

1 Measuring β -diversity by remote sensing: a
2 challenge for biodiversity monitoring

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51 **Abstract**

52 Biodiversity includes multiscalar and multitemporal structures and
53 processes, with different levels of functional organization, from genetic
54 to ecosystemic levels. One of the mostly used methods to infer bio-
55 diversity is based on taxonomic approaches and community ecology
56 theories. However, gathering extensive data in the field is difficult due
57 to logistic problems, [especially](#) when aiming at modelling biodiversity
58 changes in space and time, which assumes statistically sound sampling
59 schemes. In this [context](#), [airborne](#) or satellite remote sensing allow [in-](#)
60 [formation to be gathered](#) over wide areas in a reasonable time.

61 Most of the biodiversity maps obtained from remote sensing have
62 been based on the inference of species richness by regression analy-
63 sis. On the contrary, estimating compositional turnover (β -diversity)

64 might add crucial information related to relative abundance of dif-
65 ferent species instead of just richness. Presently, few studies have
66 addressed the measurement of species compositional turnover from
67 space.

68 Extending on previous work, in this manuscript we propose novel
69 techniques to measure β -diversity from airborne or satellite remote
70 sensing, mainly based on: i) multivariate statistical analysis, ii) the
71 spectral species concept, iii) self-organizing feature maps, iv) multi-
72 dimensional distance matrices, and the v) Rao's Q diversity. Each
73 of these measures addresses one or several issues related to turnover
74 measurement. This manuscript is the first methodological example
75 encompassing (and enhancing) most of the available methods for es-
76 timating β -diversity from remotely sensed imagery and potentially
77 relating them to species diversity in the field.

78 *Keywords:* β -diversity, Kohonen self-organising feature maps, Rao's Q
79 diversity index, remote sensing, satellite imagery, Sparse Generalized Dis-
80 similarity Model, spectral species concept.

81 1 Introduction

82 Biodiversity cannot be fully investigated without considering the spatial com-
83 ponent of its variation. In fact, it is known that the dispersal of species over
84 wide areas is driven by spatial constraints directly related to the distance
85 among sites. A negative exponential dispersal kernel is usually adopted to
86 mathematically describe the occupancy of new sites by species, as:

$$F = \sum_{K=1}^N e^{\frac{-d_{ik}}{a}} \quad (1)$$

87 where d_{ik} = distance between two locations i and k and a is a parameter
88 regulating the dispersal from localized areas (low values of a) to widespread
89 ones (high values of a , Meentemeyer et al. (2008)).

90 In this sense, distance acquires a significant role in ecology to estimate bio-
91 diversity change. Hence, spatially explicit methods have been acknowledged
92 in ecology for providing robust estimates of diversity at different hierarchical
93 levels: from individuals (Tyre et al., 2001), to populations (Vernes et al.,
94 2012), to communities (Rocchini et al., 2005).

95 When dealing with spatial explicit methods, remote sensing images repre-
96 sent a powerful tool, particularly when coupling information on compositional
97 properties of the landscape with its structure (Figure 1). Remote sensing has

98 widely been used for conservation practices including very different types of
99 data such as nightlights data (Mazor et al., 2013), Land Surface Temperature
100 estimated from MODIS data (Metz et al., 2014), spectral indices (Gillespie,
101 2005).

102 Most of the remote sensing applications for biodiversity estimation have
103 relied on the estimate of local diversity hotspots, considering land use diver-
104 sity (Wegmann et al., 2017) or continuous spatial variability of the spectral
105 signal (Rocchini et al., 2010). This is mainly grounded in the assumption
106 that a higher landscape heterogeneity is strictly related to a higher amount
107 of species occupying different niches. However, given two sites s_1 and s_2 , the
108 final diversity is not only related to the species / spectral richness of s_1 and
109 s_2 , but overall to the amount of shared species / spectral values. In other
110 words, the lower the their intersection $s_1 \cap s_2$, the higher will be the total
111 diversity, while a low total diversity will be reached when $s_1 \cap s_2 = s_1 \cup s_2$.
112 Such intersection has been widely studied in ecology, after the development
113 of β -diversity theory (Whittaker, 1960).

114 Tuomisto et al. (2003) demonstrated the power of substituting distance in
115 Eq. 1 by spectral distance to directly account for the distance between sites
116 in an environmental space, instead of a merely spatial one. However, while
117 spectral distance examples exist when measuring the β -diversity among pairs
118 of sites (e.g. Rocchini et al. (2015)), few studies have tested the possibility of
119 measuring β -diversity over wide areas considering several sites at the same
120 time (however see Alahuhta et al. (2017); Harris et al. (2015)). This is
121 especially true when considering the development of remote sensing tools
122 for diversity estimate in which the concept of β -diversity is still pioneering.

123 The aim of this paper is to present the most novel methods to measure
124 β -diversity from remotely sensed imagery based on the the most recently
125 published ecological models. In particular we will deal with: i) multivariate
126 statistical techniques, ii) the applicability of the spectral species concept,
127 iii) multidimensional distance matrices, iv) metrics coupling abundance and
128 distance-based measures.

129 This manuscript is the first methodological example encompassing (and
130 enhancing) most of the available methods for estimating β -diversity from
131 remotely sensed imagery and potentially relate them to species diversity in
132 the field.

133 2 Multivariate statistical analysis for species 134 diversity estimate from remote sensing

135 Univariate statistics have been used to directly find relations between spectral
136 and species diversity. However, the amount of variability explained by single
137 bands / vegetation indices versus species diversity is generally relatively low,
138 due to the fact that different aspects related to the complexity of habitats
139 might act in shaping diversity, from disturbance and land use at local scales
140 to climate and element fluxes at global scales.

141 Ordination techniques are designed to quantitatively describe multivari-
142 ate gradual transitions in the species composition of sampled sites. Measuring
143 the distance between two sampling sites in the multi-dimensional ordination
144 space is a good proxy of the change in species composition. When this mea-
145 sure is related to the geographical distance between the considered sites, the
146 beta diversity at this particular scale can be assessed.

147 Of the various available ordination techniques, Detrended Correspon-
148 dence Analysis (DCA, Hill and Gauch (1980)) is particularly suitable for
149 such analyses. The axes (i.e. gradients) of the DCA ordination space are
150 scaled in standard deviation (SD) units, where a distance of 4 SD is related
151 to a full species turnover. This enables a versatile analysis that easily reveals
152 whether two sampled sites still have species in common.

153 Several studies have mapped the ordination space using remote sensing
154 data (e.g., Schmidtlein and Sassini (2004); Schmidtlein et al. (2007); Feil-
155 hauer et al. (2009, 2011, 2014); Gu et al. (2015); Harris et al. (2015); Leitao
156 et al. (2015); Neumann et al. (2015)). For this purpose, the axes scores of
157 the sampled sites are regressed against the corresponding canopy reflectance
158 values extracted from air- or spaceborne image data. The resulting multi-
159 variate regression models, one per ordination axis and most often generated
160 with machine learning regression techniques, are subsequently applied on the
161 image data for a spatial prediction of ordination scores. Each pixel of the
162 image data is assigned to a specific position in the ordination space that in-
163 dicates its species composition. The resulting gradient maps are a powerful
164 tool for analyses of beta diversity across different spatial scales (Feilhauer et
165 al., 2009; Hernandez-Stefanoni et al., 2012).

166 A simple analysis of the variability of the DCA scores in a defined pixel
167 neighborhood (i.e. a moving window) results in a efficient beta diversity
168 assessment. The spatial scale of this assessment can be varied either by
169 re-sampling the gradient map to a coarser spatial resolution (i.e. pixel size) or
170 by changing the kernel size of the considered pixel neighborhood. Such tech-
171 niques have been further developed e.g. for spatial conservation prioritization

172 programmes such as [Zonation](#) (Moilanen et al., 2005, 2009).

173 Figure 2 shows an example of a DCA-based assessment of beta diversity
174 on a very local scale (10 m) following the approach described in Feilhauer et
175 al. (2009). The analyzed landscape is a mosaic of raised bogs, fens, transition
176 mires and *Molinia* meadows. For a detailed description of the data and site
177 please refer to Feilhauer et al. (2014, 2016).

