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Digital mapping of the soil available water capacity: insights for the resilience of
agricultural systems to climate change

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Dissertation presented to obtain the degree of Master in
Science. Area: Soil and Plant Nutrition

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3. Valor Shapley 4. Mudanças climáticas 5. Serviços ecossistêmicos I. Título

RESUMO

Mapeamento digital da capacidade de água disponível no solo: insights para a resiliência dos sistemas agrícolas às mudanças climáticas

A capacidade de água disponível no solo (AWC) é uma função chave para a sobrevivência e o bem-estar humano. Entretanto, sua medição direta é trabalhosa e sua interpretação espacial é complexa. Estas dificuldades têm levado ao uso de formas indiretas de estimar a AWC. Entre elas, as técnicas de mapeamento digital do solo (DSM) surgem como uma alternativa à modelagem espacial das propriedades do solo. As técnicas de DSM geralmente aplicam modelos de aprendizagem de máquinas (ML) que não são fisicamente interpretáveis, limitando a possibilidade de construir novos conhecimentos na ciência do solo. Neste contexto, visamos identificar os padrões espaciais estimados pelo algoritmo Random Forest (RF) para prever AWC e, em um estudo de caso, mostrar que os mapas AWC digitais podem apoiar o planejamento agrícola em resposta aos efeitos locais da mudança climática. Para isso, foi aplicada uma abordagem baseada em dados usando atributos de solo determinados em laboratório (argila, areia e conteúdo de matéria orgânica), juntamente com uma função de pedotransferência (PTF), sensoriamento remoto, técnicas DSM, valores Shapley (interpretação do modelo) e dados meteorológicos. O mapa digital do solo AWC e os dados da estação meteorológica foram usados para calcular o balanço hídrico climatológico do solo para os períodos entre 1917-1946 e 1991-2020. A seleção de covariáveis usando os valores Shapley como critério contribuiu para a parcimônia do modelo, obtendo-se métricas de qualidade de ajuste de R^2 0,72, RMSE 16,72 mm m^{-1} , CCC 0,83, e Bias de 0,53 sobre o conjunto de validação. As maiores contribuições para a previsão de AWC do solo foram imagens multitemporais Landsat com pixels de solo descoberto, média diurna e variação anual de temperatura. O presente estudo de caso mostra que as mudanças climáticas no local do estudo modificaram o regime pluviométrico, aumentando a quantidade de água retida no solo durante o período seco (de abril a agosto). A metodologia utilizada fornece insights para construir estratégias que permitam a adaptação dos sistemas agrícolas aos efeitos da mudança climática.

Palavras-chave: Aprendizagem de máquinas, Sensoriamento remoto, Valor Shapley, Mudanças climáticas, Serviços ecossistêmico

ABSTRACT

Digital mapping of the soil available water capacity: insights for the resilience of agricultural systems to climate change

Soil available water capacity (AWC) is a key function for human survival and well-being. However, its direct measurement is laborious and spatial interpretation is complex. These difficulties have led to the use of indirect ways of estimating AWC. Among those, digital soil mapping (DSM) techniques emerge as an alternative to spatial modeling of soil properties. DSM techniques commonly apply machine learning (ML) models which are not physically interpretable, limiting the possibility to build new knowledge in soil science. In this context, we aimed to identify the spatial patterns estimated by the Random Forest (RF) algorithm to predict AWC and, in a case study, to show that digital AWC maps can support agricultural planning in response to the local effects of climate change. To do so, a data-driven approach was applied using laboratory-determined soil attributes (clay, sand, and organic matter contents), together with a pedotransfer function (PTF), remote sensing, DSM techniques, Shapley values (model interpretation), and meteorological data. The AWC digital soil map and weather station data were used to calculate climatological soil water balances for the periods between 1917-1946 and 1991-2020. The selection of covariates using Shapley values as a criterion contributed to the parsimony of the model, obtaining goodness-of-fit metrics of R^2 0.72, RMSE 16.72 mm m⁻¹, CCC 0.83, and Bias of 0.53 over the validation set. The highest contributing covariates for soil AWC prediction were the Landsat multitemporal images with bare soil pixels, mean diurnal, and annual temperature range. The present case study shows that climate changes at the study site modified the rainfall regime, increasing the amount of water retained in the soil during the dry period (from April to August). The used methodology provides insights to build strategies that allow the adaptation of agricultural systems to the effects of climate change.

