Workshop on Visualisation in Environmental Sciences (EnvirVis) (2019)
R. Bujack and K. Feige and K. Rink and D. Zeckzer (Editors)

SOAViz: Visualization for Portable X-ray Fluorescence Soil Profiles

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Abstract

The soil is an essential element of life. It is where people grow plants for food, fibers, and other materials. It also helps to filter water and recycles wastes. Therefore, understanding soil physical/chemical characteristics and structural aggregation are of vital importance. In this project, we work closely with the soil scientists to develop a visualization solution to the rapidly gaining favor approach to soil horizon analysis using Portable X-ray Fluorescence (pXRF) devices. Our visualization, called SOAViz, aims to provide soil scientists with rapid valuable insights into soil properties both visually perceptible with graphs and imperceptible quantification features with statistical calculations from the data collected from pXRF equipment. SOAViz was developed with analysis tasks solicited from the soil scientists and validated by applying to real soil profiles collected in an Experimental Rangeland in Lubbock, TX, USA. This visual solution together with the quick scanning results from pXRF devices offers a timely means of quantifying elemental concentrations in the soil horizons in large scale at a reduced cost.

1. Introduction

Agriculture is tasked with feeding a large and increasing population with limited natural resources. In addition, soil health is gradually decreased due to unsustainable agricultural practices and environmental management [Sta06], which leaves pressures on policy maker on better solutions for managing and controlling the properties related to soil health. Because accurate soil health assessments require many different types of measurements, researchers have struggled to establish an effective unified method for quantifying soil health [WCW*15]. Sensor-based approaches may provide a cost-effective, site-specific solution for soil health monitoring and management. Recently, using proximal sensors such as portable X-ray fluorescence spectrometry (pXRF) to analyze soil horizons is gaining favor [SCMM16, GIH*18] with the ability to provide faster scanning results (in 60 to 90 seconds), it offers a rapid means of quantifying elemental concentrations in the soil [LBZ*12, PMWP15]. This paper focuses on analyzing the collected data from proximal sensors.

While the scanning time reduced significantly, the analyzing time is still a time-consuming process which may take days or weeks and involve many people with different expertise for data collection, chemical measurements, visual representation, and data analysis. Currently, soil scientists use traditional software to analyze the scanned results such as Microsoft Excel or some complicated packages such as ArcGIS and MatLab or even programming languages such as R or Python to create custom visualizations for the analysis part. Moreover, current soil data analytics approaches are limited to very few dimensions to be considered at the same time and therefore the analysis outcomes heavily rely on the skills and experiences of the soil experts. In this paper, we propose a visual prototype, called *SOAViz*, for analyzing the multidimensional data from pXRF equipment on-the-fly. Hence, the main contributions of this work are:

- We propose an approach for analyzing soil chemical data scanned by pXRF devices. The approach is implemented as a web application and is portable, so soil scientists can upload soil data to analyze on-field.
- We incorporate statistical features for detecting distribution and correlations of chemical elements identified in the soil profile [DW14b]. These features and visualizations provide scientists a lens into both visually perceptible features (with graphs) and imperceptible features (with statistical calculations) of the soil profiles.
- We apply our solution to three soil profiles collected in an Experimental Rangeland in Lubbock, TX, USA and conduct an informal user study with the soil scientists.

Overall, the tool has three overview visualizations: a) chemical elements and how they are correlated to each other b) concentration of elements across the cross 2D section's cells, and c) the concentration of elements across the cross section's horizontal levels. The interaction capabilities are restricted to low-level routine methods [AES05]. The overview visualizations might be useful to highlight outliers, and visual features [BBK*18, WAG06] in the data distribution which is an important step in data-intensive science [DW14a].

The remainder of the paper is organized as follows: we first describe the background and related research in this direction. We present the project roadmap and describe the major components. Then we give the detailed exposition of each proposed step with visual examples. Finally, we conclude the paper with future work.