178 Analyses like this require two different data sets: (1) a sample of field
179 data that is representative for the vegetation in the studied area and is used
180 to generate the ordination space; (2) image data with a sufficient spectral
181 resolution to discriminate the vegetation types within the ordination space
182 and with a spatial resolution that is in line with the sampling design of the
183 field data (Feilhauer et al., 2013).

184 Using these data, the continuous spatial variability of the spectral signal
185 in the image pixels is translated into a spatially continuous measure of species
186 composition. The advantages of this approach are obvious: since the diversity
187 analyses are conducted in the floristic gradient space, the resulting measures
188 resemble field studies and are thus easier to interpret than spectral proxies
189 and closer to the point of view of many end-users. [Furthermore](#), the analysis
190 of ordination scores in defined pixel neighborhoods is not restricted to a
191 single spatial scale but offers the opportunity to implement assessments of
192 beta diversity on multiple scales.

193 **3 The spectral species concept**

194 The spectral species concept has been proposed by Féret and Asner (2014a)
195 to map both α and β component of the biodiversity using a unique frame-
196 work. It is rooted in the convergence between two other concepts, the spec-
197 tral variation hypothesis (SVH) proposed by Palmer et al. (2002), and the
198 plant optical types proposed by Ustin and Gamon (2010), sustained by the
199 technological advances in the domain of high spatial resolution imaging spec-
200 troscopy. The SVH states that the spatial variability in the remotely sensed
201 signal, that is the spectral heterogeneity, is related to environmental hetero-
202 geneity and could therefore be used as a powerful proxy of species diversity.
203 SVH has been tested in different situations (Rocchini et al., 2010) and con-
204 clusions show that the [performance](#) of this approach is very dependent on
205 several factors, including the [instrument](#) characteristics (spectral, spatial and
206 temporal resolution), the type of vegetation investigated, and the metrics de-
207 rived from remotely sensed information to estimate spectral heterogeneity.
208 Plant optical types refer to the capacity of sensors to measure [signals that](#)
209 [aggregate](#) information about vegetation structure, phenology, biochemistry

210 and physiology. Therefore, this concept is also tightly linked to the perfor-
211 mances of the sensor and finds particular echo with the increasing use of high
212 spatial resolution imaging spectroscopy for the estimation and identification
213 of multiple vegetations properties.

214 The details provided by high spatial resolution imaging spectroscopy are
215 sufficient to perform analyses of plant optical traits at the individual tree scale
216 in order to differentiate tree species, obtain information about leaf chemical
217 traits and estimate the α component of biodiversity (Asner et al., 2008, 2015;
218 Chadwick and Asner, 2016; Clark et al., 2005; Clark and Roberts, 2012;
219 Féret and Asner, 2013; Vaglio Laurin et al., 2014). These results illustrate
220 that spectral information can be related to taxonomic or functional informa-
221 tion of the vegetation, which supports the SVH under the hypothesis that
222 the metrics used to compute spectral heterogeneity and a given component
223 of vegetation diversity are properly defined. However these applications are
224 currently limited by the important amount of field data required to train re-
225 gression or classification models, which is also directly linked to their low gen-
226 eralization ability in time and space. Unsupervised approaches then appear
227 as valuable alternatives for the analysis of ecosystem heterogeneity (Baldeck
228 and Asner, 2013; Baldeck et al., 2014; Feilhauer et al., 2011; Baldeck and
229 Asner, 2013; Féret and Asner, 2014b), as ecological indicators of α and β
230 diversity at landscape scale usually require one or several levels of abstraction
231 beyond the correct taxonomic identification (Tuomisto et al., 2006).

232 Clustering (properly pre-processed) spectral information should result in
233 pixels from the same species naturally grouping together rather than dis-
234 tributing randomly among clusters, Féret and Asner (2014a) proposed a
235 grouping method aiming at assigning labels to pixels based on multiple clus-
236 tering of spectroscopic data acquired at landscape scale. These pixels, labeled
237 with a set of so-called spectral species, can then be used straightforwardly
238 in order to compute various diversity metrics such as Shannon index for α
239 diversity, and Bray-Curtis dissimilarity for β diversity. The pre-processing
240 stage is divided into several stages. After masking all non-vegetated pixels, a
241 normalization based on **continuous** removal is applied to each pixel and over
242 the full spectral domain, then a principal component analysis is performed on
243 the **continuously** removed spectral data. The normalization **reduces** effects
244 due to changes in illumination, canopy geometry and other factors unrelated
245 to vegetation, while enhancing the signal corresponding to vegetation. The
246 components including individual-specific information are the components of
247 interest. They can be identified after visual inspection or automated routines,
248 if initial data show sufficient signal to noise ratio. Once a limited number
249 of components have been selected, k-means clustering is then applied to a
250 certain number of subsets, and for each of these subsets, centroids are com-

251 puted and each pixel in the image is labeled based on the closest centroid.
252 The repetition of clustering based on various subsets of the image tends to
253 minimize the risk of assigning centroids to irrelevant groups of pixels. Ex-
254 perimental results showed that the averaging of diversity indices computed
255 from multiple centroid maps can be seen as an analogous to signal averaging,
256 which consists in increasing signal to noise ratio by replicating measurements.
257 For each repetition, the closest centroid corresponds to the spectral species,
258 and for each spatial unit of a given size, the spectral species distribution is
259 derived in order to compute any diversity metric requiring either information
260 at the local scale, or comparison of information across spatially distant plots.

261 The concepts of spectral species and spectral species distribution have
262 been tested successfully on a limited number of situations and types of
263 ecosystems (see (Rocchini et al., 2016) for a review, and (Lausch et al.,
264 2016) for an application to similar concepts). As an example, F eret and
265 Asner (2014a) showed ability to properly estimate landscape heterogeneity
266 at moderate spatial scale, up to few dozen square kilometers over tropical
267 forests, based on high spatial resolution imaging spectroscopy (Figure 3).
268 A generic parameterization of the method showed robust performances for
269 α diversity mapping across space and time, but mapping β diversity across
270 large spatial scales using images acquired during different airborne campaign
271 remains challenging, which leads to an unsolved problem when considering
272 operational regional mapping. In the perspective of global monitoring of
273 biodiversity, and given the unprecedented remote sensing capacity allowed
274 by the Copernicus program, including the Sentinel-2 multispectral satellites,
275 several other challenges are foreseen and currently investigated. The influ-
276 ence of decreased spatial and spectral resolution on the ability to properly
277 differentiate ecologically meaningful spectral species across landscapes and
278 over regions will need to be investigated. The application of this concept be-
279 yond tropical forests and savanna ecosystems should also be investigated, as
280 it may not hold when applied on moderately diverse ecosystems or systems
281 with individuals whose individuals have dimensions well below the resolving
282 power of the instrument.

283 4 Self organizing feature maps

284 The Kohonen self-organising feature map (SOFM, Kohonen (1982)) is a neu-
285 ral network that may be used to undertake unsupervised clustering of data.
286 Critically, the input to a SOFM can be a large multi-variate data set such
287 as may be acquired on species from quadrat based field surveys. The SOFM
288 summarises the data in a low, typically two, dimensional output (Figure

289 4). In this output space the data for individual quadrats are topologically
290 ordered – with sites that are similar close together while those of highly dif-
291 ferent species composition are more distant. Because the data sites in the
292 output space are arranged by relative similarity the output space may also
293 be used to aggregate or classify a data set. As such the SOFM is attrac-
294 tive as a non-parametric clustering analysis and as a means to undertake an
295 ordination (Chon et al., 1996).

