 0.53$ in the F and $r \geq 0.77$ in

the H and F + H horizons, $p < 0.001$). SOC demonstrated a moderate negative correlation with all attributes; the correlations were still significant ($p < 0.001$), and only in the H horizon the correlation with Cu was significant at $p < 0.05$.

Figure 4: Correlation matrix among soil attributes at the horizons F + H (A), horizon F (B), and horizon H (C). *** $p < 0.001$, ** $p < 0.01$, and * $p < 0.05$

3.4. Correlation of PTEs and reflectance spectra

An easy approach to visualize spectral implications of soil attributes is to plot correlation spectra (i.e., the correlations between attributes and measured reflectance for each wavelength), which can be seen in Figure 5.

Figure 5: Correlation between soil attributes and raw spectra reflectance at different horizons.

262 The plots indicate that PTEs contribute to the reflectance of almost all
 263 wavelengths in the VIS–NIR range; the concentration of PTEs in the F and F
 264 + H horizons showed correlations in a wider range ($-0.5 < r < 0.4$) through-
 265 out the studied spectral region, as they were correlated via their high con-
 266 tent of organic matter. Figure 5 also illustrates that all toxic elements in
 267 all horizons displayed their maximum correlations in the VIS range around
 268 430–450 nm and their highest negative correlations in NIR range between
 269 around 1400 nm and 2300 nm. Moreover, correlation analysis indicated that
 270 the correlation coefficients of Cu and Pb were usually separated from the
 271 other PTEs. In spite of other elements correlating positively with VIS wave-
 272 lengths, Cu and Pb in the F + H horizons, Pb in the F horizon, and Cu
 273 in the H horizon had negative correlations across the VIS reflectance of soil
 274 spectra. The correlation coefficient of all PTEs with NIR reflectance spectra,
 275 in contrast to VIS spectra, fell totally into the negative section of the cor-
 276 relation plots, displaying relatively moderate negative spectral correlations.
 277 In general, Cr and Al had the strongest positive correlation coefficients with
 278 VIS–NIR spectra than other elements.

279 According to Figure 5, the correlation of Fe in all soil horizons was in
 280 accordance with other PTEs across the entire VIS–NIR spectra (positive
 281 correlations with VIS and negative correlations with NIR wavelengths). Fur-
 282 thermore, Fe and Cr had very similar correlation coefficient values, particu-
 283 larly in the H horizon. Correlation changes (both pattern and value) for SOC
 284 were different from all other attributes and followed an opposite trend (Fig-
 285 ure 5), negatively falling into the VIS range, but positive in the NIR region.
 286 In comparison with the examined PTEs, the correlation coefficients of SOC
 287 with VIS–NIR reflectance spectra in the F + H horizons were considerably
 288 higher, with the highest ($r = 0.6$) at around 750 nm.

289 3.5. Performance of prediction models derived from techniques

290 The performance of the selected ML techniques (PLSR, SVMR, and RF)
 291 and the DL approach (FNN) to extract soil PTEs, SOC, and total Fe cali-
 292 bration models from the spectra of forest soils can be seen in Table 3.

293 Regarding PTE prediction models and the PLSR calibration set, R^2 val-
 294 ues ranged between 0.37 (for Zn) and 0.82 (for Cr). The best predictive
 295 models were obtained for Cr ($R^2 = 0.82$ and $RMSE = 3.16$ mg/kg), followed
 296 by Al ($R^2 = 0.75$ and $RMSE = 2121.86$ mg/kg). Using the SVMR technique,
 297 again Cr and Al were the most accurately predicted PTEs, with R^2 value of
 298 0.88 and 0.82, and RMSE of 3.01 mg/kg and 1682.25 mg/kg, respectively;
 299 Zn with $R^2 = 0.40$ and $RMSE = 33.60$ mg/kg, was not predicted adequately.
 300 Likewise, the RF analysis of PTEs for Cr and Al showed the largest R^2 (0.83
 301 and 0.78, respectively) and lowest RMSE (3.08 mg/kg and 2038.11 mg/kg,
 302 respectively), although Zn again was not assessed satisfactorily. It can be
 303 seen that among all applied techniques, SVMR had the best performance,

304 with the highest R^2 and smallest error values for almost all PTEs assessed,
305 followed by RF. PLSR showed the lowest R^2 and largest RMSE values for all
306 parameters; however, it still achieved fair to good prediction of Cr and Al in
307 the Czech forested sites. Using the FNN technique, Cr and Al were the best
308 assessed elements again, with even higher R^2 and RMSE values ($R^2 = 0.89$,
309 $RMSE = 2.95$ mg/kg, and $R^2 = 0.86$, $RMSE = 1593.64$ mg/kg) compared
310 to ML algorithms.

311 The three ML modelling strategies considered in this study displayed
312 different prediction accuracy of the studied horizons (Table 3). Among the
313 explored horizons, the best predictions were found in the H horizon, except
314 for Pb and Zn, which were better assessed in the F + H horizon. In the F
315 horizon, inadequate models (low R^2 and high RMSE) were obtained for all
316 applied techniques and all PTEs, except for Al prediction. Overall, these
317 outcomes suggest the use of SVMR and the H of the horizon of Czech forest
318 soils for fair ($0.50 < R^2 < 0.80$) to good ($R^2 > 0.81$) prediction of PTEs
319 (Chang et al., 2001). Regarding FNN, the best results for all elements were
320 obtained in the F + H horizon. These results were higher than the outputs
321 of all ML methods, indicating the superiority of DL for assessing PTEs in
322 the combined F + H horizon with larger sample size over individual F and
323 H layers. For the F and H horizons, FNN-derived models provided lower
324 accuracy than SVMR and RF; however, they were still more accurate than
325 PLSR.

326 As observed in Table 3, using all techniques (ML and DL), the calibration
327 results for SOC and total Fe performed the best in the F + H horizon using
328 FNN, with $R^2 = 0.95$ and 0.81 , and $RMSE = 1.00$ mg/kg and 1415.10 mg/kg,

329 respectively, indicating excellent models (Chang et al., 2001), followed by
330 SVMR, producing outcomes with the highest prediction accuracy in the F +
331 H horizon.

Table 3: Statistical summary of soil attributes prediction developed by ML and DL techniques for each horizon’s testing set.

