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An ensemble estimate of Australian soil organic carbon using machine learning and process-based modelling

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Abstract

Spatially explicit prediction of soil organic carbon (SOC) serves as a crucial foundation for effective land management strategies aimed at mitigating soil degradation and assessing carbon sequestration potential. Here, using more than 1000 in-situ observations, we trained two machine learning models (random forest, and K-means coupled with multiple linear regression), and one process-based model (the vertically resolved MIcrobial-MIneral Carbon Stabilization (MIMICS)) to predict SOC content of the top 30 cm of soil in Australia. Parameters of MIMICS were optimized for different site groupings, using two distinct approaches, plant functional types (MIMICS-PFT), and the most influential environmental factors (MIMICS-ENV). We found that at the continental scale, soil bulk density and mean annual temperature are the dominant controls of SOC variation, and that dominant controls vary for different vegetation types. All models showed good performance in SOC predictions with R^2 greater than 0.8 during out-of-sample validation with random forest being the most accurate, and SOC in forests is more predictable than that in non-forest soils. Parameter optimization approaches made a notable difference in the performance of MIMICS SOC prediction with MIMICS-ENV performing better than MIMICS-PFT especially in non-forest soils. Digital maps of terrestrial SOC stocks generated using all the models showed similar spatial distribution with higher values in southeast and southwest Australia, but the magnitude of estimated SOC stocks varied. The mean ensemble estimate of SOC stocks was 30.08 t/ha with K-means coupled with multiple linear regression generating the highest estimate (mean SOC stocks at 38.15 t/ha) and MIMICS-PFT generating the lowest estimate (mean SOC stocks at 24.29 t/ha). We suggest that enhancing process-based models to incorporate newly identified drivers that significantly influence SOC variations in different environments could be key to reducing the discrepancies in these estimates. Our findings underscore the considerable uncertainty in SOC estimates derived from different modelling approaches and emphasize the importance of rigorous out-of-sample validation before applying any one approach in Australia.

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1. Introduction

Globally, the soil is the largest biogeochemically active terrestrial carbon pool, storing more organic carbon than plants and the atmosphere combined. The turnover of soil organic carbon (SOC) is a key function in plant growth, maintenance of soil water and nutrients, soil structure stabilization and other biogeochemical processes (Lefèvre et al., 2017). Soil can act as either a carbon sink or carbon source depending on the balance of carbon input through plant litter and root exudates and output through respiration and leaching (Terrer et al., 2021; Panchal et al., 2022). Even a small change in SOC stocks, in any direction, could significantly affect the atmospheric concentration of CO_2 and thereby climate change (Stockmann et al., 2013).

Given the importance of SOC, there is now a large and growing interest in estimating spatially explicit SOC content and stocks. SOC supports critically important soil-derived ecosystem services, and the amount of SOC indicates the degree of land and soil degradation (Lorenz et al., 2019). SOC content below a certain limit will lead to the decline of microbial diversity, water holding capacity and soil productivity (Stockmann et al., 2015). Additionally, with growing concerns about increasing anthropogenic CO_2 emissions, soil carbon sequestration has emerged as a potential strategy for climate change mitigation (Smith, 2016; Rumpel et al., 2018). Protection of existing SOC and rebuilding depleted stocks through land management are potential strategies in mitigating climate change (Bossio et al., 2020). However, effective SOC management requires accurate knowledge of its existing distribution. Reliable estimates of SOC stocks and their spatial variation serve as a reference point for assessing how close soil is to its maximum SOC storage capacity and its potential to sequester additional carbon (Six et al., 2002; Georgiou et al., 2022). Precise estimation of contemporary SOC stocks also provides a baseline map that can be used to calibrate and initialize dynamic-mechanistic models, enabling the study of how SOC will respond to climate and land-use change (Minasny et al., 2013; Viscarra Rossel et al., 2014). It is, for example, a prerequisite for accurately predicting future carbon–climate feedbacks in Earth system models (ESMs) (Todd-Brown et al., 2013).

Accurately assessing SOC storage is challenging due to the complexity of carbon formation and degradation processes in space and time (Keskin et al., 2019). Soil exists as a continuum containing organic compounds at different stages of decomposition (Lehmann and Kleber, 2015). Soil formation can be described by a function of climate, organisms, relief, parent material and time (Jenny, 1994). These factors are widely used in SOC studies for digital soil mapping (McBratney et al., 2003; Viscarra Rossel et al., 2015; Liang et al., 2019). However, the relationship between SOC storage and these driving variables is complex and spatially variable (Mishra and Riley, 2015; Viscarra Rossel et al., 2019; Adhikari et al., 2020) leading to substantial challenges and inherent uncertainties in SOC predictions.

Mechanistic process-based models and empirical models (including machine learning models) are two widely employed approaches used to predict SOC stocks and their spatial distribution. Conventional process-based models assume first-order kinetics for SOC decomposition,

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wherein the rate of C decomposition is dependent on temperature and moisture but independent of microbial biomass, and equilibrium SOC stock is proportional to carbon input and mean residence time (Abs and Ferrière, 2020; Wang et al., 2021). ESMs coupled with conventional SOC models cannot accurately predict patterns of contemporary soil carbon and show high uncertainties in projected SOC dynamics under future climate change (Todd-Brown et al., 2013; Todd-Brown et al., 2014). This is partly due to the lack of explicit representation of soil microbial activities and metabolic traits (Wieder et al., 2015). Numerous microbial models have been developed in the past few decades to improve model performance of SOC predictions (Chandel et al., 2023), but these models has rarely been incorporated into large-scale modelling frameworks partly due to the lack of rigorous validation (Luo et al., 2016). Process-based SOC models are constructed based on our understanding on the major processes governing SOC dynamics (e.g., carbon input, decomposition, and loss). However, the disagreement in projections of carbon dynamics by different models highlights the need to improve our knowledge of SOC cycling (Luo et al., 2016). Machine learning models without any process-level assumptions provide a tool to identify the most influential controls on SOC variations. Machine learning models can represent non-linear and non-smooth relationships between predictor and response variables as well as interactions between different predictors (Heung et al., 2016). Various machine learning algorithms have been successfully used in digital soil mapping to predict high-resolution spatially explicit SOC content (Lamichhane et al., 2019).

Several modelling studies of soil carbon content/stocks have been conducted in Australia. Wang et al. (2018a) trained boosted regression trees and random forest models using observations from the semi-arid rangelands of eastern Australia. Both models predicted SOC stocks moderately well based on performance metrics. The fitted models were then applied to map the spatial distribution of SOC at two soil depths (0-5 cm and 0-30 cm). Continentally, Viscarra Rossel et al. (2014) trained the CUBIST model, a form of piecewise linear decision tree, using more than five thousand observations to produce a high resolution (90 m × 90 m) baseline map of SOC stocks of Australian terrestrial systems and its uncertainty at 30 cm depth. Based on the baseline map, Walden et al. (2023) derived spatially explicit estimates of Australian SOC stocks and uncertainty including additional data from forests from southeastern Australia and coastal marine (or blue carbon) ecosystems. SOC content at multiple soil depths along with associated uncertainties were also estimated using different machine learning algorithms (Viscarra Rossel et al., 2015; Wadoux et al., 2023). Moreover, the distribution of different soil carbon compositions (i.e., the particulate, mineral-associated and pyrogenic organic carbon fractions) and the importance of environmental factors on their variations were also studied using machine learning (Viscarra Rossel et al., 2019). However, despite the progress made in SOC modelling, significant uncertainties persist in SOC estimates due to the inherent complexities of SOC variations, the lack of appropriately sampled SOC observations and the amount of data. All these continental estimates were generated using empirical modelling approaches or first-order biogeochemical models (Grace et al., 2006; Lee et al., 2021). Estimates from mechanistic SOC models with explicit representation of microbial metabolism are missing despite offering the

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potential to better constrain SOC dynamics under future climate change scenarios in a way that empirical approaches cannot.