296 A SOFM is, unlike some of the approaches used commonly in community
297 ecology, not constrained by assumptions relating the statistical distribution
298 of the data used. The SOFM uses unsupervised learning to produce a topo-
299 logically ordered output space in which the samples are arranged spatially
300 in relation to their relative similarity in species composition. The SOFM
301 thus performs a non-parametric ordination analysis (Foody, 1999). The pro-
302 duction of a classification by a SOFM comprises two main stages (Giraudel
303 and Lek, 2001). An iterative analysis, in which time-decaying parameters
304 that control network learning and the size of local neighbourhoods located
305 around output units, is used. For this, the user must specify a number of key
306 parameters such as the size and shape of the network, number of iterations of
307 the algorithm, the learning rate and its rate of decline and a neighbourhood
308 parameter. The need for such parameters can add some uncertainty to the
309 analysis. While there are no formal rules to follow in the design of a SOFM
310 there are recommendations for the determination of SOFM parameter set-
311 tings (Giraudel and Lek, 2001). A further concern is that as an unsupervised
312 classifier the classes defined may not always be the most useful for an in-
313 vestigation. In addition, the nature of the analysis means the direction of
314 the gradients cannot be controlled (Fritzke, 1995) but the analysis performs
315 well in comparison to popular ordination techniques such as PCA and DCA
316 (Foody and Cutler, 2003). The SOFM may also use a variety of different
317 data types such as presence/absence, abundance or importance values and
318 can solve complex non-linear problems (Giraudel and Lek, 2001).

319 5 Multidimensional distance matrices: GDMs 320 and SGDMs

321 One of the most widespread methods for assessing α -diversity is using distance
322 matrices (Legendre et al., 2005). Indeed, early work by Whittaker (1960) sug-
323 gested that β -diversity could be quantified by dissimilarity matrices among
324 (pairs of) sites. Furthermore, the Mantel test (Mantel and Valand, 2017),
325 designed to estimate the association between two independent dissimilarity

326 matrices, has been widely used to correlate a community composition dissim-
327 ilarity matrix with an environment dissimilarity one, thus providing useful
328 insights into community composition and turnover (Legendre et al., 2005;
329 Tahvanainen et al., 2011).

330 Generalized Dissimilarity Modelling (GDM; Ferrier (2007) can be con-
331 sidered as an extension of the Mantel test, which is able to accommodate
332 multidimensional environmental data, to be compared with the composi-
333 tional data. GDMs also allow for the prediction of compositional turnover
334 as well as for, e.g. environmental classification constrained to the compo-
335 sitional dissimilarity (Ferrier, 2007; Leathwick et al., 2011). In GDM, the
336 compositional dissimilarities between all pairs of samples are modelled as a
337 function of their respective environmental distances. This is done through a
338 linear combination of monotonic I-spline basis functions, under the assump-
339 tion that increasing environmental dissimilarity (e.g. along a gradient) can
340 only result in increasing compositional dissimilarity. This method is thus well
341 suited for measuring and mapping β -diversity, and is thus becoming widely
342 used in conservation science and macroecology, and recently been subject to
343 several developments as we describe below.

344 One such development is the phylogenetic GDM (phylo-GDM; Rosauer
345 et al. (2014)), which incorporates phylogenetic dissimilarities into GDM and
346 allows for analysing and predicting phylogenetic β -diversity, thus linking
347 ecological and evolutionary processes. This method can provide novel in-
348 sights into the mechanisms underlying current patterns of biological diversity
349 (Graham et al., 2008). Another recent development of GDM is the multi-
350 site GDM (MS-GDM; Latombe et al. (2017)), which extends GDMs from
351 pairwise to multi-site dissimilarity modelling. In such paper, the authors
352 tested MS-GDM by means of both constrained (monotonical) additive mod-
353 els and I-splines, although with no conclusive results relating to the best
354 method overall. They concluded, however, that when applying MS-GDM to
355 a high number of samples, they could better explain the drivers of species
356 turnover. Also, an important development of GDM is the Bayesian bootstrap
357 GDM (BBGDM; Woolley et al. (2017)) designed to characterize uncertainty
358 in generalized dissimilarity models. This approach allows better represent-
359 ing the underlying uncertainty in the data, by estimating the variance in
360 parameters based on the available data.

361 Finally, an implementation of GDM, which was created particularly for
362 dealing with high-dimensional (and potentially high-collinear) remote sensing
363 data as input in GDM is the Sparse Generalized Dissimilarity Model (SGDM,
364 Figure 5, Leitao et al. (2015)). This method is a two-stage approach that
365 consists of initially reducing the environmental space (e.g. reflectance data)
366 by means of a Sparse Canonical Correlation Analysis (SCCA, Figure 5; Wit-

ten et al. (2013)), and then fitting the resulting components with a GDM
 model. The SCCA is a form of penalized canonical correlation analysis based
 on the L1 (lasso) penalty function, and is thus designed to deal with high-
 dimensional data. The two algorithms are coupled in a way that the SCCA
 penalization is selected through a heuristic grid search manner, in order to
 minimize the cross-validate root mean square error in the dissimilarities pre-
 dicted by the GDM. In this procedure, the high-dimensional environmental
 data (such as coming from time series of multispectral or hyperspectral data)
 are subject to a supervised ordination approach that reduces their dimen-
 sion while capturing the axes of variation that most correlate to those of
 the community compositional matrix. SGDM has been successfully used for
 modelling and mapping the compositional turnover of both animal and plant
 species, using several different sources of remote sensing (and auxiliary) data
 (Leitao et al., 2015; Leitão et al., 2017).

6 Rao's Q diversity

Most of the previously shown metrics are based on the distance among pixel
 values in a multidimensional spectral space. None of them considers the
 relative abundance of such pixel values in a neighbourhood.

By contrast, abundance-based metrics such as the Shannon entropy could
 output similar results despite a variable distance among pixel values. As an
 example, consider a 3x3 matrix of remotely sensed data:

$$\begin{pmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{d1} & x_{d2} & x_{d3} \end{pmatrix} \quad (2)$$

composed by the following values:

$$\begin{pmatrix} 10 & 13 & 15 \\ 18 & 20 & 23 \\ 19 & 21 & 22 \end{pmatrix} \quad (3)$$

then consider a different matrix:

$$\begin{pmatrix} 10 & 121 & 227 \\ 1 & 40 & 251 \\ 7 & 100 & 149 \end{pmatrix} \quad (4)$$

From a Shannon's entropy perspective, such matrices are equal in terms of
 heterogeneity. The Shannon's entropy is indeed based on the relative abun-
 dance (and richness) of a sample, and its value is 2.197 for both the matrices.

393 This value, equalling the natural logarithm of the number of classes (pixel
394 values), is also Shannon's maximum theoretical value given a 3x3 matrix,
395 due to the lack of identical numbers in the matrices. This example explicitly
396 shows that accounting for the distance among values and their relative abun-
397 dance is crucial to discriminate among areas in terms of measured (modeled)
398 heterogeneity.

399 One of the metrics accounting for both the abundance and the pairwise
400 spectral distance among pixels is the Rao's Q diversity index, as:

$$Q = \sum \sum d_{ij} \times p_i \times p_j \quad (5)$$

401 where d_{ij} = spectral distance among pixels i and j and p = proportion of
402 occupied area.

403 Hence, Rao's Q is capable of discriminating among the ecological diversity
404 of matrices 3 and 4, turning out to be 4.59 and 90.70, respectively. Appendix
405 1 provide an example spreadsheet to perform the calculation while the com-
406 plete R code is stored in the GitHub repository
407 <https://github.com/mattmar/spectralrao>.

408 We decided to make use of a case study to highlight the importance of
409 considering the distance among pixel values in remote sense ecological appli-
410 cation. The performance of Rao's Q index in describing landscape diversity
411 was tested in a complex agro-forestry landscape located in southern Portu-
412 gal. A test site with an area of about $10 \times 10 \text{ km}^2$ (centroid located at 38°
413 $39' 10.74''$ N; $8^\circ 12' 52.30''$ W) was selected to conduct the analysis. In this
414 area, a savanna-like ecosystem called montado occupies about 40% of the test
415 site, followed by traditional olive groves, pastures, vineyards, and irrigated
416 monocultures (e.g. corn fields). Montado is spatially characterized by the
417 variability of its tree density (e.g. Godinho et al. (2016)), and the gradient
418 between low and high tree density over space can lead to different structural
419 heterogeneity and habitat diversity.

