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Foreword

Abbreviations and acronyms

BD Bulk Density

CO₂ Carbon dioxide

CRF Coarse fragments

 \mathbf{DM} Dry matter

DSM Digital soil mapping

GAUL Global Administrative Unit Layers

 \mathbf{GHG} Greenhouse gas

GSOCmap Global Soil Organic Carbon Map

GSOCseq Global Soil Organic Carbon Sequestration Potential Map

GSP Global Soil Partnership

HWSD Harmonized World Soil Database

ISCN International Soil Carbon Network

INSII International Network of Soil Information Institutions

IPBES Intergovernmental Platform on Biodiversity and Ecosystem Services

IPCC Intergovernmental Panel on Climate Change

IPR Intellectual Property Rights

ITPS Intergovernmental Technical Panel on Soils

LDN Land Degradation Neutrality

NDVI Normalized difference in vegetation index

NPP Net Primary Production

P4WG Pillar 4 Working Group

QA/QC Quality Assurance/Quality Check

RMSE Root mean square error

SDF Soil Data Facility

SDG Sustainable Development Goals

SISLAC Latin America and the Caribbean's Soil Information System

SOC Soil organic carbon

SOM Soil organic matter

SPADE/M Soil Profile Analytical Database of Europe of Measured Parameters

SWRS Status of World's Soil Resources

UNCCD United Nations Convention to Combat Desertification

WFS Web Feature Service

WoSIS World Soil Information Service

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Presentation

Soils provide ecosystem services critical to life on Earth. The Food and Agricultural Organization of the United Nations (FAO) recognizes the need to preserve soil resources from degradation and boost healthy soils. In 2012, FAO members established the Global Soil Partnership (GSP) as a mechanism to improve soil governance at global, regional and national levels. . .

Setting-up the software environment

Y. Yigini

This cookbook focuses on SOC modeling using open source digital mapping tools. The instructions in this chapter will guide the user through installing and manually configuring the software to be used for DSM procedures for Microsoft Windows desktop platform. Instructions for other platforms (e.g. Linux Flavours, MacOS) can be found through free online resources.

2.1 Use of R, RStudio and R Packages

R is a language and environment for statistical computing. It provides a wide variety of statistical (e.g. linear modeling, statistical tests, time-series, classification, clustering, etc.) and graphical methods, and is highly extensible.

2.1.1 Obtaining and installing R

Installation files and instructions can be downloaded from the Comprehensive R Archive Network (CRAN).

- 1. Go to the following link https://cran.r-project.org/ to download and install \mathbf{R} .
- 2. Pick an installation file for your platform.

2.1.2 Obtaining and installing RStudio

Beginners will find it very hard to start using **R** because it has no Graphical User Interface (GUI). There are some GUIs which offer some of the functionality of **R**. **RStudio** makes **R** easier to use. It includes a code editor, debugging and visualization tools. Similar steps need to be followed to install **RStudio**.

- 1. Go to https://www.rstudio.com/products/rstudio/download/ to download and install **RStudio**'s open source edition.
- 2. On the download page, RStudio Desktop, Open Source License option should be selected.
- 3. Pick an installation file for your platform.

2.1.3 Getting started with R

- R manuals: http://cran.r-project.org/manuals.html
- Contributed documentation: http://cran.r-project.org/other-docs.html
- Quick-R: http://www.statmethods.net/index.html

2.2 R packages

When you download \mathbf{R} , you get the basic \mathbf{R} system which implements the \mathbf{R} language. \mathbf{R} becomes more useful with the large collection of packages that extend the basic functionality of it. \mathbf{R} packages are developed by the \mathbf{R} community.

refer to: - tidyverse book (R for data science) - caret (cookbook) - https://rspatial.org/

2.2.1 Finding R packages

The primary source for \mathbf{R} packages is CRAN's official website, where currently about 12,000 available packages are listed. For spatial applications, various

packages are available. You can obtain information about the available packages directly on CRAN with the available.packages() function. The function returns a matrix of details corresponding to packages currently available at one or more repositories. An easier way to browse the list of packages is using the *Task Views* link, which groups together packages related to a given topic.

2.3 GEE - google earth engine

general info

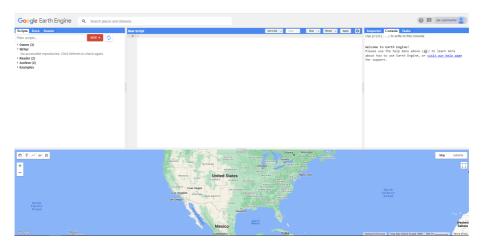


Figure 2.1: Google Earth Engine code editor.

