Investigating the Spatial Variability in Soil Geochemical and Colour Properties Across Two Contrasting Land Uses

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Abstract

Quantification and accurate assessment of the spatial variability and distribution of soil physical and biogeochemical properties are vital components of agri-environmental research and modeling, including sediment source fingerprinting. Understanding the distribution of soil properties is crucial in the development of appropriate, reliable, and efficient sampling campaigns. This study was aimed to investigate the spatial variability in soil geochemical and colour (i.e., spectral reflectance) soil properties (<63um) across two contrasting land uses. The main objectives of this study are to: 1) quantify the spatial variability of geochemical and colour properties at a field-scale (~ 40 ha) across agricultural and forested sites; 2) evaluate the spatial variability and distribution of soil properties and its relation to seven terrain attributes (e.g., catchment area, elevation). A combination of univariate analysis and geostatistical methods were applied to characterize the soil geochemistry and colour properties. This information was used to both quantify and assess the variability in soil properties. The variability and spatial autocorrelation were generally both site and soil property specific. For a selection of soil properties exhibiting some spatial autocorrelation, random forest regression was used to indentify the relative importance of terrain attributes on observed patterns of soil geochemical and colour properties. Elevation was found to explain the greatest amount of the variation in soil properties followed by the SAGA wetness index and relative slope position. These

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types of information can be used to help create efficient soil sampling designs by providing information that can inform sampling locations and number of samples collected in order to meet research needs and objectives.

Keywords: Soil geochemistry, Soil colour, Spatial analysis

1. Introduction

Variation in soil biological, chemical, and physical properties occurs across the landscape and in response to both regional and local (i.e., field-scale) variations in the five soil forming factors: parent material, relief or topography, biota, climate, and time. Superimposed on this is the influence of changes in land use and current and historic management practices which can further modify soil properties. Quantifying and understanding the patterns and drivers for this variation is an important component of many agri-environmental studies. For example, to meet the desired level of precision for agronomic and environmental nutrient management plans the spatial variability in soil nutrients will influence the soil sampling design in terms of number and locations of soil samples [1, 2].

Sediment source fingerprinting is a watershed-scale technique that is used to identify and quantify the relative proportions of sediment derived from unique sources. This technique uses natural occurring biogeochemical properties as fingerprints (i.e., tracers) to discriminate between potential sources of sediment and are linked to downstream sediment using mixing models. From a sediment fingerprinting perspective, investigating the spatial variability of soil properties at a watershed-scale can be advantageous to identify, classify, and distinguish between potential sources of sediment [3]. However, investigating spatial variability at smaller scales is less common [e.g., 4, 5, 6, 7] and remains a research priority [8].

There are three main, interconnected, ways that spatial variability in fingerprint properties are an important aspect of sediment fingerprinting. First is to adequately quantify the fingerprint properties such that it is representative of that source. For some fingerprints the variability is not random but rather varies in a more systematic way. For example, the pattern of fallout radionuclides will reflect the patterns of soil erosion and deposition [9]. Designing and implementing source sampling plans need to take this into consideration as the sampling designed used has been shown to influence the characterization of wide range of commonly used fingerprints [7].

Secondly, the issue of spatial variability of fingerprint properties is further complicated by overlying spatial variability in the rates of erosion and sediment delivery. Incorporation of both types of variability into the mixing model will provide a more reliable estimate of the proportion of sediment derived from each source. Many mixing models have well defined inputs (sources) and outputs (sediment) that are characterized by their mean and standard deviation and the spatial distribution or pattern of fingerprints are not considered. This is not ideal as the values of samples that are collected closer, and more hydrologically connected, to the stream network may in fact a better representation of that source despite potentially deviating from the mean value. This issue can be addressed by strategic sampling where the more likely to erode areas are targeted for sampling. However, a considerable amount of information and insight is lost through that approach. There has been some progress using information on erosion rates to calculate a erosion rate-weighted mean [9, 4] and using spatially interpolated maps of fingerprint values to provided a finer resolution of the fingerprint variability within each source [10].

