Accounting for taxonomic distance in accuracy assessment of soil class predictions

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Abstract

Evaluating the accuracy of allocation to classes in monothetic hierarchical soil classification systems, including the World Reference Base for Soil Classification, US Soil Taxonomy, and Chinese Soil Taxonomy, is poorly-served by binomial methods (correct/incorrect allocation per evaluation observation), since some errors are more serious than others in terms of soil properties, map use, pedogenesis, and ease of mapping. Instead, evaluations should account for the taxonomic distance between classes, expressed as class similarities, giving partial credit to some incorrect allocations. These can then be used in weighted accuracy measures, either direct measures of agreement or measures that account for chance agreement, such as the *tau* index. Similarities can be determined in one of four ways: (1) by the expert opinion of a soil classification specialist; (2) by the distance between classes in a numerical taxonomy assessment; (3) by distance within a taxonomic hierarchy; or (4) by an error loss function. Expert opinion can be from the point of view of the map user, to assess map utility, or map producer, to assess mapping skill. Examples are given of determining similarity be-

tween a subset of Chinese Soil Taxonomy classes by expert opinion and by numerical taxonomy from soil spectra, and then using these for weighted accuracy assessment. A method for assessing the accuracy of probabilistic predictions of several classes at a location is also proposed.

Keywords: soil class maps, accuracy assessment, map evaluation

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1. Introduction

Soil classes are information carriers that present a holistic view of groups of soil individuals with a definite “personality”. They have proven useful as the units of soil survey interpretation and to explain soil geography, for example using the World Reference Base for Soil Classification (WRB) (Driessen et al., 2001; FAO, 2014; Van Wambeke and Nachtergaele, 2003), US Soil Taxonomy (ST) (Buol et al., 2011; Soil Survey Staff, 2014), or Chinese Soil Taxonomy (CST) (Cooperative Research Group on Chinese Soil Taxonomy, 2001; Gerasimova, 2010). These are all monothetic hierarchical classification systems, where individuals are allocated to single classes according to sharp thresholds, so that all members of any class share a certain set of features that are not present in any members of other classes (Sneath and Sokal, 1973). This allows the construction of hierarchical keys by which a soil individual is allocated to exactly one class.

Any predictive method, for example digital (McBratney et al., 2003) or predictive (Scull et al., 2003) soil mapping (DSM, PSM) that allocates individuals to single monothetic classes is sure to produce incorrect allocations with respect the true state of nature. The producer of such a prediction is obliged to evaluate and report its accuracy, so that the map user can determine whether the map is fit for an intended use, and so that the skill of the producer may be assessed. There is an extensive literature on measures of classification accuracy (e.g., Stehman and Czaplewski, 1998). These all depend on a set of evaluation observations (often called validation observations, but see Oreskes et al. (1994) for the use of ‘evaluation’ in place of ‘validation’): the true state of nature is compared to the prediction. In the case of allocation to soil classes, the “true” state is presumed to be the allo-

27 cation assigned by the professional classifier. These observations are usually
28 presented as a *cross-classification matrix* (also called a *confusion matrix*):
29 rows represent classes as predicted, columns the reference class as presumed
30 correct, and cell entries are the number of evaluation observations for each
31 combination.

32 Most evaluations of classification accuracy consider all misallocations,
33 represented by the off-diagonal entries of the cross-classification matrix,
34 to be equally serious errors. However, when the predictions are of soil
35 classes, it is obvious that not all errors are equally serious. In the first place,
36 professional classifiers often disagree on the correct allocation in doubtful,
37 and sometimes not so doubtful, cases, as anyone who has been on a soil
38 correlation exercise can attest. Certain diagnostic features are subjective,
39 despite the efforts of the creators of the keys to make them as objective as
40 possible. For example, the Soil Taxonomy definition of a fragipan requires,
41 in part that “the layer shows evidence of pedogenesis within the horizon,
42 or at a minimum, on the faces of structural units” (Soil Survey Staff, 2014,
43 p. 13). This clearly relies on the classifier’s opinion of what constitutes
44 “evidence of pedogenesis”.

45 Second, the selection of the soil individual, typically a soil profile, for
46 evaluation is subjective, and moving a few meters one way or the other can
47 easily change the classification. For example, in the WRB a mollic horizon,
48 not directly over certain indurated materials, must have a thickness of 20 cm
49 or more. It is easy to find natural soil bodies shown as delineations on an
50 area-class map where the thickness of a horizon that would otherwise qualify
51 as mollic ranges from 18 to 22 cm. Thus the evaluation observation with
52 a calcic horizon and a dark, organic-rich, high-base saturation epipedon

would be classified as a Kastanozem if the mollic horizon is recognized, but a Calcisol otherwise. Clearly any misallocation by the predictive method can not be expected to do better than the field scientist selecting a supposedly representative individual. An extreme case was reported by Edmonds and Lentner (1986), who found profiles allocated to four Soil Taxonomy soil orders within 7 m of each other in a steep hillside map unit in the Ridge and Valley province in Virginia (USA), all with similar use potential and pedogenesis.

Third, and most importantly, the consequences of a misallocation for someone using the prediction can differ widely depending on the relation between the allocated class and the actual class. For example, in the USA if a map delineation is allocated to a soil series which is considered a so-called hydric soil, a large number of restrictions are placed on the land use (Vepraskas, 2015), so predicting a hydric soil where the soil is in fact not hydric imposes a large burden on the land user. The reverse error, i.e., predicting a non-hydric soil where the soil is in fact hydric, can lead to severe environmental problems such as agricultural chemicals in surface waters. On the other hand, if a delineation is allocated to a moderately well-drained member of a drainage sequence, when in fact the soil is dominantly well-drained, there is only a slight difference in use potential.

Our objective is thus to measure allocation accuracy, taking into account that some errors are more serious than others. This can be from the user's point of view: what is the utility of the predictions to the user who would take the prediction as correct in their decision-making? It can also be from the producer's point of view: how well did they do their job? In both cases the question is how close or how far, in some sense to be defined,

79 are the correct and incorrect allocations to each other? In this paper we
80 formalize this concept of taxonomic distance, which we define as the amount
81 of separation between classes in some feature space. We then discuss ways
82 to express and measure this distance, and its inverse, taxonomic similarity.

83 The concept of taxonomic distance has been used in several studies to
84 compare classifications (Láng et al., 2013; van Huyssteen et al., 2014), to test
85 the structure of existing classification systems (Michéli et al., 2016), as aid
86 to mapping soil classes (Taghizadeh-Mehrjardi et al., 2015), to compare tax-
87 onomic and landscape concepts of soil classes (Young and Hammer, 2000),
88 to improve estimates of pedodiversity (McBratney and Minasny, 2007), and
89 as an objective basis for classification (Carré and Jacobson, 2009; Láng
90 et al., 2016; Moore et al., 1972; Odgers et al., 2011). Phillips (2013) used
91 taxonomic adjacency, defined as classes that differ in only one criterion de-
92 fined by an arbitrary threshold value, to evaluate map unit complexity. We
93 could find only one published study, that of Dobos et al. (2014), and one
94 unpublished BSc thesis, that of van Beek (2014), which use taxonomic dis-
95 tance to evaluate mapping accuracy. The work of Dobos et al. (2014) was
96 by their own conclusion only a preliminary proof of concept; the work of
97 van Beek (2014) is explained in §3.2, below.