420 Within the test site, polyculture under small farming context (e.g. veg-
421 etable gardens, orchards, and cereal crops) is an important feature of this
422 landscape by generating a high compositional and configurational spatial
423 heterogeneity (Figure 6). The main goal in using this case study is to demon-
424 strate the potential and effectiveness of the Rao's Q index in producing ac-
425 curately remote-sensing based maps of spatial diversity over such complex
426 landscape. For this study, a cloud-free Sentinel-2A (S2A) image acquired
427 on 8 of August 2016 was used to compute the NDVI at a 10 meters spatial
428 resolution. The S2A image download, as well as the atmospheric correction
429 (DOS method) were performed using the Semi-Automatic Classification plu-
430 gin (SCP) implemented in the QGIS software (QGIS Development Team ,
431 2016(@)).

432 The NDVI was used as input data for Rao's Q index computation using
433 a window size of 3×3 pixels. The performance of the Rao's Q was compared
434 to the Shannon Entropy index (Shannon's H), which is one of the simplest,
435 and widely used, remote sensing-based diversity measures for landscape het-
436 erogeneity assessment (Rocchini et al., 2016). To investigate whether both
437 diversity indices differ between land cover types, one-way ANOVA tests were
438 performed. This approach was used for analysing the degree of dissimilarity
439 between Rao's Q and Shannon H index across two high complex land cover
440 types; i) montado, and ii) polyculture. To do so, a sample of 60 squares with
441 250×250 meters size was randomly selected over these two land cover types.
442 Each square represents a sample of 625 S2A NDVI pixels, thus corresponding
443 to a total of 37,500 pixels over the 60 squares. For the comparison between
444 both indices, the coefficient of variation (CV) was calculated for each $250 \times$
445 250 m squares. Regarding the Rao's Q performance, Figure 6 clearly points
446 to the significant improvements shown by Rao's Q index compared to the
447 Shannon H index in describing the spatial diversity. In particular, it can be
448 seen through the Figure 6, that Rao's Q index can highlight different gra-
449 dients of spatial diversity of montado areas, which present high tree density
450 variability (Figure 6), and thus high spatial heterogeneity. One-way ANOVA
451 tests revealed that both indices values were significantly different between
452 the two land cover types (montado: $F = 503.3$, $p < 0.001$; polyculture: $F =$
453 889.8 , $p < 0.001$). Overall, the obtained results demonstrate the capability of
454 Rao's Q index in producing accurate landscape diversity maps in a complex
455 landscape such as the Mediterranean agro-forestry systems.

456 7 Conclusion

457 In this paper, we showed several methods based on ecological β -diversity,
458 which can be investigated by remote sensing through the calculation of
459 ecosystem heterogeneity, to estimate the spatial variability of biodiversity.
460 When there is a wide range of heterogeneity, for example when the data
461 include homogeneous and heterogeneous zones, no single measure might cap-
462 ture all the different aspects of β -diversity (e.g. Baselga (2013)). That is why
463 we suggested in this manuscript multivariate and multidimensional methods
464 (e.g. multivariate statistics and multidimensional distance matrices) based
465 on the spectral signal and its variability over space to account for different
466 aspects of diversity, also including distance- and abundance-based methods
467 (e.g. the Rao's Q).

468 Biodiversity measured as species richness is often used for conservation
469 purposes, hence the importance of avoiding an under- or over-estimate has

470 been highlighted (Chiarucci et al., 2009). Furthermore, pairwise distance-
 471 based methods might be profitably used to detect not only diversity hotspots
 472 in an area but also the variation of biodiversity over space, and potentially
 473 over time, once multitemporal sets of images are used.

474 In this paper we focused on optimising measures of β -diversity based on
 475 remote sensing data. Such measures might be used to regress species diversity
 476 against remotely sensed heterogeneity, based on new regression techniques
 477 which maximise the possibility of predicting the zones in a study area, or at
 478 larger spatial scales, of peculiar conservation value. As an example, shrink-
 479 age regression, recently applied in biodiversity conservation (Authier et al.,
 480 2017) could allow a direct focus on habitat modelling, which is one of the
 481 major strengths of remote sensing (Gillespie et al., 2008). Moreover, such
 482 analysis might be performed in a Bayesian framework allowing to i) model
 483 multidimensional covariates with non-stationary variation over space (Ran-
 484 dell et al., 2016), such as the bands of satellite images, and ii) model the
 485 errors in the output and their variation over space (Rocchini et al., 2017).

486 As previously stated, the suggested methods for β -diversity estimation
 487 from remote sensing are mainly based on distances, but they could be effec-
 488 tively translated to relative abundance-based methods. As an example Roc-
 489 chini et al. (2013) introduced the possibility of applying generalized entropy
 490 theory to satellite images with one single formula representing a continuum
 491 of diversity measures changing one parameter. One of the best examples
 492 in this framework could be the use of Hill numbers, in which diversity is
 493 expressed as:

$${}^qD = \left(\sum_{i=1}^S p_i^q \right)^{\frac{1}{1-q}} \quad (6)$$

494 where S = number of samples / pixels and p_i = relative abundance of a
 495 species / spectral value. varying the parameter q , qD varies accordingly in
 496 several diversity indices, e.g. for $q = 0$ qD is the simple number of species,
 497 for $\lim(q) = 1$ qD equals Shannon's entropy, etc. (Hsieh et al., 2016).

498 Furthermore, connectivity analysis might also be taken into account (Moila-
 499 nen et al., 2005, 2009). For instance, a remote sensing based connectivity
 500 network among different sites, based on β -diversity measures, could be ap-
 501 plied for the estimate of landscape connectivity and consequent genetic flow,
 502 as demonstrated by Vernesi et al. (2012). It has also been shown that commu-
 503 nity related biodiversity indicators are often missing from current monitoring
 504 programmes (Vihervaara et al., 2017); thus methods such as remote sensing
 505 based Rao's Q diversity applied for various ecosystems might improve other-
 506 wise challenging monitoring of biological communities.

507 With this manuscript we hope to stimulate discussion on the available
508 methods for estimating β -diversity from remotely sensed imagery by propos-
509 ing innovative techniques grounded on ecological theory.

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514 Authors' contribution statement

515 All authors contributed to the development and writing of the manuscript.

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- 773 Figures

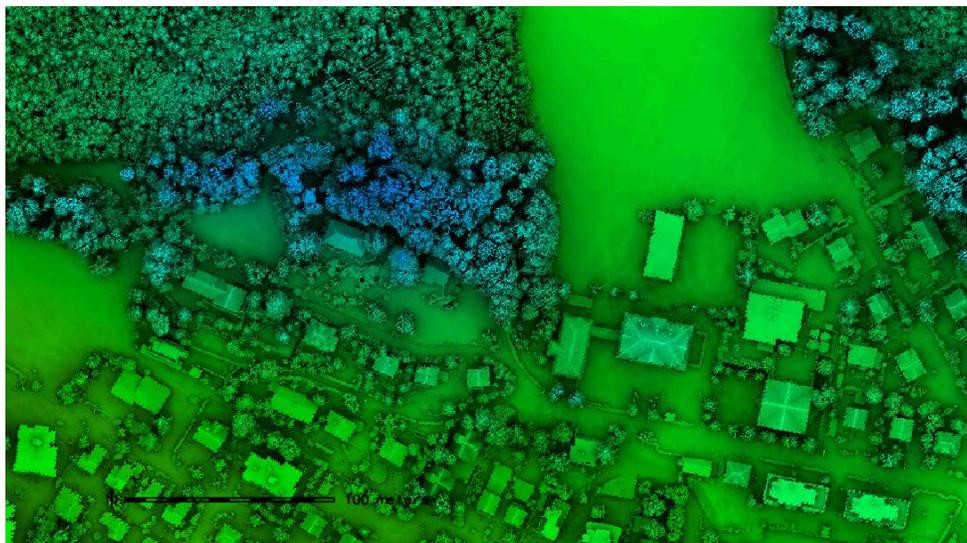


Figure 1: An example of how to couple information on compositional properties of the landscape by optical data together with structural (3D) properties by laser scanning LiDAR data.

