A new machine-learning model to partition soil organic carbon into its centennially stable and active fractions based on Rock-Eval(r) thermal analysis

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PARTYsoc v3: A new machine-learning model to partition soil organic carbon into its centennially stable and active fractions based on Rock-Eval® thermal analysis

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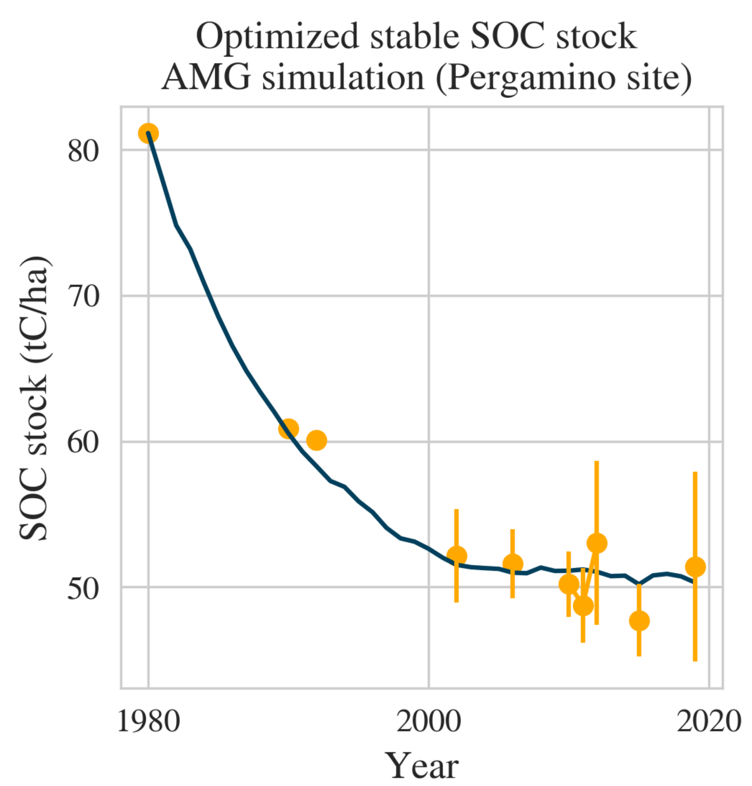
Introduction

- Accurately simulating soil organic carbon (SOC) stock evolution is crucial for assessing the role of soil in climate regulation.
- SOC evolution is often modeled by dividing SOC into kinetic pools with contrasting residence times. **Initializing such kinetic pools remains a complex** task and a source of uncertainty in SOC simulations.
- In a previous study, Cécillon et al. [1] developed a machine-learning model (PARTYsoc v2) that uses Rock-Eval® thermal analysis results as input features to quantify the proportion of centennially stable and active SOC fractions.
- These proportions have been shown to be particularly effective for initializing the AMG model, enabling very accurate simulations of SOC stock evolutions for a dozen French agricultural long-term experiments [2].
- This present work builds **a new version of PARTYsoc**, validated on a larger data set, and extends the usefulness of the AMG model initialized with PARTYsoc to different parts of the world.

Materials and methods

Data

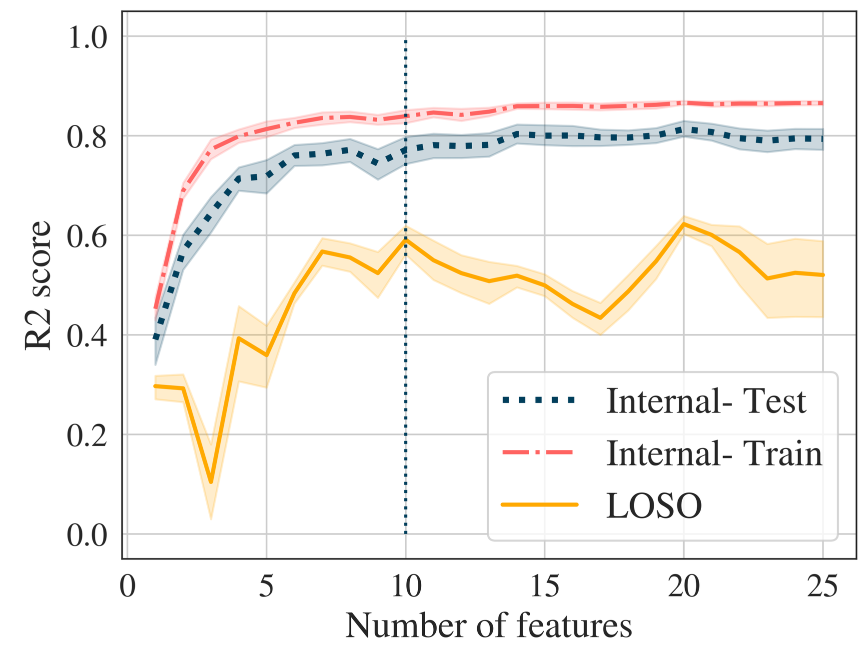
- Data collection of 18 sites with known crop yields and SOC stock evolutions and archived soil samples available for Rock-Eval® characterization.
- Sites are located in Europe and South America.
- The list of Rock-Eval® parameters [3] represents our potential **set of features**.
- The stable SOC stock size for each site is determined by optimization of the AMG model as in Clivot et al. (2019) [4].