98 Therefore the objectives of this paper are to: (1) explain how the conven-
99 tional classification accuracy assessment method using the cross-classification
100 matrix can be adjusted to account for taxonomic distance; (2) present and
101 discuss different methods for computing taxonomic distance to be used in
102 accuracy assessment. We do not explore the very important issue of how the
103 observations used to build the cross-classification matrix were obtained, i.e.,
104 the sampling plan for map evaluation (e.g., Brus et al., 2011; Stehman and

105 Czaplewski, 1998). Our objective here is simply to see how adjustments
 106 to the conventional accuracy measures can be made, taking into account
 107 taxonomic distance between classes.

108 2. The ordinary and weighted cross-classification matrices

109 The cross-classification matrix $\mathbf{X}$ is the fundamental data structure in
 110 accuracy assessment (Congalton and Green, 1999). It is constructed as fol-
 111 lows. Suppose that we have n soil profiles and that they have been allocated
 112 to r classes, which we denote i , $i = 1, 2, \dots, r$. We set up a square asymmet-
 113 ric $r \times r$ matrix $\mathbf{X}$, each row and each column of which corresponds to one
 114 class, in the same order. In each cell (i, j) we enter the number of profiles
 115 which actually are of class j that have been predicted to belong to class i .
 116 Thus the diagonals $(1, 1), (2, 2) \dots (r, r)$ represent agreement between pre-
 117 dicted and actual, and off-diagonals represent different misallocations. The
 118 asymmetry arises because there is no reason to expect that a mis-allocation
 119 of a profile actually of class j to class i will happen as frequently as the
 120 inverse misallocation

121 From this matrix we compute row sums x_{i+} , i.e., the total number allo-
 122 cated to class i , and the column sums x_{+j} , i.e., the total actually in class
 123 j . The row-wise proportion of correct allocations $C_i = x_{ii}/x_{i+}$ is commonly
 124 referred to as the *user's accuracy* for class i ; in the case of map accuracy
 125 assessment, following Brus et al. (2011) perhaps better termed *map unit*
 126 *purity*. The errors in this sense $\bar{C}_i = 1 - C_i$ are called the *errors of commis-*
 127 *sion*, i.e., the allocator committed an error in allocating an observation to
 128 class i . The column-wise proportion of correct allocations $O_j = x_{jj}/x_{+j}$ is
 129 commonly referred to as the *producer's reliability* for class j ; in the case of

map accuracy assessment, again following Brus et al. (2011) perhaps better termed *soil class representation*. The errors in this sense $\bar{O}_j = 1 - O_j$ are called the *errors of omission*, i.e., the allocator did not correctly allocate an observation to class j . The overall accuracy is $A_o = \sum_{i=1}^r x_{ii}/n$ is the proportion of all observations correctly allocated.

Our aim is to weight the cross-classification matrix when computing various accuracy statistics. Our method requires that the analyst make a second matrix $\mathbf{W}$, with the same $r \times r$ dimensions as the cross-classification matrix $\mathbf{X}$, containing the weights w_{ij} corresponding to each cell in the cross-classification matrix. The diagonals $w_{ii} \equiv 1$, giving full credit to correct allocations. The off-diagonals usually range from 0, indicating that there is no credit for this mistaken allocation, to 1, indicating that the mistake is of no consequence, i.e., that the two classes are considered identical for the purpose of accuracy assessment. It is also possible to assign a negative weight, as low as -1 , to a particularly egregious misclassification in the “expert opinion” method of assigning weights explained in §3.1, although this option should rarely be used. The weights matrix need not be symmetric, since an error of commission may be considered more or less serious than an error of omission, depending on the point of view (producer vs. user). Thus the weights matrix can be thought of as assigning partial credit, or even a demerit, for each cross-classification error.

The weighted accuracy statistics are then computed as overall agreement $A_{ow} = \sum_{i=1}^r \sum_{j=1}^r w_{ij} \cdot p_{ij}$, per-class user’s accuracy (map unit purity) $C_{i_w} = (1/p_{i+}) \cdot \sum_{j=1}^r w_{ij} \cdot p_{ij}$, and per-class producer’s accuracy (soil class representation) $O_{j_w} = (1/p_{+j}) \cdot \sum_{i=1}^r w_{ij} \cdot p_{ij}$, where i and j are the predicted and reference classes, and p_{ij} is the proportion of observations in $\mathbf{X}$

156 predicted in class i but actually in class j , i.e., x_{ij}/n .

157 **3. Operational definitions of taxonomic distance**

158 The key issue is how to create the weights matrix. Finke (2007) proposed
159 that “[w]eighting can be applied to account for errors that are considered less
160 important, for example because the two classes involved are considered to be
161 taxonomically adjacent.” However, he then says “[t]here is no agreement
162 on how such taxonomic weighting should be done.” We aim to address
163 this issue. Here is where the specifics of soil classification and soil map
164 use become relevant; a similar discussion for land use/land cover weighted
165 accuracy assessment would have other considerations than those presented
166 here. We present four alternatives; they are then compared in the Discussion
167 of §7.

168 *3.1. Expert opinion on taxonomic similarity*

169 The first method for creating the weights matrix is expert opinion on
170 how similar are each pair of classes (i, j) when the allocation is to class i but
171 the observation is actually in class j . This rating can be thought of as the
172 expert’s opinion of the partial credit to be given to the allocator who makes
173 a certain error, either of omission or commission. This is not necessarily
174 symmetric, nor transitive, i.e., there is no need to check for consistency. It
175 is strictly a pairwise assessment, filled in column-wise: the reference class
176 (column) mapped as the class given in the row. For example the partial
177 credit for allocating an observation that is really of reference class 2 to
178 class 1 is entered in cell $(1, 2) = (\text{allocated}, \text{reference})$. The asymmetry
179 could come from the error in interpretations due to misallocation, or the

180 classifier’s judgement about how similar the soils are overall, or how likely it
181 might be to make a small change in the properties and follow another branch
182 of the key at any level. The credit can be from the user’s or producer’s point
183 of view, according to whether the partial credit should reflect the utility of
184 the map to the user or the skill of the mapper.