ML techniques	Horizon	Cr			Cu			Pb			Zn			Al			Fe			SOC		
		R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²
PLSR	F + H	0.65	4.15	0.44	5.97	0.59	18.29	0.54	29.88	0.69	2295.41	0.69	2523.23	0.89	1.25							
	F	0.42	7.18	0.41	5.27	0.40	28.03	0.37	35.53	0.53	2853.02	0.46	3263.62	0.86	1.28							
	H	0.82	3.16	0.52	4.14	0.44	25.30	0.43	33.08	0.75	2121.86	0.67	2867.90	0.55	2.96							
SVMR	F + H	0.67	4.13	0.48	4.16	0.65	18.18	0.57	27.81	0.81	1727.95	0.79	1603.20	0.94	1.03							
	F	0.45	6.90	0.45	6.15	0.48	22.55	0.40	33.60	0.60	2749.29	0.69	2405.69	0.91	1.14							
	H	0.88	3.01	0.57	3.92	0.53	20.68	0.46	30.29	0.82	1682.25	0.74	1891.85	0.57	2.88							
RF	F + H	0.68	4.09	0.44	5.46	0.63	18.21	0.59	26.80	0.73	2336.24	0.71	2127.14	0.93	1.07							
	F	0.36	7.59	0.51	5.81	0.43	25.85	0.42	32.41	0.63	2701.76	0.57	3135.95	0.88	1.19							
	H	0.83	3.08	0.63	3.82	0.51	20.43	0.44	31.60	0.78	2038.11	0.70	2220.60	0.62	2.34							
FNN	F + H	0.89	2.95	0.67	3.56	0.75	17.48	0.61	25.11	0.86	1593.64	0.81	1415.10	0.95	1.00							
	F	0.36	7.51	0.42	5.48	0.46	22.00	0.42	33.12	0.51	3010.96	0.59	3007.43	0.85	1.39							
	H	0.84	3.07	0.60	3.95	0.52	21.03	0.44	31.96	0.82	1795.48	0.70	2308.30	0.57	2.92							

332 4. Discussion

333 Although Pavlu et al. (2016) found that Cu and Zn contents in Czech for-
334 est soils were higher in the F horizon, the soil analysis of the current study
335 revealed that all examined PTEs were concentrated more in the H horizon,
336 which is in agreement with the studies of Suchara & Sucharov (2002) and
337 Sucharova et al. (2011). For instance, the estimated mean concentrations of
338 Cr and Al in the H horizon (27.15 mg/kg and 8533.11 mg/kg, respectively)
339 were almost 2 times higher than those of the F horizon (Table 2). The initial
340 vertical migration of soil contaminants from upper to lower organic layers is
341 driven by washout and leaching (Fujii et al., 2014); however, the mobility
342 of PTEs in soil depends on their nature, either in particle or soluble/mobile
343 form; the mobile form attains the highest concentration in the H horizon
344 (Pavlu et al., 2016). The mobility and depth distribution of PTEs in forest
345 soil horizons are also regulated by factors such as water content, pH, temper-
346 ature, soil particle size, clay, total Fe, and Fe-oxide content (Rafferty et al.,
347 2000; Wu et al., 2007; Xie et al., 2012; Fujii et al., 2014). The bioavailability
348 of PTEs in soils besides other factors is mostly associated with accumulation
349 and decomposition of SOC (Alloway, 2013). Shand et al. (1994) mentioned
350 that higher SOC can retain higher amounts of contamination due to sorption
351 onto clay minerals, though it can cause a reduction in PTE bioavailability
352 by changing them from bioavailable form (Walker et al., 2004). This also re-
353 flects the accumulation of SOC with bonded elements in horizons with high
354 C content, as documented by Pavlu et al. (2016). In this study, the mean
355 SOC content in the F horizon (38.61%) showed high C storage in forest
356 soils of the Czech Republic, decreasing by depth in the H horizon (28.75%).

357 Therefore, we expected to observe a higher concentration of PTEs in the F
358 horizon than the H horizon; however, it was the opposite (Table 2). Suchara
359 & Sucharov (2002) explained that because of the significantly higher decom-
360 position and density of organic C in the H horizon of forest soil, the cation
361 binding capacity of this layer is very high, reaching 550 meq/100 g of the
362 humus substrate, and PTEs are easily bound to numerous free functional
363 groups of humus macromolecules. The H horizon thus keeps a much higher
364 concentration of PTEs than the F layer, which is mostly accumulated plant
365 residuals. Moreover, plants take up elements via their roots from the deeper
366 mineral soil horizons and then use leaf fall to dispose of undesired elements,
367 including PTEs. After decomposing litter, the released PTEs are absorbed
368 by humic substances in the H horizon due to the strong binding capacity of
369 humus (Reimann & Caritat, 2000). As such, the H horizon can be viewed
370 as the “memory” of the contamination history (e.g., by PTEs) of an area
371 (Sucharova et al., 2011).

372 Figure 3 shows that the spectra of all horizons had a similar typical form,
373 with the waveforms displaying an upward parabolic shape in the VIS–NIR
374 range (400–1000 nm) representing Fe-oxide and C concentration and type
375 (Sherman & Waite, 1985; Song et al., 2012). In the range of 400 nm to
376 1000 nm, the spectral pattern of the F horizon (also F + H), containing
377 less decomposed organic matter (e.g., leaves, needles, and little branches),
378 can also be related to remaining photosynthetic pigments (e.g., chlorophyll,
379 carotenoids, and xanthophylls) and vegetative cell structure (Gitelson et al.,
380 2002). These findings were similar to the results of Ogen et al. (2017), who
381 used the VIS–NIR range for soil classification and concluded that accumu-

lated roots and other plant residuals on upper soil layers affected the soil spectral pattern. In the NIR range, at wavelengths 1400 nm and 1900 nm, there were sharp absorption bands. There were also some weak features between 2000 nm and 2500 nm that resulted from overtones and combined vibrations of the organic functional groups methyl, methylene and aryl, carbonyl, ester and carboxyl C=O, cellulose C-C/C-H, C-H, and O-H groups (Ben-Dor & Banin, 1995; Viscarra Rossel & Hicks, 2015). The NIR spectra of forest organic horizons also consist of numerous overlapping peaks related to different chemical structures (Ludwig & Khanna, 2001). Therefore, it is impossible to exactly relate absorption at particular wavelengths to unique chemical compounds or groups of compounds (Chodak et al., 2007). In this study, as the content of PTE, total Fe, and SOC varied with depth, corresponding changes in the forest soil spectral intensities were seen. Chakraborty et al. (2015), Douglas et al. (2018), and Hong et al. (2019a) reported similar patterns and demonstrated that soil samples with higher PTE content showed lower spectral reflectance than soil samples with lower contamination levels, particularly in the spectral range of 700–2500 nm. It has also been proved that soil reflectance is decreased throughout the VIS–NIR region with increasing organic matter content (Kooistra et al., 2003). Nevertheless, as the soil horizon color varies due to PTE concentration (Douglas et al., 2018; Hong et al., 2019a), soil organic matter content (Ben-Dor et al., 2008), and structure (Zanella et al., 2017), it can influence soil spectra too (Gholizadeh et al., 2020). Therefore, in the H horizon, with darker color and fine and well-decomposed structure (Zanella et al., 2017), the reflectance absorbs more light energy, then the spectral curve decreases. Though intense bands in the

407 VIS–NIR spectra are not directly associated with the presence of PTEs, it
408 is clear that PTEs can bond and interact with the main spectrally active
409 components of soil such as SOC and different forms of Fe (Wu et al., 2005;
410 Song et al., 2012).