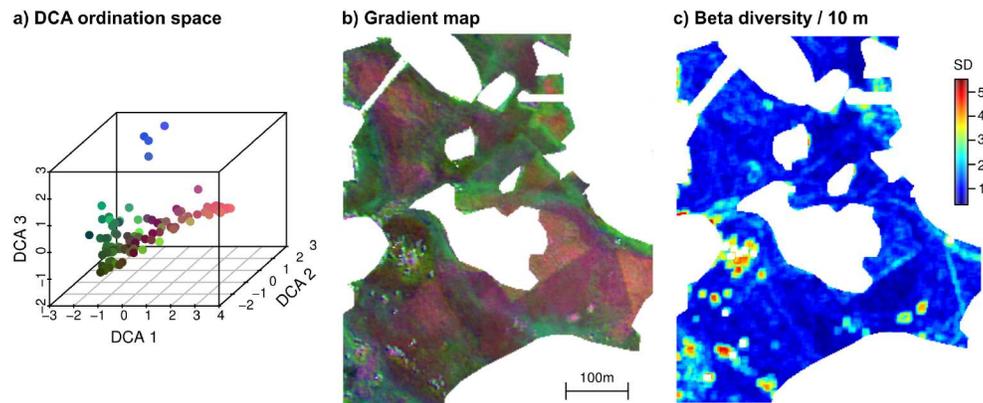


Figure 2: β -diversity assessment with a combination of ordination techniques and remote sensing. a) Three dimensional DCA ordination space of $n=100$ vegetation plots sampled in raised bogs, fens, transition mires and *Molinia* meadows in the alpine foothills of Southern Germany. An inter-plot distance of 4 SD corresponds to a full species turnover. b) Maps of the ordination axes resulting from a spatial prediction based on canopy reflectance. Each pixel has a predicted position in the ordination space that is indicated by its color. The color scheme corresponds to a). The map has a spatial resolution of 2 m x 2 m, which is in line with the sampled plot size. c) Cumulative change rates along the three DCA axes in a 5 x 5 pixel neighborhood. A high change rate indicates a high beta diversity.

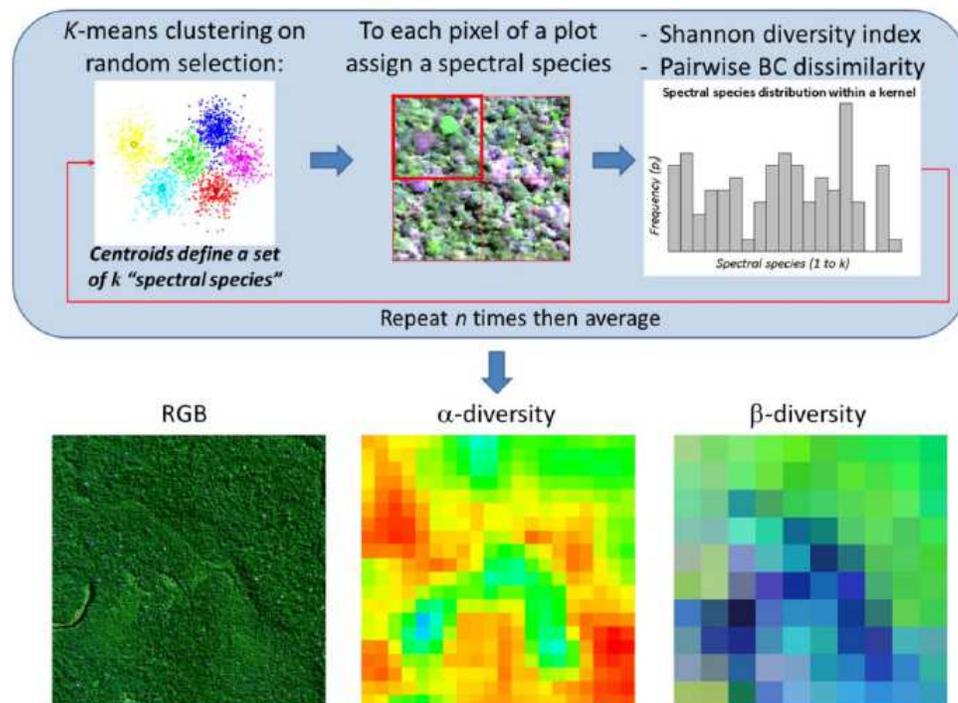


Figure 3: Spectral species can be identified in a hyper- or multi-spectral image by spatial clustering method and their distribution can be mapped. Such maps can further be used to apply local-based heterogeneity measurements (α -diversity) as well as iterative distance based methods to build β -diversity maps. Reproduced from Féret and Asner (2014a).

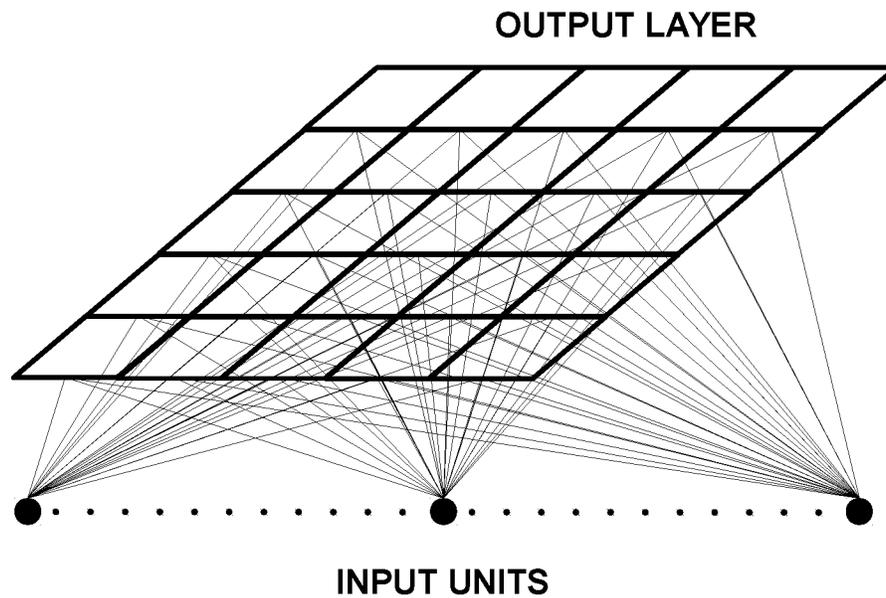


Figure 4: A self-organising feature map can be built starting from an input layer, e.g. the presence absence of a tree species or of a peculiar spectral value) which is connected to every unit in the output layer by a weighted connection. The self organising feature map uses unsupervised learning to map the location of field sites within the output space on the basis of their relative similarity in species or spectral composition. [Redrawn](#) from Foody and Cutler (2003).

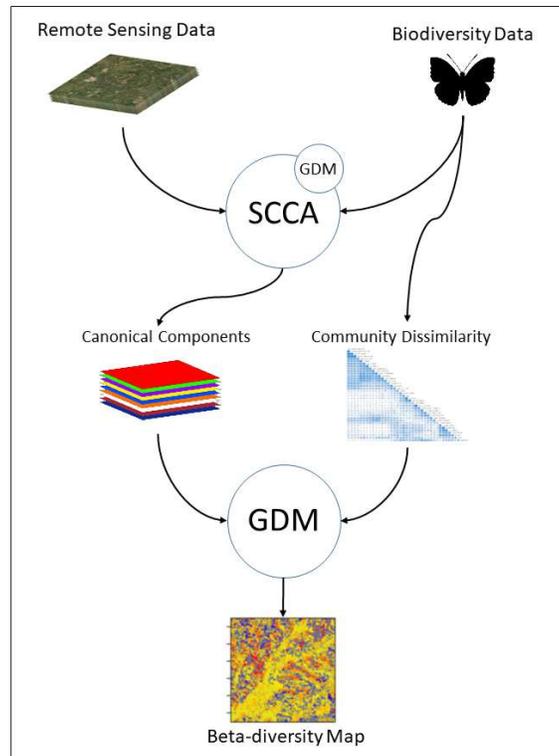


Figure 5: An example of the Sparse Generalized Dissimilarity Model (SGDM) approach. Remote sensing data and biodiversity data in the field can be coupled by Sparse Canonical Correlation Analysis to produce canonical components and a community dissimilarity matrix, which are then used to build a Generalized Dissimilarity Model to finally derived a β -diversity map.