Our primary objective in this paper is to assess the predictability of SOC stocks in Australia. We generate a range of estimates of terrestrial SOC stocks, employing both process-based and empirical modelling, and examine why these estimates might differ. First, we discern the significance of environmental predictors, both at continental and biome scales. We then evaluate the performance of random forests, k-means with multiple linear regression and the vertically resolved MIcrobial-MIneral Carbon Stabilization (MIMICS) SOC model with different parametrization approaches. Finally, we compare the spatial estimates of SOC stocks using these different approaches across Australia, and discuss their differences and potential application to future SOC projection.

2. Materials and Methods

2.1. Model descriptions

2.1.1. Vertically resolved MIMICS

The MIcrobial-MIneral Carbon Stabilization (MIMICS) model (Wieder et al., 2015; Zhang et al., 2020) is a soil carbon model that explicitly considers relationships between litter quality, functional trade-offs in microbial physiology, and the physical protection of microbial by-products in forming stable soil organic matter. There are two litter pools: metabolic (LIT_m) and structural (LIT_s) litter (Figure 1), and the partitioning of litter input into metabolic and structural pools is determined by the chemical properties of the litter. Litter and SOC turnover are governed by two microbial functional types that exhibit copiotrophic (i.e., r-selected, MIC_r) and oligotrophic (i.e., K-selected, MIC_k) growth strategies. The MIC_r is assumed to have higher growth and turnover rates, and a preference for consuming labile litter (LIT_m), while MIC_k is characterized by lower growth and turnover rates, and a greater competitive advantage when consuming low-quality litter (LIT_s) and chemically recalcitrant SOC. SOC in MIMICS is divided into three pools: physically protected (SOC_p), (bio)chemically recalcitrant (SOC_c) and available (SOC_a) carbon (Figure 1).

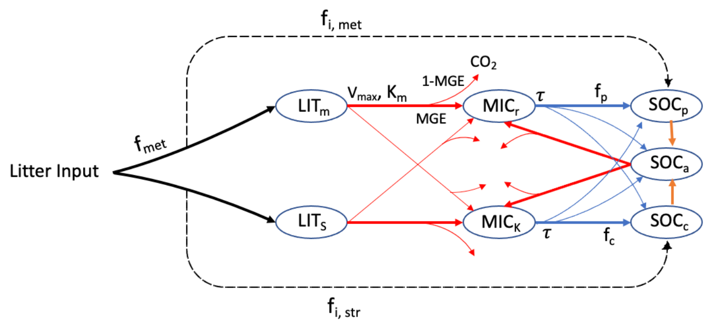

Figure 1. Soil carbon pools and fluxes represented in MIMICS (adapted from Wieder et al., (2015)). Litter inputs are partitioned into metabolic and structural litter pools (LIT_m and LIT_s) based on litter quality (f_{met}).

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Decomposition of litter and available SOC pool (SOC_a) are governed by temperature sensitive Michaelis-Menten kinetics (V_{max} (maximum reaction velocity) and K_m (half saturation constant)), shown by red lines. Microbial growth efficiency (MGE) determines the partitioning of C fluxes entering microbial biomass pools vs. heterotrophic respiration. Turnover of microbial biomass (τ, blue) depends on microbial functional types (MIC_r and MIC_k), and is partitioned into available, physically protected and chemically recalcitrant SOC pools (SOC_a, SOC_p and SOC_c, respectively).

The decomposition of litter pools and SOC pools follows temperature-sensitive Michaelis-Menten kinetics. Microbial growth efficiency (MGE) determines the partitioning of carbon fluxes entering microbial biomass pools (MIC_r and MIC_k) versus heterotrophic respiration. Access of microbial enzymes to available substrates is restricted by soil texture. The equations of MIMCS are from Wieder et al. (2015), except that the density-dependent microbial turnover was introduced to MIMCS to minimize an unrealistic oscillation (Zhang et al., 2020). To better simulate carbon turnover at different soil depths, vertical transport of soil carbon was introduced into MIMICS considering carbon transported through bioturbation and diffusion among adjacent soil layers (Wang et al., 2021).

Vertically resolved MIMICS is run using a daily time step. The soil was divided into 15 layers, each of 10 cm thickness. All the sites in this study are assumed to be at steady state (i.e., no interannual variation of SOC). Historical climate, litterfall input and soil properties were all assumed to be similar to the average conditions. At each site, the pool size was initialized within a sensible range for different pools and spun up to finally achieve steady state.

2.1.2. Machine learning

Two machine learning algorithms were applied in this study to predict SOC. First, random forest (RF) is a tree-based ensemble learning method that works by building a set of regression trees and averaging results (Breiman, 2001). Within the training procedure, the RF algorithm produces multiple trees. Each regression tree in the forest is independently constructed based on a unique bootstrap sample (with replacement) from the original training data set. The response, as well as the predictor variables are either categorical (classification trees) or numeric (regression trees). Bootstrap sampling makes RF less sensitive to overfitting and allows for robust error estimation based on the remaining test set, the so-called Out-Of-Bag (OOB) sample (Wiesmeier et al., 2014). We used the "ranger" package R (version 4.2.0) for RF computation. We trained the RF model with different numbers of trees and observed that the model's performance remained similar regardless of the number of trees used. The number of regression trees generated in the forest (num.trees) was finally set as 200, and the number of predictors randomly selected at each node (mtry) was set as default, which was 2.

Multiple linear regression (MLR) is widely used in SOC studies but found to be less effective than machine learning algorithms (Lamichhane et al., 2019). Here, instead of applying MLR directly with all environmental factors as predictors, our approach involved a preliminary step where we partitioned all observations into distinct clusters using K-means, an unsupervised

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machine learning algorithm. K-means aims to segregate the data into a predefined number of clusters (k), with the objective of maximizing the similarity among data within each cluster. The underlying assumption here was that sites sharing similar environmental conditions would exhibit comparable SOC concentration. In cases where certain clusters had fewer observations than five times the number of predictors, we augmented these clusters by incorporating observations from other clusters. This augmentation process was guided by the Euclidean distance between the observation and the cluster centre, ensuring a more robust construction of the linear regression model. To determine the number of clusters, we applied the coupled K-means and MLR with varying number of clusters. The selection of the optimal number of clusters was based on the criterion of producing the smallest root mean square error during independent out-of-sample validation.

2.2. Identification of dominant controllers on SOC concentration

RF-based measures of variable importance have gained widespread popularity as tools for evaluating the contributions made by predictor variables within a fitted random forest model (Debeer and Strobl, 2020). In the context of this study, we employed permutation variable importance (PVI) within the random forest framework to gauge the significance of predictors in predicting SOC concentration.