Secondly, understanding the geomorphic, hydrologic, and biochemical processes that have led to the observed patterns in spatial variability helps in the selection of robust and reliable fingerprints and/or guide the sampling design for source characterization. In selecting fingerprints that provide good discrimination between sources many studies typically used a statistical-based approach [11]. However, there are concerns that this approach may result in the inclusion of false positives (i.e., type I error) or non-conservative fingerprints [12]. Consequently, there has been a call for the inclusion of a process-based (e.g., weathering, erosion) or geologic/lithologic-based explanation of the fingerprints selected to address these concerns [8]. Furthermore, there is also a lack of standardization in how sediment source areas are sampled (e.g., judgement, random, transect, grid, stratified) and it can be difficult to have an efficient sampling design without prior knowledge of why and how soil properties vary across the landscape [7]. Prior knowledge of the spatial variability of soil fingerprint properties would be beneficial; however, in practice this can be difficult, particularly with geochemical properties as routine lab analysis often return information on more than 50 elements. The spatial patterns of some soil properties are well studied because of their agronomic importance or ability to infer other important soil properties and processes and can include fallout radionuclides [e.g., ^{137}Cs, ^{7}Be; [13]], plant nutrients [e.g., N, P; [14]], soil colour [e.g., hue, value; [15]], major non-acid forming cations [e.g., Ca, Na; [16]]. In contrast, other soil properties including rare Earth elements and trace metals the processes leading to their distribution across the landscape is less studied or it is difficult to make generalizations (i.e., site specific).

Terrain attributes such as elevation, slope curvature, slope position, and soil wetness have been shown to be useful information in the understanding and modelling of a range of soil properties including soil moisture [17], texture [18], colour [19], organic matter [20], conductivity [21], and geochemistry [22]. Similar techniques may provide additional insight into the pedologic and geomorphic processes that drive the observed patterns of fingerprint properties within a given source. This information can be used to guide sampling design and interpret the data it provides.

This study builds on the previous work of Luna Miño [7] where the impact of three different sampling designs on the characterization of source materials, within the framework of the sediment fingerprinting approach, was assessed.

This study expands that study by using the data from grid sampling approach to assess the spatial autocorrelation, create iso-fingerprint maps, and identify important terrain attributes driving the observed patterns. The objectives of this study were (1) to investigate the spatial variability of a range of soil colour and geochemical properties in an agricultural and forested site; and (2) to assess the relative importance and correlation of terrain attributes with the spatial distribution of these soil properties.

2. Methods

2.1. Site description

Two sites of contrasting land uses located in the Wilson Creek Watershed (WCW), near McCreary, Manitoba, Canada were selected to investigate the spatial variability in fingerprint properties. The headwaters of the WCW are located on top of the Manitoba Escarpment within the boundary of Riding Mountain National Park. There is a ~300m drop in elevation crosses the escarpment where the streams become deeply incised. At the base of the escarpment is a large alluvial fan situated in the lacustrine deposits of glacial lake Aggasiz where the main stem has a meandering form. However, beyond the national park boundary the stream flows straight through an engineered drain until it reaches the Turtle river (Figure 1). Both sites are both hydrologicaly connected to the mainstem of the Wilson Creek

The first site was a mixedwood forest including white and black spruce (Picea glauca, Picea mariana), balsam fir (Abies balsamea), larch (Larix laricina) and young stands of deciduous trees including trembling aspen (Populus tremuloides). The forested site is located within the boundaries of the national park where there is little disturbance beyond recreational hiking trails. The soil within the park are not well mapped but likely are part of the Grey Wooded soil association (Luvisol) consisting of fine sandy loam to clay loam soils developed on boulder till of mostly shale with some limestone, and granitic rocks [23]. The second site is under agricultural production and includes rotations of grain crops and forage. The site is mapped to the Edwards Soil Series (Cumulic Regosol) consisting of silty clay loam to silty clay soil developed on recent alluvial deposits [23].

The Köppen-Geiger climate classification of the WCW is cold, without dry season, and with warm summer (Dfb) [24]. The average annual precipitation is ~539 mm, with approximately 27% falling as snow with a mean annual temperature is 3.0°C [25]. The hydrology of the watershed is snowmelt dominated with ~ 80% of the cumulative runoff occurring during the spring season (May and June) [26].