DOI: 10.2312/envirvis.20191102

2. Related Work

Visible and near-infrared (VisNIR) diffuse reflectance spectroscopy (DRS) is a promising hyperspectral scanning technology that has become popular for rapidly quantifying and identifying multiple soil parameters simultaneously [RWM*06]. By comparison, VisNIR spectroscopy utilizes reflectance patterns from visible and near-infrared light emitted from a contact probe or mug lamp to make determinations of soil properties. This hyperspectral technique has achieved wider acceptance in soil science, owing to its cost-effectiveness and advantages over other analytical spectroscopic and wet chemistry methods. VisNIR spectroscopy perfectly complements many of the “gaps” not easily read by PXRF [Wei16]. Emerging proximal sensor technologies such as diffused reflectance spectroscopy (DRS) and portable XRF (PXRF) can efficiently quantify soil salinity, total C/total N, and other soil properties [ZWZ11, CWD*17]. Coupled with georeferencing, the combined use of DRS and PXRF enables us to predict multiple soil properties in a single day on-site with non-destructive scans [WBZ14, CMd*18]. This paper focuses on proximal sensor technologies, particularly the on-the-field collected data via portable XRF devices [MWC*18].

In this section, we do not attempt to survey all visualizations solutions for analyzing soil horizon data coming from pXRF devices but to provide general tools that soil scientists often use for their analysis. The pXRF devices, such as Vanta Handheld XRF Series (Olympus Corporation) and the Handheld XRF analyzers (Hitachi High-Tech Analytical Science), provide some basic statistics (simple listing) incorporated into their device screens. However, these are mostly tabular format data displays or basic charts and usually does not scale well with the data sizes. Figure 1 shows two typical screens from Vanta Handeld XRF Series built-in interface adapted from Vanta Family X-Ray Fluorescence Analyzer User’s Manual [Ana16]. In many cases, soil scientists need to create their own visualizations to suit their analysis purposes which highlight the trends and patterns in a large amount of collected data. In these cases, the solutions could be generally categorized into three main approaches as using a traditional method, advanced software, or custom programming code.

The conventional approach to analyzing pXRF soil pedon scanning results is using Microsoft Excel [ZWZ11]. Some advanced software packages such as Global Mapper (Blue Marble Geographics, Hallowell, ME), ArcGIS (ESRI, The Redlands, CA), NCSS 8 (NCSS, Kaysville, UT) [PMWP15, GIH*18], MDI Jade v9.1.1 [CWD*17], GeoChem, and SAGA GIS [CMd*18] require a reasonable training time before being able to use them. In many cases, soil scientists even need to use complicated programming languages/packages like MatLab, R, and Python to analyze their data [WORD13]. These visual representations customized for individual cases based on the data collection settings and tasks are time-consuming to be generated and usually required experiences and skills in using the software packages and/or programming languages. For the same task, the analysis process can be repetitive over the years. As the availability of pXRF devices, soil pedon data are easier and faster to collect. Therefore, it is desirable for a unified framework for analyzing this type of data with consistency, high performance, and reduced cost. Our *SOAViz* prototype is designed to fill in this gap.

Figure 1: *Vanta Handheld XRF series built-in interface. This figure is adapted from Vanta Family X-Ray Fluorescence Analyzer User’s Manual [Ana16].*

3. *SOAViz* Stages

Our prototype aims to provide visual representations for the collected data. The visualization can be generated on-the-fly so that obvious mistakes in data collection can be corrected while the soil scientists are still on the field (which otherwise very expensive or irreversible). Figure 2 depicts the major phases of our system: data importing, data processing, visualization, and interactions.

1. **Data processing**: The data processing stage consists of several modules for data cleaning, adding of some important soil compounds, and statistical calculations for the correlations of the concentrations of the detected chemical elements (details are described in Section 3.1).
2. **Data visualizations**: There are several interconnected graphs to show the spatial chemical element distributions in the pedon, and the statistical correlations among these elements are also displayed (details are discussed in Section 3.2).
3. **Interactions**: Interactions allow selecting individual soil profile to analyze, picking different chemical elements (or their compounds) to compare their correlations and/or changing display properties such as contour types, color ranges, and plot opacity (details are described in Section 3.3).

While developing this visualization solution, we worked closely with the soil scientists to implement the following analysis tasks [CGM*17, CAS*18] required while analyzing pXRF soil horizon scanning data:

- **T1**: Provide an overview of all detected chemical elements and/or their compounds in the soil profile [KPS04].
- **T2**: Show and quantify the relationship between any two selected chemical elements and/or their compounds [GE03].