- upload assets to GEE
- Explain how to import uploaded assets (?) ...

2.4 rgee - Extension to use google earth engine in R

The rgee package enables users to interact with the GEE servers using the R language. The package makes use of the Python language to interact with GEE. The package can be downloaded easily either directly from the GitHub repository or via CRAN.

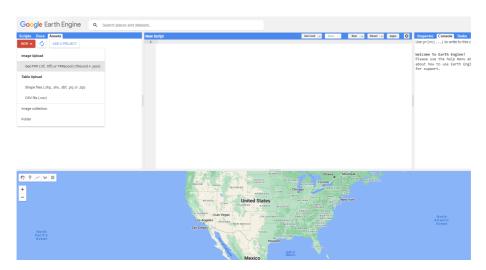


Figure 2.2: Select files and filetype to be uploaded as GEE assets.

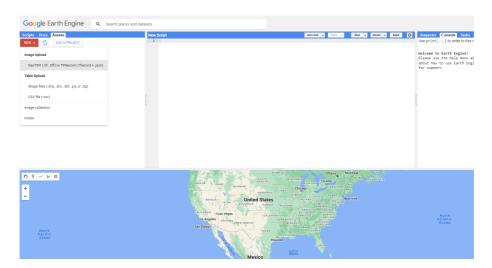


Figure 2.3: Upload interface.

```
# Source: https://yabellini.github.io/curso_rgee/index.html
# Yanina Bellini Saibene

#install.packages('remotes')
# remotes::install_github("r-spatial/rgee")
```

To be able to interact with the GEE via Python, it is necessary to install certain R packages but also the so-called "Miniconda" commmand prompt which acts as Python interpreter mediating between R and GEE. The 'ee_install()' function automatically downloads and install all the software that is needed.

```
# load rgee package and install dependencies
library(rgee)
# ee_install() # installs miniconda
```

Once the dependencies are installed, it is necessary to initialize rgee by providing the user credentials of our GEE account. The ee_Initialize command must be run every time we want to use rgee.

```
# Initialize Google Earth Engine! (you need to create a user account)
# ee_Initialize()

# Useful functions

#ee_check() # check the dependencies that do not belong to R
#ee_clean_credentials() # to remove the user credentials
#ee_clean_pyenv() # Delete variables of the system
```

Introduction to Digital Soil Mapping

Digital soil mapping (DSM) is a methodological framework to create soil attribute maps on the basis of the quantitative relationships between spatial soil databases and environmental covariates. The quantitative relations can be modelled by different statistical approaches, most of them considered machine learning techniques. Environmental covariates are spatially explicit proxies of soil-forming factors that are employed as predictors of the geographical distribution of soil properties. The methodology has evolved from the theories of soil genesis developed by Vasil Dokuchaev in his work the Russian Chernozems (1883), which later were formalised by Jenny (1941) with the equation of the soil-forming factors. The conceptual equation of soil-forming factors has been updated by McBratney, Santos and Minasny (2003) as follow:

$$S = f(s, c, o, r, p, a, n)$$
(3.1)

Where S is the soil classes or attributes (to be modelled) as a function of "s" as other soil properties, "c" as climatic properties, "o" as organisms, including land cover and human activity, "r" as terrain attributes, "p" as parent material, "a" as soil age, and "n" as the geographic position.

Digital soil mapping has been used to produce maps of soil nutrients. For

instance, Hengl et al. (2017) predicted 15 soil nutrients at a 250 m resolution in Africa, using a random forest model (Wright and Ziegler, 2016), topsoil nutrient observations at point locations and a set of spatially-explicit environmental covariates. In 2021, Hengl et al. applied the same modelling approach to estimate total phosphorus in semi-natural soils at the global scale, as well.

In this technical manual, we present a DSM frameworks to map soil properties, including soil nutrients. One approach for soil observations with latitude and longitude data (point-support) (Figure 3.1).

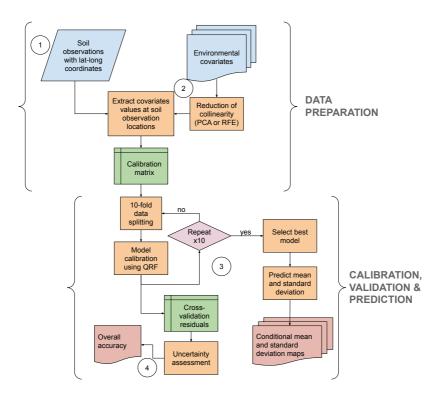


Figure 3.1: Digital soil mapping approach for point-support data. Circles are the steps.

