Spatial interpolation quality assessment for soil sensor transect datasets

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Abstract

Near-ground geophysical soil sensors provide valuable information for precision agriculture applications. Indeed, their readings can be used as proxy for many soil parameters. On-the-go soil sensor surveys are, typically, carried out intensively (e.g., every 2 m) over many parallel transects. Two types of soil sensors measurements are considered in this paper: apparent electrical conductivity (4 fields in California, USA) and reflectance (1 field in Italy). Two types of spatial interpolations are carried out, universal kriging (model-based) and inverse distance weighting (deterministic). Interpolation quality assessment is usually carried out using leave-one-out (loo) resampling. We show that loo resampling on transect sampling datasets returns overly-optimistic, low interpolation errors, because the left-out data point has values very close to that of its neighbors in the training dataset. This bias in the map quality assessment can be reduced by removing the closest neighbors of the validation observation from the training dataset, in a (spatial) h-block (SHB) fashion. The results indicate that, for soil sensor data acquired along parallel transects: (i) the SHB resampling is a useful tool to test the performance of interpolation techniques and (ii) the optimal (i.e., rendering the same errors of un-sampled locations between transects) SHB threshold distance (h.dist) for neighbor-exclusion is proportional to the semi-vario-gram range and partial sill. This procedure provides research scientists with an improved means of understanding the error of soil maps made by interpolating soil sensor measurements.

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1. Introduction

The benefits of using on-the-go sensors as proxies for soil properties is well recognized (Adamchuk et al., 2004). The increased coverage provided by geospatial sensor measurements enables the spatial structure of the target soil property to be characterized more accurately than when a limited set of soil samples are used (Corwin and Lesch, 2005a). In order to obtain information across the entire field, spatial interpolation techniques (e.g., kriging, inverse distance weighing) are employed. Once the map is made, it is essential to properly quantify its prediction uncertainty. Indeed, interpolation error is often the greatest contribution to the overall prediction error in a soil map (Nelson et al., 2011).

To assess the quality of the spatial interpolations, leave-one-out (loo) resampling techniques are usually employed (Robinson and Metternicht, 2006). The loo resampling is particularly effective when removing a single observation allows estimating the interpolation error over the farthest-away-as-possible (in terms of distance and/or value) location from the observed data (i.e., where the highest prediction uncertainties are expected). Unfortunately this does not always apply to soil sensor data. On-the-go soil sensors are, generally, used to acquire data intensively (e.g., every 2 m), along many parallel transects. Unless the transect spacing is narrow enough for the sampling scheme to be considered a discrete grid, transect sampling is clustered (i.e., large difference between average nearest neighbor and transect spacing). In clustered sampling, neighboring measurements tend to be very similar. Therefore, removing a single location may not provide comprehen-
sive information on the error at un-sampled locations. Unrealistically low error estimates may, then, be expected (Ruß and Brenning, 2010; Brenning, 2012).

To overcome this issue in the interpolation quality assessment, nearly identical neighbors of the validation observation can be removed from the training dataset. This particular case of loo is called h-block (HB) resampling (Burman et al., 1994; Telford and Birks, 2009). Spatial HB (SHB) resampling is generally used to remove the spatial bias in the evaluation of the performance of different spatial regression models. The SHB is generally employed in large-scale (e.g., hundreds of km) applications, to select/validate spatial models, mostly, in ecology studies. Here, we propose a version of the SHB resampling for spatial interpolation quality assessment at the field-scale (e.g., hundreds of m). The proposed application specifically targets the interpolation of intense transect surveys carried out with on-the-go proximal soil sensors.

2. Materials and methods

2.1. Sensor data

On-the-go soil sensing was carried out by electromagnetic induction (EMI) over four fields in California, USA and with an active radiometer over one field in northeastern Italy (Supplemental Fig. A.1).