185 As an example from the WRB, consider allocating a deep soil mainly of
186 coarse fragments, fine earth fraction sandy loam, with a cambic horizon (“a
187 subsurface horizon showing evidence of pedogenetic alteration that ranges
188 from weak to relatively strong”). If the mapper estimates that the require-
189 ment “< 20% (by volume) fine earth, averaged over a depth of 75 cm from
190 the soil surface” from the definition of Leptosols is met, this would be al-
191 located to the Cambic Skeletic Leptosols. Suppose that the volume of fine
192 earth is in fact somewhat higher, 20 – 60 % (40 – 80 % coarse fragments),
193 so it does not quality as Leptosol (5th in key order). It will fall through
194 the keys to the Cambisols (29th in key order) and be classified as a Skeletic
195 Cambisol, meeting the qualifier requirement for Skeletic: “having $\geq 40\%$
196 (by volume) coarse fragments averaged over a depth of 100 cm from the soil
197 surface”. This is an easy misallocation to make, especially because estimat-
198 ing coarse-fragment volume in the field is notoriously unreliable¹. So the
199 expert may rate this misallocation as a minor error (1) for interpretations
200 (soil functions), (2) for pedogenesis, (3) for ease of making the mistake in
201 the keys due to imprecise and inconsistent measurement of diagnostic prop-
202 erties, and may assign a partial credit of 0.9 to a predicted Cambic Skeletic

¹This could be determined on a weight basis and converted using particle density for coarse fragments and overall soil bulk density, but the latter would be difficult to measure with so many coarse fragments

203 Leptosol which is in fact a Skeletic Cambisol. The other direction may
204 receive the same partial credit, if similarity is based on concepts of pedo-
205 genesis, but may well be less (say, 0.8) since the use potential of Cambic
206 Skeletic Leptosol is poorer than most Skeletic Cambisols, due to the higher
207 proportion of coarse fragments.

208 This approach is unwieldy for many classes. In a recent study² soil ob-
209 servations were allocated to 8 orders, 12 suborders, 23 groups and 49 sub-
210 groups of CST. These would require $(8*7)=56$ (asymmetric) or $(8*7/2)=28$
211 (symmetric) comparisons just at the order level; for subgroups this would
212 be $(49*48)=2352$ or $(49*48/2)=1176$ comparisons. However, in practice not
213 all pairs of classes are confused. For any pairs where the cross-classification
214 matrix has a zero, there is no need to assign weight, since it will not affect
215 computations.

216 The obvious criticism of this approach is its subjectivity. This can be
217 partially offset by consulting several experts and (1) agreeing on the criteria
218 for similarity (use potential, pedogenesis, ease of misallocation or a com-
219 bination of these), (2) asking the experts to independently assign weights;
220 (3) comparing these for consistency. If consistent, there is no problem; if
221 not, either average the expert opinions or ask the experts to discuss their
222 reasoning and reach a consensus. An advantage of this approach is that the
223 result is *per se* acceptable to the experts.

²R. Zeng *et al.* "Numerical classification based on whole-profile spectra and soil properties as a complement to hierarchical soil classification", submitted to Geoderma 06-December-2016

224 *3.2. Distance between classes in a numerical taxonomy assessment*

225 The second method for creating the weights matrix is to use numerical
226 taxonomy to establish taxonomic distances between entities as a symmetric
227 distance matrix. Classes may be compared by computing the distances
228 between single representatives of each class, e.g., a modal profile, whether
229 an actual profile on the landscape or a synthetic central concept. They may
230 also be compared from sets of individuals representing each class, in which
231 case the distances may be computed as the average of individual Euclidean
232 or other single-linkage distances between the several representatives of each
233 class, or as Mahalanobis distances between these, which take into account
234 the intra-class variances as well as the distances between classes.

235 The advantage of using numerical taxonomy is that similarities are based
236 on measured soil properties. Numerical taxonomists working in biological
237 systematics (e.g., Sneath, 1995; Sneath and Sokal, 1973) advise selecting a
238 large number of properties to avoid bias, despite the obvious problems of
239 intercorrelation and previous selection of properties to be measured (Smith,
240 1986, §1.22.7). We illustrate this with visible-near infrared (VNIR) spectra
241 in §5.2, below.

242 Another approach is to select those properties considered relevant for the
243 purpose. For example, Bidwell and Hole (1964) in their study of Kansas soils
244 selected properties that had been used in the then-current USA classification
245 system, so that the computed distances were directly interpretable in terms
246 of that system. A similar approach was taken by Minasny et al. (2010) in
247 their study of global pedodiversity, where they selected indicators used in
248 the studied classification system, in their case the WRB.

249 A particular problem with soil profiles is how to compare profiles of

different thicknesses. Various solutions are compared by Beaudette et al. (2013); we explain one that we adopted in §5.2, below. Thus the apparent objectivity of numerical taxonomy is subject to intervention by the analyst; however this can be an advantage if the properties are selected specifically for the purposes of similarity according to some criteria of interest, and the selection criteria are transparent to the user of the accuracy statistics.

There are a wide variety of distance measures that can be used. These are discussed thoroughly in many sources (e.g., de Gruijter, 1977; Sneath and Sokal, 1973). A common choice is that of Gower (1971), in which similarity between objects i and j is defined as the average score taken over all possible k attribute comparisons: $S_{ij} = \sum_{k=1}^v s_{ijk} / \sum_{k=1}^v \delta_{ijk}$, where δ_{ijk} is an indicator which shows whether attribute k is present in both objects and thus can be compared. The per-attribute similarities s_{ijk} for each of the v possible attributes may be computed for dichotomous (e.g., present or absent), qualitative (classes), or quantitative variables. In the most common case of a quantitative variable, e.g., a spectral reflectance in a single band, similarity is computed as $s_{ijk} = 1 - (|x_i - x_j|/R_k)$, where R_k is the range of the variable within the sample or the population from which the sample was taken.

Taxonomic distances may be based on a set of indicators that are assumed to adequately characterize each class, and to have equal weight for that purpose. This was proposed by Minasny et al. (2010) in their study of global pedodiversity, and applied to the 30 reference groups of the WRB. They coded the presence of 21 diagnostic soil and environmental conditions as the indicators “present” (1) or “absent” (0) in the definition of the reference group. The taxonomic distance between classes i and j was then

276 computed as $d_{ij} = \sqrt{(\mathbf{x}_i - \mathbf{x}_j)^T(\mathbf{x}_i - \mathbf{x}_j)}$, where $\mathbf{x}$ is the vector of indica-
 277 tors, either 0 or 1. Lower values of this measure are more similar, i.e., more
 278 common 0's and 1's. For example, Solonetz and Solonchaks agree in 14
 279 of the 21 indicators, so their distance is $\sqrt{7} \approx 2.65$; perhaps surprisingly
 280 Solonetz and Ferralsols agree in 17 of the indicators, so their distance by this
 281 measure is only 2. Van Beek (2014) then used these distances as weights
 282 to prepare weighted accuracy measures for three class maps of African soils
 283 (HWSD, S-World, and SoilGrids1km), using the Africa Soil Information
 284 Service (AfSIS) profile database (Leenaars, 2013) as the reference classes.
 285 Each entry of the cross-classification matrix was multiplied by the associ-
 286 ated taxonomic distance, as we propose here, and then subtracted from an
 287 assumed perfect accuracy: $A_{ow} = 1 - \sum_{i=1}^r \sum_{j=1}^r p_{ij} \cdot d_{ij}$. The computed
 288 accuracy of the three products increased from 0.33, 0.27 and 0.28 to 0.57,
 289 0.55, and 0.58, respectively, i.e., more or less doubled. Our contention is
 290 that these weighted accuracies better represent the usefulness of the maps,
 291 when their users base decisions or model inputs on the mapped classes.