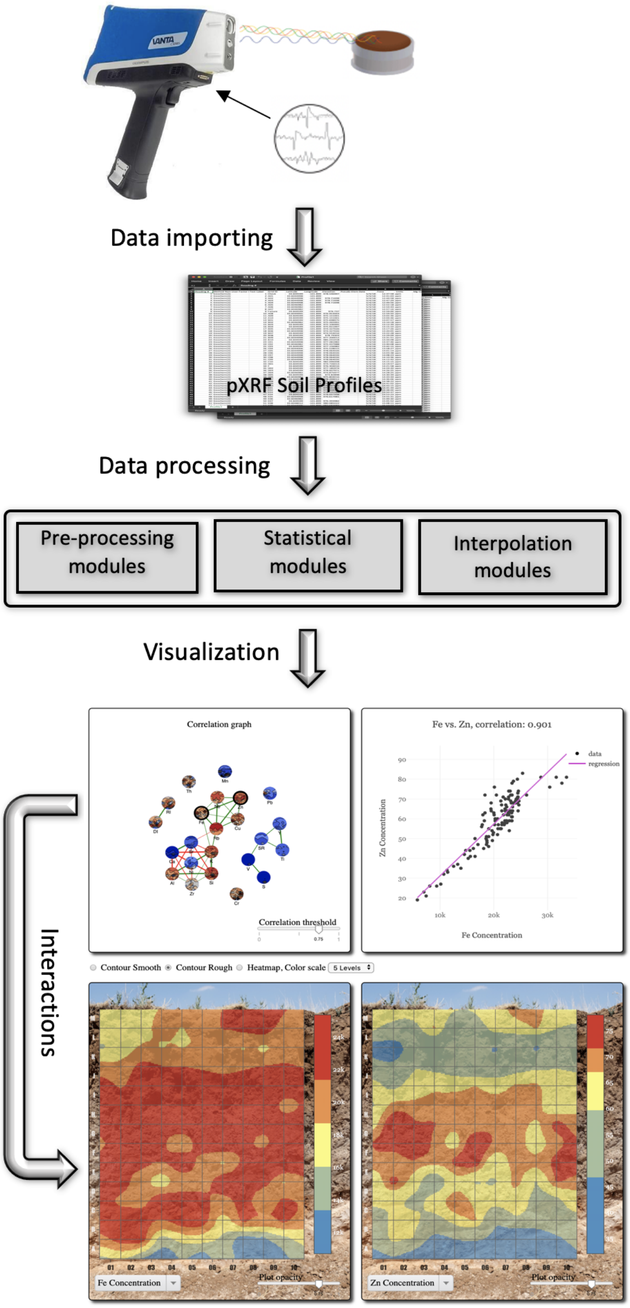

Figure 2: *Major stages in SOAViz roadmap: data importing, processing, data visualizing, and interactions.*

- **T3**: Show and compare the spatial distributions of any two selected chemical elements and/or their compounds over the 2-D surface of the pedon.
- **T4**: Quantify the distributions of any two selected chemical elements and/or their compounds over the pedon horizons.
- **T5**: Show and quantify the difference between the traditional (6-horizons) soil profile approach and the newly exploring (10-cm-horizon across 13 horizons) approach to soil profiling.
- **T6**: Detect and alert outlying data points [WAG05] that might be caused by the mistakes happened during on-field soil scanning.

3.1. Data processing

The soil scientists provided us three soil profiles to evaluate and develop this visualization solution. The soil profiles were located on an Experimental Rangeland in Lubbock, TX, USA. The soil pits at each site were excavated to a depth of 1.2m. Before the morphological process, strings were used to set up a grid across the entire pedon; each grid cell was 10cm^2. A column and row numbering system was applied, such that each grid cell had a unique identifier. Then, a Vanta Series M pXRF (Olympus Corporation) was used to scan the soil in each cell in situ.

After the data is imported from the pXRF devices, the data is then cleaned such as removing missing or lower than *"LOD"* (Limit of Detection) values. The remained pXRF elements detected in these soil horizons include 20 elements (*Al, Ca, Cr, Cu, Fe, K, Mn, Nb, Ni, Pb, Rb, S, Si, Sr, Th, Ti, V, Y, Zn, and Zr*). Besides the reported values on individual chemical elements, several important soil compounds such as *Ruxton Weathering Index* (SiO_2/Al_2O_3), *Desilication Index* ($SiO_2/(Al_2O_3+Fe_2O_3+TiO_2)$), and *Stable Ratio* ($Ti/Zr$) [SCMM16] are also calculated and added to the soil profile to aid the soil properties analysis.