Transect EMI surveys were used to measure apparent electrical conductivity (ECa), following the ECa survey protocols of Corwin and Lesch (2005b), over the 0–1.50 m soil depth in four agricultural fields in California, USA (Supplemental Fig. A.1 and Table A.1): Fields 1, 2, 3 in the western San Joaquin Valley, and Field 4 in the San Jacinto Valley. Data for Fields 1, 2, and 4 were taken from Scudiero et al. (2014). Data for Field 4 was taken from Corwin et al. (2010). Measurements were carried out using an EM38 (Geonics Ltd., Mississauga, Ontario, Canada) sensor, connected to a Trimble (Sunnyvale, CA, USA)2 GPS system with decimeter precision in horizontal positioning and mounted on a non-metallic sled (as shown in Fig. 5 of Corwin and Lesch, 2005b). Field 1 (20.7 ha) was surveyed with 111 transects, on average ~6 m apart, totaling 13,440 ECa readings (Fig. 1). Field 2 (6.4 ha) was surveyed with 8 transects, on average ~9 m apart, totaling 1311 ECa readings (Supplemental Fig. A.2). Field 3 (40.5 ha) was surveyed with 18 transects, on average ~32 m apart, totaling 1204 ECa readings (Supplemental Fig. A.3). Field 4 (6.9 ha) was surveyed with 44 transects, on average ~4 m apart, totaling 3502 ECa readings (Supplemental Fig. A.4).

For Field 5, on-the-go bare-soil reflectance at 590 ± 5.5 nm (VIS) and at 880 ± 5.5 nm (NIR) was measured with an active spectrometer (ACS-210-CropCircle, Holland Scientific, Lincoln, NE, USA) linked with a Trimble (Sunnyvale, CA, USA)2 GPS system with decimeter precision in horizontal positioning over a 25.8-ha field in Chioggia, Italy (Supplemental Fig. A.1 and Table A.1). The NIR and VIS readings were used to calculate the normalized difference vegetation index (NDVI) (Rouse et al., 1973):

\[
\text{NDVI} = \frac{\text{NIR} - \text{VIS}}{\text{NIR} + \text{VIS}}
\]

The survey at Field 5 was carried out over 22 transects, on average ~27 m apart, totaling 7403 NDVI readings (Supplemental Fig. A.5). Data for Field 5 was taken from Scudiero et al. (2013).

2.2. Spatial interpolations specifications

In this paper, we discuss the quality assessment of model-based (i.e., universal kriging) and deterministic (i.e., inverse distance weighting) spatial interpolation techniques.

2.2.1. Kriging

At all fields, ECa and bare-soil NDVI data were characterized by the presence of spatial trend and were interpolated using Universal Kriging (UK). Data for Field 1 and 3 were normalized using square-root transformation and Field 4 was normalized with natural logarithm transformation. To carry out the interpolation, the spatial correlation structures of ECa and of bare-soil NDVI were modeled by an isotropic penta-spherical semi-variogram, \( \gamma(h) \):

\[
\gamma(h) = \begin{cases} 
\gamma_0 + \frac{1}{2} \frac{h^2}{R^2} - \frac{1}{2} \frac{h^2}{R^2} \left( \frac{h}{R} \right)^2 + \frac{1}{2} \left( \frac{h}{R} \right)^3 & \text{for } h \leq R \\
\gamma_0 & \text{for } h > R
\end{cases}
\]

where \( \gamma_0 \) represents the nugget variance, \( \sigma \) the spatial variance component (partial sill), \( h \) the lag distance, and \( r \) the range. Semi-variograms were considered accurate when the loo resampling average kriging standard error (i.e., the squared-root average of the kriging variance at all locations) was very close to the RMSE (Robinson and Metternicht, 2006). Semi-variogram specifications are reported in Table 1 (for Field 1) and Supplemental Table A.3 (for the other fields). Kriging interpolations were performed using a maximum of 40 neighbors.

2.2.2. Inverse distance weighting

Inverse distance weighting (IDW) estimates values at un-sampled locations as weighted average of the known data points within a selected number of neighbors of the un-sampled location:

\[
x_0 = \frac{\sum_{i=1}^{n} x_i \times d_i^{-w}}{\sum_{i=1}^{n} d_i^{-w}}
\]

where \( x_0 \) is the value to be estimated, \( x_i \) is the known value at location \( i \) within the neighborhood of \( n \) known points (i.e., \( n = 40 \)), \( d \) is the distance of \( x_0 \) to \( x_i \), and \( w > 0 \) is the IDW weighting exponent. The lower \( w \), the more uniformly the \( n \) neighbors are incorporated into the calculation of \( x_0 \). Contrarily, with high weighting exponent values, the estimation of \( x_0 \) is mainly determined by the closest \( x_i \) values (Robinson and Metternicht, 2006). The Model Optimization feature in Arc Map’s (version 10.1; ESRI, Redlands, CA, USA) Geostatistical Analyst was used to determine the best \( w \) by minimizing the loo resampling residual sum of squares.