Step 1: soil data preparation

Soil data consist of measurement at a specific geographical location, time and soil depth. Therefore, it is necessary to arrange the data following the format shown in Table 4.1.

Table 4.1: Format example of a soil dataset

Profile ID	Horizon ID	Lat	Long	Year	Top	Bottom	Soil property	Value	Lab method
1	1_1	12.123456	1.123456	2018	0	20	SOC	3.4	W&B
1	1_2	12.123456	1.123456	2018	20	40	SOC	2.1	W&B
2	2 1	23.123456	2.123456	2019	0	30	SOC	2.9	W&B

Profile ID = unique profile identifier; Horizon ID = unique layer identifier; Lat = latitude in decimal degrees; Long = longitude in decimal degrees; Year = sampling year; Top = upper limit of the layer in cm; Bottom = lower limit of the layer in cm; Soil property = name of the soil property; Value = numerical value of the measure; Lab method = name of the laboratory protocol used for measuring the soil property.

Soil data usually require a preprocessing step to solve common issues such as, arranging the data format, fixing soil horizon depth consistency, detecting unusual soil property measurements, among others issues. Once the original dataset is clean and consistent, data harmonisation is needed to produce synthetic horizons (such as 0-30 cm layer), as well as to make compatible measurements from different lab methods. Horizon harmonisation will be done with the mass preserving spline function (Bishop, McBratney and Laslett, 1999; Malone et al., 2009) fitted to each individual soil profile, which requires more than a layer per profile. In the cases of single-layer samples, which is common in sampling for nutrient determination, a pedotransfer function locally calibrated should be

applied. Pedotransfer functions will be also required to harmonise the laboratory methods. Experts from GLOSOLAN will provide advice in this regard.

Step 2: environmental covariates

5.1 Environmental covariates

The SCORPAN equation (Eq. 3.1) refers to the soil-forming factors that determine the spatial variation of soils. However, these factors cannot be measured directly. Instead, proxies of these soil forming factors are used. One essential characteristic of the environmental covariates is that they are spatially explicit, covering the whole study area. Table 2 shows a summary of the environmental covariates that can be implemented under the DSM framework.

Table 5.1: Environmental covariates

Factor	Description	Code	Resolution
Temp-	Mean air temperature (annual)	bio1	1000
erature			
	Mean daily temperature of warmest	bio5	1000
	month		
	Mean daily temperature of coldest	bio6	1000
	month		
Precipi-	Total precipitation (annual)	bio12	1000
tation			

	Mean precipitation of wettest month	bio13 1000
	Mean precipitation of driest month	bio14 1000
	Mean monthly precipitation of wettest	bio16 1000
	quarter	
	Mean monthly precipitation of driest	bio17 1000
	quarter	
Evapotrans	pMean monthly PET	pet_penman_meail000
iration		
	Minimum monthly PET	$pet_penman_min 1000$
	Range monthly PET	pet_penman_rang@000
	Maximum monthly PET	$pet_penman_max1000$
Wind	Minimum monthly wind speed	sfcWind_min 1000
	Maximum monthly wind speed	$sfcWind_max$ 1000
	Range monthly wind speed	sfcWind_range 1000
Growing	Number of days with mean daily air	ngd10 1000
season	temperature 10 °C	
Vegetation	NDVI (MOD13Q1), mean March-May	ndvi_030405_mea 2 50
Indices	from 2000-2022	
	NDVI (MOD13Q1), mean June-	$ndvi_060708_mea 250$
	August from 2000-2022	
	NDVI (MOD13Q1), mean September-	ndvi_091011_mea 2 50
	November from 2000-2022	1
	NDVI (MOD13Q1), mean December- February from 2000-2022	ndvi_120102_mea 2 50
	NDVI (MOD13Q1), standard devia-	ndvi_030405_sd 250
	tion March-May from 2000-2022	11411_030100_54 200
	NDVI (MOD13Q1), standard devia-	ndvi_060708_sd 250
	tion June-August from 2000-2022	
	NDVI (MOD13Q1), standard devia-	ndvi_091011_sd 250
	tion September-November from 2000-	
	2022	
	NDVI (MOD13Q1), standard devia-	ndvi_120102_sd 250
	tion December-February from 2000-	
	2022	
FPAR	Fraction of photosynthetically ac-	fpar_030405_mear500
-	tive radiation (FPAR) (MOD15A2H),	
	mean March-May from 2000-2022	
	v	