The statistical modules help to calculate several statistics while analyzing soil profiles. Sample correlations [SC80] among the elements are used to show the relationships among them. Box-plot statistics [HN98] are calculated to show the distributions of element contamination in the thirteen measured horizons. R-squared scores [Nag07] are used to quantify the goodness of fit between the exploring 10-cm-horizon across 13 levels approach versus the traditional 6-horizon-levels approach to soil profiling. We use the R-squared score in this case because it gives an estimate of the relationship between the movements of the two measurement approaches. The R-squared score of 1.0 represents a perfect match, and the R-squared score of 0.0 represents a not good match (simply fitting a curve to its mean value resulted in R-squared score of 0.0). Also, it provides sufficient generality [CW97] to cover reasonably the correlation between these two non-linear curves of measured data.

The scanned pedon is divided into 13 (indexed from A to M) by 10 (indexed from 1-10) discrete cells of 10cm by 10cm each. Also, in some cases, outlying data in these discrete cells might be removed due to the mistake during scanning. On the visualizations, the soil scientists would like to have a smooth view of the chemical element contamination distributed on the pit. Therefore, we use Krigging algorithm [VB05] to interpolate the data. This method is widely used in the spatial analysis which is governed by the Gaussian process regression to give better smoothness of the data distribution.

3.2. Data visualizations

To realize the analysis tasks required by the soil scientists (as described earlier in Section 3), coordinated multiple views [Rob07] is adapted to show a different perspective of chemical elements: the correlation graphs, the scatter plots and linear regression line, the contour-map/heat-map, the box-plots, and the goodness of fit graphs. These views are linked.

The correlation graphs: To give an overview of all detected chemical elements and their relationships (task **T1** and task **T2**), *SOAViz* calculates the sample correlations among the elements and the compounds to generate a force-directed network graph [BOH11], as shown in Figure 3. Each vertex represents a chemical element (or a chemical compound) and overlaid by its contamination contour to guide users during the exploration process. A link indicates the correlation between two nodes: the thicker the link, the higher the correlation. The color of the links encodes positive/negative correlations. Notice that the highly connected vertices represent similar contour patterns. Users can use the slider provided at the bottom right corner to refine the relationship network and focus on the strongly correlated chemical element. As we explore the different soil profile, the relationship network varies significantly across different profiles since they are collected from various locations and hence represent different soil classifications. *Ruxton Weathering Index Desilication Index*, and *Stable Ratio* are abbreviated as *Ri*, *Di*, and *Ti* in the network view. As shown on the top of Figure 3, *Ri* and *Di* are positively correlated in this soil profile.

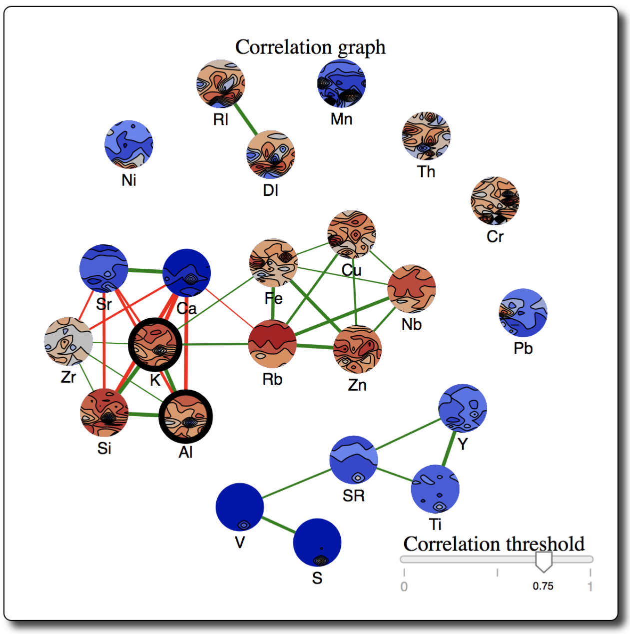

Figure 3: *The correlation network of chemical elements and their compounds in a soil profile. The vertex thumbnails show their chemical contamination maps.*

To verify the correlation of any two chemical elements or the compounds (visualization task **T2**), a scatterplot is generated on demand. As depicted in Figure 4, each data point is an instance (or a pXRF shot) on the 2D soil profile grid. A linear regression line [NWK89] is plotted as a reference for the estimated correlation. Furthermore, the *Pearson* correlation score can be displayed on top of the scatterplot to quantify and compare the relationship between any two selected chemical elements.