292 The distance matrix is expressed on some arbitrary scale depending on
 293 the number of properties, their measurement scales and ranges across the
 294 set of entities, and the method of accounting for covariance. One method to
 295 standardize the distances is to divide each dissimilarity d by the maximum
 296 dissimilarity in the set $\max\{\mathbf{D}\}$. The distance matrix measures dissimi-
 297 larity: higher numbers represent greater differences. To use in weighted
 298 accuracy assessment, the matrix must be converted to a similarity matrix
 299 $S = 1 - (\mathbf{D} / \max\{\mathbf{D}\})$.

300 3.3. *Distance within the taxonomic hierarchy*

301 The third method for creating the weights matrix is to use distance
302 within a hierarchical system: how far in the hierarchy one must go to match
303 classifications. For example, a Soil Taxonomy Fragiudept and a Dystrudept
304 differ in the presence of a fragipan, and the designers of Soil Taxonomy
305 decided that this difference is important at the third level of the classifica-
306 tion. A misallocation between these could be assigned a similarity of $2/3$,
307 since they agree at the second, but not the third, level. In the same way,
308 a difference in the predicted moisture regime at suborder level within the
309 same order, e.g., Udepts vs. Ustepts, would be assigned a similarity of $1/2$.
310 A complication is if the name at the target or next lower level implies an
311 intergrade to the property that caused the difference at the target level. For
312 example, the Pawnee series (Oxyaquic Vertic Argiudolls) differs from the
313 Wymore series (Aquertic Argiudolls) at the subgroup level, implying a sim-
314 ilarity of $3/4$. These are geographically-associated soil series on hillslopes
315 of loess-mantled dissected till plains in Nebraska and Kansas, USA (USDA-
316 NRCS, N.D.). However, ‘aquertic’ implies ‘vertic’, and ‘oxyaquic’ is just
317 one drainage class above ‘aquic’ (as used in Aquertic). Thus rather than a
318 similarity of $3/4$ (in different subgroups of the Arigudolls great group) per-
319 haps the similarity is more like $5/6$. This kind of refinement would have to
320 be established by expert rules, for example identifying related intergrades
321 expressed as subgroup modifiers.

322 This method assumes that the hierarchical levels represent degrees of
323 similarity, and this was certainly the aim of the designers of hierarchical
324 systems. This may be true for the lower levels, e.g., families and subgroups,
325 but has less justification at higher categories, because these are so broad as

326 to include individuals that are intergrades to adjacent classes. In the exam-
 327 ple of the Udepts vs. Ustepts, in transitional regions between these moisture
 328 regimes the use potential of these soils are quite similar, whereas at the
 329 extremes of these regimes (transition to aridic and perudic regimes, respec-
 330 tively) the use potential of the soils are quite different. Further, this method
 331 does not account for similarity of concepts at the same level. Fragiudepts
 332 have a fragipan, which has a large influence on land use, so the contrast
 333 with a Dystrudept is fairly strong. Another contrast at the same taxonomic
 334 level, Humudepts (with mollic or umbric epipedon) and Eutrudepts (high
 335 base status) seems much weaker, as both have indications of high natural
 336 soil fertility. Another contrast is even stronger: Sulfudepts vs. Eutrudepts.
 337 Rating all these contrasts as 2/3 the same similarity does not capture the
 338 functional distance between them, nor the ease of misallocation.

339 To apply this method to WRB 2014 (FAO, 2014) the principal, sec-
 340 ondary, and supplementary qualifiers of the second level (below the refer-
 341 ence groups) could be considered as three levels. However, all of these can
 342 be multiple, and rules would have to be developed to assign a difference
 343 within one of the qualifier groups when classes have different numbers of
 344 qualifiers.

345 3.4. *Error loss function*

346 The fourth method for creating the weights matrix is to use a loss func-
 347 tion which is or can be converted to a monetary value. This is appropriate
 348 if the allocation will be used to make class-based management decisions.
 349 In this case the loss due to a misallocation can serve as the weighting: the
 350 more loss, the less credit that can be given for a misallocation. This does

351 not have to be symmetric.

352 As an example, consider the site index (Avery and Burkhart, 2015, §15)
353 for an adapted forest species, one of the interpretations provided by the US
354 Natural Resources Conservation Service (NRCS) for each USA soil series.
355 This is supposed to be a linear measure of the growth of the species over
356 time, leading to the economically useful timber volume per unit land area,
357 and is established by calibration plots of the species. If the soil map is used
358 to locate suitable planting sites for a species, there would be an economic
359 loss in planting in less-than-ideal sites, which should correspond to the dif-
360 ference between site indices of the two classes. This could be asymmetric,
361 for example to give partial credit for mapping a less-productive soil, but
362 not vice-versa. The user will get an unexpected bonus if the site turns out
363 to be better than mapped, but will make a decision to plant or not based
364 on the map.

365 An example from the middle coastal plain of North Carolina illustrates
366 this method. Loblolly pine (*Pinus taeda*) is an important softwood timber
367 species of the southern USA. In its range of adaptation this species pro-
368 duces best on poorly-drained upland sites with thick argic horizons. Table
369 1 shows the soil series along a drainage sequence from poorly (Rains) to
370 excessively (Wagram) well-drained series in related families of Ultisols, as
371 well as a a geographically-associated series (Tarboro) of Psamments on a
372 lower geomorphic surface, well-drained and with a sandy profile throughout,
373 thus more prone to drought. Site indices and classification in Soil Taxon-
374 omy per the Official Series Descriptions were taken from Web Soil Survey
375 (USDA-NRCS, 2013).

376 ** Table 1 about here.

377 The site index drops quickly from the optimum 94 (Rains) to 86 for the
378 somewhat poorly drained member of the sequence (Lynchburg), but then
379 reduces on gradually on better-drained members of this sequence of thick
380 fine-loamy Ultisols³.

381 Predicting a more productive soil than actually found always results in
382 an economic loss, thus a reduction in similarity. For example, predicting
383 Norfolk (84) when in fact Tarboro (72) would over-estimate productivity.
384 Loss is $(84 - 72) / 84 = 0.143\%$. Thus, similarity would be $(1 - 0.143) = 0.857$
385 in the weights matrix. These losses could be converted to monetary values
386 by the methods of economic land evaluation (Rossiter, 1995). In the case
387 of tree species, the loss can be due to slower growth to harvestable volume,
388 or lower volume at a fixed time of harvest.