2.3. Interpolation quality assessment: spatial h-block (SHB) resampling

In the SHB, each observation is removed from the dataset and used for validation. Then, according to an arbitrary threshold neighborhood size, neighboring locations to the validation observation are removed. The threshold neighborhood is, in this manuscript, a circular area of radius of size \( h \text{dist} \). The remaining observations (i.e., training dataset) are used to interpolate the selected variable at the validation location. The interpolated prediction is then compared to the observed (left-out) value. Similar to the classical loo resampling, the above described procedure is repeated for every observation of the dataset. Finally, the size of the error of the SHB predictions from the actual observed data is used as the metric to evaluate the quality of the spatial interpolation model (i.e., interpolation prediction errors). In this work, we analyze the resampling root mean square error (RMSE) of spatial interpolations.

The SHB procedure for UK and IDW was carried out in the R (version 3.2.0, R Core Team, 2015) environment. For each valida-
tion location, a training dataset is created with the splitting function provided by Le Rest et al. (2014). This function removes from the data frame (data) all the neighbors of the validation location which are closer than the SHB threshold distance (h.dist):

```r
splitting <- function(data, x.lab, y.lab, h.dist){
  dist.matrix <- as.matrix(dist(data[,c(x.lab,y.lab)], diag=T, upper=T))
  training <- list()
  for(i in 1:nrow(dist.matrix)){
    num.cell <- which(dist.matrix[i,] > h.dist)
    training[[i]] <- num.cell
  }
  return(training)
}
```

We present, as an example, the SHB procedure for the UK interpolations. After reading the data and creating the training sets, a data frame (shb) that will hold the UK predictions is initialized. The new data frame has columns x, y, var1.pred (the prediction at the validated location), and var1.var (for kriging only – the kriging variance at the validated location):

```r
dataframe <- read.table(file="example.txt", header=TRUE)
H.DIST <- 25
training <- splitting(data=dataframe, x.lab='x', y.lab='y', h.dist=H.DIST)
ndata <- nrow(dataframe)
shb <- data.frame(x=numeric(ndata), y=numeric(ndata), var1.pred=numeric(ndata), var1.var=numeric(ndata))
```

Next, each observation (stored in column ‘z’) in the dataset is SHB cross-validated, with the sp and gstat libraries (Bivand et al., 2008) used for the interpolations:
The predictions \texttt{shb[, ‘varl.pred’]} can be compared with measurements \texttt{dataframe[, ‘z’]} in order to calculate goodness-of-fit measurements such as RMSE and $R^2$. To test the differences between using a SHB approach rather than the classical loo, the actual error in un-sampled locations should be known; especially between transects, where the largest interpolation errors are expected. To do so, we selected data from transect surveys that could be divided into two (or more) sub-groups of transects (e.g., see Fig. 1) having very similar frequency statistics and spatial structure. Similarity among sub-groups is essential for an unbiased comparison between transect groups, as error measurements done with RMSE (and $R^2$) are a function of minimum, maximum, and variance of samples. Practically, while a subgroup of data was used for the interpolation, the other sub-group(s) was(were) used for independent validation at un-sampled locations. In the independent validation, only transects included in the map were considered (no extrapolation of the models was carried out). When data transformation was carried out to meet normality, interpolation quality assessment (independent validation, and loo and SHB resampling) is presented for the back-transformed data (i.e., EC$_a$ in dS m$^{-1}$).