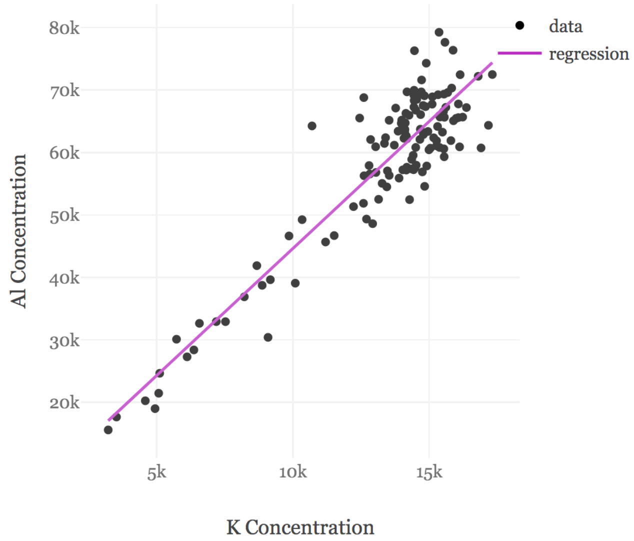

Figure 4: *The scatterplot and the linear regression line of two selected chemical elements (K vs. Al) from the network in Figure 3.*

Figure 5 shows the scatterplot matrices [DAW13] of all pairwise correlation between 21 chemical elements in the two sample soil profile collected via the portable XRF device. The scatterplots are color-coded by their *Pearson* correlation scores: red for high correlation, green for no association. The variables (chemical elements) have been ordered so that high correlated variables appear on the top of the matrix triangles.

The contour maps/heatmaps: Relying on the string settings that were used to physically impose a grid across the profile during the on-field scanning, a contour-map or heatmap (can be made interchangeably on the user selection from the menu at the top of our visualization tool) is generated to mimics the actual spatial distributions of the element concentrations over the 2D surface of the pit (task **T3**). In case of the contour map as shown in Figure 6(a), the data is first interpolated using the Krigging algorithm (as described in section 3.1) to have smooth data over the pit. On the other hand, the discrete heat-map shows the discrete data scanned from the corresponding cells as in Figure 6(b). Notice that pXRF devices iteratively shot at the center of each cell.

The box-plots: The box-plots are used to show distributions of the selected elements across the soil horizons of the pedon (visualization task **T4**) as shown in Figure 7. Box-plots are the standardized methodology the soil scientists use to graphically visualize the statistical distributions of the concentrations of the chemical elements across the soil horizons. In particular, boxplot displays the distribution of data based on a five number summary: minimum, first quartile, median, third quartile, and maximum [Wil17]. It also shows the outliers which are not in the