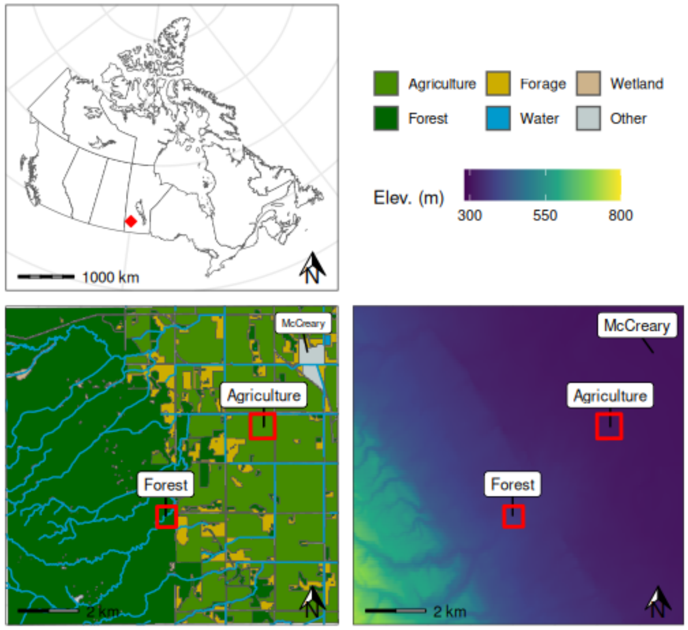

Figure 1: Map showing the location of the study sites within Canada, and the regional land use and topography.

Source: Research Site Locations

2.2. Soil sampling and analysis

This study uses samples and data collected as part of the grid sampling design outlined in Luna Miño [7]. Briefly, at each site 49 samples were collected using a soil auger on a 7x7 grid at a 100m spacing. Within the forested surface soil samples were collected below the LFH layer to a depth of 5cm, and the agricultural site was sampled to a depth of 15cm to account for the regular mixing of the soil due to tillage and other field operations.

Samples were dried, homogenized with a motar and pestle, and sieved through a 63 m sieve to remove the sand fraction. The sand fraction was removed in an effort to reduce the differences in grain size and organic matter content between the two sites [27]. Samples were analyzed for a broad suite geochemical element using inductively coupled plasma mass spectrometry (ICP-MS) following a microwave-assisted digestion with aqua-regia (ALS Mineral Division, North Vancouver, BC, Canada). Spectral measurements were made with a spectroradiometer (ASD FieldSpecPro Malvern Panalytical Inc Westborough MA 01581, United States). Spectral reflectance measurements were taken in 1 nm increments over the 0.4-2.5 m wavelength range. Both samples and Spectralon standard (white reference) were illuminated with a white light source using a halogen-based lamp (12 VDC, 20 Watt). Following the method outlined in Boudreault et al. [28], fifteen colour coefficients (R, G, B, x, y, Y, X, Z, L, a*, b*, u*, v*, c*, h*) were calculated for each sample [29]. Based on the results of Luna Miño [7], a composite fingerprint consisting of 10 geochemical elements (Ca, Co, Cs, Fe, Li, La, Nb, Ni, Rb, and Sr) and five colour coefficients (a, b, c, h, and x) were identifying as providing a strong discrimination between the agricultural and forested surface soils. These fifteen soil properties are the focus of the detailed spatial analysis detailed in this study.

2.3. Geospatial and terrain analysis

All geostatistics were performed with ArcGIS Pro [v 3.3.0 30]. Semivariograms were used to quantify spatial correlation for each of the 15 soil properties. The optimization tool, based on minimizing the mean square error, was used to parameterize the semivariogram model. Kriging was used to interpolate and generate maps of each soil property. The exploratory interpolation tool (Geostatistical Analyst extension) was used to select the kriging type with the highest ranked prediction accuracy.

A Digital Elevation Model (DEM) for the forested site was acquired from publicly available data [31]. A DEM for the agricultural site was generated by photogrammetry using UAV imagery, including the use of ground control and check points, with Agisoft Metashape Professional [v1.8.2 32]. Ordinary kriging was used to calculate a 1 m gridded digital elevation model for each site. Geographic information software [SAGA v2.1.4 33] was used to calculate six additional terrain attributes and included plan and profile curvatures, saga wetness index, catchment area, relative slope position, vertical channel network distance.