411 Based on Figure 4, the relationships of total Fe and SOC with PTE
412 exhibited different rates, which reflect different metal dependency in different
413 circumstances and horizons (Xie et al., 2012). The significant correlations
414 between total Fe and PTE for the datasets were moderate to high ($0.53 \leq$
415 $r \leq 0.89$), increasing by depth. SOC also displayed significant correlations
416 with all PTEs, with higher values in the F horizon. This difference between
417 horizons can be explained by the higher content of total Fe and SOC in
418 the H and F horizons, respectively (Table 2), and their capability of metal-
419 sorption (Wu et al., 2005). These findings reveal that these two soil properties
420 cannot be neglected during the PTE modelling process. In general, total Fe
421 showed higher correlations with the studied PTEs than SOC, showing in this
422 study that PTEs were more closely bound to Fe. Therefore, Fe significantly
423 influenced the estimation of PTE concentration from the reflectance spectra
424 of the forest soil samples. Thus, in the VIS–NIR spectral estimation of PTEs
425 in Czech forested sites, total Fe had higher priority to interact with the five
426 PTEs than with SOC. These results were similar to the results of Kemper
427 & Sommer (2002) in estimating Pb, as well as the results of Khosravi et al.
428 (2017) and Khosravi et al. (2018) in estimating As, Pb, and Zn. In contrast,
429 Chen et al. (2014) and Hong et al. (2019b) showed a higher correlation of SOC
430 with Zn and Pb compared to Fe forms. The differences in these mechanisms
431 may be caused by different soil-forming environments and land-use types in

432 various areas (Hong et al., 2019a).

433 In order to confirm our findings, the correlation coefficients between VIS–
434 NIR reflectance and PTEs across the spectral range (Figure 5) were assessed,
435 which represent the primary mechanism of estimating toxic elements by spec-
436 troscopy (Rathod et al., 2015; Khosravi et al., 2018). It can be seen that the
437 concentrations of toxic elements and total Fe in all horizons followed the same
438 pattern, with similar peaks and valleys, in their correlations with the VIS–
439 NIR reflectance of soil spectra. The highest positive correlations of PTEs
440 were in the VIS region (at about 460–590 nm), which are mainly attributed
441 to the presence of Fe-oxide (Ben-Dor, 2002; Xie et al., 2012; Gholizadeh et al.,
442 2018a). Similar results were also reported by Wu et al. (2005) and Wu et al.
443 (2007) regarding the substantial role of Fe in the spectral relation of PTEs.
444 These findings emphasize the importance of Fe in the spectral estimation of
445 PTEs in this study area, especially in the H and F + H horizons with high
446 concentrations of total Fe. Few SOC correlation features (specifically in the
447 F horizon) were consistent with those of PTE. In addition, the high negative
448 correlation of PTEs with the spectra was mainly identified at wavebands
449 of 1380–1450 nm and 1860–2000 nm (Xie et al., 2012), which are mostly
450 governed by the content of SOC and darkness of humic acid (Knadel et al.,
451 2013; Shi et al., 2015). Thus, the SOC related spectral features also need to
452 be considered in study of PTEs, suggesting that the role of SOC cannot be
453 ignored in the spectral modelling procedure of the examined PTEs in forest
454 soils of the Czech Republic. It should also be noted that the differences be-
455 tween soil horizons mirror the effects of the various soil attribute contents
456 and metal-sorption by Fe and SOC concentration.

457 The effectiveness of various ML predicting algorithms (PLSR, SVMR,
 458 and RF) and the DL technique (FNN) to extract PTE calibration models
 459 from the reflectance spectra of forest soil horizons in the VIS–NIR range was
 460 compared (Table 3). Different prediction accuracies were obtained, and their
 461 adequacy was evaluated based on maximal R^2 and minimal RMSE. Accord-
 462 ing to the evaluation criterion, among the studied PTEs, Cr and Al were
 463 the best predicted elements, whether they were based on ML or DL meth-
 464 ods. This was expected based on the strong positive correlation coefficients
 465 of these elements with VIS–NIR spectra (Figure 5). This may be linked to
 466 their high concentration and their strong internal relations with spectrally
 467 active soil components (Ben-Dor, 2002; Xie et al., 2012), especially total Fe
 468 in this study (Figure 5). For Zn and Cu, the R^2 and RMSE values of differ-
 469 ent methods were not as good as they were for the other elements, implying
 470 that the prediction models derived from VIS–NIR spectra were not able to
 471 handle Zn and Cu in forest soils of the Czech Republic (Table 3). Chodak
 472 et al. (2007), Xie et al. (2012), and Gholizadeh et al. (2015) obtained com-
 473 parable results when assessing these elements using VIS–NIR spectra using
 474 various ML methods. Chodak et al. (2007) mentioned that, since deposited
 475 PTEs can exist in an inorganic form (e.g., contained in deposited dust), they
 476 cannot be determined by VIS–NIR. Similarly, Siebielec et al. (2004) found
 477 that VIS–NIR spectroscopy underestimated the Zn and Cu contents in heav-
 478 ily polluted soils of Poland and ascribed the imprecise predictions of these
 479 elements to the presence of a large proportion of dustborne PTEs. Consid-
 480 ering forest soil horizons, it can be noticed that the H layer with high SD of
 481 PTE concentration (Table 2) was the most accurately assessed horizon using

482 ML algorithms. Kuang & Mouazen (2011) found that variability in the con-
483 centration range of PTEs significantly affects the performance of calibration
484 models, and a wider range and larger SD lead to higher accuracy. Of the
485 horizons, the H horizon had the largest SD values, which might explain its
486 high accuracy. Applying the FNN approach, the best prediction performance
487 was seen for the combined horizon (F + H). Due to the nature of DL, this
488 can be related to the bigger sample size (LeCun et al., 2015; Padarian et al.,
489 2018) at this merged dataset.

490 Compared to FNN, SVMR, and RF, PLSR showed the lowest modelling
491 accuracy in all cases. The reason is that PLSR is a linear method and does
492 not perform well in solving nonlinear-linear problems (Wei et al., 2019). It
493 is also apparent in Table 3 that among ML approaches, the best predictions
494 in nearly all cases, regardless of the soil element, were achieved by SVMR.
495 One may justify the superior performance of SVMR by its capability to ap-
496 proximate nonlinear functions between multidimensional space (Bilgili et al.,
497 2010; Gholizadeh et al., 2016). This algorithm can also derive linear hyper-
498 planes as a decision function for nonlinear problems, which reduces problems
499 with heterogeneity and nonlinearity and can be considered as another reason
500 for the method’s excellence (Clairotte et al., 2016). The superiority of the
501 SVMR technique has been proved in several studies related to soil parameter
502 prediction in general (Viscarra Rossel & Behrens, 2010; Araujo et al., 2014;
503 Jiang et al., 2019), and soil PTE assessment in particular (Gholizadeh et al.,
504 2015; Khosravi et al., 2017).

505 Considering the FNN results in Table 3, it can be noticed that in terms
506 of prediction capability, this DL method had the best predictability when

507 the number of samples was higher (F + H horizon), which indicates the
 508 robustness of FNN using larger sample sizes. In the individual layers (F
 509 and H), the model accuracy obtained from FNN was lower than (although
 510 comparable to) predictive models of SVMR and RF but still higher than
 511 PLSR. According to Jiang et al. (2019), the reason is that the SVMR and RF
 512 methods achieve maximum reliability for the prediction of smaller samples.
 513 Generally speaking, regarding the obtained results in the Czech Republic's
 514 forested sites, the examined DL technique (FNN) was considered to be the
 515 best theory for assessing PTEs (particularly Cr and Al) based on national
 516 spectral data when a large number of samples is accessible. However, if a
 517 small sample size is involved, it is better to couple SVMR with spectral data
 518 for modelling of PTEs. Nevertheless, future studies should still focus on
 519 better exploring the effects of different soil sample sizes, especially higher
 520 numbers of samples, on the performance of ML and DL calibration models
 521 using spectral data. Additionally, other DL architectures and algorithms
 522 need to be investigated to obtain better prediction accuracy.