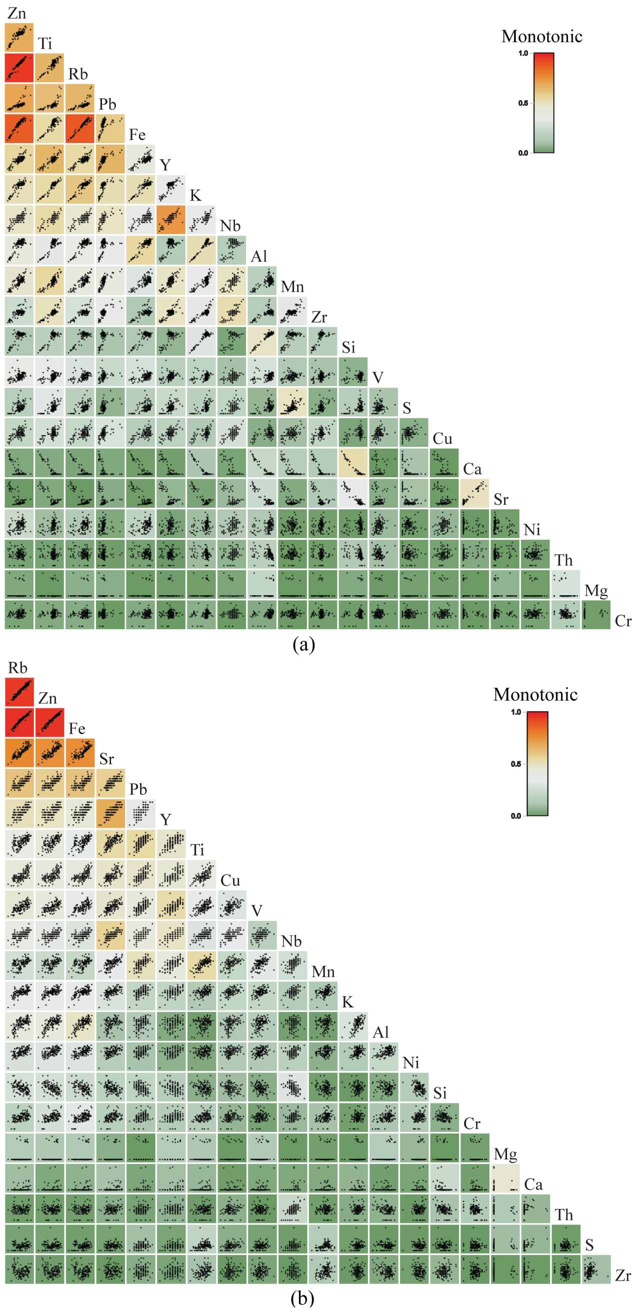

Figure 5: *Overview of all chemical pairwise correlations in two soil profiles. Each data point is an multidimensional instance (on the 2D soil profile grid) collected via a pXRF shot.*

