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Evaluating the prediction success of soil organic carbon stock in pasture land using different modeling performance metrics

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Abstract

Many national and international initiatives depend on detailed spatial data on changes in soil organic carbon stock (SOC stock) at various scales to support policies aimed at land degradation neutrality and climate change mitigation Developing tools to accurately model the spatial distribution of SOC_{stock} at national scales is a priority for both monitoring soil organic carbon (SOC) changes and contributing to global carbon cycle studies. The primary goal of this study was to evaluate and compare various spatial performance metrics used to assess the accuracy of predicting soil SOC and SOCstock content in a semi-arid pasture. Soil samples were taken from 0-20 cm soil depth at 150 random sampling points. Spatial structure of SOC_{stock} and SOC were modelled by ordinary kriging The soil pH varied from slightly acidic (6.34) to neutral (7.19), and salinity was not an issue in the study area. Lime content, with an average of 2.04%, stands out as the most variable soil property, with a coefficient of variation (CV) of 61.76%. The carbon stock ranged from 23.46 to 65.36 tons ha^{-1}, with an average carbon stock of 43.28 tons ha^{-1} calculated. In the study area, SOC (%) and stoniness (%) had the shortest autocorrelation distance (21.00 m), while bulk density had the longest (27.00 m). The prediction errors indicated that parameters in the random sampling did not result in better predictions using the OK technique.The results indicated that SOC content can exhibit significant spatial variability even within a small area, highlighting the need for site-specific management in semi-arid pastures. In order to achieve high accuracy and success in modeling, metrics of the performance such as RRMSE, RMSE and MAPE should be used that minimize the effect of the relevant soil property measurement unit.

Keywords: Soil organic carbon, geostatistics, spatial variability, kriging, pasture.

Introduction

Digital mapping of pasture soil organic carbon (SOC) aids in the development of sustainable grazing management and in monitoring its effects on climate change (Garcia-Franco et al., 2021). SOC has commonly been assumed that plays an important role in determining grassland quality affecting soil quality and grass growth (Wang et. al., 2022). Recent studies indicate that increasing plant species richness in grasslands enhances soil carbon storage (Yang et al., 2019; Zhou et al., 2019). As determining soil organic carbon stock (SOC_{stock}) requires extensive sampling effort, time-consuming and high cost, it is not possible to observe at every point in the field (Bhunia et al., 2018). Therefore, the interest in predicting the amount of soil organic carbon stock is growing rapidly. Spatial interpolation analysis has been commonly used to predict SOC_{stock} at non-sampling points by various forms of kriging algorithms for estimating continuous attributes procedure (Isaaks and Srivastava, 1989). Ordinary kriging is an interpolation method estimating surface data from point data, based on the distances between sampling points (Rutter et al., 1991) and minimizing the estimation variance (Li and Heap, 2011). Evaluating the accuracy of modeling predictions in environmental sciences becomes important. The objective of this study was to predict soil carbon content using kriging methods and to assess the accuracy of the estimation through various performance metrics.

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Material and Methods

The study site was in semi-arid climate condition which is highly grazed site in North-Central Anatolia, Corum province in Turkey (Figure 1). The study area is 10 ha and the altitude is 1650 m above sea level. The area is flat and nearly middle slope (0-5%) in the northwest border of the Corum Plain. Long-term (2013-2023) annual average temperature of the study area is 12.30 °C. This region is defined by a semi-arid climate, with an average annual precipitation of 371.65 mm.