2.4. Data analysis

All subsequent statistical analysis was undertaken using R statistical Software v4.4.0 [34] through RStudio Integrated Development Environment v2024.04.2 [35]. Plots and maps were created using the R package `ggplot2` v `r packageVersion("ggplot2")` [36]. Skewness was categorized as values between -0.5 and 0.5 considered approximately symmetric, -1.0 to -0.5 or 0.5 to 1 as moderately skewed, and $<$ -1.0 or $>$ 1.0 as highly skewed. Coefficient of variation (CV) thresholds were categorized as low (<15%), moderate (15–35%), high (35–75%), and very high (>75%) .Interpolated soil property and terrain attribute data were resampled to a 10 m resolution prior to analysis [`terra` v`r packageVersion("terra")` 37]. Random Forest Regression [`randomForest` v`r packageVersion("randomForest")` 38] was used to assess the relative importance of the terrain attributes on the spatial distribution of soil properties. The dataset was randomly split into training, validation, and testing datasets. Multicollinearity among the terrain attributed was assessed using the Variance Inflation Factor with a threshold of eight and correlated terrain attributes were removed [`usdm` v`r packageVersion("usdm")` 39]. The number of variables randomly sampled as candidates at each split within the random forest model was tuned using the training and validation data sets [`caret vr packageVersion("caret")` 40]. The number of trees to grow was set to 500 and assessed using the Root Mean Square Error for both the Out of Bag Error and the validation data sets. To test the model, actual and predicted values were plotted and the R^2 was calculated.

3. Results

3.1. Univariate summary

Overall, the agricultural site had soil colour and geochemical properties that exhibited lower variability and more symmetrical data distributions as compared to the forested site. Considering all 15 colour properties measured it was observed that all the colour properties for both sites exhibit an approximate symmetric distribution. All 15 colour properties for the agriculture site had a low CV and the forested site had slightly greater variability with 10 colour properties the a low CV and five with a moderate CV. Overall, the agricultural site had lower variability and the distribution of data for each element were generally more symmetrical as compared to the forest site. Of the 44 geochemical concentrations measured at the agricultural site, nine elements exhibited moderately skewed distributions, while five displayed highly skewed distributions. Additionally, 12 elements had moderate coefficients of variation (CV), and five had high CV. At the forested site, seven elements showed moderately skewed distributions and 14 exhibited highly skewed distributions. Furthermore, 28 elements had moderate CV, six had high CV, and two had very high CV.

Table 1: Summary univariate statistics of selected geochemical and colour soil properties for each site (n = 49).

Property	Mean	SD	Max	Min	Skewness	CV
			Agriculture			
Ca	4.00	2.19	8.78	0.95	0.28	54.66
Co	8.76	0.83	10.60	7.50	0.52	9.48
Cs	0.75	0.15	1.07	0.47	0.18	19.93
Fe	1.92	0.09	2.11	1.71	−0.25	4.70
Li	15.62	1.42	19.80	12.80	0.62	9.11
La	18.23	1.22	20.20	15.50	−0.29	6.71
Nb	0.59	0.06	0.73	0.46	0.45	9.67
Ni	29.63	2.72	35.70	25.00	0.36	9.17
Rb	18.43	4.33	26.70	10.20	0.24	23.48
Sr	91.31	38.98	163.50	38.60	0.09	42.69
a*	3.38	0.32	4.15	2.59	−0.03	9.53
b*	8.84	0.97	10.59	6.69	−0.18	11.00
c*	9.47	1.02	11.32	7.17	−0.19	10.74
h*	1.20	0.01	1.23	1.18	0.19	1.12
x	0.47	0.00	0.48	0.47	0.06	0.46

Table 1: Summary univariate statistics of selected geochemical and colour soil properties for each site (n = 49).

Property	Mean	SD	Max	Min	Skewness	CV
			Forest			
Ca	1.89	1.53	5.46	0.47	1.07	81.12
Co	6.76	1.39	9.60	4.00	0.03	20.62
Cs	0.55	0.12	0.78	0.34	0.25	21.73
Fe	1.18	0.13	1.46	0.83	−0.58	11.24
Li	6.47	0.90	8.60	4.30	−0.02	13.89
La	15.00	2.60	21.80	10.30	0.33	17.31
Nb	0.37	0.06	0.56	0.17	−0.68	17.10
Ni	18.09	3.90	28.00	11.00	0.33	21.55
Rb	13.83	1.85	18.10	9.90	0.27	13.40
Sr	32.43	12.60	64.20	15.30	0.98	38.87
a*	5.73	0.41	6.56	4.41	−0.38	7.10
b*	12.47	2.01	15.91	8.02	0.22	16.11
c*	13.74	1.94	17.00	9.15	0.15	14.15
h*	1.13	0.05	1.23	1.06	0.34	4.13
x	0.49	0.00	0.49	0.48	−0.21	0.47

Source: Univariate summary

Table 2: Summary statistics for the interpoloated values (10m resolution) for slected geochemical and colour soil properties and terrain attributes for each site.