523 **Conclusions**

524 This study explored the potential of the combined use of soil VIS–NIR
 525 spectroscopy and learning algorithms (ML and DL) in organic horizons of
 526 the Czech Republic's forested sites to model soil PTEs (Cr, Cu, Pb, Zn, and
 527 Al). PTE content was higher in the H horizon and the reflectance spectra
 528 decreased with increased soil PTE concentration. The darker color and well-
 529 decomposed structure of the H horizon and its capability of metal-sorption
 530 caused the absorbance of more light energy and the decline of the spectral

531 curve. PTEs showed the highest positive correlation with VIS–NIR spectra
 532 in the VIS region (at about 460–590 nm). The highest correlation among the
 533 studied parameters was observed between PTEs and total Fe content. These
 534 results highlight the importance of Fe in the spectral prediction of PTEs in
 535 this study area, particularly in the H and F + H horizons with higher total
 536 Fe content compared to the F layer. Among all PTEs, Cr and Al were the
 537 most accurately predicted elements regardless of the applied learning tech-
 538 nique, and the successful mechanism of their estimation by using reflectance
 539 spectroscopy was mainly described by their high correlation and close re-
 540 lationship with SOC and especially Fe as soil spectrally active attributes.
 541 Using the ML methods and a smaller sample size ($n = 1080$), SVMR and
 542 the H layer were the best algorithm and horizon for predicting PTEs ($R^2 =$
 543 0.88 and $RMSE = 3.01$ mg/kg, and $R^2 = 0.82$ and $RMSE = 1682.25$ mg/kg
 544 for Cr and Al, respectively). The FNN approach had the best performance
 545 in predicting PTEs (mainly Cr and Al: $R^2 = 0.89$ and $RMSE = 2.95$ mg/kg,
 546 and $R^2 = 0.86$ and $RMSE = 1593.64$ mg/kg, respectively) in the combined
 547 F + H horizon due to the larger sample size ($n = 2160$), which is a prereq-
 548 uisite for training in DL. In the F horizon, inadequate models (low R^2 and
 549 high RMSE) were obtained using all techniques. All in all, the proposed
 550 FNN model in this paper coupled with spectral data indicate the feasibility
 551 of modeling PTEs (Cr and Al) based on national spectral data in the forests
 552 of the Czech Republic.

553 Acknowledgement

554 The authors like to thank the financial support of the Czech Science
555 Foundation (project No. 18-28126Y). The authors also thank the Central
556 Institute for Supervising and Testing in Agriculture for providing the samples
557 and data. The kind efforts of Mr. Josef Kratina and Mr. Karel Nemecek
558 for soil spectra measurement and providing the study area detailed map are
559 greatly appreciated.

560 References

- 561 Aggarwal, C. C. (2013). Outlier ensembles: position paper. *ACM SIGKDD*
562 *Explorations Newsletter*, 14, 49. doi:10.1145/2481244.2481252.
- 563 Ahmed, A. M., Duran, O., Zweiri, Y., & Smith, M. (2019). Quantification of
564 Hydrocarbon Abundance in Soils Using Deep Learning with Dropout and
565 Hyperspectral Data. *Remote Sensing*, 11, 1938. doi:10.3390/rs11161938.
- 566 Alloway, B. J. (2013). Sources of heavy metals and metalloids in soils. In B. J.
567 Alloway (Ed.), *Heavy Metals in Soils: Trace Metals and Metalloids in Soils*
568 *and their Bioavailability* (pp. 11–50). Dordrecht: Springer Netherlands.
569 doi:10.1007/978-94-007-4470-7-2.
- 570 Araujo, S. R., Wetterlind, J., Dematt, J. A. M., & Stenberg, B. (2014).
571 Improving the prediction performance of a large tropical visNIR spectro-
572 scopic soil library from Brazil by clustering into smaller subsets or use of
573 data mining calibration techniques. *European Journal of Soil Science*, 65,
574 718–729. doi:10.1111/ejss.12165.

- 575 Arellano, P., Tansey, K., Balzter, H., & Boyd, D. S. (2015). Detect-
 576 ing the effects of hydrocarbon pollution in the Amazon forest using hy-
 577 perspectral satellite images. *Environmental Pollution*, 205, 225–239.
 578 doi:10.1016/j.envpol.2015.05.041.
- 579 Baciak, M., Warmiski, K., & Bes, A. (2015). The effect of selected gaseous
 580 air pollutants on woody plants. *Forest Research Papers*, 76, 401–409.
 581 doi:10.1515/frp-2015-0039.
- 582 Behrens, T., Schmidt, K., MacMillan, R. A., & Viscarra Rossel, R. (2018).
 583 Multi-scale digital soil mapping with deep learning. *Scientific Reports*, 8,
 584 15244. doi:10.1038/s41598-018-33516-6.
- 585 Bellon-Maurel, V., Fernandez-Ahumada, E., Palagos, B., Roger, J.-M., &
 586 McBratney, A. (2010). Critical review of chemometric indicators com-
 587 monly used for assessing the quality of the prediction of soil attributes by
 588 NIR spectroscopy. *TrAC Trends in Analytical Chemistry*, 29, 1073–1081.
 589 doi:10.1016/j.trac.2010.05.006.
- 590 Ben-Dor, E. (2002). Quantitative remote sensing of soil properties. In
 591 *Advances in Agronomy* (pp. 173 – 243). Academic Press volume 75.
 592 doi:10.1016/S0065-2113(02)75005-0.
- 593 Ben-Dor, E., & Banin, A. (1995). Near-Infrared Analysis as a Rapid Method
 594 to Simultaneously Evaluate Several Soil Properties. *Soil Science Society*
 595 *of America Journal*, 59. doi:10.2136/sssaj1995.03615995005900020014x.
- 596 Ben-Dor, E., Heller, D., & Chudnovsky, A. (2008). A Novel Method of