### 3. Results and discussion

Due to the consistency of the results across fields and sensors and for brevity, this section will mainly focus on data from Field 1. Details for the other fields can be found in the Supplemental Appendix A. The EC$_a$ data at Field 1 was divided in three transect groups as shown in Fig. 1. The three groups consisted of 33 transects each, comprising 4479, 4532, 4429 EC$_a$ measurements, respectively, for groups 1.A, 1.B, and 1.C (Supplemental Table A.2). Transects were, on average, 18-m apart in all three groups. The average nearest transect (neighbor) was 17.6 (2.53), 17.1 (2.48), and 17.3 (2.57) m for groups 1.A, 1.B, and 1.C, respectively. After normalization (Supplemental Table A.2), the mean (standard deviation) values for groups 1.A, 1.B, and 1.C were 1.73 (1.73), 1.71 (1.73), and 1.72 (1.74), respectively. The three groups were normally distributed, with skewness values of 0.00 (1.A), 0.03 (1.B), and –0.07 (1.C). The three groups showed similar frequency distributions (Fig. 1) and were not significantly different ($p$ level 0.05) according to the Kruskal–Wallis rank-test. Moreover, according to Table 1, the three transect groups for Field 1 were characterized by similar spatial structure. This similarity within transect sub-groups at Field 1 (as well as at the other fields) allowed their use for independent validation of the kriging interpolations. As stated earlier, great similarity in the frequency statistics and semi-variogram specifications between sub-datasets were observed at the other fields too. Only at Field 3 the two selected sub-datasets were dissimilar in semi-variogram range. Sub-group 3.A had $r = 238.4$ m and sub-group 3.B had $r = 124.6$ m (Supplemental Table A.3).

#### 3.1. Interpolation quality assessment

For the UK interpolations, at all four fields, the loo resampling RMSEs were significantly lower than the independent validation RMSEs. On average (between dataset sub-groups), the independent validation RMSEs were 181 (Field 1), 93 (Field 2), 33 (Field 3), 37 (Field 4), and 660 (Field 5) % bigger than the loo resampling RMSEs (Table 1 and Supplemental Table A.3). This clearly indicates that loo resampling provides unrealistic low RMSEs for kriging interpolations of transect soil sensor data. Consequently, when evaluating the quality of soil maps produced using such sampling technique, the spatial bias in the loo resampling should be addressed.

When using the SHB resampling, the kriging RMSE increases as the $h$ dist increases (Fig. 2). As expected, when an appropriate $h$ dist is selected, the SHB methodology produces resampling RMSEs of the same magnitude as the independent validations. In particular, for the three sub-datasets at Field 1, the SHB resampling returned the same RMSE values as the independent validations with $h$ dist around 14.2 m (for 1.A), 13.2 m (for 1.B), and 13.5 m (for 1.C). See Supplemental Table A.3 for specifications of semi-variogram modeling, loo resampling, independent validation, and best SHB $h$ dist for the other four fields.

The weighting exponents at the five fields (transect group in parenthesis) were fairly high 5.41 (1.A), 5.47 (1.B), 5.15 (1.C), 5.75 (2.A), 6.06 (2.B), 4.85 (3.A), 3.62 (3.B), 5.77 (4.A), 6.22 (4.B), 5.56 (5.A), and 2.37 (5.B). The objective selection of the IDW weight exponent gave high weight to very close neighbors in the estimation of un-sampled locations. Consistent with the very-low semi-variogram nugget values observed at the five fields, the high weight indicates a strong spatial autocorrelation of the soil-sensor data at very short distances.

For the IDW interpolations, the loo resampling RMSEs were also significantly lower than the independent validation RMSEs, at all fields (Table 2 and Supplemental Table A.4). Indeed, the independent validation RMSEs were, on average, 258 (Field 1), 80 (Field 2), 54 (Field 3), 20 (Field 4), and 583 (Field 5) % bigger than the loo resampling RMSEs.

Additionally, the observed-predicted $R^2$ values for both UK and IDW loo resampling are always considerably higher than those of the independent validation (Supplemental Table A.5). The most remarkable drop in $R^2$ was observed at Field 5 (transect spacing ~54 m; average nearest neighbor ~1.2 m), there loo resampling $R^2$ values were ~0.99 but the independent validations were characterized by $R^2$ of about 0.90–0.88.