Property	Mean	SD	Max	Min	Skewness	C
			Agriculture			
Ca	4.12	2.10	8.76	0.918	0.0727	51
Co	8.75	0.664	10.6	7.52	0.431	7.
Cs	0.729	0.123	1.07	0.458	0.376	16
Fe	1.92	0.0644	2.10	1.73	−0.450	3.
Li	15.7	1.16	19.3	13.2	0.551	7.
La	18.2	0.817	19.8	16.5	−0.268	4.
Nb	0.593	0.0550	0.740	0.459	0.569	9.
Ni	29.9	2.23	34.5	26.3	−0.0100	7.
Rb	18.0	3.94	26.1	11.5	0.498	21
Sr	93.4	38.6	167	36.3	0.00105	41
a*	3.34	0.211	3.83	2.88	0.0621	6.
b*	8.73	0.707	10.2	6.98	−0.162	8.
c*	9.34	0.762	11.0	7.41	−0.158	8.
h*	1.20	0.00977	1.23	1.18	−0.0603	0.8
x	23.1	1.31	26.6	18.6	−0.501	5.
Plan Curvature	1.65×10^{-6}	1.36×10^{-4}	6.57×10^{-4}	-5.07×10^{-4}	3.54×10^{-1}	8.24

Table 2: Summary statistics for the interpoloated values (10m resolution) for slected geochemical and colour soil properties and terrain attributes for each site.

Property	Mean	SD	Max	Min	Skewness	C
Profile Curvature	-7.64×10^{-6}	1.53×10^{-4}	5.83×10^{-4}	-6.47×10^{-4}	9.51×10^{-2}	−2.00
SAGA Wetness Index	9.64	0.704	11.2	7.77	−0.122	7.
Catchment Area	475	1,010	10,100	4.35	4.76	2
Rel. Slope Position	0.718	0.288	1.20	0.0221	−0.946	40
Vert. Dist. Channel	5.98×10^{-2}	4.10×10^{-2}	2.92×10^{-1}	4.25×10^{-3}	1.21	6.85
Elevation	310	0.593	312	309	0.615	0.1
			Forest			
Ca	1.88	0.769	3.61	0.787	0.202	40
Co	6.80	0.632	8.66	4.93	−0.200	9.
Cs	0.551	0.0737	0.714	0.423	0.297	13
Li	6.43	0.694	8.46	4.39	−0.136	10
La	15.0	1.57	18.5	11.5	−0.0324	10
Nb	0.370	0.0356	0.440	0.278	−0.436	9.
Ni	18.2	2.49	24.9	14.3	0.314	13
Sr	31.6	8.50	53.1	18.1	0.716	26
h*	1.13	0.0371	1.22	1.06	0.257	3.
x	19.7	3.92	30.5	10.8	0.362	19
Plan Curvature	3.97×10^{-4}	3.27×10^{-3}	2.89×10^{-2}	-2.62×10^{-2}	7.91×10^{-1}	8.22
Profile Curvature	-1.83×10^{-4}	9.47×10^{-3}	6.37×10^{-2}	-7.37×10^{-2}	-5.31×10^{-1}	−5.18
SAGA Wetness Index	6.00	0.988	8.48	2.21	−0.430	16
Catchment Area	571	1,940	25,400	3.44	6.60	3
Rel. Slope Position	0.222	0.232	0.993	0.00617	1.56	10
Vert. Dist. Channel	4.15×10^{-1}	4.43×10^{-1}	3.66	2.02×10^{-2}	2.96	1.07
Elevation	369	3.34	377	359	−0.184	0.9

Source: Univariate summary

3.2. Spatial analysis

Table 3: Geostatistical parameters of the fitted semivariogram models of selec
geochemical properties within the agricultural and forested sites.