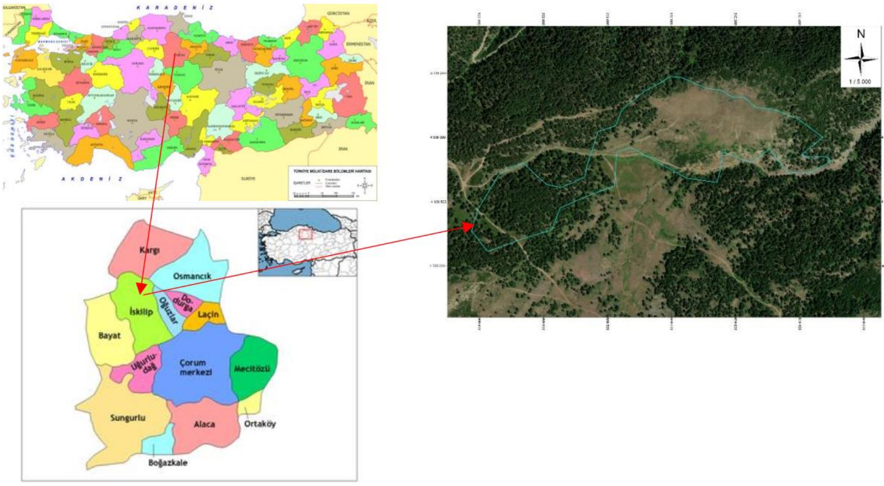

Figure 1. Location of the study area.

Soil sampling and analysis

Field sampling was conducted between May and July 2021 in a natural grassland, with 150 experimental points randomly selected. Soil samples were collected as both undisturbed and disturbed from a depth of 0-20 cm. Soil texture was determined using the hydrometer method (Bouyoucous, 1951). Soil pH and electrical conductivity (EC) were measured using a 1:2.5 soil-water ratio following the method of Hendershot et al. (2007), and the calcium carbonate content (% $CaCO_3$) was determined according to Kacar (1994). Bulk density (BD) was measured using cylindrical cores (100 cm^3) from a 0-20 cm soil depth, as described by Blake and Hartge (1986). Soil organic matter (SOM) content was analyzed using the Walkley-Black wet digestion method (Nelson and Sommers, 1982), while organic carbon was determined by oxidizing carbon with an acidic dichromate solution, as this method is both simple and requires minimal equipment (Nelson and Sommers, 1982). Soil organic carbon stock was calculated by considering soil bulk density, organic carbon concentration, and soil depth, using the formula provided in Equation 1 (Lu and Liao, 2017).

$$SOC_{stock} = 100 \times SOC \times BD \times (1\text{-}CF) \times (Top\text{-}Bottom) \qquad (1)$$

In Equation (1), SOCstock is the soil organic carbon stock (ton/ha), SOC is the SOC content (wt. %), BD is the bulk density (g cm-3), CF is the proportion of coarse fragments (vol. %), (Top-Bottom) is the thickness of the given sampling soil depth (cm) and 100 is used for unit conversion.

Spatial modelling

Descriptive statistics were calculated with SPSS 11.0. Following Lark (2000) holds the view that necessary transformations should be made in non-normally distributed data sets to make a successful geostatistical modeling. Although necessary transformations were made according to Webster's (2001) criteria in order to better model the data that did not show normal distribution, semivariogram models were not affected. For this reason, geostatistical modeling was continued without transforming the data sets. Ordinary kriging (OK) was used because it provides the best linear unbiased estimate of the predicted spatial variable while minimizing the variance of the prediction errors. Unlike other interpolation methods, OK takes into account the spatial autocorrelation between sample points, meaning that it considers how values at one location are related to values at nearby locations (Isaaks and Srivastava, 1989). The geostatistical software GS+ was employed to examine the spatial structure of the data for soil properties as well as to model the semivariogram..Variable lag distances were also applied for semivariogram selection, ensuring a minimum of ten lags with at least 30 data pairs in each lag.. In determining the most suitable semivariogram, it was decided that the R^2 (coefficient of determination) should be close to 1, and RSS (residual sum of squares) and nugget value should be close to 0. (Isaaks and Srivastava, 1989). An experimental semivariogram was generated by calculating semivariance values for each pair of sample points and then averaging these values across increasing lag intervals (h).