When using the SHB resampling, the IDW RMSE increases as the $h$ dist increases (Fig. 2b). Consistent with the quality assessment of UK interpolations, the selection of an appropriate $h$ dist, allows understanding the actual map error at un-sampled locations. At Field 1, the SHB resampling returned the same RMSE values than the independent validations with $h$ dist around 13.5 m (for 1.A), 12.5 m (for 1.B), and 13.0 m (for 1.C). See Supplemental Table A.4 for specifications on loo resampling, independent validation, and best SHB $h$ dist for the other four fields. Note that UK and IDW were characterized by very similar values of $h$ dist, (Fig. 3).

Unfortunately, it is not possible to know the appropriate $h$ dist value a priori. It is, however, reasonable to expect the $h$ dist to be a function of the spatial structure of the modeled variable. For model-based interpolation methods, with multiplicative error, the error at un-sampled locations should be a function of the semi-variance and the error of the theoretical semi-variogram in describing the experimental spatial variability, at the considered lag distance. From the experimental data for the five study sites,
we observed that $h_{\text{dist}}$ (meters) for the UK interpolations can be empirically quantified as a linear function of the semi-variogram $\gamma$ (standardized as % of total sill, i.e., nugget + partial sill) and $r$:

$$h_{\text{dist}}_{\text{UK}} = 18.3 \pm 1.9 \times \frac{r}{\gamma} - 13.2 \pm 3.1$$ (4)

The regression had $R^2 = 0.91$ and significant $F = 91.7$ ($P > F$ at $<0.001$). Intercept and slope, reported in Eq. (4) with their respective standard error, were highly significant ($p < 0.001$). Note that $h_{\text{dist}} R^2$ with $r$ and $\gamma$ (standardized as % of total sill) were equal to 0.89 ($p < 0.01$) and 0.39 ($p < 0.05$), respectively. Supplemental Table A.6 presents a correlation matrix for $h_{\text{dist}}$ and semi-variogram statistics and sampling specifications (e.g., transect spacing).

Similarly, for the IDW interpolations, $h_{\text{dist}}$ (meters) could be estimated as follows:

$$h_{\text{dist}}_{\text{IDW}} = 18.0 \pm 2.1 \times \frac{r}{\gamma} - 13.0 \pm 3.5$$ (5)
The regression had $R^2 = 0.89$ and significant $F = 70.5$ ($P > F$ at <0.001). Intercept and slope were highly significant ($p < 0.001$).

The two equations were characterized by similar slope and intercept coefficients, allowing using a single model to estimate the ideal $h_{dist}$ (meters), regardless of the interpolation method (Fig. 4):

$$h_{dist} = 18.2 \pm 1.4 \times \frac{r}{\sigma} = 13.1 \pm 2.2$$ (6)

The regression had $R^2 = 0.90$ and significant $F = 176.78$ ($P > F$ at <0.001). Intercept and slope were highly significant ($p < 0.001$).

More soil sensors and a wider interval of the $r$ to $\sigma$ ratio should be tested to consolidate the relationship in Eq. (6). Unfortunately, estimating the error at un-sampled locations is very hard, as sensor surveys that can be divided into sub-datasets having similar frequency statistics are not common. Eq. (6) is, however, derived from an analysis carried out over five fields for two different sensors in two different continents. Therefore, at the tested range values, the use of Eq. (6) should provide accurate $h_{dist}$ estimates. However, semi-variogram modeling is a partially subjective practice. Even though semi-variogram parameters can be optimized objectively, model selection is subjective. This can result in different $r$ and $\sigma$ parameter values if different models are used (e.g., exponential vs. spherical). To cope with this uncertainty in $r$ and $\sigma$ determination, we suggest that $h_{dist}$, calculated using Eq. (6), should be arbitrarily increased by some safety margin (e.g., 5–10%).

4. Summary and conclusion

Providing decision makers with the best spatial information on natural resources is a challenge for scientists. Part of the decision making process includes being aware of the error hidden in the maps. When spatial variability of soil properties is properly characterized, farmers can make educated decisions on whether or not to use a site-specific management approach on a particular field (rather than managing it homogeneously).

When testing the performance of both model-based and deterministic spatial interpolation techniques, leave-one-out (loo) resampling is generally used. Because of inherent spatial autocorrelation, locations used for the loo resampling are very similar to their neighbors used in the training dataset. A spatial $h$-block (SHB) resampling is provided to address this issue in intense proximal soil sensors transect data.

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Appendix A. Supplementary material

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References