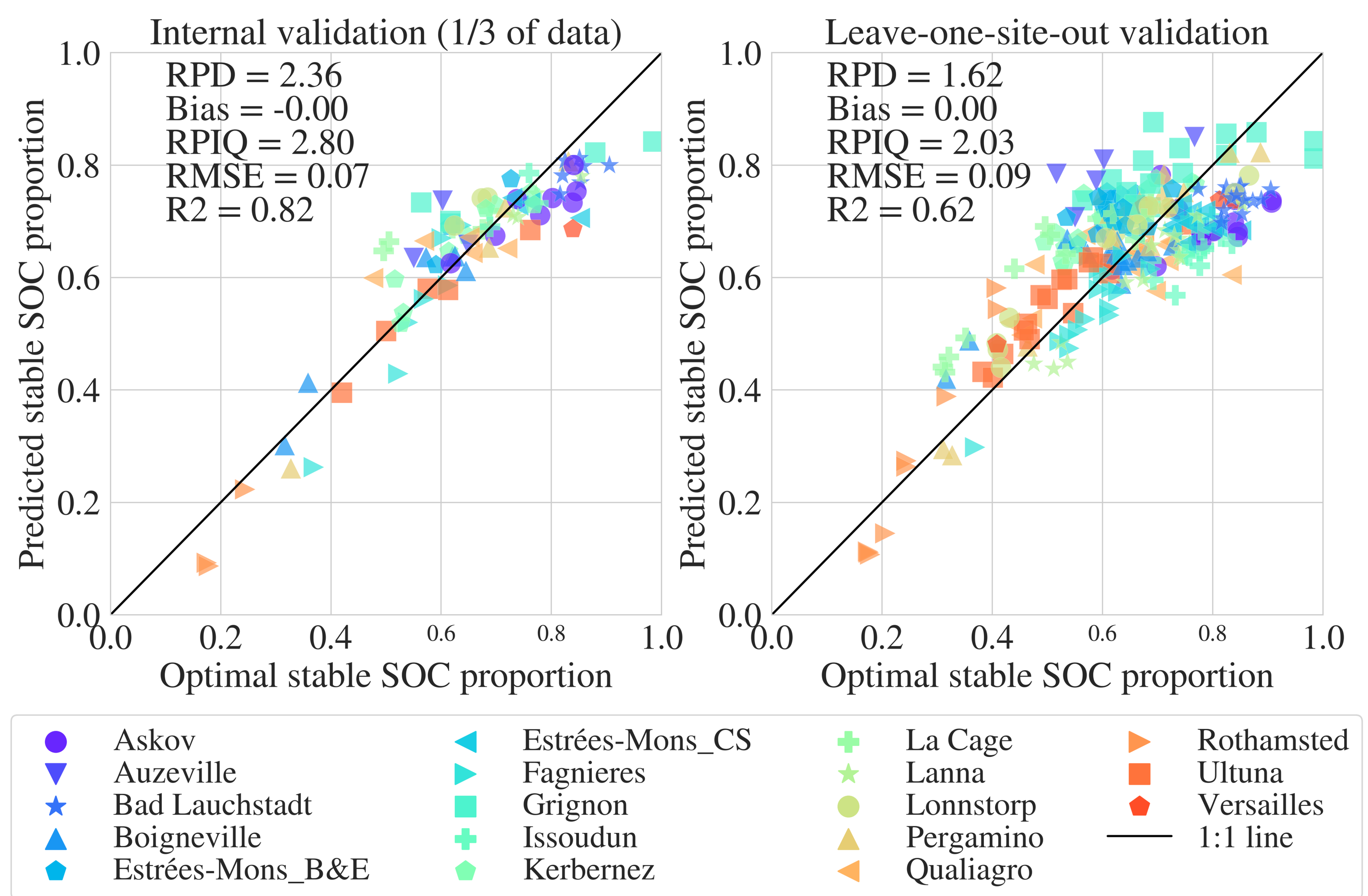
- Using the optimal stable SOC stock values, we calculate the stable SOC proportion of each sample from each site, representing our **target variable**.
- We reserve 1/3 of the data for testing, and use 2/3 for training.