The permutation variable importance entails measuring the reduction in a RF model's performance score upon random shuffling of a single variable values. By doing so, the inherent relationship between the variable and the SOC concentration is disrupted. Consequently, the disparity in prediction accuracy observed in a random forest model before and after such shuffling serves as a quantitative representation of the significance of the particular predictor in predicting SOC concentration. The greater the importance of the predictor, the higher its corresponding PVI value becomes.

2.3. Parameter optimization

MIMICS parameters were derived from (Zhang et al., 2020; Wang et al., 2021), except that five parameters (Table 1) which directly control the organic carbon decomposition were optimized. An effective global optimization algorithm called the shuffled complex evolution (SCE-UA, version 2.2) method (Duan et al., 1993) was applied for parameter optimization. Parameters were optimized by minimizing the sum of squared residuals between the observed and modelled values.

Vertically resolved MIMICS simulated SOC concentration for 15 soil layers. As observations only provide one measurement for the top 30 cm soil, we computed the average of the modelled values spanning the 0-10 cm, 10-20 cm, and 20-30 cm soil layers. This average was then adopted as the modelled SOC concentration for top 30 cm soil, serving as the basis for evaluating the difference between observations and simulations.

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Table 1. The optimized model parameters and their value range

Parameter	Definition	Range
a_v	A scaling factor for V_{max}	0-30
a_k	A scaling factor for K_m	0-20
xdesorp	A scaling factor for SOC desorption rate	0-3
xbeta	An exponent of the biomass density dependent mortality rate of microbes	1.05-2
xdiffsoc	A scaling factor for SOC diffusion coefficient in soil	0-30

Parameters were optimized for distinct groups divided based on two approaches. The first approach involved categorizing all observations into four groups based on plant functional types (PFTs). The second approach was taking the most influential abiotic variables as predictors (as outlined in Section 2.2) and dividing all observations into 6 clusters using the K-means algorithm. The determination of the optimal number of clusters was achieved through the minimization of the sum of the within-cluster-sum-of-squares-of-all-clusters (WCSSE), a process facilitated by the "ClusterR" package in R (version 4.2.0). This clustering aimed to ensure the highest possible similarity among the environmental factors within each cluster. It was anticipated that SOC ranges within each cluster would be narrow due to the high similarity of environmental predictors.

2.4. Data

2.4.1. Predictors of SOC concentration

MIMICS requires gridded mean annual temperature (MAT), carbon input and clay content as driving variables for a spatial simulation. Soil bulk density is also required for conversion between SOC concentration (g C/kg soil) and SOC stocks (t/ha). Gridded mean annual precipitation (MAP) and vegetation types were also used during calibration and when understanding the drivers and spatial variability of SOC. Details of gridded data can be found in Table 2.

Gridded daily maximum temperature, minimum temperature, and precipitation at 0.05° resolution were obtained from the SILO database of Australian climate data. Mean daily temperature was approximated as the average of maximum and minimum daily temperature. MAT was calculated from mean daily temperature from 1991 to 2020, and MAP was calculated from daily precipitation from 1991 to 2020.

Carbon input was represented by NPP. Gridded mean annual NPP at 500 m was calculated based on annual NPP from 2001 to 2020 obtained from MODIS (MOD17A3HGF V6.1). NPP was partitioned to above-/belowground part by multiplying by the root/shoot ratio for different vegetation types (Mokany et al., 2006).

The distribution of vegetation types at 3” resolution was obtained from National Vegetation Information System (NVIS, version 6.0). Pixels of non-vegetated regions were removed and types were aggregated to just 4 PFTs: forest, woodland, shrubland and grassland.

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Soil bulk density and clay content were obtained from Soil and Landscape Grid National Soil Attributes Maps (SLGA – Release 2). Soil properties were predicted based on machine learning at depths 0-5 cm, 5-15 cm, 15-30 cm, 30-60 cm, 60-100 cm, and 100-200 cm in SLGA. Bulk density and clay content were estimated for top 30 cm soil as weighted average of first 3 layers in SLGA.

The initial spatial resolution of the gridded data was maintained when extracting the required environmental factors for each SOC observation. All data were then resampled to 0.05° resolution using bilinear interpolation for estimation of terrestrial SOC stocks at continental scale.

Table 2. Information of gridded data used in this study.

	Source	Spatial Scale	Temporal Scale	Unit	Time Period	Ref.
Maximum Temperature	SILO	~5 km	daily	°C	1991-2020	(Jeffrey et al., 2001)
Minimum Temperature	SILO	~5 km	daily	°C	1991-2020	(Jeffrey et al., 2001)
Precipitation	SILO	~5 km	daily	mm	1991-2020	(Jeffrey et al., 2001)
NPP	MODIS	500 m	annually	g C/m^2	2001-2020	(Running and Zhao, 2021)
Vegetation Types	NVIS	100 m	/	/	/	
Soil Bulk Density	SLGA	~90 m	/	kg/m^3	/	(Grundy et al., 2015; Viscarra Rossel et al., 2015)
Soil Clay Content	SLGA	~90 m	/	%	/	(Grundy et al., 2015; Viscarra Rossel et al., 2015)

2.4.2. Soil organic carbon observations

SOC observations for top 30 cm soil in Australia were collected from two datasets. The first one, VR dataset, is described in (Viscarra Rossel et al., 2014; Viscarra Rossel et al., 2019). We removed the observations collected from croplands based on the land-use record in the dataset and removed those from unvegetated regions based on NVIS vegetation map (see above). Observations at 1070 sites remained. SOC stocks were reported in t/ha and converted to SOC concentration (g C/kg soil) using soil bulk density (BD, kg/m^3) and soil depth (m),

$$SOC_{concentration} = SOC_{stock}/(BD \times depth) \times 100 \tag{1}$$

Clay content and soil bulk density were reported in this dataset and also in Viscarra Rossel et al. (2015). To better represent SOC distribution in forest, we obtained more forest SOC observations from a second dataset, the Biomes of Australian Soil Environments (BASE) described in (Bissett et al., 2016). Here, SOC concentration was reported for 0-10 and 20-30 cm, and we estimated the SOC concentration for 20-30 cm soil using the algorithm (Jobbágy and Jackson, 2000) below,

$$\log_{10} C = S \log_{10} d + I \tag{2}$$

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Where *C* represents the SOC stocks (t/ha), and *d* represents depth. *S* and *I* are parameters of the model. We took the average SOC concentration of three layers as the value for top 30 cm soil. Clay content was reported in this dataset and bulk density was extracted from SLGA (see above).

The spatial distribution of SOC concentration observations from different PFTs is shown in Figure 2a. SOC concentration in top 30 cm is positively skewed, ranging from 1.36 to 59.73 g C/kg soil with mean value at 9.97 g C/kg soil and median value at 6.11 g C/kg soil. SOC concentration in grassland, shrubland and woodland show similar distribution patterns (Figure 2b), while SOC concentration in forest is more variable with a standard deviation at 15.92 g C/kg soil.