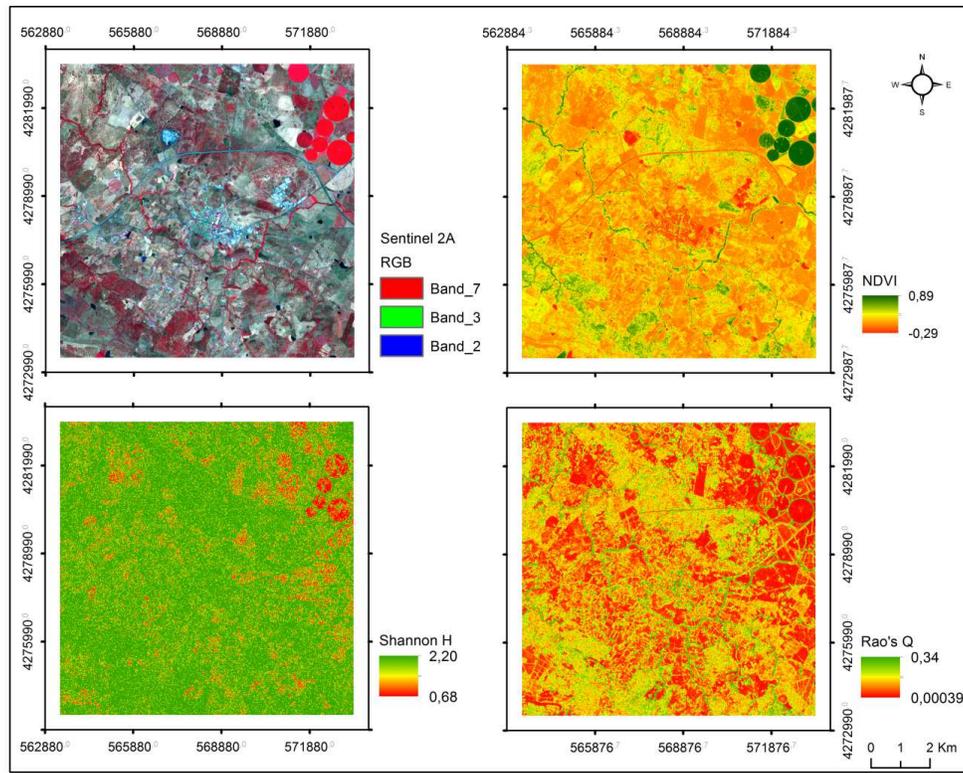


Figure 6: Upper panels: Sentinel-2A scene (8 August 2016) and derived NDVI for the agro-forestry systems test site located in southern Portugal. Lower panels: results from Shannon's H and Rao's Q indices computation. Shannon index tends to overestimate the landscape diversity when compared to the Rao's Q index.

1 Measuring β -diversity by remote sensing: a
2 challenge for biodiversity monitoring

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51 **Abstract**

52 Biodiversity includes multiscalar and multitemporal structures and
53 processes, with different levels of functional organization, from genetic
54 to ecosystemic levels. One of the mostly used methods to infer bio-
55 diversity is based on taxonomic approaches and community ecology
56 theories. However, gathering extensive data in the field is difficult due
57 to logistic problems, [especially](#) when aiming at modelling biodiversity
58 changes in space and time, which assumes statistically sound sampling
59 schemes. In this [context](#), [airborne](#) or satellite remote sensing allow [in-](#)
60 [formation to be gathered](#) over wide areas in a reasonable time.

61 Most of the biodiversity maps obtained from remote sensing have
62 been based on the inference of species richness by regression analy-
63 sis. On the contrary, estimating compositional turnover (β -diversity)

64 might add crucial information related to relative abundance of dif-
65 ferent species instead of just richness. Presently, few studies have
66 addressed the measurement of species compositional turnover from
67 space.

68 Extending on previous work, in this manuscript we propose novel
69 techniques to measure β -diversity from airborne or satellite remote
70 sensing, mainly based on: i) multivariate statistical analysis, ii) the
71 spectral species concept, iii) self-organizing feature maps, iv) multi-
72 dimensional distance matrices, and the v) Rao's Q diversity. Each
73 of these measures addresses one or several issues related to turnover
74 measurement. This manuscript is the first methodological example
75 encompassing (and enhancing) most of the available methods for es-
76 timating β -diversity from remotely sensed imagery and potentially
77 relating them to species diversity in the field.

78 *Keywords:* β -diversity, Kohonen self-organising feature maps, Rao's Q
79 diversity index, remote sensing, satellite imagery, Sparse Generalized Dis-
80 similarity Model, spectral species concept.

81 1 Introduction

82 Biodiversity cannot be fully investigated without considering the spatial com-
83 ponent of its variation. In fact, it is known that the dispersal of species over
84 wide areas is driven by spatial constraints directly related to the distance
85 among sites. A negative exponential dispersal kernel is usually adopted to
86 mathematically describe the occupancy of new sites by species, as:

$$F = \sum_{K=1}^N e^{\frac{-d_{ik}}{a}} \quad (1)$$

87 where d_{ik} = distance between two locations i and k and a is a parameter
88 regulating the dispersal from localized areas (low values of a) to widespread
89 ones (high values of a , Meentemeyer et al. (2008)).

90 In this sense, distance acquires a significant role in ecology to estimate bio-
91 diversity change. Hence, spatially explicit methods have been acknowledged
92 in ecology for providing robust estimates of diversity at different hierarchical
93 levels: from individuals (Tyre et al., 2001), to populations (Vernesi et al.,
94 2012), to communities (Rocchini et al., 2005).

95 When dealing with spatial explicit methods, remote sensing images repre-
96 sent a powerful tool, particularly when coupling information on compositional
97 properties of the landscape with its structure (Figure 1). Remote sensing has

98 widely been used for conservation practices including very different types of
99 data such as nightlights data (Mazor et al., 2013), Land Surface Temperature
100 estimated from MODIS data (Metz et al., 2014), spectral indices (Gillespie,
101 2005).

102 Most of the remote sensing applications for biodiversity estimation have
103 relied on the estimate of local diversity hotspots, considering land use diver-
104 sity (Wegmann et al., 2017) or continuous spatial variability of the spectral
105 signal (Rocchini et al., 2010). This is mainly grounded in the assumption
106 that a higher landscape heterogeneity is strictly related to a higher amount
107 of species occupying different niches. However, given two sites s_1 and s_2 , the
108 final diversity is not only related to the species / spectral richness of s_1 and
109 s_2 , but overall to the amount of shared species / spectral values. In other
110 words, the lower the their intersection $s_1 \cap s_2$, the higher will be the total
111 diversity, while a low total diversity will be reached when $s_1 \cap s_2 = s_1 \cup s_2$.
112 Such intersection has been widely studied in ecology, after the development
113 of β -diversity theory (Whittaker, 1960).

114 Tuomisto et al. (2003) demonstrated the power of substituting distance in
115 Eq. 1 by spectral distance to directly account for the distance between sites
116 in an environmental space, instead of a merely spatial one. However, while
117 spectral distance examples exist when measuring the β -diversity among pairs
118 of sites (e.g. Rocchini et al. (2015)), few studies have tested the possibility of
119 measuring β -diversity over wide areas considering several sites at the same
120 time (however see Alahuhta et al. (2017); Harris et al. (2015)). This is
121 especially true when considering the development of remote sensing tools
122 for diversity estimate in which the concept of β -diversity is still pioneering.

123 The aim of this paper is to present the most novel methods to measure
124 β -diversity from remotely sensed imagery based on the the most recently
125 published ecological models. In particular we will deal with: i) multivariate
126 statistical techniques, ii) the applicability of the spectral species concept,
127 iii) multidimensional distance matrices, iv) metrics coupling abundance and
128 distance-based measures.

129 This manuscript is the first methodological example encompassing (and
130 enhancing) most of the available methods for estimating β -diversity from
131 remotely sensed imagery and potentially relate them to species diversity in
132 the field.