389 Predicting a less productive soil than actually found is more complicated;
390 there are three possibilities. First, such an error could be considered to be
391 no loss, since the land user would get an unexpected benefit if deciding to
392 plant the tree species on that land. In that case the (asymmetric) similarity
393 between series would be 1. Second, the error could be symmetric to the
394 previous case, in that the difference in rating distorts any calculation that
395 the planner would make based on the soil map. Finally, the similarity could
396 be rated as zero if the site index as predicted is so low that the site would
397 not be used; the land user suffers complete loss for not using a suitable
398 resource. For example, suppose the user defines a minimum site index of
399 80 to plant the tree species. Then predicting the Tarboro series ($72 < 80$)
400 when in fact the Norfolk series is found on the landscape ($84 \geq 80$) would

³The discrepancy where Goldsboro is rated higher than Lynchburg is unexplained and may represent a recording error.

401 result in complete loss, similarity 0.

402 4. Computation

403 Once the cross-classification matrix (from the evaluation sample) and
404 the weights matrix (as outlined above) are created, accuracy statistics can
405 be computed as presented in §2. The obvious statistics for a map or allo-
406 cation user are naïve statistics, a direct measure of the agreement between
407 predicted and reference classes. The user’s statistics from these are the ac-
408 curacy that the user can expect, and the producer’s are measures of how
409 successfully the producer identified the correct class. However, if the tax-
410 onomic distances are based on the differences in utility to the map user,
411 the weighted accuracy statistics give a more realistic indication of the map
412 accuracy. This is certainly the case if an error loss function or numerical
413 taxonomy was used to compute the distances, and also if expert opinion on
414 similarity from the point of view of map interpretation was used.

415 If the accuracy assessment is to evaluate the skill of the allocator or
416 mapper, many studies use Cohen’s *kappa* (Cohen, 1960) for the producer’s
417 statistics and overall accuracy. This modifies the naïve or weighted statistics
418 to adjust for chance agreement, and is especially relevant if the reference
419 data has only a few classes or if some classes occur much more frequently
420 than others. It suffers from a major conceptual flaw, namely the assumption
421 that the reference and allocations are independent and that both the user’s
422 and producer’s marginal class probabilities are known *a priori* before the al-
423 location. These assumptions are needed to compute the effect of a random
424 allocation of observations to classes, according to the known conditional
425 probabilities. These may be satisfied in the case of independent observers

426 in clinical psychology, with equal subjective prior probabilities of each pos-
 427 sible clinical diagnosis; this was the original application for which *kappa* was
 428 developed. In our application of allocating observations to soil classes, the
 429 producer's marginals (column proportions of the cross-classification matrix)
 430 of the reference observations may be considered to be known *a priori*, since
 431 they are independently-determined by field sampling. However, the user's
 432 marginals (row proportions of the cross-classification matrix) are often not
 433 known until the independent classifier (human or automatic) completes its
 434 work, i.e., these marginals are *a posteriori*. In this case we should assume
 435 no prior information, i.e., equal *a priori* probabilities for each class. But,
 436 in an automatic procedure that uses prior probabilities based on the refer-
 437 ence data, or on training data with a similar class distribution (e.g., linear
 438 discriminant analysis, machine learning algorithms such as random forests),
 439 the user's marginals are indeed *a priori* equal to the producer's marginals,
 440 so that the reference and allocation are not independent. Thus the specific
 441 context dictates the proper *a priori* user's conditional probabilities.

442 Ma and Redmond (1995) proposed the *tau* index of agreement, sym-
 443 bolized as τ , to allow the specification of prior probabilities for the user's
 444 marginals. In the absence of specific information, these may all be set to
 445 $1/r$, i.e. equal probability for each of the r classes, in which case, τ is
 446 the same as the modified *kappa* proposed by Foody (1992). If the user's
 447 marginals are equal to the producer's, τ reduces to Cohen's *kappa*.

448 The *tau* index is computed as follows:

$$\tau = \frac{\theta_1 - \theta_2}{1 - \theta_2}, \text{ where } \theta_1 = \sum_{i=1}^r p_{ii}, \theta_2 = \sum_{i=1}^r p_i \cdot p_{+i} \quad (1)$$

449 Note the use of the *a priori* probabilities of class membership p_i , instead

450 of the post-allocation row proportions p_{i+} as in *kappa*, to represent the row
 451 proportions. These are assigned by the analyst, with the obvious restriction
 452 that $\sum_i p_i = 1, \forall i$. The first coefficient, θ_1 , is the overall naïve accuracy A_o .
 453 The second, θ_2 , is the expected overall accuracy if allocations were made
 454 randomly to reference classes, taking into account prior probabilities of each
 455 reference class. So τ is the ratio between the actual proportional errors to
 456 the proportion of errors expected by chance allocation, taking into account
 457 the prior probabilities of allocation. This can even be less than 0 for a
 458 worse-than-random allocation.

459 As with the naïve statistics, *tau* can be weighted, symbolized as τ_w . This
 460 is computed as:

$$\theta_{w1} = \sum_{i=1}^r \sum_{j=1}^r w_{ij} \cdot p_{ij}, \quad \theta_{w2} = \sum_{i=1}^r \sum_{j=1}^r w_{ij} \cdot p_i \cdot p_{+j} \quad (2)$$

461 and these modified coefficients substituted into Equation 1.

462 The revised coefficient θ_{w1} (overall accuracy) includes the partial credit
 463 for errors; if all the off-diagonals of the weights matrix are zero, this reduces
 464 to θ_1 . Similarly, θ_{w2} (chance agreement) accounts for partial credit, i.e.,
 465 increases the chance agreement if any off-diagonal is not zero.

466 We have implemented the calculation of naïve and *tau* statistics in
 467 the R function `tau.w`, which results can be summarized by R function
 468 `summary.tau.w`. These are provided in file `WeightedAccuracy.R` as sup-
 469plementary material.

470 5. Examples

471 In this section we illustrate weighted accuracy assessment with examples
 472 of various kinds of similarity estimates.

473 5.1. *Expert opinion*

474 In the first example we evaluate the taxonomic distance by expert opin-
475 ion. The cross-classification matrix is from Zeng et al. (2016), who evalu-
476 ated how well VNIR spectra could distinguish observations from a set of soil
477 classes. We chose this example because it has a small matrix, with which
478 we can easily illustrate the computations. Allocation was to subgroups in
479 Chinese Soil Taxonomy, the subgroups coded as AV (Aquic Vertosols), AC
480 (Aquic Cambosols), UC (Udic Cambosols), UA (Udic Argosols), SA (Stag-
481 nic Argosols) and OP (Orthic Primosols). The results of the allocation from
482 the VNIR spectra are shown in Table 2. From the user’s perspective, the
483 Aquic Vertosols were never correctly predicted, and Aquic Cambosols pre-
484 dictions were distributed among four incorrect reference classes as well as
485 the correct one. From the producer’s perspective, actual Aquic Cambosols
486 were predicted to be in three incorrect reference classes, in addition to the
487 correct one.

488 ** Table 2 about here.