Each point in a semivariance was calculated from Equation (2):

$$\gamma(\mathrm{h}) = \frac{1}{2N\,(h)}\sum_{\mathrm{i}=1}^{N}[z(x_i+h)-zx_i]^2 \tag{2}$$

Where $z(x_i+h)$ is the z value at location (x_i+h), zx_i is the z value at a location separated from x_i by distance h and N is number of sampling pairs separated by distance h (lag) (Webster and Oliver, 2008). After determining the appropriate semivariogram model, cross-validation analysis was used to determine accuracy of the interpolation technique by graphing the predicted values with the observed values. An unknown sample point in kriging is calculated as seen in equation (3) as:

$$z_0=\sum z_i \times \mathrm{w} \tag{3}$$

where z_0 is a known predicted value, z_i is observed value. The parameter w is kriging weight (Isaaks and Srivastava 1989). The errors calculated by subtracting observed values from predicted values were used to evaluate performance OK (Burrough and McDonnell, 1998). Spatial distribution maps for each variable were created using the best parameters obtained from the semivariogram models and cross-validation process. The geostatistical extension of ArcGIS 10.2.1 was utilized to generate kriging maps of soil properties.

Results and Discussion

Descriptive statistics

Descriptive statistics for SOC_{stock} and other soil properties are given Table 1. SOC and SOC_{stock} contents were % 2.45, 43.27 (ton ha^{-1}) at 20 cm soil depth, respectively. On the other hand, in contrary with our results, some researchers observed that SOC_{stock} was higher (Szatmári et al., 2019; Zhu et al., 2019; Li et al., 2022; Ma et al., 2023). According to Webster (2001), bulk density, $CaCO_3$ (%), and EC are positively skewed, while clay (%) is negatively skewed. Webster defined a distribution with skewness greater than ±1.0 as strongly skewed. These strong positive skewness-values indicate proportional effect, wherein the variability is greater in sample points with high values compared to those with low values corrupting spatial modeling. Modeling performance increases significantly when the distribution of variable follows a normal or near-normal distribution.

Table 1. Descriptive statistics for the soil variables (N:150)

Soil variable	Min	Max	Mean	Std dev	Skewness	Kurtosis	CV%	DT
BD (g cm^{-3})	1.03	1.58	1.18	0.08	1.00	1.90	6.78	NN
Sand (%)	24.00	64.00	43.46	7.22	0.18	0.19	16.61	NN
Clay (%)	4.00	44.00	32.85	5.51	-0.84	3.96	16.77	NN
Silt (%)	7.00	49.00	23.70	5.71	-0,12	3,30	24.09	NN
Stoniness (%)	0.00	40.00	25.00	0.09	0.13	-0.75	35.81	NN
CF (%)	60.00	100.00	75.00	0.09	-0.13	-0.75	11.79	NN
$CaCO_3$ (%)	0.89	8.27	2.04	1.26	2.35	0.19	61.76	NN
OM (%)	2.51	5.49	4.23	0.87	-0.52	-1.06	20.57	NN
SOC (%)	1.46	3.19	2.45	0.50	-0.52	-1.06	20.41	NN
SOC_{stock} (ton ha^{-1})	23.46	65.36	43.28	9.01	0.20	-0.37	20.81	NN
pH	6.34	7.19	6.70	0.16	0.32	-0.19	2.39	N
EC (ds m^{-1})	0.026	0.231	0.088	47.85	1.07	0.71	53.89	NN

N—Number of soil samples, Min—Minimum value, Max—Maximum value, Std dev—Standard deviation, CV—Variation of coefficient, DT—Distribution type, N—Normal distribution, NN—Abnormal distribution, BD—Bulk density, CF—proportion of coarse fragments, OM—Organic matter, SOC—Soil organic carbon, SOC_{stock}—Soil organic carbon stock, EC—Electrical conductivity, CV—Variation of coefficient.