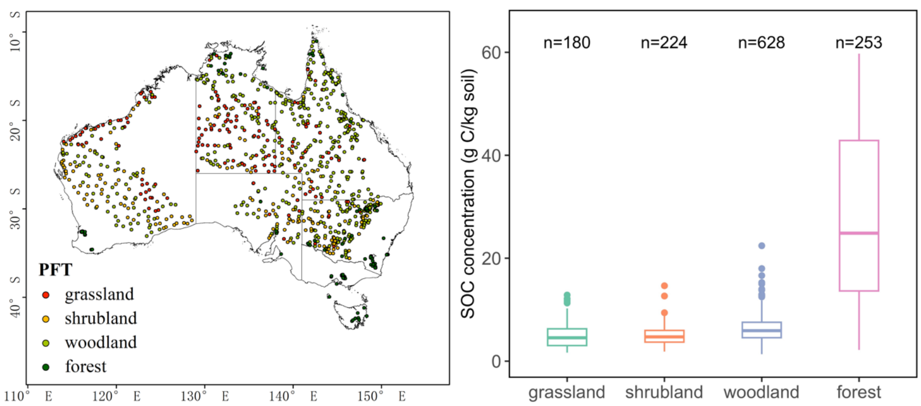

Figure 2. Spatial distribution of 1285 soil organic carbon concentration observations used in this study and the plant functional types which they belong to (a); boxplots of SOC concentration distributions for each plant functional type (b). For boxplots, centre lines represent the median value, and upper and lower box boundaries represent third and first quartile. Whiskers extend to the smallest and largest values within 1.5 times the interquartile range.

2.5. Model evaluation

For machine learning models, all observations were separated to a training and test dataset randomly with 70% used to train the model and the remaining 30% used to validate the predictions of SOC concentration. For vertically resolved MIMICS, parameters were optimized for each group, and we again randomly selected 70% of observations in each group to train the model and used the remaining 30% for validation. To cross-validate, the procedure was repeated 10 times.

The performance of models was evaluated using four metrics. Mean Absolute Error (MAE) indicates how close the average predictions are to average observations. Root Mean Square Error (RMSE) measures the overall accuracy combining mean, standard deviation differences

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(across sites) and (spatial) correlation. Coefficient of determination (R^2) measures the percentage of variation explained by the model. Lin's Concordance Correlation Coefficient (LCCC) (Lawrence and Lin, 1989) measures the level of agreement between predictions and observations following the 1:1 line. A good model will have MAE and RMSE close to 0 and R^2 and LCCC close to 1.

2.6. Estimation of terrestrial SOC stocks

To examine terrestrial SOC stocks and their continental-scale spatial distribution, we generated pixel-based SOC maps utilizing the four models validated within this study. In the cases of MIMICS-PFT and MIMICS-ENV, the initial step involved segregating all pixels into four distinct plant functional groups or six environmental clusters. Since cross-validation was performed, the machine learning and process-based models were evaluated using test data, and the models with the optimal performance were subsequently employed at each pixel to estimate terrestrial SOC stocks. The map of ensemble estimate of SOC stocks was also produced as the average of four models at each pixel.

3. Results

3.1. Dominant environmental controls of SOC concentration

Using the Permutation Variable Importance (PVI) in random forest, we identified the significance of environmental factors in predicting SOC. At the continental scale, soil bulk density is the most influential driver of SOC concentration variations, following by MAT, NPP and MAP (Figure 3). Soil clay content and plant functional type exhibit relatively lesser significance in this regard.

The relative predictor importance for forests and grasslands aligns with the importance at continental scale. In shrubland and woodland, NPP and MAP emerge as the pivotal factors. Collectively, across both continental and regional scales, soil bulk density, MAT, and MAP are the three most influential abiotic factors.

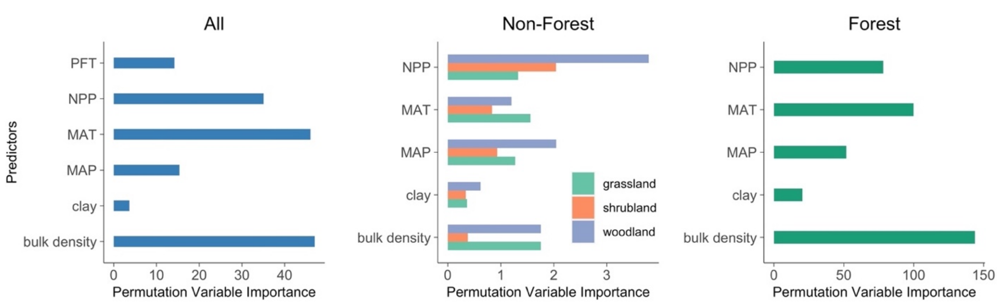

Figure 3. Importance of predictors on SOC concentration for different plant functional types.

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3.2. Data clustering based on environmental factors

To develop the calibration groups for MIMICS-ENV, we partitioned the top three important abiotic factors, which are soil bulk density, MAT and MAP, into six distinct clusters using K-means (see Section 2.3). The resulting characteristics and SOC distributions for these six clusters are illustrated in Figure 4.

Notably, a substantial majority of forests were assigned to clusters 2 and 6 (Figure 4a), while woodland, shrubland, and grassland observations were distributed across the remaining four clusters. Among these clusters, cluster 5 exhibits the lowest SOC concentration, while SOC of cluster 1 and 3 display a comparable pattern but spread across different biomes. Conversely, distribution of SOC concentration in clusters 2, 4, and 6 shows more pronounced variability (Figure 4b).

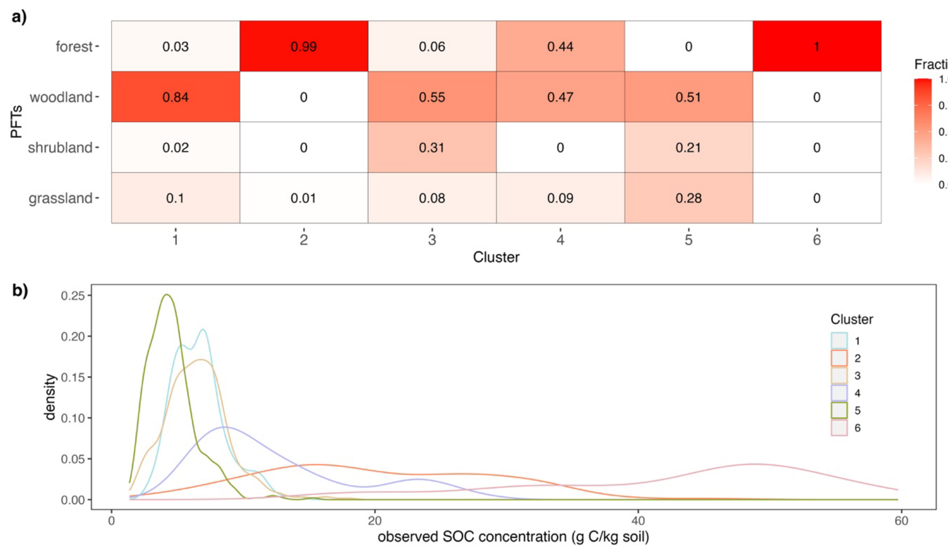

Figure 4. Fraction of different PFTs in each cluster divided based on environmental factors (a) and density plot of observed SOC concentration for different clusters (b).

3.3. Evaluation of model performance

All models employed in this study (RF, K-means + MLR, MIMICS-PFT and MIMICS-ENV) predicted SOC concentration well for both training data and test data (Figure 5). As anticipated, performance for both process-based model and machine learning models degrade using out-of-sample data versus in-sample training or calibration data. When using test data, the mean value of R^2 for all models ranges from 0.82 to 0.94, mean LCCC ranges from 0.90 to 0.97, mean RMSE ranges from 2.88 to 4.51 g C/kg soil, and mean MAE ranges from 1.55 to 2.57 g C/kg soil.