489 Table 3 shows the partial credit assigned to each misallocation, in the
490 expert opinion of an experienced soil classifier from the Nanjing Soil Science
491 Research Institute, Chinese Academy of Sciences. Interestingly, the similar-
492 ities assigned by the expert are not symmetric. For example, misallocating
493 an actual Aquic Cambosol as a Stagnic Argosol is given the highest partial
494 credit (0.35), while the reverse misallocation only is given a partial credit
495 of 0.30.

496 ** Table 3 about here.

497 The resulting accuracy assessment from applying the computation meth-
 498 ods of §4 for both the unweighted and weighted case is shown in Table 4.
 499 Since the automatic classifier did not use any information on the relative
 500 proportion of reference classes, the prior probabilities for τ were set as the
 501 inverse of the number of classes, i.e., equal prior probabilities. Accounting
 502 for partial credit leads to a slight increase in overall accuracy, from 0.763
 503 to 0.804. User’s accuracy increased for all classes, because all classes had
 504 errors of commission, and all errors received some partial credit. The largest
 505 increase in user’s accuracy was for for the Aquic Vertosols: from 0 (nothing
 506 correct) to 0.12. This is because the eight misallocations of Aquic Vertosols
 507 as Stagnic Argosols (4) or Aquic Cambosols (4) were given a partial credit
 508 of 0.1 and 0.15, respectively. The expert considered the aquic or stagnic
 509 moisture regimes to be important control land use, the Argosols to by defi-
 510 nition have high clay as do the Vertosols, and that most of the Cambosols
 511 in this study area are fairly clayey. However these similarities only resulted
 512 in a small amount of partial credit, because the vertic properties were not
 513 recognized in the two erroneously-allocated classes. Per-class producer’s
 514 accuracy increased most for this same class. Here the misallocations were
 515 to the Aquic Vertosols (8) from the Stagnic Argolsols (3), Udic Argosols
 516 (1) and Aquic Cambosols (4), all with some partial credit. The τ statistic
 517 increased only slightly, from 0.716 to 0.725. These are not much less than
 518 the corresponding naïve statistics, because the classifier mostly identified
 519 the large and small classes, and this is an improvement from the equal prior
 520 probabilities.

521 ** Table 4 about here.

522 5.2. Numerical taxonomy

523 In the second example we use similarity as distance in property space as
524 computed by the techniques of numerical taxonomy. We illustrate this with
525 spectral space as the soil properties to be used as an objective quantitative
526 measure; the same technique could be used with a set of field and laboratory
527 quantitative soil properties. Soil spectra are especially suited for numerical
528 taxonomy because of the large amount of quantitative information, which
529 is influenced by many soil properties. This approach to allocation has been
530 used successfully by, among others, Viscarra Rossel and Webster (2011).
531 Our example dataset contains 189 soil profiles from a field campaign in the
532 Heihe River watershed, northwestern China, with a combined 830 genetic
533 horizons (average 4.4 horizons per profile), from the Zeng *et al.* manuscript
534 mentioned in §4. Each profile had been classified to CST orders by experts
535 in the CST.

536 Samples from each field-identified and sampled genetic horizon were
537 scanned with a Cary 5000 spectrometer under controlled laboratory con-
538 ditions, providing 2151 bands in the visible and near infrared (VNIR) range
539 of 350-2500 nm. The profiles were scaled to one meter thickness, i.e., either
540 expanded or contracted according to the original thickness; their constituent
541 horizons were proportionally scaled within this one meter. The 830 2151-
542 band spectra were reduced with standardized principal components anal-
543 ysis (sPCA); four components explained 98% of the total variance. This
544 shows the large amount of redundancy among spectral bands and between
545 horizons in a given profile. The first four principal components were then
546 stacked into profiles using the `slab` function of the `aqp` “Algorithms for
547 Quantitative Pedology” R package (Beaudette et al., 2013) to convert per-

548 horizon values to average values for a set of standard depth slices, in this
 549 case those specified by the GlobalSoilMap.net project (GlobalSoilMap.net
 550 Science Committee, 2012). This function performs weighted averaging. For
 551 each user-specified depth slice with upper and lower depth limits (z_u, z_l) it
 552 finds the n horizons $h_i, i \in [1 \dots n]$ that are contained within or overlap
 553 (completely or partially) these limits. These each represent a proportion
 554 $p_i; \sum p_i = 1$ of the thickness $(z_l - z_u)$ of the target slab. The attribute
 555 values x_i (in this case the reflectances) from the n source layers are then
 556 combined as weighted averages $\sum_i p_i \cdot x_i$ to give a value for the target slice.
 557 These stacked profiles, all with the same horizon limits, were then used as
 558 input to linear discriminant analysis (LDA) of the soil orders (highest level
 559 in CST), using the `lda` function of the **MASS** R package. Prior probabili-
 560 ties for LDA were set to the distribution of the profiles into CST orders.
 561 This considers the principal component values at all slices, but not their
 562 sequence from top to bottom. Also, because of the standardisation to one
 563 meter thickness, the original thickness of the profiles is not represented in
 564 the LDA. The distance between LDA centroid means was computed using
 565 the `dist` R function and converted to similarities as explained in §3.2.

566 ** Figure 1 about here.

567 The similarity matrix shown in Figure 1(a) accords with intuition. For
 568 example, Aridosols and Halosols are the most similar, while Aridosols are
 569 completely dissimilar to Isohumosols. Primosols and Cambosols are also
 570 quite similar.

571 These objectively-computed similarities, based on class centroids in the
 572 linear discriminant space, can be directly used as weights in a weighted ac-

573 curacy assessment. To illustrate this, we repeated the LDA on a training set
 574 of 126 profiles from the set of 189, selected by stratified random sampling
 575 of 2/3 from each order, using the `strata` function of the `sampling` R pack-
 576 age, and used these class centroids to allocate the remaining 63 evaluation
 577 profiles, not used to construct the class centroids, to a class based on the
 578 nearest centroid. We also re-computed the distance between LDA centroid
 579 means, using only the training set, and used these as the weights matrix for
 580 weighted accuracy statistics; these are shown in Figure 1(b). The resulting
 581 cross-classification matrix is shown in Table 5 and the naïve and weighted
 582 accuracy statistics in Table 6. Overall unweighted accuracy is only 67%;
 583 the largest error is prediction of known Cambosols as Aridosols. Weighting
 584 increases the overall accuracy considerably, to 83%, because of the many
 585 medium to high similarities in Figure 1, including for the off-diagonals with
 586 the most mis-classifications: Aridosols and Cambosols (0.3239) and Ari-
 587 dosols and Halosols (0.7259). The per-class accuracies increase correspond-
 588 ingly.

589 The τ statistics are much lower, because of the unbalanced reference
 590 class distribution, i.e., mostly Aridosols and Cambosols. The *a priori* class
 591 probabilities were set equal to the reference class distribution in the training
 592 set, since these probabilities were used in the discriminant analysis, and
 593 these show a high probability of the two dominant classes. Therefore, the
 594 weighted $\tau_w = 0.5337$ even decreases slightly compared to the unweighted
 595 $\tau = 0.5432$. All these statistics would change somewhat with different
 596 training and evaluation sets; the point here is that the weighted statistics
 597 give a more realistic view of the value to the user of the use of spectroscopy
 598 to allocate unknown profiles to established classes by numerical taxonomy.