	Fraction of photosynthetically active radiation (FPAR) (MOD15A2H), mean June-August from 2000-2022	fpar_060708_mear 5 00
	Fraction of photosynthetically active radiation (FPAR) (MOD15A2H), mean September-November from 2000-2022	fpar_091011_meai500
	Fraction of photosynthetically active radiation (FPAR) (MOD15A2H), mean December-February from 2000-2022	fpar_120102_mean 500
	Fraction of photosynthetically active radiation (FPAR) (MOD15A2H), standard deviation March-May from 2000-2022	fpar_030405_sd 500
	Fraction of photosynthetically active radiation (FPAR) (MOD15A2H), standard deviation June-August from 2000-2022	fpar_060708_sd 500
	Fraction of photosynthetically active radiation (FPAR) (MOD15A2H), standard deviation September-November from 2000-2022	fpar_091011_sd 500
	Fraction of photosynthetically active radiation (FPAR) (MOD15A2H), standard deviation December-February from 2000-2022	fpar_120102_sd 500
LST	Land Surface Temperature Day (MOD11A2), mean March-May from	lstd_030405_meanl000
	2000-2022 Land Surface Temperature Day (MOD11A2), mean June-August from 2000-2022	lstd_060708_meanl000
	Land Surface Temperature Day (MOD11A2), mean September- November from 2000-2022	lstd_091011_meanl000
	Land Surface Temperature Day (MOD11A2), mean December-February from 2000-2022	lstd_120102_meanl000

	Land Surface Temperature Day	lstd 030405 sd 1000
	(MOD11A2), standard deviation	
	March-May from 2000-2022	
	Land Surface Temperature Day	lstd_060708_sd 1000
	(MOD11A2), standard deviation	
	June-August from 2000-2022	
	Land Surface Temperature Day	$lstd_091011_sd 1000$
	(MOD11A2), standard deviation	
	September-November from 2000-2022	
	Land Surface Temperature Day	$lstd_120102_sd$ 1000
	(MOD11A2), standard deviation	
	December-February from 2000-2022	
NDLST	Normalised Difference between LST	$ndlst_030405_meal 1000$
	Day and LST Night (MOD11A2),	
	mean March-May from 2000-2022	
	Normalised Difference between LST	$ndlst_060708_meal 1000$
	Day and LST Night (MOD11A2),	
	mean June-August from 2000-2022	11
	Normalised Difference between LST	$ndlst_091011_meal 1000$
	Day and LST Night (MOD11A2),	
	mean September-November from 2000-	
	2022	11 / 100100 1000
	Normalised Difference between LST	$ndlst_120102_meah000$
	Day and LST Night (MOD11A2),	
	mean December-February from 2000-	
	2022 Normalised Difference between LST	ndlat 020405 ad 1000
	Day and LST Night (MOD11A2),	ndlst_030405_sd 1000
	standard deviation March-May from	
	2000-2022	
	Normalised Difference between LST	ndlst 060708 sd 1000
	Day and LST Night (MOD11A2),	ndist_000708_sd 1000
	standard deviation June-August from	
	2000-2022	
		11
	Normalised Difference between LST	ndlst 091011 sd 1000
	Normalised Difference between LST Day and LST Night (MOD11A2).	ndlst_091011_sd 1000
	Normalised Difference between LST Day and LST Night (MOD11A2), standard deviation September-	ndlst_091011_sd 1000