133 2 Multivariate statistical analysis for species 134 diversity estimate from remote sensing

135 Univariate statistics have been used to directly find relations between spectral
136 and species diversity. However, the amount of variability explained by single
137 bands / vegetation indices versus species diversity is generally relatively low,
138 due to the fact that different aspects related to the complexity of habitats
139 might act in shaping diversity, from disturbance and land use at local scales
140 to climate and element fluxes at global scales.

141 Ordination techniques are designed to quantitatively describe multivari-
142 ate gradual transitions in the species composition of sampled sites. Measuring
143 the distance between two sampling sites in the multi-dimensional ordination
144 space is a good proxy of the change in species composition. When this mea-
145 sure is related to the geographical distance between the considered sites, the
146 beta diversity at this particular scale can be assessed.

147 Of the various available ordination techniques, Detrended Correspon-
148 dence Analysis (DCA, Hill and Gauch (1980)) is particularly suitable for
149 such analyses. The axes (i.e. gradients) of the DCA ordination space are
150 scaled in standard deviation (SD) units, where a distance of 4 SD is related
151 to a full species turnover. This enables a versatile analysis that easily reveals
152 whether two sampled sites still have species in common.

153 Several studies have mapped the ordination space using remote sensing
154 data (e.g., Schmidtlein and Sassini (2004); Schmidtlein et al. (2007); Feil-
155 hauer et al. (2009, 2011, 2014); Gu et al. (2015); Harris et al. (2015); Leitao
156 et al. (2015); Neumann et al. (2015)). For this purpose, the axes scores of
157 the sampled sites are regressed against the corresponding canopy reflectance
158 values extracted from air- or spaceborne image data. The resulting multi-
159 variate regression models, one per ordination axis and most often generated
160 with machine learning regression techniques, are subsequently applied on the
161 image data for a spatial prediction of ordination scores. Each pixel of the
162 image data is assigned to a specific position in the ordination space that in-
163 dicates its species composition. The resulting gradient maps are a powerful
164 tool for analyses of beta diversity across different spatial scales (Feilhauer et
165 al., 2009; Hernandez-Stefanoni et al., 2012).

166 A simple analysis of the variability of the DCA scores in a defined pixel
167 neighborhood (i.e. a moving window) results in a efficient beta diversity
168 assessment. The spatial scale of this assessment can be varied either by
169 re-sampling the gradient map to a coarser spatial resolution (i.e. pixel size) or
170 by changing the kernel size of the considered pixel neighborhood. Such tech-
171 niques have been further developed e.g. for spatial conservation prioritization

172 programmes such as [Zonation](#) (Moilanen et al., 2005, 2009).

173 Figure 2 shows an example of a DCA-based assessment of beta diversity
174 on a very local scale (10 m) following the approach described in Feilhauer et
175 al. (2009). The analyzed landscape is a mosaic of raised bogs, fens, transition
176 mires and *Molinia* meadows. For a detailed description of the data and site
177 please refer to Feilhauer et al. (2014, 2016).

178 Analyses like this require two different data sets: (1) a sample of field
179 data that is representative for the vegetation in the studied area and is used
180 to generate the ordination space; (2) image data with a sufficient spectral
181 resolution to discriminate the vegetation types within the ordination space
182 and with a spatial resolution that is in line with the sampling design of the
183 field data (Feilhauer et al., 2013).

184 Using these data, the continuous spatial variability of the spectral signal
185 in the image pixels is translated into a spatially continuous measure of species
186 composition. The advantages of this approach are obvious: since the diversity
187 analyses are conducted in the floristic gradient space, the resulting measures
188 resemble field studies and are thus easier to interpret than spectral proxies
189 and closer to the point of view of many end-users. [Furthermore](#), the analysis
190 of ordination scores in defined pixel neighborhoods is not restricted to a
191 single spatial scale but offers the opportunity to implement assessments of
192 beta diversity on multiple scales.

193 **3 The spectral species concept**

194 The spectral species concept has been proposed by Féret and Asner (2014a)
195 to map both α and β component of the biodiversity using a unique frame-
196 work. It is rooted in the convergence between two other concepts, the spec-
197 tral variation hypothesis (SVH) proposed by Palmer et al. (2002), and the
198 plant optical types proposed by Ustin and Gamon (2010), sustained by the
199 technological advances in the domain of high spatial resolution imaging spec-
200 troscopy. The SVH states that the spatial variability in the remotely sensed
201 signal, that is the spectral heterogeneity, is related to environmental hetero-
202 geneity and could therefore be used as a powerful proxy of species diversity.
203 SVH has been tested in different situations (Rocchini et al., 2010) and con-
204 clusions show that the [performance](#) of this approach is very dependent on
205 several factors, including the [instrument](#) characteristics (spectral, spatial and
206 temporal resolution), the type of vegetation investigated, and the metrics de-
207 rived from remotely sensed information to estimate spectral heterogeneity.
208 Plant optical types refer to the capacity of sensors to measure [signals that](#)
209 [aggregate](#) information about vegetation structure, phenology, biochemistry

210 and physiology. Therefore, this concept is also tightly linked to the perfor-
211 mances of the sensor and finds particular echo with the increasing use of high
212 spatial resolution imaging spectroscopy for the estimation and identification
213 of multiple vegetations properties.

214 The details provided by high spatial resolution imaging spectroscopy are
215 sufficient to perform analyses of plant optical traits at the individual tree scale
216 in order to differentiate tree species, obtain information about leaf chemical
217 traits and estimate the α component of biodiversity (Asner et al., 2008, 2015;
218 Chadwick and Asner, 2016; Clark et al., 2005; Clark and Roberts, 2012;
219 Féret and Asner, 2013; Vaglio Laurin et al., 2014). These results illustrate
220 that spectral information can be related to taxonomic or functional informa-
221 tion of the vegetation, which supports the SVH under the hypothesis that
222 the metrics used to compute spectral heterogeneity and a given component
223 of vegetation diversity are properly defined. However these applications are
224 currently limited by the important amount of field data required to train re-
225 gression or classification models, which is also directly linked to their low gen-
226 eralization ability in time and space. Unsupervised approaches then appear
227 as valuable alternatives for the analysis of ecosystem heterogeneity (Baldeck
228 and Asner, 2013; Baldeck et al., 2014; Feilhauer et al., 2011; Baldeck and
229 Asner, 2013; Féret and Asner, 2014b), as ecological indicators of α and β
230 diversity at landscape scale usually require one or several levels of abstraction
231 beyond the correct taxonomic identification (Tuomisto et al., 2006).

232 Clustering (properly pre-processed) spectral information should result in
233 pixels from the same species naturally grouping together rather than dis-
234 tributing randomly among clusters, Féret and Asner (2014a) proposed a
235 grouping method aiming at assigning labels to pixels based on multiple clus-
236 tering of spectroscopic data acquired at landscape scale. These pixels, labeled
237 with a set of so-called spectral species, can then be used straightforwardly
238 in order to compute various diversity metrics such as Shannon index for α
239 diversity, and Bray-Curtis dissimilarity for β diversity. The pre-processing
240 stage is divided into several stages. After masking all non-vegetated pixels, a
241 normalization based on **continuous** removal is applied to each pixel and over
242 the full spectral domain, then a principal component analysis is performed on
243 the **continuously** removed spectral data. The normalization **reduces** effects
244 due to changes in illumination, canopy geometry and other factors unrelated
245 to vegetation, while enhancing the signal corresponding to vegetation. The
246 components including individual-specific information are the components of
247 interest. They can be identified after visual inspection or automated routines,
248 if initial data show sufficient signal to noise ratio. Once a limited number
249 of components have been selected, k-means clustering is then applied to a
250 certain number of subsets, and for each of these subsets, centroids are com-

251 puted and each pixel in the image is labeled based on the closest centroid.
252 The repetition of clustering based on various subsets of the image tends to
253 minimize the risk of assigning centroids to irrelevant groups of pixels. Ex-
254 perimental results showed that the averaging of diversity indices computed
255 from multiple centroid maps can be seen as an analogous to signal averaging,
256 which consists in increasing signal to noise ratio by replicating measurements.
257 For each repetition, the closest centroid corresponds to the spectral species,
258 and for each spatial unit of a given size, the spectral species distribution is
259 derived in order to compute any diversity metric requiring either information
260 at the local scale, or comparison of information across spatially distant plots.