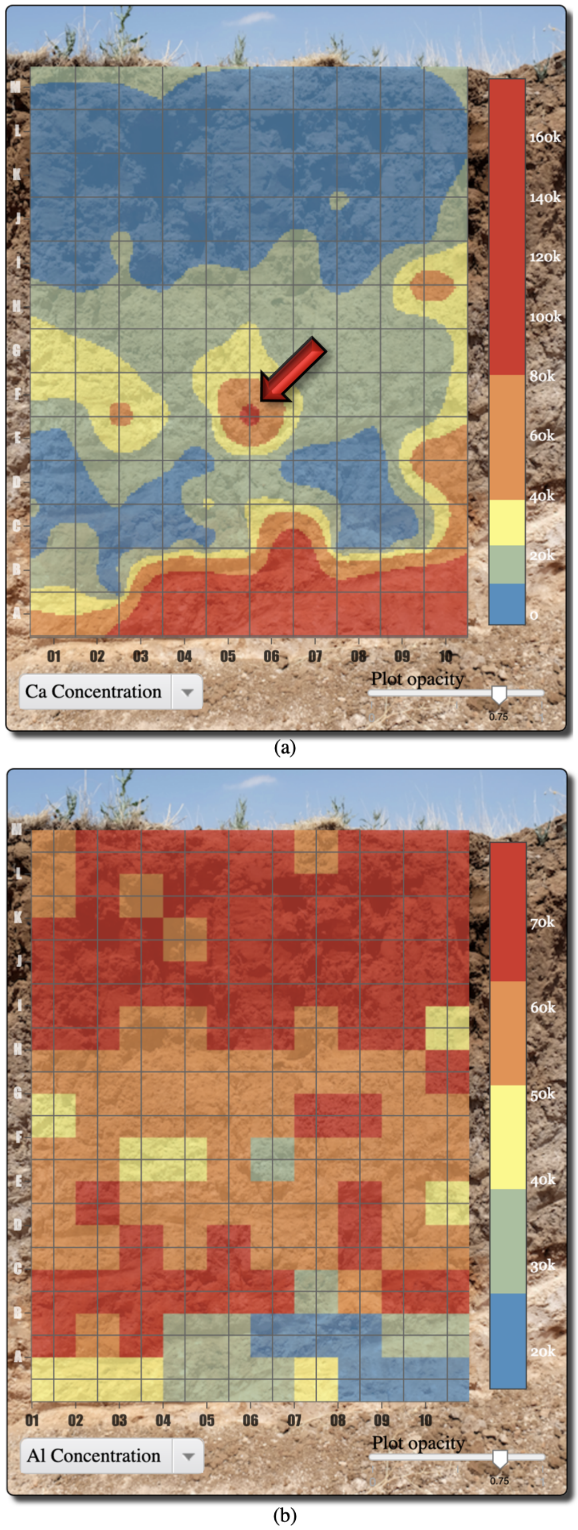

Figure 6: *The spatial distributions of the contamination of the detected chemical elements: (a) contour map (b) heatmap.*

range from minimum to maximum (visualization task **T6**). Moreover, remove outlying data before applying other analysis techniques are recommended by many works in the soil research field ([ZTLX09, FZZ*16, BEA18]), as to improve the accuracy of the soil profile analysis. We can quickly notice that the chemical concentrations vary significantly as we go deeper.

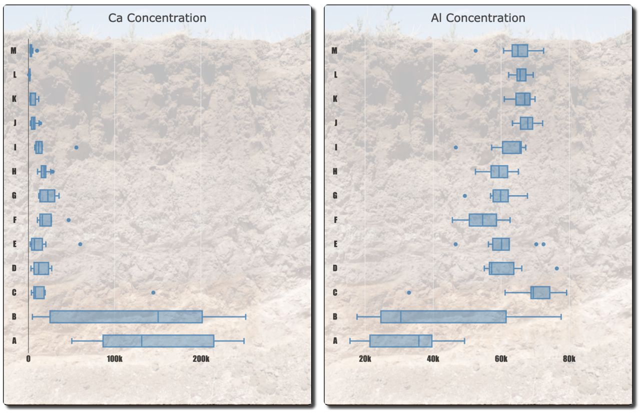

Figure 7: *The box-plots to show the distribution of the element contamination over the horizons of the pedon. The Ca and Al concentrations vary significantly as shown in the last two rows.*

The goodness-of-fit graphs: With the availability of the pXRF devices and its improvement in getting the faster scanning results, the soil scientists would like to explore a new approach to soil horizon analysis using 10cm horizons (across 13 horizons) instead of the traditional 6-level horizon approach. Comparing to the traditional approach, the newly exploring strategy provides finer details of the chemical element contamination distribution over the pit and better accuracy by having higher sampling frequencies in the horizontal and vertical directions. Figure 8 displays the curves to visually represent the goodness-of-fit of the averaged concentration values of these two approaches (task **T5**). To quantify the goodness-of-fit between the two curves, the R-squared score (described in section 3.1) is calculated and displayed on top of the element profile.

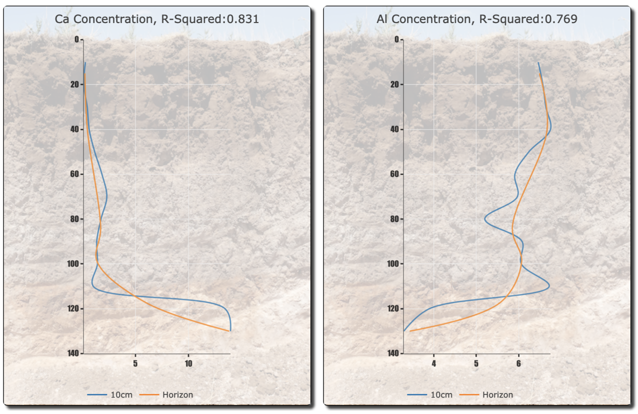

Figure 8: *Goodness-of-fit graphs to show the difference/similarity between the traditional 6-level-horizon approach and 10cm-horizon across 13 horizons approach to soil horizon analysis.*

3.3. Interactions

Users can select any uploaded pXRF soil horizon profile to visualize from the top menu of the visualization. All the visualization views are interconnected, for instance, users can choose any two nodes on the network graph visualization in Figure 3, the selected nodes will be highlighted (with black borders), and all the views will be updated to compare the two selected elements. Similarly, users could also choose individual chemical elements (or compounds) by names to analyze from the selection boxes at the bottom of the contour-map/heat-map views as in Figure 6 and all other views will be updated accordingly.