Feature engineering and model training

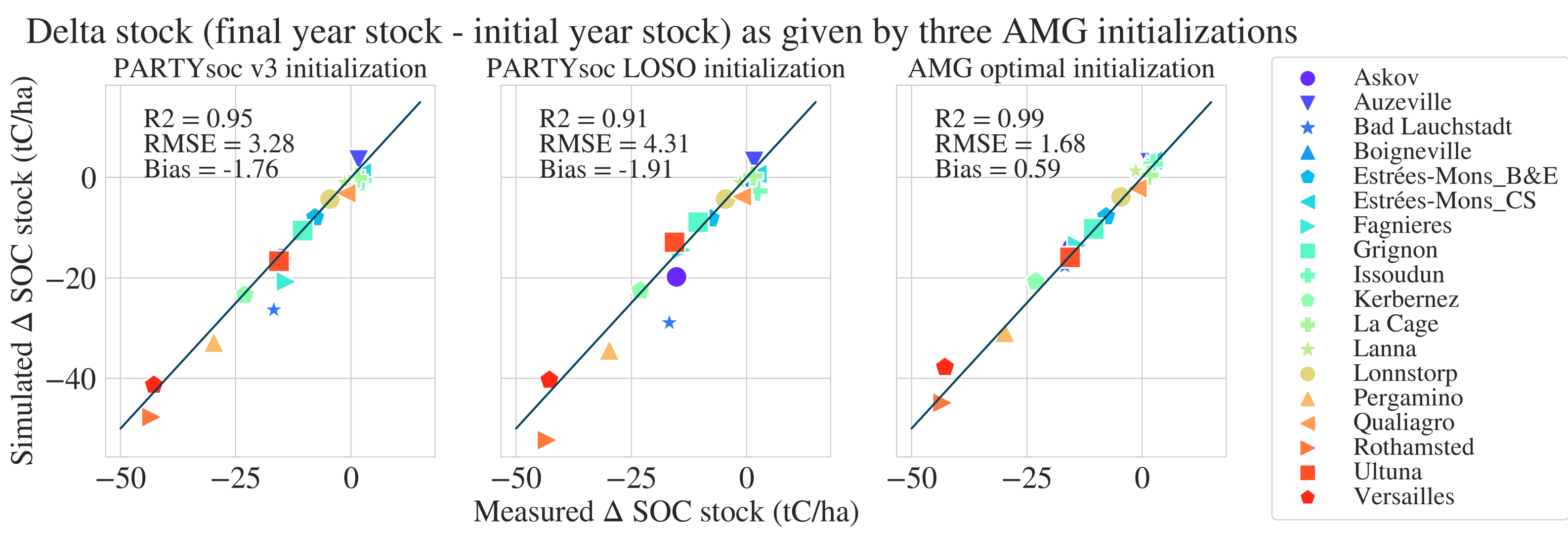
- We remove the highly correlated Rock-Eval® features using Spearman's correlation and a threshold of 0.9.
- We use AutoFeatureCorrelation and permutation importance to **rank the features according to their impact on the predicted target**.
- We run 30 repetitions of 5-fold cross-validation to find the **optimal number of features** for prediction on the test set and in Leave-One-Site-Out (LOSO) validation.
- The final model is a **combination of a Support Vector Machine (SVM) and a Beta regression**, trained using 10 Rock-Eval® features.



Results



- On average, we obtain an $R^2 = 0.78$ and RMSE = 0.07 in internal validation, and $R^2 = 0.59$ and RMSE = 0.09 in LOSO validation.



- Using PARTYsoc v3 (LOSO) values to initialize AMG simulations offers comparable results to initializing with optimal AMG values.

Conclusions and forthcoming research

- The proposed new PARTYsoc v3 builds upon and improves the original PARTYsoc v2 by incorporating a larger data set covering a **wider geographic area**, and a **and more parsimonious machine-learning model** (10 vs. 18 Rock-Eval® features in PARTYsoc v2).
- We are currently working on extending the data set as well as stabilizing the processes of feature selection and model parameterization.

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