It is common for SOC data to be positively skewed (Liang et al., 2019; Szatmári et al., 2019, 2021; Wang et al., 2021). However, in this study area, the SOC data exhibited a slight negative skew.Regarding Table 1, the values of variation coefficient vary between 2.39% and 61.76%, and among all soil properties examined, $CaCO_3$ (%) was a more variable soil property than others. According to (Cambardella et al., 1994), the coefficient of variation (CV) can be categorized into three groups: low (<15%), medium (15% to 35%), and high (>35%).

The CV of SOC_{stock} in different studies was represented by high (Rodríguez Martín et al., 2016; Szatmári et al., 2021; Li et al., 2022) unlike our study.

Geostatistical analyses characteristics of the SOC and its components

Semivariogram analysis was applied separately to quantify the spatial structure of SOC_{stock} and other soil properties The semivariogram charts related to the soil properties under investigation are presented in Figure 2. The spatial distribution SOC_{stock} and SOC were better described with spherical model (Figure 2). In other studies, quite different nugget values for SOC have been reported, such as Mishra et al. (2009) 294.5, 294.5, Li et al. (2023) 0.33 and Kingsley et al. (2021) 0.19.

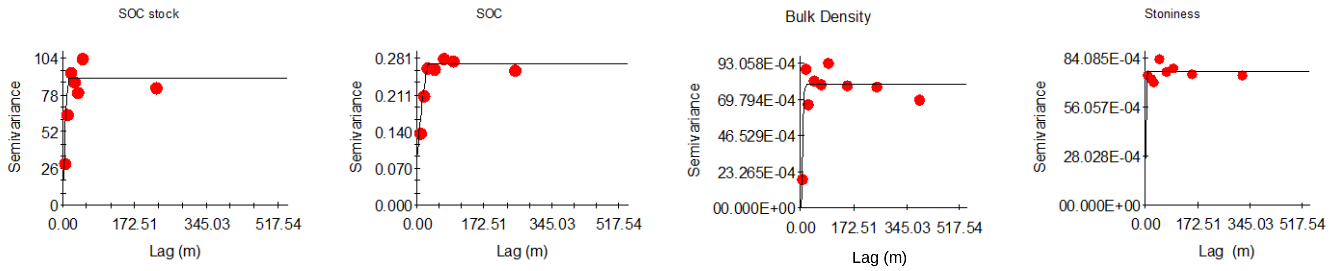

Figure 2. Semivariograms of soil properties

The high nugget value observed for SOC_{stock} implies a substantial level of random variance within the study area. This indicates that samples taken from nearby and distant locations exhibit distinct values. The higher sill value for SOCstock (77.56), compared to stoniness (0.007) and bulk density (0.007), suggests greater variability between sampling points and lower prediction accuracy at finer scales (Table 2).

Table 2. Semi-variogram parameters of soil properties of the grassland (Turkıye)

Soil parameters	Model type	Nugget C_o	Sill $C_o + C$	Range A_0 (m)	Spatial dependence (%)	RSS	R^2
SOC_{stock} (ton ha^{-1})	Spherical	21.6	77.56	25.00	27.84	228	0.89
BD (g cm^{-3})	Spherical	0.001	0.007	27.00	12.82	1.32E-06	0.92
SOC (%)	Spherical	0.09	0.257	21.00	194.55	3.29	0.97
Stoniness (%)	Exponential	0.0037	0.007	21.00	52.85	1.34E-06	0.62

SOC_{stock}: Soil organic carbon stock, BD: Bulk density, SOC: Soil organic carbon, RSS: Residual sum of squares, R^2: Coefficient of determination

A nugget-to-sill ratio of <25% signifies strong spatial dependence, typically due to intrinsic factors like soil texture and mineralogy; 25-75% indicates moderate dependence from both intrinsic and extrinsic factors; and >75% suggests weak spatial dependence, often due to extrinsic factors such as uncontrolled grazing and hoofprints (Cambardella et al., 1994). According to this classification, spatial variations of soil SOC_{stock}, SOC, BD, and stoniness were characterized as moderately, strongly, weakly, and moderately spatially dependent, respectively (Table 2). This dependency was not large enough to confirm geostatistical methods to predict examined soil properties, irrespective of the sampling intervals. The nugget/sill ratio for SOC% was 194.55, indicating a very weak spatial dependency according to reported by (Blackburn et al., 2022). Table 2 results indicate minimal nugget effect, suggesting that variation is not due to sampling error but rather to short-range spatial variability beyond the sampling intervals.