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The machine learning models outperformed MIMICS in predicting SOC concentration, regardless of the optimisation approach taken. Particularly, the random forest algorithm demonstrated the most accurate predictions characterized by higher R^2 and LCCC values and lower RMSE and MAE values for both training and test data. While MIMICS-ENV displayed performance similar to that of MIMICS-PFT in SOC concentration predictions based on RMSE and MAE, the former exhibited slightly superior median R^2 and LCCC values (Figure 5).

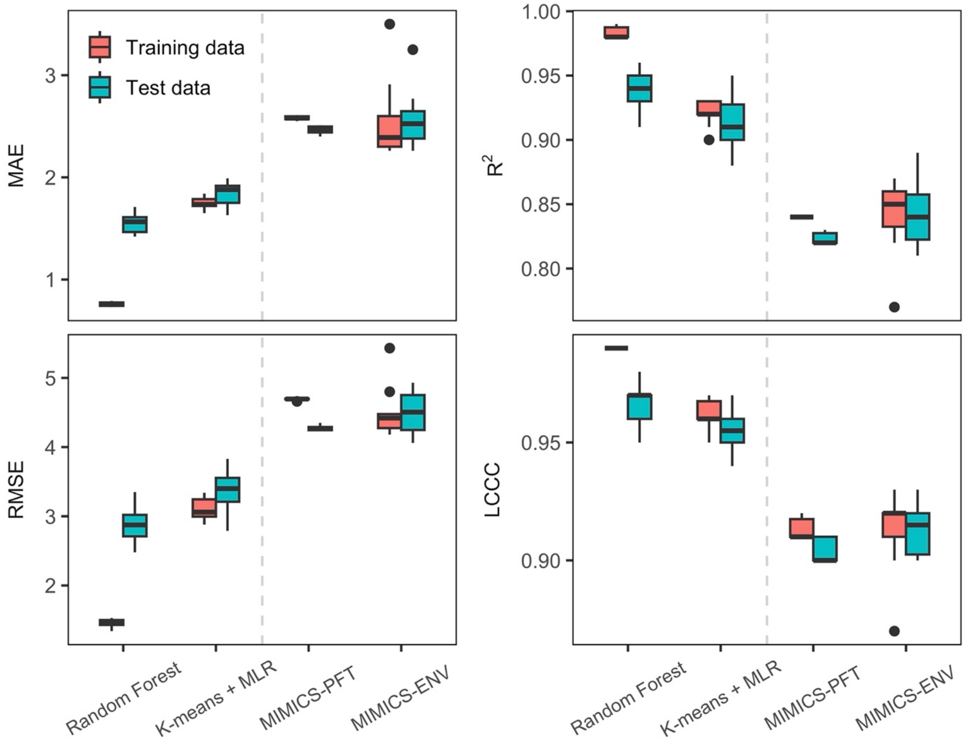

Figure 5. Performance metrics of SOC concentration predictions. Units for MAE and RMSE are g C/kg. Centre line represents median value, and upper and lower box boundaries represent third and first quartile. Whiskers extend to the smallest and largest values within 1.5 times the interquartile range.

SOC concentration in forest soil exhibited significantly higher predictability than those in non-forest (woodland, shrubland and grassland) soil, evidenced by higher R^2 (ranging from 0.58 to 0.91) and LCCC (ranging from 0.75 to 0.95) for test data (Figure 6). Machine learning algorithms surpassed MIMICS in predicting SOC for both forest and non-forest soils. Notably, MIMICS-ENV outperformed MIMICS-PFT in SOC predictions, particularly in non-forest soils.

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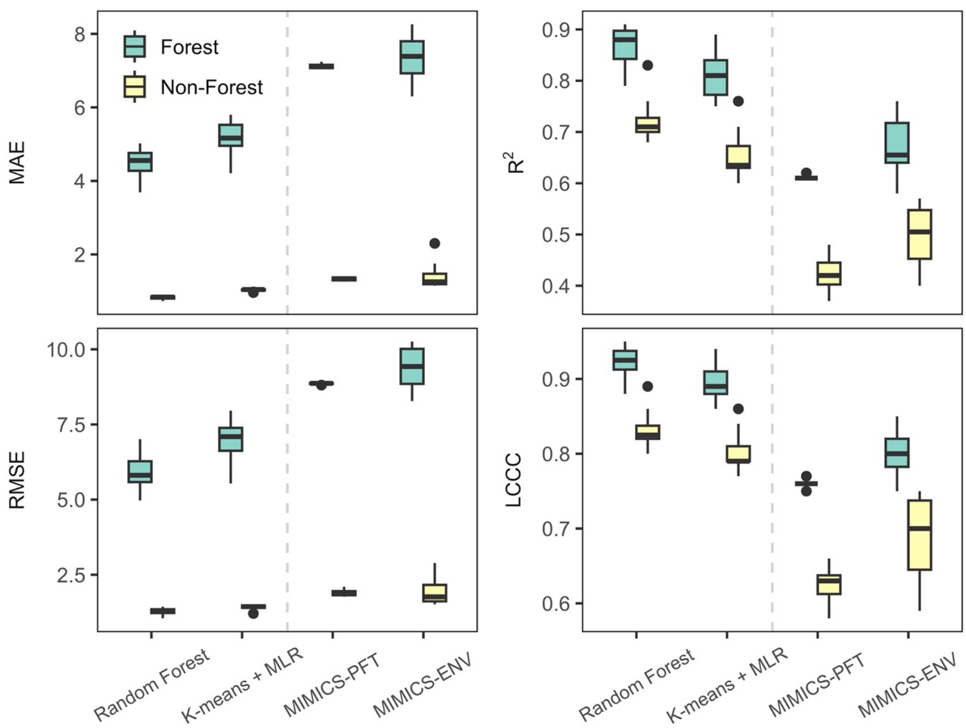

Figure 6. Performance metrics of SOC concentration predictions for forest and non-forest (woodland, shrubland and grassland) soils in test (out-of-sample) data. Unit for MAE and RMSE is g C/kg soil. Centre line represents median value, and upper and lower box boundaries represent third and first quartile. Whiskers extend to the smallest and largest values within 1.5 times the interquartile range.

3.4. Estimations of terrestrial SOC stocks

Descriptive statistics of predicted terrestrial SOC stocks at 0-30 cm soil depth are shown in Table 3. Forests have the largest mean SOC stocks ranging from 70.3 to 113.9 t/ha by all models, and shrubland is estimated to have the lowest mean SOC stocks. The distributions of predicted continental SOC stocks by all models are positively skewed with most estimated SOC stocks less than 50 t/ha (Figure 7a), and SOC stocks at peak density predicted by MIMICS-ENV and MIMICS-PFT are smaller than those predicted by machine learning approaches. The maximum value of SOC stocks predicted by all models vary considerably.

As expected, all models consistently projected greater SOC stocks in the southeast region, southwest corner and Tasmania, and consistently indicated lower SOC stocks in central and western Australia (Figure 7b). Notably, MIMICS-ENV depicted a pronounced deficit of SOC in central Australia, a distinctive pattern compared to the predictions of other models. Among the models, K-means coupled with multiple linear regression consistently provided the highest SOC estimations across all vegetation types, while MIMICS-PFT model consistently yielded the lowest mean SOC stocks.