- 597 Classifying Soil Profiles in the Field using Optical Means. *Soil Science*
598 *Society of America Journal*, 72, 1113. doi:10.2136/sssaj2006.0059.
- 599 Bilgili, A. V., Es, H. v., Akbas, F., Durak, A., & Hively, W. (2010). Visible-
600 near infrared reflectance spectroscopy for assessment of soil properties in
601 a semi-arid area of Turkey. *Journal of Arid Environments*, 74, 229–238.
602 doi:10.1016/j.jaridenv.2009.08.011.
- 603 Boruvka, L., Sramek, V., Cupr, P., Fadrhonsova, V., Hofman, J., Houska, J.,
604 Sanka, O., Slavikova, A. A., Sindelarova, L., Tejnecky, V., Vasckova, J.,
605 Sanka, M., Cechmankova, J., Drabek, O., Frankova, A., Horvathova, V.,
606 Rotter, P., Skala, J., Novotny, R., Shudoma, M., Vacha, R., & Jurkovska,
607 L. (2015). *Srovnávací hodnoty pro hodnocení kontaminace lesních půd: cer-*
608 *tifikovaná metodika. - Strnady: Výzkumný ústav lesního hospodářství a*
609 *myšlivosti*. Strnady: Vzkumn stav lesního hospodství a myšlivosti.
- 610 Boska, E., Lasota, J., Szuszkiewicz, M., ukasik, A., & Klamerus-Iwan, A.
611 (2016). Assessment of forest soil contamination in Krakow surroundings
612 in relation to the type of stand. *Environmental Earth Sciences*, 75, 1205.
613 doi:10.1007/s12665-016-6005-7.
- 614 Chakraborty, S., Weindorf, D. C., Li, B., Aldabaa], A. A. A., Ghosh,
615 R. K., Paul, S., & Ali], M. N. (2015). Development of a hybrid
616 proximal sensing method for rapid identification of petroleum contam-
617 inated soils. *Science of The Total Environment*, 514, 399 – 408.
618 doi:10.1016/j.scitotenv.2015.01.087.
- 619 Chang, C.-W., Laird, D. A., Mausbach, M. J., & Hurburgh, C. R. (2001).

- 620 Near-Infrared Reflectance Spectroscopy-Principal Components Regression
621 Analyses of Soil Properties. *Soil Science Society of America Journal*, 65,
622 480–490. doi:10.2136/sssaj2001.652480x.
- 623 Chen, Y., Lin, Z., Zhao, X., Wang, G., & Gu, Y. (2014). Deep Learning-
624 Based Classification of Hyperspectral Data. *IEEE Journal of Selected*
625 *Topics in Applied Earth Observations and Remote Sensing*, 7, 2094–2107.
626 doi:10.1109/jstars.2014.2329330.
- 627 Chodak, M., Khanna, P., Horvath, B., & Beese, F. (2004). Near Infrared
628 Spectroscopy for Determination of Total and Exchangeable Cations in
629 Geologically Heterogeneous Forest Soils. *Journal of Near Infrared Spec-*
630 *troscopy*, 12, 315–324. doi:10.1255/jnirs.440.
- 631 Chodak, M., Nikliska, M., & Beese, F. (2007). Near-infrared spectroscopy
632 for analysis of chemical and microbiological properties of forest soil organic
633 horizons in a heavy-metal-polluted area. *Biology and Fertility of Soils*, 44,
634 171–180. doi:10.1007/s00374-007-0192-z.
- 635 Clairotte, M., Grinand, C., Kouakoua, E., Thbault, A., Saby, N. P., Bernoux,
636 M., & Barths, B. G. (2016). National calibration of soil organic carbon
637 concentration using diffuse infrared reflectance spectroscopy. *Geoderma*,
638 276, 41–52. doi:10.1016/j.geoderma.2016.04.021.
- 639 ČSN EN ISO 11267 (2014). *Kvalita pudy - Inhibice reprodukce chvostoskoku*
640 *(Folsomia candida) látkami znečišťujícími pudy.*
- 641 Czech Statistical Office (2019). Surveying, mapping and cadastre. URL:
642 <https://vdb.czso.cz>.

- 643 Douglas, R., Nawar, S., Alamar, M., Mouazen, A., & Coulon, F.
644 (2018). Rapid prediction of total petroleum hydrocarbons concen-
645 tration in contaminated soil using vis-nir spectroscopy and regression
646 techniques. *Science of The Total Environment*, 616-617, 147 – 155.
647 doi:10.1016/j.scitotenv.2017.10.323.
- 648 Du, C., & Zhou, J. (2011). Application of Infrared Photoacoustic Spec-
649 troscopy in Soil Analysis. *Applied Spectroscopy Reviews*, 46, 405–422.
650 doi:10.1080/05704928.2011.570837.
- 651 Ferreira, E. C., Milori, D. M. B. P., Ferreira, E. J., Silva, R. M. D., &
652 Martin-Neto, L. (2008). Artificial neural network for Cu quantitative deter-
653 mination in soil using a portable Laser Induced Breakdown Spectroscopy
654 system. *Spectrochimica Acta Part B: Atomic Spectroscopy*, 63, 1216–1220.
655 doi:10.1016/j.sab.2008.08.016.
- 656 Fiala, P., Reininger, D., Samek, T., Nemec, P., & Susil, A. (2013). *Pružkum*
657 *vyzivy lesa na uzemi Ceske Republiky 19962011*. Technical Report Central
658 Institute for Supervising and Testing in Agriculture.
- 659 Fujii, K., Ikeda, S., Akama, A., Komatsu, M., Takahashi, M., & Kaneko, S.
660 (2014). Vertical migration of radiocesium and clay mineral composition in
661 five forest soils contaminated by the Fukushima nuclear accident. *Soil Sci-*
662 *ence and Plant Nutrition*, 60, 751–764. doi:10.1080/00380768.2014.926781.
- 663 Gholizadeh, A., Boruvka, L., Saberioon, M., & Vasat, R. (2016). A Memory-
664 Based Learning Approach as Compared to Other Data Mining Algorithms

665 for the Prediction of Soil Texture Using Diffuse Reflectance Spectra. *Re-*
666 *mote sensing*, 8. doi:10.3390/rs8040341.

667 Gholizadeh, A., Boruvka, L., Vat, R., Saberioon, M., Klement, A., Kratina,
668 J., Tejnecky, V., & Drabek, O. (2015). Estimation of Potentially Toxic
669 Elements Contamination in Anthropogenic Soils on a Brown Coal Mining
670 Dumpsite by Reflectance Spectroscopy: A Case Study. *PLoS ONE*, 10.
671 doi:10.1371/journal.pone.0117457.

672 Gholizadeh, A., & Kopackova, V. (2019). Detecting vegetation stress as a
673 soil contamination proxy: a review of optical proximal and remote sensing
674 techniques. *International Journal of Environmental Science and Technol-*
675 *ogy*, 16, 2511–2524. doi:10.1007/s13762-019-02310-w.

676 Gholizadeh, A., Saberioon, M., Ben-Dor, E., & Borvka, L. (2018a). Mon-
677 itoring of selected soil contaminants using proximal and remote sens-
678 ing techniques: Background, state-of-the-art and future perspectives.
679 *Critical Reviews in Environmental Science and Technology*, (pp. 1–36).
680 doi:10.1080/10643389.2018.1447717.

681 Gholizadeh, A., Saberioon, M., Carmon, N., Boruvka, L., & Ben-Dor, E.
682 (2018b). Examining the Performance of PARACUDA-II Data-Mining En-
683 gine versus Selected Techniques to Model Soil Carbon from Reflectance
684 Spectra. *Remote Sensing*, 10, 1172. doi:10.3390/rs10081172.