The nugget-to-sill ratio represents the interaction between random and structural factors, reflecting the proportion of spatial heterogeneity due to autocorrelation within the overall spatial heterogeneity (Li et al., 2021). Structural factors such as climate, parent material, terrain, and soil composition contribute to significant spatial correlation among spatial variables. Conversely, random factors like fertilization, grazing and cultivation contribute to a reduction in spatial correlation. To better understand spatial dependence can best be treated under three distinct types using percentage of nugget/sill ratio (Cambardella et al., 1994). Although nugget values of SOC_{stock} was high, its spatial dependence was at a moderate level which might be attributed to extrinsic factors like soil forming processes and intrinsic factor like uncontrolled grazing. As regards range is the maximum distance over which spatial dependence or autocorrelation exists. Range distances are presented in Table 2 reveals that there has been a slight decreased respectively in the range distance of soil properties. Range distances were indicated that the optimum sampling interval did not vary greatly among different soil properties. According to Rossel and McBratney (2008), R^2 values are classified as follows: ≥0.81 is very good, 0.61–0.80 is good, 0.41–0.60 is moderate, and <0.40 is weak (Viscarra Rossel et al., 2016). According to the definition above, the R^2 values obtained for SOC_{stock}, SOC, and BD were higher. Consistent with this, researchers have reported similar results (Rostaminia et al., 2021; Zhang et al., 2022).

Kriging

Spatial distribution maps obtained using ordinary kriging was presented in Figure 2. The maps illustrating spatial distribution facilitated the assessment of both the extent and magnitude of soil properties in the study area. A gradual increase in SOC_{stock} was noted from the northeast to the southwest of the study area, with the percentage of SOC_{stock} ranging from 29.88% to 58.71% in the 0-20 cm soil depth (Figure 3). The similar observation was also reported by Liu et al (2023). Compared to the spatial structure of SOC_{stock}, stoniness and bulk density displayed a non-uniform distribution.