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The ensemble estimate of SOC stocks (Figure 7c) shows a similar distribution pattern as that generated by single approach. The SOC stocks of the ensemble range from 9.3 to 180.4 t/ha with an average value of 30.1 t/ha. The standard deviation across the four estimates (Figure 7d) is positively correlated with the ensemble mean estimate. That is, soils with higher SOC stocks exhibit greater variability in SOC predictions among different models. Note also that the variability of estimates tends to be smaller in areas with denser numbers of observations.

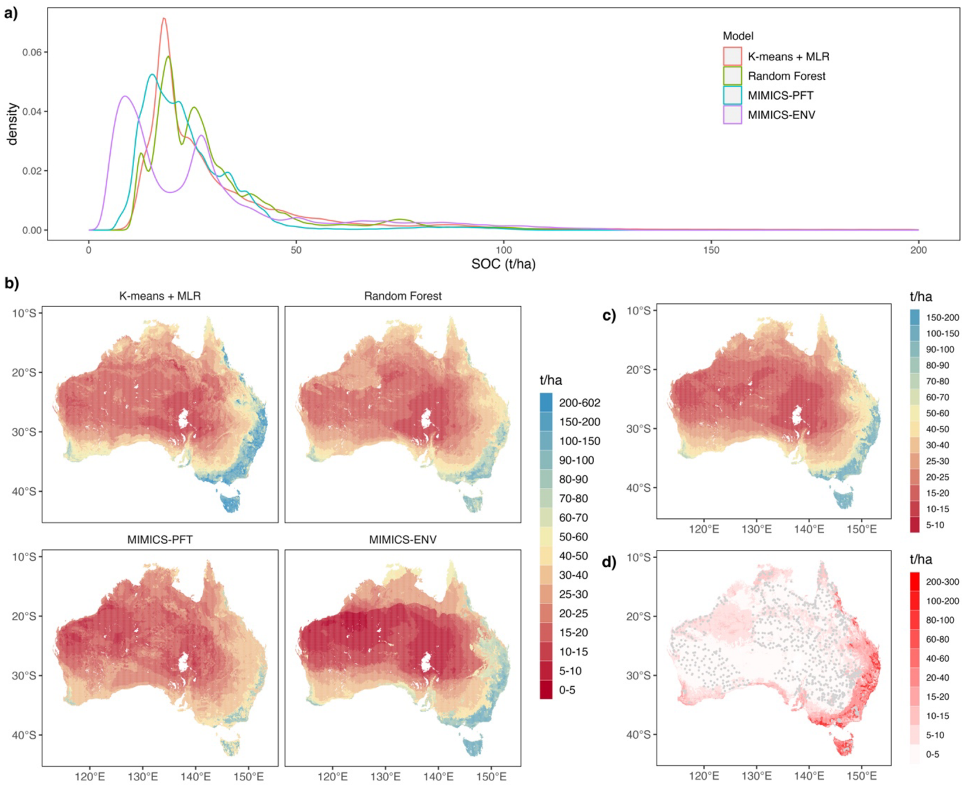

Figure 7. Predicted Australian terrestrial SOC stocks (t/ha) for top 30 cm soil and ensemble statistical characteristics: a) density plot of estimated terrestrial SOC stocks by all models, noting that only stocks less than 200 t/ha are shown for better comparison of the distribution; b) Predicted SOC stocks for each model; c) Predicted SOC stocks of the ensemble; d) standard deviation stocks within the ensemble. Grey points represent locations of SOC observations.

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Table 3. Descriptive statistics of predicted terrestrial SOC stocks (t/ha) at 0-30 cm soil. Min. and Max. are minimum and maximum value, respectively. 1st Qu and 3rd Qu are first and third quartile, respectively.

	PFT	Min.	1st Qu	median	mean	3rd Qu	Max.
K-means + MLR	grassland	4.2	17.9	21.2	41.5	42.5	601.1
	shrubland	7.2	16.4	19.3	23.6	24.4	472.2
	woodland	7.1	20.1	26.1	33.3	33.7	483.1
	forest	18.0	51.3	95.2	113.9	153.4	474.0
	all	4.2	18.1	23.6	38.2	16.7	601.1
Random Forest	grassland	10.4	18.5	26.0	30.4	37.2	125.3
	shrubland	10.3	17.0	19.6	21.4	24.4	104.4
	woodland	10.5	20.3	25.8	28.2	32.4	122.1
	forest	29.3	55.0	82.3	78.4	97.0	161.7
	all	10.3	18.9	25.0	29.8	33.7	161.7
MIMICS-PFT	grassland	10.8	16.4	24.1	25.1	33.3	58.7
	shrubland	6.5	12.2	15.5	16.5	20.6	56.5
	woodland	7.8	17.4	21.2	22.1	25.9	61.4
	forest	17.9	44.5	77.4	70.3	88.5	109.9
	all	6.5	15.7	21.2	24.3	28.9	109.9
MIMICS-ENV	grassland	4.2	7.9	15.4	26.9	37.6	124.0
	shrubland	4.4	9.9	13.4	18.6	25.3	131.9
	woodland	4.9	14.7	26.3	28.4	31.3	131.6
	forest	9.6	53.1	92.4	81.6	106.5	134.1
	all	4.2	10.5	21.9	28.1	33.2	134.1

4. Discussion

4.1. Relative importance of predictors on SOC variations

Extensive research has been conducted to discern the factors that govern SOC content/stocks. Among the commonly employed predictors for SOC variations, climate, organisms, topography, parent material, and soil properties are prominent (Wiesmeier et al., 2019). Within this study, we conducted a comparative assessment of the significance of key variables, namely MAT, MAP, NPP, soil clay content and bulk density, in driving variations in SOC in Australia. While the number of predictors utilized in our approach is fewer than that employed in most digital mapping methodologies, its strength lies in the potential for a more direct comparison between empirical and process-based models.

Soil bulk density is the most important driver of SOC concentration at the continental scale (Figure 3). The role of soil bulk density in SOC has been noted before in eastern Australia (Hobley et al., 2015). Soil bulk density is mainly a function of the parent material, soil genesis as well as soil aggregate formation (Don et al., 2007). A soil with reduced density exhibits superior structural organization and an expanded surface area, facilitating enhanced retention of organic carbon (Lobsey and Viscarra Rossel, 2016). Subsequently, with a slightly lower value of importance than soil bulk density, MAT emerges as the second most influential factor governing SOC variations, followed by NPP, MAP, and clay content. This sequence of significance diverges from the findings of Walden et al. (2023), where the order of importance was observed as NPP > clay content > MAP > MAT on a continental scale in Australia. The

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number of predictors used in their study is much more than that in our study, which may affect the contribution of given predictors in SOC variation (Guo et al., 2019). This discrepancy might however be attributable to the utilization of observations encompassing both terrestrial and blue carbon ecosystems in their study. Clay emerges as key driver mainly in the groups where aquatic plants (e.g., seagrass, tidal marsh) appeared. The more extensive dataset encompassing the eastern coastline, characterized by greater variability and abundance of NPP input, potentially elevates NPP to a dominant role in influencing SOC variations within their study.