685 Gholizadeh, A., Saberioon, M., Viscarra Rossel, R., Boruvka, L., & Kle-
686 ment, A. (2020). Spectroscopic measurements and imaging of soil colour

687 for field scale estimation of soil organic carbon. *Geoderma*, 357, 113972.
688 doi:10.1016/j.geoderma.2019.113972.

689 Gholizadeh, A., ZiZala, D., Saberioon, M., & Borvka, L. (2018c). Soil organic
690 carbon and texture retrieving and mapping using proximal, airborne and
691 Sentinel-2 spectral imaging. *Remote Sensing of Environment*, 218, 89–103.
692 doi:10.1016/j.rse.2018.09.015.

693 Gitelson, A. A., Zur, Y., Chivkunova, O. B., & Merzlyak, M. N.
694 (2002). Assessing Carotenoid Content in Plant Leaves with Re-
695 flectance Spectroscopy. *Photochemistry and Photobiology*, 75, 272–281.
696 doi:10.1562/0031-8655(2002)0750272ACCIPL2.0.CO2.

697 Gomez, C., Gholizadeh, A., Borvka, L., & Lagacherie, P. (2016). Us-
698 ing legacy data for correction of soil surface clay content predicted from
699 VNIR/SWIR hyperspectral airborne images. *Geoderma*, 276, 84–92.
700 doi:10.1016/j.geoderma.2016.04.019.

701 Hang, X., Wang, H., Zhou, J., Ma, C., Du, C., & Chen, X. (2009). Risk
702 assessment of potentially toxic element pollution in soils and rice (*Oryza*
703 *sativa*) in a typical area of the Yangtze River Delta. *Environmental Pol-*
704 *lution*, 157, 2542–2549. doi:10.1016/j.envpol.2009.03.002.

705 Hastie, T., Tibshirani, R., & Friedman, J. (2009). *The Elements of Statistical*
706 *Learning: Data Mining, Inference and Prediction*. New York, NY, USA:
707 Springer.

708 Hong, Y., Shen, R., Cheng, H., Chen, S., Chen, Y., Guo, L., He, J., Liu,
709 Y., Yu, L., & Liu, Y. (2019a). Cadmium concentration estimation in

- 710 peri-urban agricultural soils: Using reflectance spectroscopy, soil auxil-
 711 iary information, or a combination of both? *Geoderma*, *354*, 113875.
 712 doi:10.1016/j.geoderma.2019.07.033.
- 713 Hong, Y., Shen, R., Cheng, H., Chen, Y., Zhang, Y., Liu, Y.,
 714 Zhou, M., Yu, L., Liu, Y., & Liu, Y. (2019b). Estimating lead
 715 and zinc concentrations in peri-urban agricultural soils through re-
 716 flectance spectroscopy: Effects of fractional-order derivative and ran-
 717 dom forest. *Science of The Total Environment*, *651*, 1969 – 1982.
 718 doi:https://doi.org/10.1016/j.scitotenv.2018.09.391.
- 719 ISO 11466:1995 (1995). *Soil Quality Extraction of Trace Elements Soluble*
 720 *in Aqua Regia*. Standard International Organization for Standardization
 721 Geneva, CH.
- 722 Jiang, H., Rusuli, Y., Amuti, T., & He, Q. (2019). Quantitative assessment of
 723 soil salinity using multi-source remote sensing data based on the support
 724 vector machine and artificial neural network. *International Journal of*
 725 *Remote Sensing*, *40*, 284–306. doi:10.1080/01431161.2018.1513180.
- 726 Kemper, T., & Sommer, S. (2002). Estimate of Heavy Metal Contamination
 727 in Soils after a Mining Accident Using Reflectance Spectroscopy. *Environ-*
 728 *mental Science & Technology*, *36*, 2742–2747. doi:10.1021/es015747j.
- 729 Khosravi, V., Ardejani, F. D., & Yousefi, S. (2017). Spectroscopic-based as-
 730 sessment of the content and geochemical behaviour of arsenic in a highly
 731 heterogeneous sulphide-rich mine waste dump. *Environmental Earth Sci-*
 732 *ences*, *76*, 459. doi:10.1007/s12665-017-6793-4.

- 733 Khosravi, V., Ardejani, F. D., Yousefi, S., & Aryafar, A. (2018). Monitoring
734 soil lead and zinc contents via combination of spectroscopy with extreme
735 learning machine and other data mining methods. *Geoderma*, *318*, 29–41.
736 doi:10.1016/j.geoderma.2017.12.025.
- 737 Knadel, M., Viscarra Rossel, R., Deng, F., Thomsen, A., & Greve, M. H.
738 (2013). VisibleNear Infrared Spectra as a Proxy for Topsoil Texture and
739 Glacial Boundaries. *Soil Science Society of America Journal*, *77*, 568–579.
740 doi:10.2136/sssaj2012.0093.
- 741 Kooistra, L., Wanders, J., Epema, G., Leuven, R., Wehrens, R., & Buy-
742 dens, L. (2003). The potential of field spectroscopy for the assessment
743 of sediment properties in river floodplains. *Analytica Chimica Acta*, *484*,
744 189–200. doi:10.1016/s0003-2670(03)00331-3.
- 745 Kuang, B., & Mouazen, A. (2011). Calibration of visible and near in-
746 frared spectroscopy for soil analysis at the field scale on three European
747 farms. *European Journal of Soil Science*, *62*, 629–636. doi:10.1111/j.1365-
748 2389.2011.01358.x.
- 749 LeCun, Y., Bengio, Y., & Hinton, G. (2015). Deep learning. *Nature*, *521*,
750 436. doi:10.1038/nature14539.
- 751 Li, J., Xi, B., Li, Y., Du, Q., & Wang, K. (2018). Hyperspectral Classification
752 Based on Texture Feature Enhancement and Deep Belief Networks. *Remote*
753 *Sensing*, *10*, 396. doi:10.3390/rs10030396.
- 754 Liu, M., Wang, T., Skidmore, A. K., & Liu, X. (2018a). Heavy metal-
755 induced stress in rice crops detected using multi-temporal Sentinel-

- 756 2 satellite images. *Science of The Total Environment*, 637, 18–29.
757 doi:10.1016/j.scitotenv.2018.04.415.
- 758 Liu, X., Liu, F., Huang, W., Peng, J., Shen, T., & He, Y. (2018b).
759 Quantitative Determination of Cd in Soil Using Laser-Induced Break-
760 down Spectroscopy in Air and Ar Conditions. *Molecules*, 23, 2492.
761 doi:10.3390/molecules23102492.
- 762 Ludwig, B., & Khanna, P. (2001). Use of near infrared spectroscopy to
763 determine inorganic and organic carbon fractions in soil and litter. In
764 R. Lal, J. Kimble, R. Follett, & B. Stewart (Eds.), *Assessment methods*
765 *for soil carbon*. (pp. 361–370). CRC/Lewis Publishers.
- 766 Ng, W., Minasny, B., & McBratney, A. (2019). Convolutional Neu-
767 ral Network for soil microplastic contamination screening using in-
768 frared spectroscopy. *Science of The Total Environment*, (p. 134723).
769 doi:10.1016/j.scitotenv.2019.134723.
- 770 Ogen, Y., Goldshleger, N., & Ben-Dor, E. (2017). 3D spectral analysis in
771 the VNIRSWIR spectral region as a tool for soil classification. *Geoderma*,
772 302, 100–110. doi:10.1016/j.geoderma.2017.04.020.
- 773 Padarian, J., Minasny, B., & McBratney, A. (2018). Using deep learning to
774 predict soil properties from regional spectral data. *Geoderma Regional*,
775 16, e00198. doi:10.1016/j.geodrs.2018.e00198.
- 776 Panchenko, T., Pradivlyana, A., & Ursul, O. (2018). Estimation of the
777 influence of thermal energy objects on the environment. In *Materialy*