Property	Kriging Type[1]	Nugget (Co)	Sill (Co + C)	C/(C + Co) (%)	Range (m)	r^2
					Agriculture	
Ca	Universal	0.0	7.2	100	580	0.9
Co	Simple	0.0	0.7	100	208	0.4
Cs	Ordinary	0.0	0.0	100	210	0.5
Fe	Ordinary	0.0	0.0	100	185	0.2
Li	Universal	0.3	1.5	81	185	0.6
La	Simple	0.4	1.0	56	308	0.5
Nb	Universal	0.0	0.0	91	210	0.7

Table 3: Geostatistical parameters of the fitted semivariogram models of selec
geochemical properties within the agricultural and forested sites.

Property	Kriging Type[1]	Nugget (Co)	Sill (Co + C)	C/(C + Co) (%)	Range (m)	r^2
Ni	Ordinary	1.4	8.9	84	352	0.6
Rb	Ordinary	1.4	27.6	95	551	0.9
Sr	Ordinary	0.9	900.2	100	220	1.0
a*	Ordinary	0.4	1.0	59	288	0.3
b*	Simple	0.2	0.9	83	199	0.3
c*	Simple	0.1	0.9	87	199	0.3
h*	Simple	0.0	1.1	100	185	0.2
x	Simple	0.4	1.0	58	220	0.1
					Forest	
Ca	Ordinary	1.6	2.7	41	269	0.2
Co	Ordinary	0.0	2.1	100	298	0.1
Cs	Ordinary	0.0	0.0	83	237	0.2
Li	Ordinary	0.0	0.8	100	222	0.3
La	Ordinary	3.1	7.4	59	176	0.1
Nb	Ordinary	0.0	0.0	51	224	0.2
Ni	Universal	6.7	15.8	57	187	0.2
Sr	Simple	0.4	1.0	65	229	0.4
h*	Universal	0.0	0.0	100	230	0.3
x	Ordinary	0.0	39.2	100	312	0.2

[1] Models are all isotropic.

[2] Strong spatial dependency (C/(C + Co) % >75); Moderate spatial dependency (C/(C + Co) % between 75