For SOC in different vegetation types (Figure 3), soil bulk density and MAT are more important than other factors in forest, and all factors except clay content showed similar importance in driving SOC in grassland. NPP and MAP dominate the SOC variations in woodland and shrubland. Climate conditions exert their impact on SOC in all vegetation types. It was proposed that the primary climatic determinant of SOC variation hinges on the primary constraint affecting SOC production and turnover (Hobley et al., 2016). In this study, most shrublands and woodlands are distributed in arid and semi-arid regions characterized by limited precipitation, which leads to water stress in surface soil, limiting plant productivity and reducing soil C input (Hobley et al., 2015). Consequently, MAP and NPP exhibited relatively higher influence on SOC variations. In contrast, forest SOC observations are mainly distributed in areas with relatively lower temperatures, therefore experience constrained microbial metabolism, leading to reduced decomposition rates and the high accumulation of SOC (Wynn et al., 2006). Consequently, MAT emerges as a key factor influencing SOC variations in forests. Furthermore, it is noteworthy that soil bulk density plays a crucial role in determining SOC distribution within forest ecosystems, where it is significantly lower compared to other vegetation types. This lower soil bulk density likely facilitates the formation of microaggregates and enhances the preservation of SOC within the soil matrix (Bronick and Lal, 2005). Consequently, it effectively contributes to elevated SOC concentration levels in forested areas.

PFTs are the only categorical predictor for SOC concentration in this study. SOC is mainly derived from plant C input through above-/belowground tissues, and SOC turnover and storage are influenced by plant traits like plant growth rate and chemical and physical composition (De Deyn et al., 2008; Faucon et al., 2017). With shared representation of similar plant traits, PFTs are widely used in process-based models (Poulter et al., 2015; Famiglietti et al., 2023). It was found that the vertical distribution of SOC is highly related to PFTs due to the different root distribution and above- and belowground allocation (Jobbágy and Jackson, 2000). However, our study is limited by the absence of SOC observations at multiple soil depths, restricting the analysis to the spatial distribution of SOC at 30 cm soil depth. The influence of PFTs on SOC concentration at this particular depth appears relatively insignificant (Figure 3), casting doubt on the effectiveness of optimizing parameters of process-based model for individual PFTs (Cranko Page et al., 2023). Considering this, employing the top 3 influential abiotic predictors, soil bulk density, MAT, and MAP, we partitioned all observations into six distinct clusters using K-means. It was anticipated that SOC ranges within each cluster would be narrow due to the high similarity of these three predictors within each group. However, the distribution of SOC

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in clusters 2, 4, and 6 exhibited considerable variability (Figure 4). Given that these clusters are predominantly composed of forest ecosystems, it becomes apparent that these three abiotic factors alone are insufficient to fully characterize the intricacies of forest SOC concentration. It was found that elevation and evapotranspiration also drive the variation of forest SOC in Australia (Walden et al., 2023), and taking them into account might potentially increase the predictability of forest SOC.

4.2. Model evaluation and comparison

Although the predictors used for machine learning models are not exactly same as the inputs of MIMICS, the missing factors (e.g., MAP) were used for parameter optimization of MIMCS-ENV, making the predictions dependent on similar information and so comparable to some extent. Besides, our study presented clear evaluation metrics for out-of-sample validation, enabling a more robust assessment of model performance when applied to new datasets.

Based on the performance metrics of test data, the machine learning models performed remarkably well (Figure 5). The R^2 suggest that both two machine learning models can explain more than 90% of SOC variability across sites, and random forest did the best job with greatest R^2 and LCCC, and lowest MAE and RMSE. Random forest algorithms were widely adopted in predicting spatial-temporal SOC dynamics and produced moderate well performance regionally and globally. For example, Wang et al. (2022) applied random forest to estimate SOC stocks in south-eastern Australia and explained 69% of the variation of current SOC stocks. Nyaupane et al. (2023) trained a random forest model using global SOC observations and explained 61% of SOC variation. The good performance of random forest might be attributed to reduced susceptibility to over-fitting and better capacity to manage the hierarchical non-linear relationships that exit between SOC and environmental predictors (Wang et al., 2018b). Other machine learning methods have been applied to predict continental SOC stocks in Australia. For example, Walden et al. (2023) trained regression-tree algorithm CUBIST to predict SOC stocks at 30 cm soil using the harmonised datasets. The mean LCCC and RMSE for out-of-sample validation in their study was 0.78 and 0.20 respectively when $\log_{10}$ transformed SOC (t/ha) values used. Wadoux et al. (2023) applied quantile regression forest to predict SOC stocks at multiple soil depths. The prediction accuracy decreased dramatically for deeper depth intervals with the greatest R^2 (0.53) at 0-5 cm soil. The better results in this study may be attributed to the removal of cropland ecosystems, which are clearly highly managed and so less predictable. Agricultural practices greatly affect SOC content in Australia and add the complexity to the relationship between SOC and environmental factors (Luo et al., 2010). Models using environmental predictors without representation of land use management are unlikely to be able to fully capture the SOC dynamics in croplands (Abramoff et al., 2022).

Although MIMICS made less accurate estimations of SOC than machine learning models, it did well at continental scale with mean R^2 at 0.82 and 0.84 for MIMICS-PFT and MIMICS-ENV, respectively (Figure 5). Georgiou et al. (2021) found that there was a mismatch between

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observations and MIMICS in the role of environmental controls in explaining SOC variability at global scale. NPP and MAT had the most explanatory power for SOC stocks from MIMICS, while clay content had the most explanatory power for SOC observations, which limits the predictability of SOC using MIMICS in their study. However, in our study, NPP and MAT rather than clay content played a greater role in observed SOC variations, perhaps contributing to a better performance of MIMICS in Australia. The modest performance of MIMICS relative to machine learning models could potentially be attributed to the absence of explicit representation of MAP. The augmentation of MAP within parameter optimization in MIMICS-ENV did allow improved performance compared to MIMICS-PFT, particularly within non-forest regions where the importance of MAP rivals or surpasses that of temperature. Precipitation is a determinant of plant productivity, especially in arid and semi-arid regions. Besides, arid regions with limited precipitation are characterized by lower weathering rate limiting the formation of mineral-associated soil carbon (Doetterl et al., 2015). Hence, we assume that introducing the effect of moisture to MIMICS could contribute to more accurate prediction of SOC, as compared with just taking MAP into account for parametrization, especially in arid and semiarid regions.

All models produced lower MAE and RMSE for non-forest SOC but higher R^2 and LCCC for forest SOC (Figure 6). SOC in forest is more abundant and variable compared to SOC in other vegetation types even when climate conditions are similar, which constrains the accuracy of forest SOC estimation. However, the higher R^2 and LCCC mean that all models show higher ability to predict forest SOC using environmental predictors. Forests, given they are less perturbed ecosystems, might afford greater SOC predictability due to the reduced influence of direct anthropogenic disturbances. This stands in contrast to ecosystems like grasslands, shrublands, and woodlands, predominantly situated in Australian rangelands where extensive grazing constitutes the predominant agricultural practice. Primarily, grazing leads to a reduction in soil carbon influx originating from aboveground biomass. Moreover, the cascading effects of grazing extend to potential alterations in plant composition and structural attributes, inducing consequential shifts in litter properties that modulate soil carbon decomposition kinetics (Lunt et al., 2007; Bai and Cotrufo, 2022). This intricate interplay of grazing-induced disturbances introduces a layer of complexity to SOC predictions. The disturbances triggered by grazing manifest in soil carbon pools, leading to a state of disequilibrium rather than adhering to the assumption of SOC convergence toward equilibrium, as embraced in this study's framework. Notably, forests, as relatively undisturbed natural ecosystems, demonstrate a better coherence with the equilibrium assumption, rendering their SOC more amenable to prediction through environmental drivers.