There are also several interactions to customize individual views while analyzing the data. On the correlation network graph in Figure 3, users can use the slider at the bottom to set the correlation threshold, the network graph will only show the links for nodes with an absolute value of the correlation greater than or equal to this threshold. The soil scientists would often like to refer back the digital photo taken of the pedon surface while observing the distributions of the contamination of the chemical elements. At the bottom of the contour map/heatmap views, there are sliders for the user to set the opacity of these graphs. Users can lower the opacity to view the soil color and content in the digital photo in the background. Another essential analysis task is that the soil scientists would like to have different views of the contamination levels on the contour-map/heat-map views, so we provide three different color ranges as coarse (5 color ranges), fine (10 color ranges), and smooth (20 color ranges) to select from the top of the system.

4. Implementation

For portability, ease of use, and multiple platform compatibility, *SOAViz* is implemented as JavaScript based web application using D3.js [BOH11] and Plotly.js [SPH*17] libraries. The source codes, video, and the web demo of our visualization are available on our Github project at `https://github.com/iDataVisualizationLab/Soil`.

5. Evaluation and discussion

While developing this visualization solution, we worked closely with two senior soil scientists: One post-doc researcher and a senior Professor with more than ten years of experience in analyzing soil horizons and soil profiling with pXRF devices. With their experiences in this field, they provided us with clear, concrete, and important soil horizon analysis tasks and we worked together to form visualizations, interactions, and statistics for the tasks. We frequently meet to solicit analysis tasks required and validate proposed visualizations and interactions with application to the real soil profiles provided by the soil scientists.

The soil scientists are currently using our solution in analyzing soil horizon profiles in their lab. They reported to us a good use-case regarding analyzing *Profile1* (out of the three soil horizon profiles given to us), *SOAViz* helps to highlight the extremely high value of *Ca* concentration in the cell *F*6 visually in the contour map as shown at the red arrow in the panel (a) of Figure 6. The soil scientists explained that it could be due to an error that the pXRF equipment was hitting directly to rock in this cell during the scanning time. This outlying cell was then removed from soil horizon *Profile1* for better accuracy of the analysis.

Current visualization solution receives positive feedback from these experts as it provides a common framework for analyzing soil horizon scanning data using pXRF devices. Also, they stated that pairing between fast scanning results using pXRF devices and more rapid analysis process using *SOAViz* is promising solution to enable us to create soil profiles for a large number of pedons at consistent results, lower cost, and shorter time.

To complete this promising solution, there are several directions that these experts expected us to incorporate in future developments. The first one is being able to connect and pull data directly from pXRF devices using various wireless communication channels such as WiFi and Bluetooth. This helps to reduce the data importing process. The second direction is about enabling the users to define more custom color ranges due to different soil profile would have different ranges of chemical contamination values. The current solution of fixing 5, 10, or 20 color levels may work in many general cases as default settings but would still be better to allow users to set color ranges for some specific cases.

We have also initiated several interviews with four soil survey staff from the United States Department of Agriculture (USDA), Natural Resources Conservation Service at Lubbock County, and received positive feedback from them. However, in the future, we will continue to work more with the soil survey staff to make this project become a standard framework in analyzing soil horizons using pXRF devices.

6. Conclusion and Future work

In this project, we worked closely with two senior soil scientists to develop an on-the-fly visualization solution to help to analyze the soil horizon pXRF scanning results which otherwise may takes days. The solution supports several visualizations and interactions to provide perceptions about the data. Also, to quantify the data correlation, several statistical calculations are computed and displayed on the solution. Interactions are provided to aid the analysis tasks. The system allows the user to navigate through different profiles or compare individual elements or change display properties such as opacity and color. We also applied our solution to three soil horizon profiles provided by the soil scientists and received positive feedback from the soil scientists and the soil survey staff from USDA.

In the future, we will continue to work on several essential features such as connecting to the pXRF devices using WiFi or Bluetooth connection to pull data directly from them to improve time and convenience and to enable on-field analysis. One another direction to speed up the analysis process would be being able to deploy our solution directly in the pXRF devices. Also, we will work more with the soil survey staff from USDA to make this project become a standard framework in analyzing soil horizons using pXRF equipment.

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