- 778 *XLVII Naukovo-Tekhnichnoyi Konferentsiyi Pidrozdiliv VNTU, Vinnytsya*
 779 *sya* (p. 4574). URL: [https://conferences.vntu.edu.ua/index.php/](https://conferences.vntu.edu.ua/index.php/all-fksa/all-fksa-2018/paper/view/4574)
 780 [all-fksa/all-fksa-2018/paper/view/4574](https://conferences.vntu.edu.ua/index.php/all-fksa/all-fksa-2018/paper/view/4574).
- 781 Pavlu, L., Drbek, O., Borvka, L., Nikodem, A., & Nmeek, K. (2016). Degrada-
 782 tion of forest soils in the vicinity of an industrial zone. *Soil and Water*
 783 *Research*, 10, 65–73. doi:10.17221/220/2014-swr.
- 784 Percy, K. E., & Ferretti, M. (2004). Air pollution and forest health: to-
 785 ward new monitoring concepts. *Environmental Pollution*, 130, 113–126.
 786 doi:10.1016/j.envpol.2003.10.034.
- 787 Plyatsuk, L. D., Chernysh, Y. Y., Ablicieva, I. Y., Yakhnenko, O. M., Batalt-
 788 sev, E. V., Balintova, M., & Hurets, L. L. (2019). Remediation of Soil
 789 Contaminated with Heavy Metals. *Journal of Engineering Sciences*, 6,
 790 h1–h8. doi:10.21272/jes.2019.6(1).h1.
- 791 Qian, N. (1999). On the momentum term in gradient descent learning algo-
 792 rithms. *Neural Networks*, 12, 145 – 151. doi:10.1016/S0893-6080(98)00116-
 793 6.
- 794 Rafferty, B., Brennan, M., Dawson, D., & Dowding, D. (2000). Mechanisms
 795 of ¹³⁷Cs migration in coniferous forest soils. *Journal of Environmental*
 796 *Radioactivity*, 48, 131–143. doi:10.1016/s0265-931x(99)00027-2.
- 797 Rathod, P. H., Mller, I., Meer, F. D. V. d., & Smeth, B. d. (2015). Analysis
 798 of visible and near infrared spectral reflectance for assessing metals in soil.
 799 *Environmental monitoring and assessment*, 188, 558. doi:10.1007/s10661-
 800 016-5568-9.

- 801 Reimann, C., & Caritat, P. d. (2000). Intrinsic Flaws of Element Enrichment
802 Factors (EFs) in Environmental Geochemistry. *Environmental Science &*
803 *Technology*, *34*, 5084–5091. doi:10.1021/es001339o.
- 804 Ren, H.-Y., Zhuang, D.-F., Singh, A., Pan, J.-J., Qiu, D.-S., & Shi, R.-
805 H. (2009). Estimation of As and Cu Contamination in Agricultural Soils
806 Around a Mining Area by Reflectance Spectroscopy: A Case Study. *Pe-*
807 *dosphere*, *19*. doi:10.1016/S1002-0160(09)60167-3.
- 808 Savitzky, A., & Golay, M. (1964). Smoothing and Differentiation of
809 Data by Simplified Least Squares Procedures. *Analytical Chemistry*, *36*.
810 doi:10.1021/ac60214a047.
- 811 Shand, C. A., Cheshire, M. V., Smith, S., Vidal, M., & Rauret, G. (1994).
812 Distribution of radiocaesium in organic soils. *Journal of Environmental*
813 *Radioactivity*, *23*, 285–302. doi:10.1016/0265-931x(94)90067-1.
- 814 Sherman, D. M., & Waite, T. D. (1985). Electronic spectra of Fe^{3+} oxides and
815 oxyhydroxides in the near infrared to ultraviolet. *American Mineralogist*,
816 *70*, 1262–1269.
- 817 Shi, T., Guo, L., Chen, Y., Wang, W., Shi, Z., Li, Q., & Wu, G. (2018).
818 Proximal and remote sensing techniques for mapping of soil contam-
819 ination with heavy metals. *Applied Spectroscopy Reviews*, *53*, 1–23.
820 doi:10.1080/05704928.2018.1442346.
- 821 Shi, T., Wang, J., Chen, Y., & Wu, G. (2016). Improving the prediction
822 of arsenic contents in agricultural soils by combining the reflectance spec-

823 troscopy of soils and rice plants. *International Journal of Applied Earth Ob-*
824 *servation and Geoinformation*, *52*, 95–103. doi:10.1016/j.jag.2016.06.002.

825 Shi, Z., Ji, W., Viscarra Rossel, R. A., Chen, S., & Zhou, Y. (2015). Pre-
826 diction of soil organic matter using a spatially constrained local partial
827 least squares regression and the chinese visnir spectral library. *European*
828 *Journal of Soil Science*, *66*, 679–687. doi:10.1111/ejss.12272.

829 Siebielec, G., McCarty, G. W., Stuczynski, T. I., & Reeves, J. B. (2004).
830 Near- and Mid-Infrared Diffuse Reflectance Spectroscopy for Measuring
831 Soil Metal Content. *Journal of Environmental Quality*, *33*, 2056–2069.
832 doi:10.2134/jeq2004.2056.

833 Sihag, P., Keshavarzi, A., & Kumar, V. (2019). Comparison of different
834 approaches for modeling of heavy metal estimations. *SN Applied Sciences*,
835 *1*, 780. doi:10.1007/s42452-019-0816-6.

836 Smith, P., House, J. I., Bustamante, M., Sobock, J., Harper, R., Pan, G.,
837 West, P. C., Clark, J. M., Adhya, T., Rumpel, C., Paustian, K., Kuikman,
838 P., Cotrufo, M. F., Elliott, J. A., McDowell, R., Griffiths, R. I., Asakawa,
839 S., Bondeau, A., Jain, A. K., Meersmans, J., & Pugh, T. A. M. (2015).
840 Global change pressures on soils from land use and management. *Global*
841 *change biology*, *22*, 1008–28. doi:10.1111/gcb.13068.

842 Song, Y., Li, F., Yang, Z., Ayoko, G. A., Frost, R. L., & Ji, J. (2012). Diffuse
843 reflectance spectroscopy for monitoring potentially toxic elements in the
844 agricultural soils of Changjiang River Delta, China. *Applied Clay Science*,
845 *64*, 75–83. doi:10.1016/j.clay.2011.09.010.