599 6. Assessing the accuracy of probabilistic predictions

600 The previous sections of this paper have considered the case when a
601 single class is predicted at each location. Some digital soil mapping ap-
602 proaches predict not only the most likely soil class, but also the probability
603 of occurrence of every class in a classification system. This is the approach
604 taken in the SoilGrids project (Hengl et al., 2014), which at the time of the
605 cited paper used multinomial logistic regression to predict the probability
606 of occurrence of each Soil Taxonomy suborder and WRB reference group
607 with one second-level qualifier. In recent versions SoilGrids uses separate
608 binary logistic regressions which are then normalized to sum to one.

609 The accuracy measures of the previous sections can be used if just the
610 most probable class is taken as the single prediction. However, the mul-
611 tiple predictions allow for more information about map accuracy. The
612 uncertainty of allocation to this most probable class can be measured by
613 Shannon entropy of the probabilities p_i for each of the n predicted classes
614 $-\sum_{i=1}^n p_i \cdot \log_2(p_i)$, substituting 0 for $\log_2(0)$ for any classes that are not pre-
615 dicted. On the one hand, the most probable class may not be correct, while
616 the correct class is predicted with some probability; the mapping method
617 should get some credit for this. On the other hand, even if the most probable
618 class is correctly predicted, high probabilities of other classes, as shown by
619 high Shannon entropy, should reduce the apparent success of the prediction.
620 This adjustment should also account for class similarity, i.e, taxonomic dis-
621 tance between the several predicted classes. If the classes predicted with the
622 highest probabilities are similar, the reported accuracy should increase to
623 reflect the actual value of the map to the user, and the skill of the mapping
624 method.

625 We extend the computations of §4 to the case where n classes are pre-
626 dicted, each with probability p_i . Weighted accuracy of a single prediction
627 is then computed as $A = (\sum_{i=1}^n p_i \cdot w_{ia}) / \sum_{i=1}^n p_i$, where w_{ia} is the similarity
628 between predicted class i and the actual class a ; $w_{aa} \equiv 1$. The denomi-
629 nator normalizes the weighted sum, in case of separate predictions. These
630 accuracies can then be summarized either overall or categorized by actual
631 class.

632 We illustrate this computation with an example of a profile located at ge-
633 ographic coördinates (118.8016°E, 32.13815°N), collected as part of a project
634 to define soil series, classified as a CST Typic Hapli-Udic Argosol, equivalent
635 to a Soil Taxonomy Udalf. At this location SoilGrids predicts⁴ the probabil-
636 ity of occurrence of 67 Soil Taxonomy suborders, of which 31 are non-zero.
637 Shannon entropy is quite high, 4.29, showing the uncertainty of prediction.
638 The first six predictions are Udalfs ($p = 0.18$), Udults ($p = 0.16$), Ochrepts
639 ($p = 0.06$), Udepts, Ustalfs and Ustolls (all $p = 0.05$); this despite the fact
640 that Ochrepts are no longer a suborder in Soil Taxonomy 2014. Although
641 the most probable class is the correct one, the large uncertainty should be
642 included in the accuracy assessment. To do this, a similarity matrix must be
643 prepared by one of the methods of the previous section. Supposing that the
644 similarity between the Udalfs (correct class) and the other listed classes are
645 0.8, 0.1, 0.3, 0.2 and 0, respectively, the weighted accuracy would be 0.34,
646 almost double the naïve accuracy 0.18.

647 A second example profile from the same project located at geographic
648 coördinates (131.9806°E, 45.65152°N) is a CST Albic Argi-Udic Isohumosol
649 with a frigid temperature regime, equivalent to a Soil Taxonomy Boroll.

⁴<https://rest.soilgrids.org/>, 23-Dec-2016

At this location SoilGrids predicts the probability of occurrence of 67 Soil Taxonomy suborders, of which 24 are non-zero. Shannon entropy is again quite high, 4.12. The most probable class is Aquents ($p = 0.14$), which is quite dissimilar from the Borolls. Of the first ten most probable classes only the Borolls (second most probable, $p = 0.13$), Aquolls (fourth, $p = 0.07$) and Udolls (tenth, $p = 0.04$) have any similarity to the correct class. Supposing that the similarity between the Borolls (correct class) and the other two classes with partial credit are 0.2 (Aquolls) and 0.8 (Udolls), the weighted accuracy would be 0.18, an increase from the naïve accuracy 0.13, i.e., the probability assigned to the correct class.

7. Discussion

We have presented four possible methods to compute taxonomic similarity for the purpose of giving partial credit for misclassifications in a weighted accuracy assessment: expert opinion, distance between classes in a numerical taxonomy assessment, distance within taxonomic hierarchy, and an error loss function.

Of these, the error loss function is the best representation of the effects of a misclassification from the map user’s point of view, and can best be converted to a monetary value, and so we prefer it. The difficulty is in formulating the loss function. In the example given above a large amount of tree stand information had to be collected in order to determine the relative yields as site indices. This is only feasible if there is a similar long-term effort, and is especially difficult if the user has multiple objectives. If a land index such as the Storie index (O’Geen et al., 2008) or taxation land value *bonitierung* system (Rothkegel, 1950) is available and is considered to

675 fairly represent the multi-functional value of a soil unit, then these values
676 could be used to determine the relative losses.

677 The distance in the taxonomic hierarchy is unwieldy and depends on the
678 vagaries of the classification system.

679 Numerical taxonomy is not as objective as it may first appear, because
680 of choices made in selection of properties and their intercorrelation. These
681 issues have been thoroughly discussed since the pioneering work of Sneath
682 and Sokal (1973), with the conclusion that selecting a large number of prop-
683 erties tends to smooth out any differences, resulting in similar taxonomic
684 distances. In this regard we especially like the use of spectroscopy, which
685 integrates many soil properties in a single spectral signature with thousands
686 of bands. This does not however account for horizon thickness and sequence,
687 and does not include properties destroyed in sampling for spectroscopy, no-
688 tably soil structure.

689 Expert opinion is often inconsistent among supposed experts. Especially
690 when evaluating the skill of a soil classifier, the expert opinion of, for ex-
691 ample, a regional correlator, is a reasonable way to judge the severity of
692 misallocations. As in any expert judgement, we can guard against extremes
693 by having a panel of experts independently assign partial credits, and then
694 remove the extremes and average the rest. This system is used to judge the
695 skill of gymnasts and divers.

696 The accuracy measures developed in this paper take the reference class,
697 the so-called ground truth, as correct. It is well-known that some allocation
698 decisions are more difficult than others or more subject to observer bias,
699 also that some allocations depend on measured values close to thresholds
700 used as the so-called taxonomic chop in monothetic classification systems;

701 as Butler (1980) pointed out, these introduce taxonomic noise that are the
702 result of human concepts being imposed on natural variation. However, we
703 suppose the user makes decisions based on the predicted class, i.e., consults
704 its description and interpretations. So this assumption of a true reference
705 class does not affect the validity of our procedure.