4.3. Spatial prediction of SOC stocks

We produced gridded SOC stocks across Australia using the models validated in this study and an ensemble estimate as the average of four models (Figure 7). Among the models, K-means coupled with multiple linear regression produced the largest mean SOC stocks both at continental scale and for all vegetation types. In contrast, random forest and MIMICS with different parameterization approaches produced more conservative SOC stock estimations. The mean terrestrial SOC stocks estimated by random forest and MIMICS are comparable with that estimated by Australian baseline map, which was generated using machine learning algorithm, reporting the mean SOC stocks at 29.7 t/ha with 95% confidence limits of 22.6 and 37.9 t/ha (Viscarra Rossel et al., 2014). However, SOC stocks might be underestimated by these methods because of the scarcity of data from the most productive temperate forest both in the baseline map (Bennett et al., 2020) and in our study. Parameter optimization process of MIMICS and the training process of random forest are greatly affected by data used to train the model. Most SOC observations in this study were sourced from arid and semiarid regions, characterized by limited SOC content. As a result, the models' ability to predict SOC stocks beyond the observed data range is somewhat constrained. PFTs was found to be less important than other environmental factors in driving spatial SOC variations (Figure 3), so it was perhaps not surprising that applying parameters optimized for each plant functional type to the regions with same PFT but broader climate conditions led to inferior results than applying parameters optimized for each environmental group.

The utilization of linear regression in K-means + MLR generated SOC estimates beyond the range of observations, particularly in eastern Australia where environmental conditions deviate from the training data. The mean SOC stocks estimated by K-means + MLR (38.2 t/ha) are higher than those of the other models employed in this study, and align closely with the mean value 36.2 t/ha reported by Walden et al. (2023) who updated the Australian baseline SOC map (Viscarra Rossel et al., 2014) by incorporating additional SOC observations from forests and coastal marine ecosystems. However, caution is required when interpreting extreme values derived from the K-means + MLR, such as the instance of grassland SOC stocks reaching 601 t/ha (Table 3). These values raise concerns about the reliability of this approach when extrapolating out-of-sample. Though there is a positive relationship between NPP and SOC observations in this study, SOC accumulation cannot continuously increase linearly in the regions where environmental conditions seem highly conducive to SOC formation. The greater amount of carbon input in eastern Australia might trigger the acceleration of microbial decomposition because of a priming effect, and lead to a decreased accumulation of SOC stocks (Ren et al., 2022). The existence of SOC saturation also implies that SOC cannot be accumulated without limit (Georgiou et al., 2022; Viscarra Rossel et al., 2023). In light of these complexities, applying linear regression to predict SOC content, especially under the extreme environmental conditions, should be undertaken with care.

Continentally, higher SOC was estimated for the southwest corner and southeast Australia (Figure 7), aligning with other SOC maps for Australia (Wadoux et al., 2023; Walden et al., 2023). These regions are characterized by lower temperature and higher precipitation, therefore high SOC accumulation appeared because of stimulation of NPP by moisture and the constrained microbial metabolism in low temperatures. Forest has the largest mean SOC stocks ranging from 70.3 to 113.9 t/ha estimated by four models in this study. Around 75% of the forest

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SOC is from soil under Eucalypt open forest, and mean SOC stocks under this type of forest were estimated to be 87.5 t/ha (63.8 -119.6 t/ha for 95% confidence interval) (Walden et al., 2023). Shrublands are estimated to have the lowest mean SOC stocks, and more than 90% of shrub SOC observations are from soil under Acacia shrubland and Chenopod shrubland, which rank at the bottom of SOC stocks among different vegetation types (Walden et al., 2023). The low SOC in shrubland is probably due to low carbon input because of limited rainfall (MAP < 280 mm). Though the mean SOC stocks in non-forest regions are much smaller than that for forest, the greater area of vegetation cover results in considerable total SOC stocks, highlighting the importance of carbon building and maintaining via improved managements in these areas. Greater variability of SOC estimates among different models appears in the regions where SOC stocks are higher (Figure 7). The sparsity of SOC observations is a primary contributor to the uncertainties associated with SOC estimates in these regions, highlighting the importance on continual collection of data to better constrain models' behaviour. This imperative is especially pronounced in regions covered by forests, as forested soils exhibit substantial SOC stocks, amplifying the significance of abundant and accurate data acquisition in these specific ecosystems.

5. Conclusion

We compared the performance of two machine learning models, and one process-based microbial model employing distinct parameterization approaches, to explore the diversity of SOC estimates within a 30 cm soil depth across Australia. Results highlight soil bulk density and MAT as predominant factors governing SOC concentration variations, both on a continental scale and within forest and grassland ecosystems. Conversely, NPP and MAP exhibit greater significance in driving SOC variations within shrubland and woodland soil. Our study underscores the importance of including the influence of appropriate environmental factors in process-based models in different environments.

Validation results affirm that with appropriate filtering of data (e.g. removing highly managed crop ecosystems) models can predict SOC at a continental scale with reasonably high reliability, achieving explained variances exceeding 80% for out-of-sample test data, with random forest showing highest prediction accuracy. Notably, all models show higher R^2 in prediction of SOC under forest than under non-forest vegetations. MIMICS, with parameters optimized for different environmental clusters, performed better in SOC prediction than MIMICS with parameters optimized for different PFTs, especially in non-forest regions.

All models broadly agree on the spatial distribution of SOC, with higher SOC stocks concentrated in the southeast and southwest regions of Australia. However, the variations in estimated values need to be acknowledged, particularly in highly productive regions. Among these estimates, K-means algorithm coupled with multiple linear regression yields the highest mean SOC stocks estimate, while the MIMICS-PFT model generates the most conservative estimate. Considerable disagreement of the maximum and minimum SOC stock values

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predicted by all models exists partly because models are less constrained by observations in these environments, highlighting the need for continued observational campaigns.

Our investigation has revealed significant disparities in estimated SOC stocks when different methodologies were employed. This highlights the need for a critical re-evaluation of land management strategies that heavily depend on SOC estimates derived from a single approach. The incorporation of an ensemble of SOC estimates is more likely to effectively capture elements of the uncertainty associated with SOC estimations, providing a more robust basis for informing strategies in soil carbon management and climate change mitigation.

Code availability

Source Code of vertically resolved MIMICS can be accessed at the CSIRO data portal https://doi.org/10.25919/843a-w584 (Wang et al., 2021). Codes for data analysis and machine learning can be accessed by contacting the correspondence author.

Data availability

The SOC observations from VR dataset are not publicly available but are available from Raphael A. Viscarra Rossel (r.viscarra-rossel@curtin.edu.au) on reasonable request. All other data used in this study are publicly accessible and the specific references of these databases are provided in Section 2.4.

Author contribution

Conceptualization: LW, GA, Y-PW, AP; Methodology: LW, GA, Y-PW; Investigation: LW, RAVR; Formal analysis and Visualization: LW; Writing-original draft preparation: LW; Writing-review & editing: LW, GA, Y-PW, AP, RAVR.

Competing interests

The co-author Raphael A. Viscarra Rossel is a member of the editorial board of SOIL.

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