

Use of machine learning methods to study the availability of nutrients and the distribution of toxic metals in agricultural Mediterranean soils.

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The group of toxic elements includes heavy metals and certain metalloids, which are a cluster of inorganic chemical hazards. The most common elements in contaminated soils are lead (Pb), chromium (Cr), arsenic (As), zinc (Zn), cadmium (Cd), copper (Cu), and nickel (Ni). Soils are the main reservoir of pollutants released into the environment mainly from anthropogenic activities and, unlike organic pollutants which are oxidized to CO₂, most metals do not undergo microbial or chemical degradation and their total concentration in soils remains for a long time.

Nevertheless, there are often changes in their chemical forms and consequently in their bioavailability. Heavy metal contamination of soil can pose risks and hazards to humans and the ecosystem through the following mechanisms: direct ingestion or contact with contaminated soil; the food chain (soil-plant-human or soil-plant-animal-human); consumption of contaminated groundwater; degradation of food quality (safety and marketability) through phytotoxicity; and the continued reduction in the potential use of land for agricultural production causing food insecurity and poverty.

Iron (Fe) is one of the 16 essential elements for plant growth and reproduction. The most abundant form of Fe in the soil is iron oxide (Fe₂O₃) or hematite, which is highly insoluble and gives the soil a red color (rust). The oxide form is usually hydrated. Under oxidizing conditions, i.e. in aerobic soils, the oxide, hydroxide, and phosphate forms control the concentration of Fe in solution and its availability to plants. Under reducing conditions - the addition of H⁺ or other reducing substances - the solubility of Fe increases. Therefore, Fe can be bound to the soil as an exchangeable ion. In certain soil conditions, carbonate or sulphide compounds can be formed with Fe. If sulphates are abundant in the soil, they become a source of oxygen for bacteria and black iron sulphide is formed.

Organic matter in soils plays an important role in the availability of Fe to plants. Many organic compounds and organic acids (aliphatic acids or amino acids) and complex polymers (humic and fulvic acids) can form soluble complexes with Fe or act as chelating agents and thus increase the availability of Fe to plants (chelating agents are organic compounds that form complexes with Fe and help to retain Fe in more soluble forms). Cadmium (Cd) on the other hand is one of the most toxic pollutants ranked seventh position among all environmental pollutants because of its potential to cause unfavorable effects on living populations. It can be highly toxic even at lower concentrations with a half-life of more than 30 years. Its main characteristic is that it is persistent in soil for thousands of years.

It is therefore particularly important to know the physico-chemical parameters that determine the availability of nutrients and trace elements as well as toxic elements such as heavy metals. Using machine learning methods, an attempt was made to create prediction models that could be used for optimal management of nutrients and toxic elements in Mediterranean soils.

The following figures visualize the correlation of the Cd and Fe soil concentration with two soil parameters. The prediction models were obtained with multivariate regression analysis and a robust iterative algorithm for the parameter estimation. Specifically, figure 1 depicts the relationship between the concentrations of the toxic element Cd and the physicochemical properties of the study soils. Figure 2 illustrates the relationship between the total Fe concentration and soil pH, cation exchange capacity and the presence of additional elements such as Co.

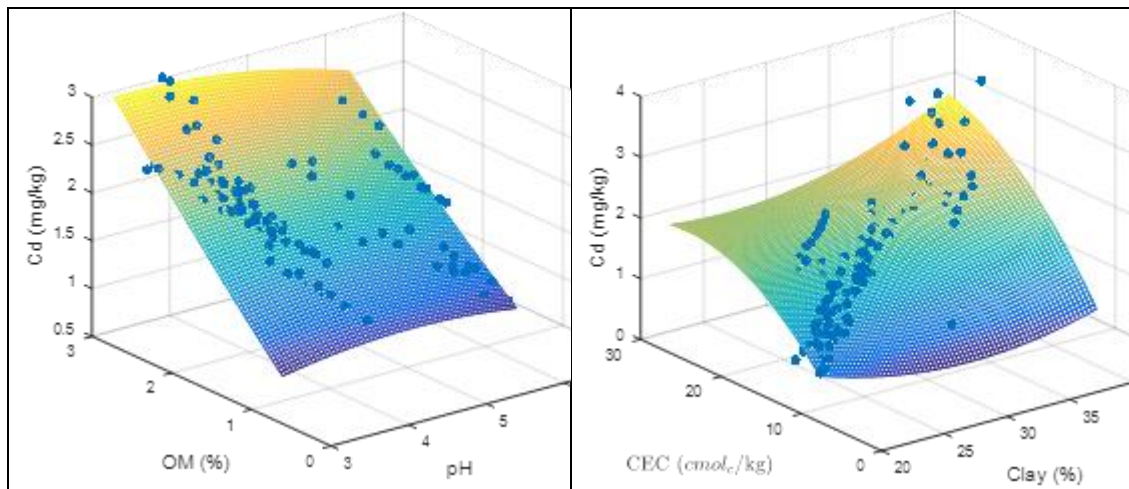


Figure 1. 3-D plots of the regression curves that relate the Cd concentrations with one or two soil parameters (predictors) in each soil order.

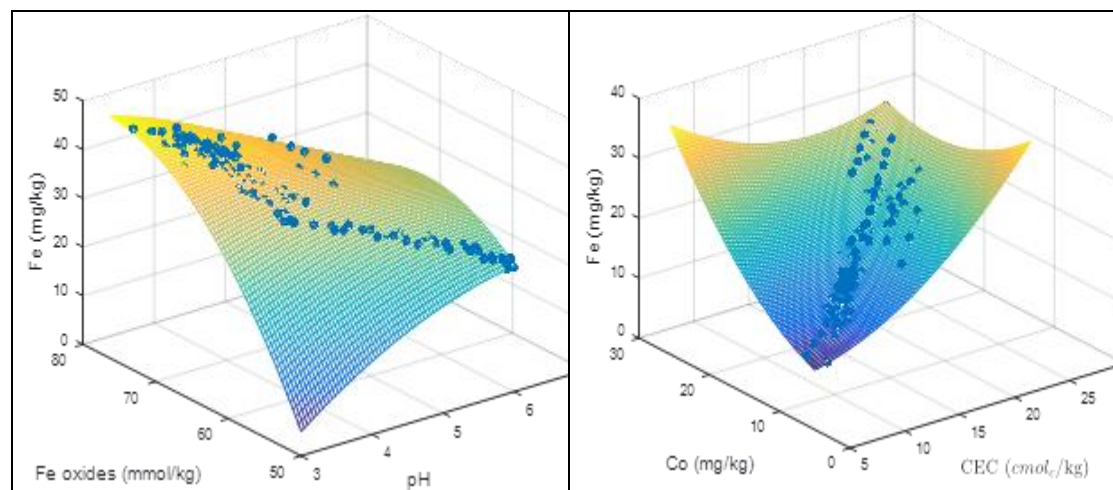


Figure 2. 3-D plots of the regression curves that relate the Fe concentrations with one or two soil parameters (predictors) in each soil order.

The present research was carried out in Greek agricultural soils but the proposed methodology could easily be extended to other regions and soil classes with similar climatic conditions. There is of course a need to collect additional data in the future, so that the proposed prediction equations can be verified, further optimized or even proven to be accurate enough to serve as a useful tool for pollution monitoring and for the rational use of fertilizers.

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