706 The methods described in the previous sections apply to cross-classifi-
707 cation matrices, where each evaluation observation is allocated to exactly
708 one reference class. Another approach to assessing misallocation in a mono-
709 thetic system is to blur the boundaries between classes. This approach is
710 known as fuzzy accuracy assessment, and is based on fuzzy allocation of
711 each observation to each class, i.e., each observation has a possibility (not
712 a probability) of being allocated to each reference class. This approach was
713 developed by Gopal and Woodcock (1994) and applied to land cover clas-
714 sification by these authors (Woodcock and Gopal, 2000) and Laba et al.
715 (2002). It requires that each evaluation observation be rated from 1 (al-
716 location completely wrong) to 5 (allocation completely correct) for each
717 possible reference class. If the number of classes is large, the rating of each
718 observation is tedious. For example, even at the most general level of a
719 hierarchical soil classification system (order or reference group), this would
720 require rating each evaluation observation 12 (Soil Taxonomy), 16 (CST),
721 or 14 (WRB) times. For that reason Laba et al. (2002) only rated a 10%
722 subsample of their 9 745 land cover plots representing only 22 of 29 land
723 cover types. However, this method has the advantage that the analysis can
724 report accuracy at various levels of possibility.

725 This paper could perhaps be considered as evidence in favour of aban-
726 doning monothetic soil classification, echoing the lament of Webster (1968).

727 Many of the misallocations that are corrected for by partial credit can be
728 attributed to the taxonomic chop of Butler (1980), imposed by the rigid
729 limits of diagnostic properties and horizons, when in fact individuals only
730 differ a small amount from one or more limits. This does not occur in poly-
731 thetic systems, where classes are based on overall similarity. But as long as
732 studies use monothetic hierarchical systems, we feel that weighted accuracy
733 measures give a more useful estimate of the success of any allocation or
734 mapping method that produces predictions of classes in these systems.

735 A final point is that decisions which affect the modified accuracy mea-
736 sure, i.e., how properties were selected and the weights matrix computed,
737 should be explicitly stated, i.e., transparent to whoever is judging the map
738 or allocation accuracy. There should be no attempt to manipulate results
739 to make them more favourable. Any positive weighting will raise the un-
740 weighted accuracy measures; indeed, giving full partial credit to all misal-
741 locations would result in a weighted accuracy of 100%, in which case one
742 might wonder why any allocation was done at all, since all results would
743 be equally useful. Rather, the aim is to report accuracy measures that
744 fairly represent the discrepancy between prediction and reality, according
745 to the needs of the map user or producer. We maintain that if the weighting
746 is fit for the purposes of the evaluation, the weighted measure is a better
747 evaluation of the success of the class predictions.

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Series	Soil Taxonomy family	Site index
Rains	Fine-loamy, siliceous, semiactive, thermic Typic Paleaquults	94
Lynchburg	Fine-loamy, siliceous, semiactive, thermic Aeric Paleaquults	86
Goldsboro	Fine-loamy, siliceous, subactive, thermic Aquic Paleudults	88
Norfolk	Fine-loamy, kaolinitic, thermic Typic Kandiudults	84
Wagram	Loamy, kaolinitic, thermic Arenic Kandiudults	81
Tarboro	Mixed, thermic Typic Udipsamments	72

Table 1: Some North Carolina soil series and their site indices for *Pinus taeda*

Suborder	OP	SA	UA	UC	AV	AC
OP	2	1	0	5	0	0
SA	1	74	2	1	3	6
UA	0	5	8	6	1	3
UC	6	1	3	91	0	0
AV	0	4	0	0	0	4
AC	0	6	2	2	4	38

Table 2: Confusion matrix of predictions for suborder level

OP = Orthic Primosols; SA = Stagnic Argosols; UA = Udic Argosols; UC = Udic Cambosols; AV = Aquic Vertosols; AC = Aquic Cambosols

Rows: as allocated; columns: reference class.

Suborder	OP	SA	UA	UC	AV	AC
OP	1	0.05	0.05	0.15	0.05	0.15
SA	0.05	1	0.05	0.05	0.05	0.35
UA	0.05	0.05	1	0.20	0.15	0.15
UC	0.15	0.05	0.25	1	0.10	0.25
AV	0.05	0.10	0.15	0.10	1	0.15
AC	0.20	0.30	0.10	0.25	0.20	1

Table 3: Weights matrix based on expert opinion

OP = Orthic Primosols; SA = Stagnic Argosols; UA = Udic Argosols; UC = Udic Cambosols; AV = Aquic Vertosols; AC = Aquic Cambosols

Rows: as allocated; columns: reference class.

Unweighted accuracy A_o : 0.7634

Weighted accuracy A_{ow} : 0.8039

Unweighted τ τ : 0.7161

Weighted τ τ_w : 0.7253

	UA	UA(W)	PA	PA(W)
OP	0.25	0.35	0.22	0.33
SA	0.85	0.88	0.81	0.84
UA	0.35	0.44	0.53	0.60
UC	0.90	0.92	0.87	0.89
AV	0.00	0.12	0.00	0.14
AC	0.73	0.79	0.75	0.81

Table 4: Accuracy statistics based on expert weighting; equal prior probabilities

Per class: UA, PA = User's, Producer's accuracy; (W) = weighted

Order	Anthrosols	Aridosols	Cambosols	Halosols	Isohumosols	Primosols
Anthrosols	2	0	1	0	0	0
Aridosols	1	14	5	3	0	3
Cambosols	0	2	17	0	1	1
Halosols	0	0	0	2	0	2
Isohumosols	0	0	1	0	1	0
Primosols	0	1	0	0	0	6

Table 5: Cross-classification matrix, evaluation of linear discriminant analysis of 126 training spectra on 63 evaluation profiles.

Rows: as allocated; columns: reference class.

Unweighted accuracy A_o : 0.6667

Weighted accuracy A_{ow} : 0.8269

Unweighted τ τ : 0.5432

Weighted τ τ_w : 0.5337

	UA	UA(W)	PA	PA(W)
Anthrosols	0.67	0.83	0.67	0.87
Aridosols	0.54	0.76	0.82	0.89
Cambosols	0.81	0.91	0.71	0.83
Halosols	0.50	0.73	0.40	0.83
Isohumosols	0.50	0.79	0.50	0.79
Primosols	0.86	0.91	0.50	0.73

Prior probabilities for τ from training set: Anthrosols 0.0322; Aridosols 0.2903; Cambosols 0.3871; Halosols 0.0645; Isohumosols 0.0326; Primosols 0.1935

Table 6: Accuracy statistics based on spectral similarity according of Figure 1

908 **Figures**

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(a)

(b)

Figure 1: Taxonomic similarity between class centroids determined by linear discriminant analysis on spectra, based on (a) all 189 profiles; (b) training set of 126 profiles.