Keywords: Machine learning, Remote sensing, Shapley value, Climate change, Soil functions, Ecosystem services

INTRODUCTION

Soil available water capacity (AWC) is a key function for human survival and well-being (Keesstra et al., 2016). The AWC concept is defined as the difference between field capacity (FC) and permanent wilting point (PWP). The PWP is usually considered as the water content corresponding to a pressure head of -150 m (Garg et al., 2020), standardized for any weather and crop conditions. The FC is defined as the water content in the soil after saturation without evapotranspiration when free drainage reaches a negligible flow (Veihmeyer and Hendrickson, 1931). It is sometimes assumed to correspond to a specific pressure head, and the most common values used in this context are -0.6, -1 or -3.3 m.

The direct evaluation of AWC is laborious since it implies undisturbed sampling and analysis in specialized laboratories. Therefore, AWC is most commonly estimated indirectly, e.g. using pedotransfer functions (PTF) correlating readily available soil information such as particle size distribution and organic matter (OM) content with soil hydraulic properties (Barros et al., 2013; Inforsato and de Jong van Lier, 2021). While these approaches provide a specific point notion, the efficient management of water resources in agricultural areas requires a spatial and temporal understanding.

The understanding of land surface and atmospheric processes and their parameterization for agricultural water resources management advanced in recent years (Chartzoulakis and Bertaki, 2015). Earth observation techniques using different parts of the electromagnetic spectrum have been used for over three decades to monitor the Earth's surface (Weiss et al., 2020). These techniques are now being transferred to operational applications like agricultural land management, offering the opportunity for new observational and modeling perspectives (Bouma et al., 2015). In this context, Digital Soil Mapping (DSM) emerges as a technique to obtain explicit spatial information on soil properties at different scales (McBratney et al., 2003).

Despite significant advances in understanding soil spatial variability through pedometric and DSM techniques, there is a need to refine the methods of obtaining relevant soil data, in addition to an interpretation of the Machine Learning (ML) models used in DSM approaches (Wadoux et al., 2021). The ML models are "black boxes" of low interpretability since they find the correlations that best describe the patterns between soil properties and the covariates used in the modeling in a merely statistical manner (McBride, 2021). ML model interpretation techniques that emerged in other areas of knowledge were adapted recently to soil science in DSM approaches (Padarian et al., 2020; Wadoux et al., 2020). In that context, the game theory proposed by Shapley (1953) and adapted by

Lundberg and Lee (2017) is a helpful approach for the interpretation of ML models used in DSM (Wadoux and Molnar, 2022).

The predictions made by ML models should be associated with the soil-forming factors to drive new knowledge in soil science (Wadoux et al., 2020). In that context, our goals were i) to identify the spatial patterns detected by the Random Forest (RF) algorithm for the prediction of soil AWC using a data-driven approach and Shapley values, and ii) to demonstrate that AWC digital soil maps coupled with meteorological data can be used to detect trends in soil water retention caused by climate change. The following hypotheses were constructed: i) the soil AWC is related to covariates that represent soil-forming factors; ii) in this context, game theory can be applied as a covariate reduction method to build a parsimonious model.

To pursue the objectives and test the hypotheses, the approach used to estimate the soil water AWC at each sampling point is described. Subsequently, the RF predictor model and the covariates used in its training are presented. Then, the model interpretation method is introduced, and the results are discussed. Finally, a case study is presented using the elaborated soil AWC map and a historical series of meteorological data to produce a normal soil water balance to support agricultural planning (sowing/planting and harvesting time) in response to the local effects of climate change.

CONCLUSIONS

Our results, obtained in a tropical scenario context, indicate that the RF algorithm captures spatially discriminant patterns of soil AWC when using climate and pedogenesis-related covariates retrieved from freely available datasets, platforms, and software. Multitemporal Landsat images with bare soil pixels, and mean diurnal and annual temperature ranges are promising covariates for modeling soil water dynamics.

Covariate refinement using SHAP value as a criterion is a useful strategy within DSM approaches as it allows the creation of parsimonious models and reduces the risk of overfitting. Although the constructed model showed robustness and high predictive power, the predictions made in soils with high textural gradients developed from siltstone presented higher values of uncertainty (~ 17 at 23 mm m^{-1}).

Finally, the proposed approach provides relevant insights for adaptive management and crop yield improvements in response to the local effects of climate change through adaptations of traditional planting and harvesting times and soil management practices.

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