SWIR	Normalised Difference between LST Day and LST Night (MOD11A2), standard deviation December-February from 2000-2022 Black-sky albedo for shortwave broadband (MCD43A3), mean June-August from 2000-2022	ndlst_120102_sd swir_060708_mea	
Snow	MODIS Snow Cover (MOD10A1)	snow_cover	500
cover	mean		
Land cover	Dynamic World 10m near-real-time (NRT) Land Use/Land Cover (LULC) dataset. Mean estimated probability of complete coverage by trees	trees	250
	Dynamic World 10m near-real-time (NRT) Land Use/Land Cover (LULC) dataset. Mean estimated probability of complete coverage by shrub and scrub	shrub_and_scrub	250
	Dynamic World 10m near-real-time (NRT) Land Use/Land Cover (LULC) dataset. Mean estimated probability of complete coverage by flooded vegetation	flooded_vegetatio	n250
	Dynamic World 10m near-real-time (NRT) Land Use/Land Cover (LULC) dataset. Mean estimated probability of complete coverage by grass	grass	250
	Dynamic World 10m near-real-time (NRT) Land Use/Land Cover (LULC) dataset. Mean estimated probability of complete coverage by bare	crop	250
Terrain	Profile curvature	curvature	250
	Downslope curvature	downslopecurvatu	
	Uplslope curvature	upslopecurvature	250
	Deviation from Mean Value Deviation from Mean Value	dvm	250
	Deviation from Mean Value Elevation	dvm2 elevation	$250 \\ 250$
	Melton Ruggedness Number	mrn	$\frac{250}{250}$
	Menon reasseances manner	111111	200

Negative openness	neg-openness	250
Possitive openness	por-openness	250
Slope	slope	250
Topographic position index	tpi	250
Terrain wetness index	twi	250
Multirresolution of valley bottom flat-	vbf	250
ness		

Apart from the environmental covariates mentioned in Table 5.1, other types of maps could also be included, such as Global Surface Water Mapping Layers and Water Soil Erosion from the Joint Research Centre (JRC). At national level there may be very significant covariates that could complement or replace the covariates of Table 5.1.

Since environmental covariates are available at different resolutions and coordinate reference systems (CRS), they have to be harmonised at a common resolution and CRS. The target resolution in GSNmap is 250 m x 250 m, therefore, all covariates were aggregated (from higher to lower resolution) or disaggregated (from lower to higher resolution) to 250 m. This process involved a raster resampling method, which is usually implemented by a bilinear approach for continuous covariates, and by the nearest-neighbour approach for categorical covariates (not included in the current list).

Note that the target resolution of GSNmap has been set at 250 m, which can be considered a moderate resolution for a global layer. However, those countries that require a higher resolution are free to develop higher resolution maps and aggregate the resulting maps to the target resolution of GSNmap for submission.

5.2 Reducing collinearity in environmental covariates

Multicollinearity is usually present in remote sensing data and terrain attributes. While this was an issue for multiple linear regression models, current models such as random forest can deal with high dimensionality. However, the main reasons to reduce the number of environmental covariates are that a model with fewer predictors can be interpreted more easily, thus extracting new knowledge, redundant information increasing the computational demand, and improve prediction results (Behrens et al., 2014).

Covariate selection can be done by supervised or unsupervised methods (Behrens et al., 2010). Supervised methods work on the basis of prediction results, hence they are based on a given dataset. For instance, recursive feature elimination (RFE) in caret R package (Kuhn, 2022) provides a tool for selecting covariates according to their predicting contribution. Instead, unsupervised methods are used to reduce the dimensionality of the dataset by removing redundant information without taking into account a particular target variable. Principal component analysis is one of the most widely used for this purpose, however, it does not ensure that specific discriminant features are kept within the main factors (Behrens et al., 2014). Another drawback of this technique is that model interpretation can be reduced when using factors instead of the original covariates.

5.3 Merging soil data and environmental covariates

A calibration dataset consists of soil observations and a matrix of predictors, where each row is a soil observation paired with the values of the corresponding covariates for the given spatial location. Some common issues and solution when merging soil observations and covariates are:

- Mismatch of coordinate reference system (CRS): it requires to convert the CRS of point data to the raster or polygon covariate CRS.
- Categorical covariates: some covariates may be categorical, such as land use/cover, legacy soil maps or geological maps. A common problem in this case is that some classes may not be sampled with any soil observation, causing an error when using the layer for prediction, since the model cannot predict over a class that was not part of the model calibration step. Also, because of the cross-validation procedure, it is advised to have, at least, three soil samples per class for the same reason.

Step 3: Mapping continuous soil properties

6.1 Setting up repeated k-fold cross validation

Cross validation is one of the most used methods in DSM for assessing the overall accuracy of the resulting maps (Step 8, Figure 3). Since this is implemented along with the model calibration step, we explain the process at this stage.