- 846 Sparks, D. (1996). *Methods of Soil Analysis. Part 3 Chemical Methods..*
 847 Madison, WI, USA: Soil Science Society of America, American Society of
 848 Agronomy.
- 849 Srivastava, V., Sarkar, A., Singh, S., Singh, P., Araujo, A. S. F. d., & Singh,
 850 R. P. (2017). Agroecological Responses of Heavy Metal Pollution with
 851 Special Emphasis on Soil Health and Plant Performances. *Frontiers in*
 852 *Environmental Science*, 5, 64. doi:10.3389/fenvs.2017.00064.
- 853 Stevenson, F. (1994). *Humus Chemistry. Genesis, Composition, Reactions.*
 854 John Wiley & Sons.
- 855 Su, C., Jiang, L., & Zhang, W. (2014). A review on heavy metal contamina-
 856 tion in the soil worldwide: Situation, impact and remediation techniques.
 857 *Environmental Skeptics and Critics*, 3, 24–38.
- 858 Suchara, I., & Sucharov, J. (2002). Distribution of Sulphur and Heavy Met-
 859 als in Forest Floor Humus of the Czech Republic. *Water, Air, and Soil*
 860 *Pollution*, 136, 289–316. doi:10.1023/a:1015235924991.
- 861 Sucharova, J., Suchara, I., Hola, M., Reimann, C., Boyd, R., Filzmoser, P., &
 862 Englmaier, P. (2011). Linking chemical elements in forest floor humus (Oh-
 863 horizon) in the Czech Republic to contamination sources. *Environmental*
 864 *Pollution*, 159, 1205–1214. doi:10.1016/j.envpol.2011.01.041.
- 865 Sun, Y., Zhou, Q., Xie, X., & Liu, R. (2009). Spatial, sources and risk
 866 assessment of heavy metal contamination of urban soils in typical re-
 867 gions of Shenyang, China. *Journal of hazardous materials*, 174, 455–62.
 868 doi:10.1016/j.jhazmat.2009.09.074.

- 869 Tziolas, N., Tsakiridis, N., Ben-Dor, E., Theocharis, J., & Zalidis, G. (2020).
870 Employing a multi-input deep convolutional neural network to derive soil
871 clay content from a synergy of multi-temporal optical and radar imagery
872 data. *Remote sensing*, *12*. doi:10.3390/rs12091389.
- 873 Tzvetkova, N., Malinova, L., Doncheva, M., Bezlova, D., Petkova, K., Kara-
874 toteva, D., & Venkova, R. (2016). Soil contamination in forest and indus-
875 trial regions of bulgaria. In *Soil Contamination - Current Consequences*
876 *and Further Solutions*. doi:10.5772/64716.
- 877 Viscarra Rossel, R., & Behrens, T. (2010). Using data mining to
878 model and interpret soil diffuse reflectance spectra. *Geoderma*, *158*.
879 doi:10.1016/j.geoderma.2009.12.025.
- 880 Viscarra Rossel, R., & Hicks, W. S. (2015). Soil organic carbon and its
881 fractions estimated by visible/near infrared transfer functions. *European*
882 *Journal of Soil Science*, *66*, 438–450. doi:10.1111/ejss.12237.
- 883 Viscarra Rossel, R., Lee, J., Behrens, T., Luo, Z., Baldock, J., & Richards,
884 A. (2019). Continental-scale soil carbon composition and vulnerability
885 modulated by regional environmental controls. *Nature Geoscience*, *12*,
886 547–552. doi:10.1038/s41561-019-0373-z.
- 887 Walker, D. J., Clemente, R., & Bernal, M. P. (2004). Contrasting effects
888 of manure and compost on soil pH, heavy metal availability and growth
889 of *Chenopodium album* L. in a soil contaminated by pyritic mine waste.
890 *Chemosphere*, *57*, 215–224. doi:10.1016/j.chemosphere.2004.05.020.

- 891 Wall, D. H., Nielsen, U. N., & Six, J. (2015). Soil biodiversity and human
892 health. *Nature*, *528*, 69–76. doi:10.1038/nature15744.
- 893 Wei, L., Yuan, Z., Yu, M., Huang, C., & Cao, L. (2019). Estimation of Arsenic
894 Content in Soil Based on Laboratory and Field Reflectance Spectroscopy.
895 *Sensors*, *19*, 3904. doi:10.3390/s19183904.
- 896 Wilding, L. (1985). Spatial variability: its documentation, accomodation
897 and implication to soil surveys. In J. PBouma, & D. R. Nielsen (Eds.),
898 *Workshop on Soil spatial variability*.
- 899 Wu, Y., Chen, J., Ji, J., Gong, P., Liao, Q., Tian, Q., & Ma., H. (2007). A
900 mechanism study of reflectance spectroscopy for investigating heavy metals
901 in soils. *Soil Sci. Soc. Am. J.*, *71*, 918–926. doi:10.2136/sssaj2006.0285.
- 902 Wu, Y., Chen, J., Wu, X., Tian, Q., Ji, J., & Qin, Z. (2005). Pos-
903 sibilities of reflectance spectroscopy for the assessment of contaminant
904 elements in suburban soils. *Applied Geochemistry*, *20*, 1051–1059.
905 doi:10.1016/j.apgeochem.2005.01.009.
- 906 Xie, X.-L., Pan, X.-Z., & Sun, B. (2012). Visible and Near-Infrared Diffuse
907 Reflectance Spectroscopy for Prediction of Soil Properties near a Copper
908 Smelter. *Pedosphere*, *22*. doi:10.1016/S1002-0160(12)60022-8.
- 909 Yang, J., Xu, J., Zhang, X., Wu, C., Lin, T., & Ying, Y. (2019). Deep
910 learning for vibrational spectral analysis: Recent progress and a practical
911 guide. *Analytica Chimica Acta*, . doi:10.1016/j.aca.2019.06.012.
- 912 Zanella, A., Ponge, J.-F., Jabiol, B., Sartori, G., Kolb, E., Gobat, J.-M.,
913 Bayon, R.-C. L., Aubert, M., Waal, R. D., Delft, B. V., Vacca, A.,

- 914 Serra, G., Chersich, S., Andreetta, A., Cools, N., Englisch, M., Hager, H.,
915 Katzensteiner, K., Brthes, A., Nicola, C. D., Testi, A., Bernier, N., Graefe,
916 U., Juilleret, J., Banas, D., Garlato, A., Obber, S., Galvan, P., Zampedri,
917 R., Frizzera, L., Tomasi, M., Menardi, R., Fontanella, F., Filoso, C., Di-
918 bona, R., Bolzonella, C., Pizzeghello, D., Carletti, P., Langohr, R., Cat-
919 taneo, D., Nardi, S., Nicolini, G., & Viola, F. (2017). Humusica 1, article
920 4: Terrestrial humus systems and formsSpecific terms and diagnostic hori-
921 zons. *Applied Soil Ecology*, 122, 56–74. doi:10.1016/j.apsoil.2017.07.005.
- 922 Zhang, X.-Y., Bengio, Y., & Liu, C.-L. (2017). Online and offline handwrit-
923 ten Chinese character recognition: A comprehensive study and new bench-
924 mark. *Pattern Recognition*, 61, 348–360. doi:10.1016/j.patcog.2016.08.005.