Source: Semivariograms

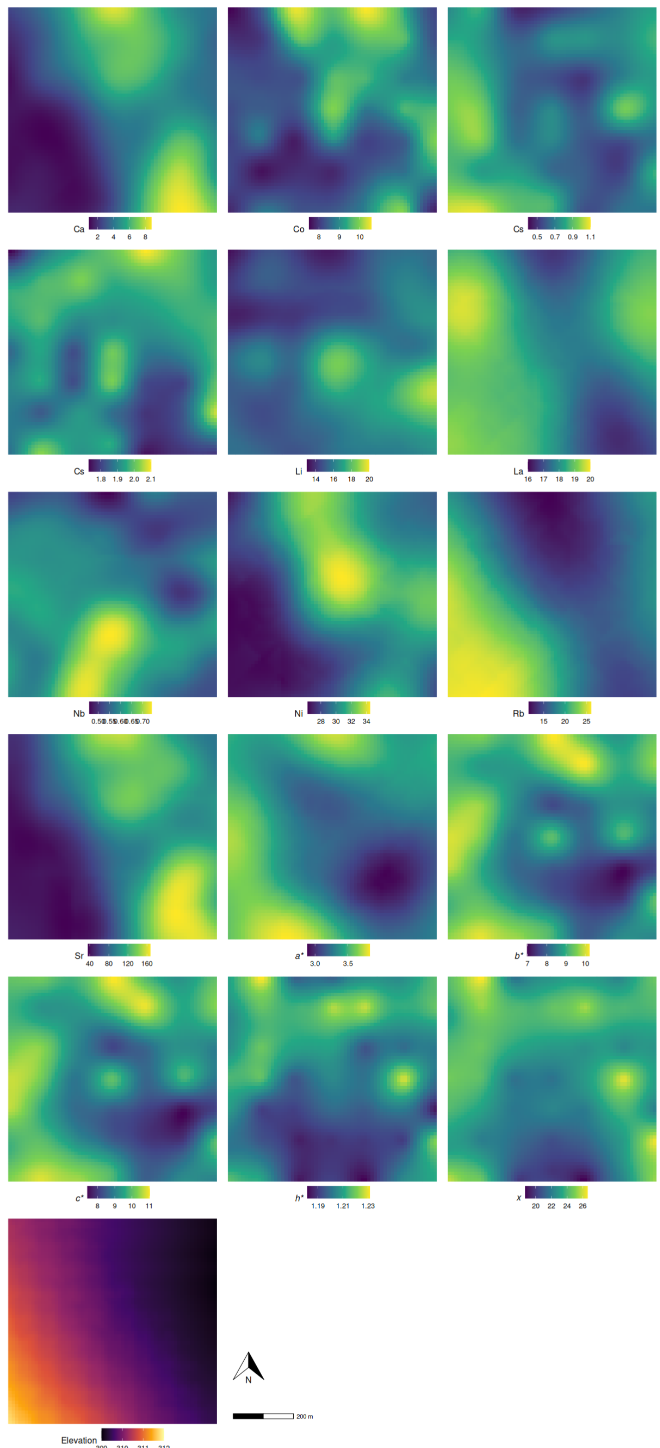

Figure 2: Kriged maps of select colour and geochemical properties and elevtion across the agricultural site.

Source: Soil property mapping

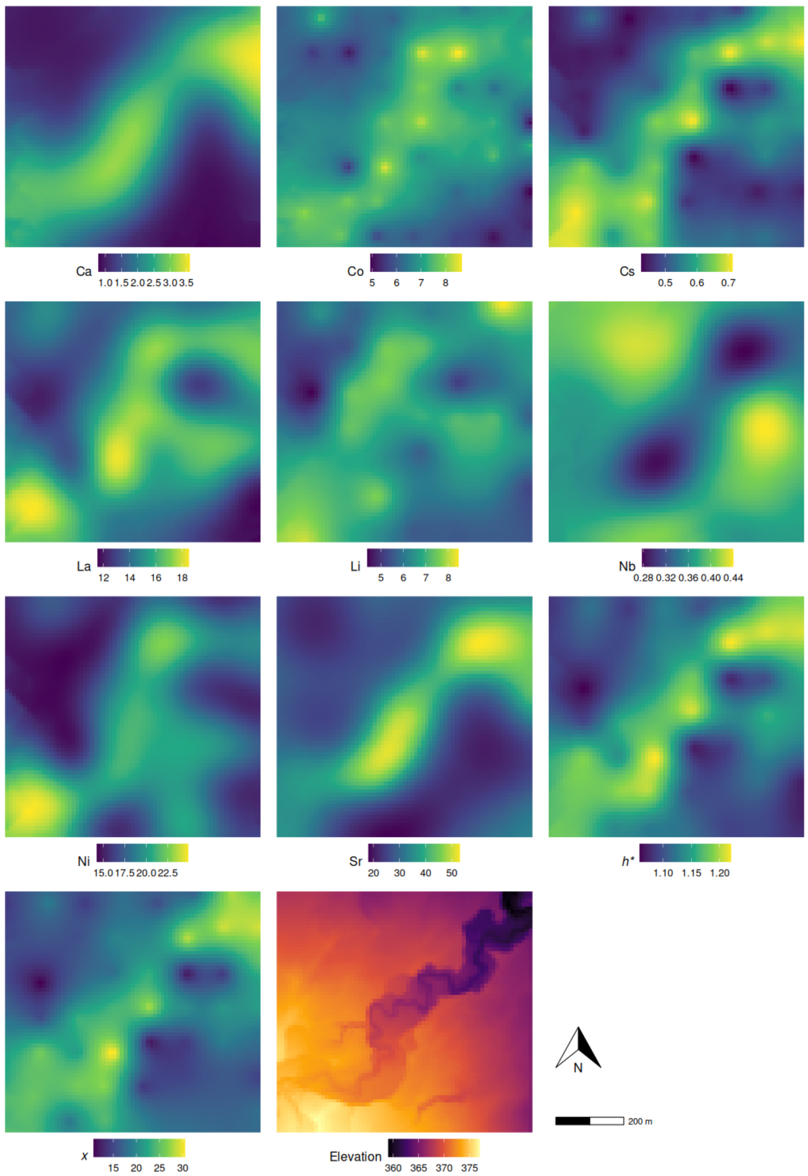

Figure 3: Kriged map of select colour and geochemical properties and elevation across the forested site.