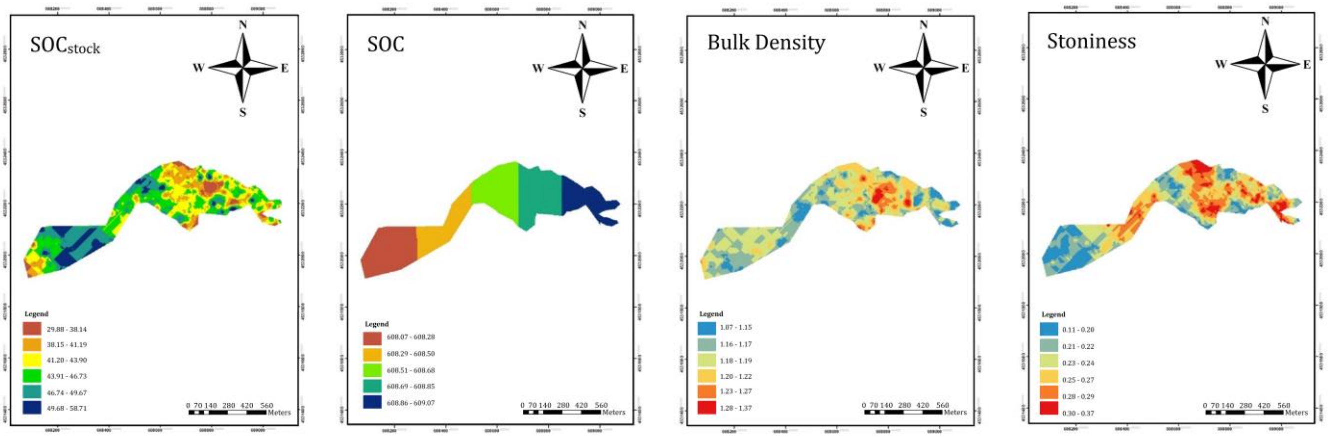

Figure 3. Spatial distribution maps for soil properties

As can be seen in Table 3, different metrics of interpolation performance were calculated to evaluate the fitting accuracy of the models. According to the data, the absolute value of the Mean Error (ME) was far from 0, while Root Mean Square Error (RMSE) and Mean Square Error (MSE) exhibited the biggest values.

Table 3. Metrics used to assess the performance of spatial interpolation methods

Performance Metrics	SOC_{stock}	BD	SOC	Stoniness
ME	-0.16	0.003	0.004	0.005
MPE	4.28	0.71	5.18	16.79
MAE	7.70	0.06	0.43	0.07
MSE	87.90	0.008	0.26	0.007
RMSE	9.37	0.08	0.51	0.08
RMAE	0.18	0.05	0.20	0.37
MSRE	35.92	0.23	1.86	0.36
RMSSE	39.52	30.60	1.35	1.37
RRMSE	24.41	7.10	26.04	49.95
ASE	6.34	1.08	1.56	0.50
MAPE	18.99	5.69	20.25	37,36
Willmott's D	0.23	0.38	0.28	0.27
EF	0.98	0.99	0.98	0.96

The magnitude of these metrics is contingent upon the unit or scale of the primary variable being considered. For instance, the magnitude of MAE is typically less than 1% for soil organic matter, but it can beyond 100 mm for rainfall or even exceed 1000 mm for tropical regions. The unit of measurement for variables can influence the magnitude of these metrics of performance (Li and Heap, 2011). Therefore, it becomes essential to compare the performance of kriging methods across various studies, especially when variables are observed in different units or scales. This problem is tackled by introducing two new performance metrics: Relative Mean Absolute Error (RMAE) and Relative Root Mean Square Standardized Error (RRMSE). These metrics of performance aim to mitigate the impact of measurement units and maintain sensitivity regardless of changes in units or scale. Model accuracy is classified as excellent if RRMSE is below 10%, good if RRMSE is between 10% and 20%, fair if RRMSE is between 20% and 30%, and poor if RRMSE exceeds 30% (Despotovic et al., 2016). Based on this classification, model accuracy of soil SOC_{stock}, BD, SOC, and stoniness were characterized as fair, excellent, fair, poor, respectively. The mean percent error (MPE) suggests a superior model as its value approaches zero, indicating improved accuracy. RMSE provides an observe of error size, but the main problem with RMSE is its sensitivity to outliers, as it assigns significant weight to large errors. This means that the presence of several large errors can cause the value of RMSE to increase. RMSE is a commonly used metric for assessing modeling performance, and similar to the findings of (Rostaminia et al., 2021), our study obtained a high RMSE value (3.37) for SOC_{stock} suggesting the model's prediction accuracy is low. A value of RMSSE greater than 1 means the model underpredicts values observed in this study. The reason why RMSE takes a value greater than 1 the model underpredicts the observed values in this study. RMSE and MAE are considered to comparable metrics, offering predicts of the average error; however, they do not offer insights into the relative magnitude of the average difference or the characteristics of the differences that make them up. Nevertheless, some researchers argue that RMSE and MAE are among the most comprehensive indicators of model performance as they summarize the average disparity between observed and predicted values in their respective units (Willmott, 1982). The value of MAE was closest to ASE therefore, we can draw a conclusion from the Table 3 mentioned that a model was considered better Mean Square Error (MSE) values approach zero and Root Mean Square Error (RMSE) was smaller. According to this, the highest values observed for MSE and RMSE indicate that the accuracy of interpolation is the poorest. Considering Table 3, ASE < RSME means the model underpredicts the observed values. MSE encounters similar limitations to RMSE, whereas MAE demonstrates reduced sensitivity to extreme values and indicates the extent to which the predict can be in error. RMSE and MAE are some of the most effective observes for evaluating model performance, as they encapsulate the average discrepancy between the units of observed and predicted values. MSE shares the same limitations as RMSE, while MAE is less affected by extreme values and indicates the extent to which the predict can be in error.