Cross validation consists of randomly splitting the input data into a training set and a testing set. However, a unique testing dataset can bias the overall accuracy. Therefore, k-fold cross validation randomly splits the data into k parts, using 1/k part of it for testing and k-1/k part for training the model. In order to make the final model more robust in terms of parameter estimations, we include repetitions of this process. The final approach is called repeated k-fold cross-validation, where k will be equal to ten in this process. A graphical representation of the 10-fold cross validation is shown in Figure 6.1. Note that green balls represent the samples belonging to the testing set and yellow balls are samples of the training set. Each row is a splitting step of the 10-folds, while each block (repetitions) represent the repetition step.

Step 5 in Figure 3 represents the repeated cross-validation, but note that after each single splitting step (the rows in Figure 4) the training data go to model

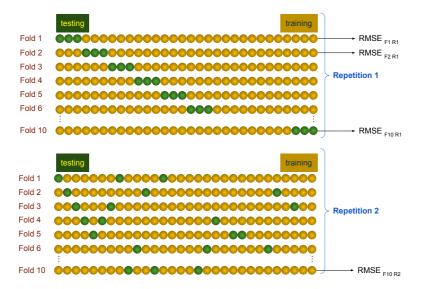


Figure 6.1: Schematic representation of the repeated cross-validation process.

calibration, which will be explained in Step 6 (next Section), and the testing data will be used with the calibrated model to produce the residuals (Step 8, Section 2.2.8). Repeated cross validation has been nicely implemented in the caret R package (Kuhn, 2022), along with several calibration methods.

6.2 Model calibration

The model calibration step involves the use of a statistical model to find the relations between soil observations and environmental covariates. One of the most widely used models in DSM is random forest (Breiman, 2001). Random forest is considered a machine learning method which belongs to the decision-tree type of model. Random forest creates an ensemble of trees using a random selection of covariate. The prediction of a single tree is made based on the observed samples mean in the leaf. The random forest prediction is made by taking the average of the predictions of the single trees. The size of the number

of covariates at each tree (mtry) can be fine-tuned before calibrating the model.

Quantile regression forests (QRF, Meinshausen (2006)) are a generalisation of the random forest models, capable of not only predicting the conditional mean, but also the conditional probability density function. This feature allows one to estimate the standard deviation of the prediction, as well as the likelihood of the target variable falling below a given threshold. In a context where a minimum level of a soil nutrient concentration may be decisive for improving the crop yield, this feature can play an important role for the GSNmap initiative.

Model calibration will be implemented using the caret package (Kuhn, 2022). While we suggest to use QRF, caret provides a large set of models https://topepo.github.io/caret/available-models.html#) that might perform better in specific cases. In this regard, it is up to the user to implement a different model, ensuring the product specifications (Section Product Specifications).

6.3 Predicting soil attributes

After calibrating the model, caret will select the best set of parameters and will fit the model using the whole dataset. Then, the final model can be used to predict the target soil properties. The process uses the model and the values of the covariates at target locations. This is generally done by using the same input covariates as a multilayer raster format, ensuring that the names of the layers are the same as the covariates in the calibration dataset. In this step we will predict the conditional mean and conditional standard deviation at each raster cell.

Step 4: uncertainty assessment

7.1 Introduction

Accuracy assessment is an essential step in digital soil mapping. One aspect of the accuracy assessment has been done in Step 7 by predicting the standard deviation of the prediction, which shows the spatial pattern of the uncertainty. Another aspect of the uncertainty is the estimation of the overall accuracy to measure the model performance. This will be measured using the model residuals generated by caret during the repeated cross validation step.

The residuals produced by caret consist of tabular data with observed and predicted values of the target soil property. They can be used to estimate different accuracy statistics. Wadoux, Walvoort and Brus (2022) have reviewed and evaluated many of them. While they concluded that there is not a single accuracy statistic that can explain all aspect of map quality, they recommended the following: mean prediction error (ME), that estimates the prediction bias; mean absolute prediction error (MAE) and root mean squared prediction error (RMSE) to estimate the magnitude of the errors; and model efficiency coefficient (MEC) (Janssen and Heuberger, 1995) as an estimator of the proportion of variance explained by the model.

While solar diagrams (Wadoux, Walvoort and Brus, 2022) are desired, we propose to produce a scatterplot of the observed vs predicted values maintaining the same range and scale for the X and Y axes.

Finally, note that accuracy assessment has been discussed in Wadoux *et al.* (2021), since the spatial distribution of soil samples might constrain the validity of the accuracy statistics. This is especially true in cases where the spatial distribution of observations is clustered. The authors recommended creating a kriging map of residuals before using them for assessing the map quality.

Reporting results

Compendium of R scripts

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