Source: Soil property mapping

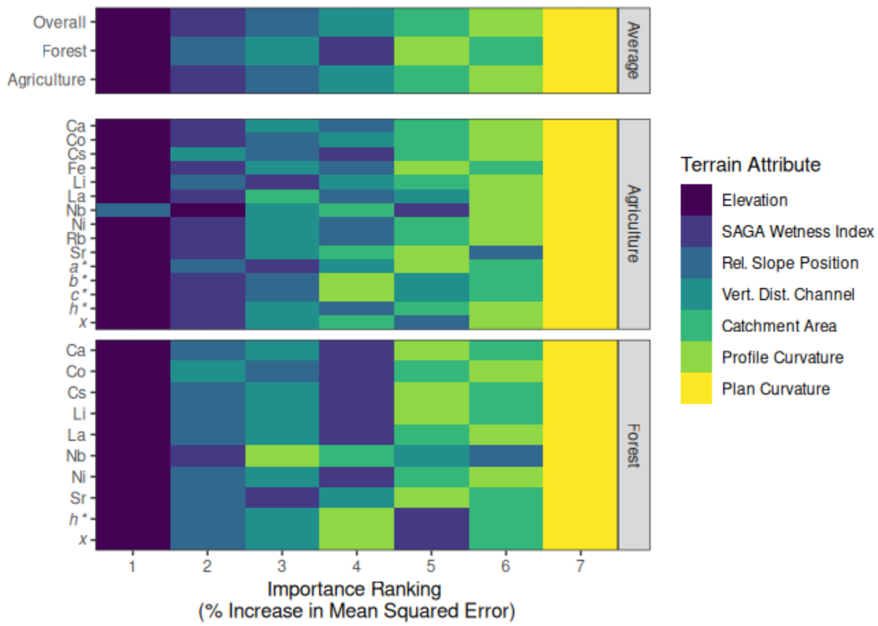

Figure 4: Heat map of the Random Forest regresssion results showing the ranking of the importance of terrain attributes (based on % increase in Mean Squared Error) in explaining the spatial variabilty of selected colour and geochemical properties within the agricultural and forested sites. Top panel shows an average ranking for each site and across both sites.

Source: Random Forest summary

Table 4: Model summary and performance statistics for the random forest regression using the training, validation, and test data sets.

Property	MSETraining[1,2]		MSETesting[1,2]		{{R^2}}Testing
		Agriculture			
Ca	0.374	91.6	0.359	91.8	0.91
Co	0.089	79.8	0.080	82.5	0.80
Cs	0.002	85.7	0.002	86.4	0.85
Fe	0.001	69.6	0.001	70.9	0.69
Li	0.538	59.3	0.533	59.8	0.64
La	0.048	93.0	0.044	93.1	0.93
Nb	0.001	57.3	0.001	59.1	0.55
Ni	0.338	93.1	0.335	93.7	0.93
Rb	0.733	95.3	0.643	96.1	0.95
Sr	97.221	93.5	93.970	93.6	0.93
a*	0.007	85.0	0.006	86.9	0.85
b*	0.136	72.5	0.120	75.3	0.72

Table 4: Model summary and performance statistics for the random forest regression using the training, validation, and test data sets.

Property	MSETraining[1] [2]		MSETesting[1] [2]		{{R^2}}Testing
c*	0.155	73.2	0.136	75.9	0.73
h*	0.000	58.3	0.000	58.6	0.56
x	0.628	61.9	0.701	61.8	0.59
			Forest		
Ca	0.231	61.1	0.231	60.7	0.63
Co	0.244	39.1	0.234	42.9	0.48
Cs	0.002	64.1	0.002	67.1	0.66
Li	0.278	41.3	0.282	42.0	0.46
La	1.401	43.3	1.323	47.5	0.48
Nb	0.001	55.0	0.001	55.9	0.58
Ni	2.819	55.2	2.806	56.0	0.55
Sr	29.427	59.4	29.663	59.1	0.59
h*	0.001	58.8	0.001	60.3	0.62
x	5.646	62.6	5.810	63.4	0.64

[1] Mean square error

[2] Percent variance explained

Source: Random Forest summary

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