ME is employed to assess the level of deviation in the predicted value, with predictions being more stronger as the value approaches zero (Wang et al., 2021). The smallest ME suggests that the predicted value is closest to the observe values. ME is employed for determining the degree of bias in predicts and is often referred to as "bias"(Hohn, 1991) but it should be used cautiously as an indicator of accuracy. Although MAE is less affected by extreme values and indicates the degree to which the estimate may be inaccurate. The main weakness with ME is that negative and positive predicts counteract each other and the resultant ME tends to be lower than observe error. Meanwhile, it would be optimal if the Mean Error (ME) and Mean Square Error (MSE) approached zero. However, there was a noticeable numerical deviation in MSE from the value of 1. The agreement index, known as Willmott's D, is scaled according to the magnitude of the variable, maintains average information, and does not magnify outliers (Willmott, 1982). The closer Willmott's D is to 1, the more accurate the method is considered. There have been proposed by some researcher (Greenwood et al., 1985), an accuracy measurement known as model efficiency (EF). The fact that the EF metric value is close to zero indicates that the average value of observations is more reliable than predictions. (Li and Heap, 2011).

As far as the Mean Absolute Percentage Error (MAPE) is concerned, it is a good metric used to assess model performance in the presented stud. Regarding the Mean Absolute Percentage Error (MAPE), it serves as a valuable metric for evaluating model performance in the study presented. MAPE is often considered one of the most effective indicators among error metrics (Moreno et. al., 2013; Gunal et. al., 2023). The MAPE value < 10% indicates highly accurate (excellent estimator), while the value 10-20 % indicates moderately accurate (good predictor), and if the value ranges 20-50 % the model's accuracy is considered low, but its outputs are still acceptable (Lewis, 1982). According to this classification model accuracy of soil BD, SOC, SOC_{stock}, and stoniness were characterized as high, moderately, low estimation, respectively (Table 3). The (%) MAPE value of stoniness was higher than other soil properties. The results can be attributed to the significant variability in the data, as the MAPE error metric exhibits very low tolerance for extreme values.

Conclusion

The soil organic carbon is a soil property characterized by high spatial variability, yet it is relatively straightforward to observe. One potential explanation for this phenomenon is the diverse range of plant communities and soil properties found within grasslands. Additionally, certain soil properties exhibit considerable variability over short distances due to uncontrolled grazing practices. As a result, estimating carbon sequestration in grasslands can be more challenging compared to cultivated agricultural areas. The limiting factors of this study include that the random sampling design has led to a low success rate in geostatistical modeling of soil organic carbon. This study indicated that SOC_{stock} and SOC vary significantly over very short distances. We evaluated the advantages and disadvantages of different spatial performance metrics can be used to estimate SOC_{stock} effectively and efficiently in terms of accuracy. The unit of measurement and the high variability of the examined soil properties are important factors that should be considered in geostatistical modeling. The observations should include at least MAPE, RRMSE or RMSE to compare the model success across different variables in dissimilar units. The MAPE is a performance evaluation metric that effectively mitigates the impact of measurement units. Here, we recommend that future studies clearly report in their publications information about why the metrics used in model performance evaluation are used and their advantages and disadvantages. Additionally, future studies should consider using systematic sampling and increasing sample density to improve the accuracy of SOC predictions.

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