261 The concepts of spectral species and spectral species distribution have
262 been tested successfully on a limited number of situations and types of
263 ecosystems (see (Rocchini et al., 2016) for a review, and (Lausch et al.,
264 2016) for an application to similar concepts). As an example, F eret and
265 Asner (2014a) showed ability to properly estimate landscape heterogeneity
266 at moderate spatial scale, up to few dozen square kilometers over tropical
267 forests, based on high spatial resolution imaging spectroscopy (Figure 3).
268 A generic parameterization of the method showed robust performances for
269 α diversity mapping across space and time, but mapping β diversity across
270 large spatial scales using images acquired during different airborne campaign
271 remains challenging, which leads to an unsolved problem when considering
272 operational regional mapping. In the perspective of global monitoring of
273 biodiversity, and given the unprecedented remote sensing capacity allowed
274 by the Copernicus program, including the Sentinel-2 multispectral satellites,
275 several other challenges are foreseen and currently investigated. The influ-
276 ence of decreased spatial and spectral resolution on the ability to properly
277 differentiate ecologically meaningful spectral species across landscapes and
278 over regions will need to be investigated. The application of this concept be-
279 yond tropical forests and savanna ecosystems should also be investigated, as
280 it may not hold when applied on moderately diverse ecosystems or systems
281 with individuals whose individuals have dimensions well below the resolving
282 power of the instrument.

283 4 Self organizing feature maps

284 The Kohonen self-organising feature map (SOFM, Kohonen (1982)) is a neu-
285 ral network that may be used to undertake unsupervised clustering of data.
286 Critically, the input to a SOFM can be a large multi-variate data set such
287 as may be acquired on species from quadrat based field surveys. The SOFM
288 summarises the data in a low, typically two, dimensional output (Figure

289 4). In this output space the data for individual quadrats are topologically
290 ordered – with sites that are similar close together while those of highly dif-
291 ferent species composition are more distant. Because the data sites in the
292 output space are arranged by relative similarity the output space may also
293 be used to aggregate or classify a data set. As such the SOFM is attrac-
294 tive as a non-parametric clustering analysis and as a means to undertake an
295 ordination (Chon et al., 1996).

296 A SOFM is, unlike some of the approaches used commonly in community
297 ecology, not constrained by assumptions relating the statistical distribution
298 of the data used. The SOFM uses unsupervised learning to produce a topo-
299 logically ordered output space in which the samples are arranged spatially
300 in relation to their relative similarity in species composition. The SOFM
301 thus performs a non-parametric ordination analysis (Foody, 1999). The pro-
302 duction of a classification by a SOFM comprises two main stages (Giraudel
303 and Lek, 2001). An iterative analysis, in which time-decaying parameters
304 that control network learning and the size of local neighbourhoods located
305 around output units, is used. For this, the user must specify a number of key
306 parameters such as the size and shape of the network, number of iterations of
307 the algorithm, the learning rate and its rate of decline and a neighbourhood
308 parameter. The need for such parameters can add some uncertainty to the
309 analysis. While there are no formal rules to follow in the design of a SOFM
310 there are recommendations for the determination of SOFM parameter set-
311 tings (Giraudel and Lek, 2001). A further concern is that as an unsupervised
312 classifier the classes defined may not always be the most useful for an in-
313 vestigation. In addition, the nature of the analysis means the direction of
314 the gradients cannot be controlled (Fritzke, 1995) but the analysis performs
315 well in comparison to popular ordination techniques such as PCA and DCA
316 (Foody and Cutler, 2003). The SOFM may also use a variety of different
317 data types such as presence/absence, abundance or importance values and
318 can solve complex non-linear problems (Giraudel and Lek, 2001).

319 5 Multidimensional distance matrices: GDMs 320 and SGDMs

321 One of the most widespread methods for assessing α -diversity is using distance
322 matrices (Legendre et al., 2005). Indeed, early work by Whittaker (1960) sug-
323 gested that β -diversity could be quantified by dissimilarity matrices among
324 (pairs of) sites. Furthermore, the Mantel test (Mantel and Valand, 2017),
325 designed to estimate the association between two independent dissimilarity

326 matrices, has been widely used to correlate a community composition dissim-
327 ilarity matrix with an environment dissimilarity one, thus providing useful
328 insights into community composition and turnover (Legendre et al., 2005;
329 Tahvanainen et al., 2011).

330 Generalized Dissimilarity Modelling (GDM; Ferrier (2007) can be con-
331 sidered as an extension of the Mantel test, which is able to accommodate
332 multidimensional environmental data, to be compared with the composi-
333 tional data. GDMs also allow for the prediction of compositional turnover
334 as well as for, e.g. environmental classification constrained to the compo-
335 sitional dissimilarity (Ferrier, 2007; Leathwick et al., 2011). In GDM, the
336 compositional dissimilarities between all pairs of samples are modelled as a
337 function of their respective environmental distances. This is done through a
338 linear combination of monotonic I-spline basis functions, under the assump-
339 tion that increasing environmental dissimilarity (e.g. along a gradient) can
340 only result in increasing compositional dissimilarity. This method is thus well
341 suited for measuring and mapping β -diversity, and is thus becoming widely
342 used in conservation science and macroecology, and recently been subject to
343 several developments as we describe below.

344 One such development is the phylogenetic GDM (phylo-GDM; Rosauer
345 et al. (2014)), which incorporates phylogenetic dissimilarities into GDM and
346 allows for analysing and predicting phylogenetic β -diversity, thus linking
347 ecological and evolutionary processes. This method can provide novel in-
348 sights into the mechanisms underlying current patterns of biological diversity
349 (Graham et al., 2008). Another recent development of GDM is the multi-
350 site GDM (MS-GDM; Latombe et al. (2017)), which extends GDMs from
351 pairwise to multi-site dissimilarity modelling. In such paper, the authors
352 tested MS-GDM by means of both constrained (monotonical) additive mod-
353 els and I-splines, although with no conclusive results relating to the best
354 method overall. They concluded, however, that when applying MS-GDM to
355 a high number of samples, they could better explain the drivers of species
356 turnover. Also, an important development of GDM is the Bayesian bootstrap
357 GDM (BBGDM; Woolley et al. (2017)) designed to characterize uncertainty
358 in generalized dissimilarity models. This approach allows better represent-
359 ing the underlying uncertainty in the data, by estimating the variance in
360 parameters based on the available data.

361 Finally, an implementation of GDM, which was created particularly for
362 dealing with high-dimensional (and potentially high-collinear) remote sensing
363 data as input in GDM is the Sparse Generalized Dissimilarity Model (SGDM,
364 Figure 5, Leitao et al. (2015)). This method is a two-stage approach that
365 consists of initially reducing the environmental space (e.g. reflectance data)
366 by means of a Sparse Canonical Correlation Analysis (SCCA, Figure 5; Wit-

367 ten et al. (2013)), and then fitting the resulting components with a GDM
 368 model. The SCCA is a form of penalized canonical correlation analysis based
 369 on the L1 (lasso) penalty function, and is thus designed to deal with high-
 370 dimensional data. The two algorithms are coupled in a way that the SCCA
 371 penalization is selected through a heuristic grid search manner, in order to
 372 minimize the cross-validate root mean square error in the dissimilarities pre-
 373 dicted by the GDM. In this procedure, the high-dimensional environmental
 374 data (such as coming from time series of multispectral or hyperspectral data)
 375 are subject to a supervised ordination approach that reduces their dimen-
 376 sion while capturing the axes of variation that most correlate to those of
 377 the community compositional matrix. SGDM has been successfully used for
 378 modelling and mapping the compositional turnover of both animal and plant
 379 species, using several different sources of remote sensing (and auxiliary) data
 380 (Leitao et al., 2015; Leitão et al., 2017).

381 6 Rao's Q diversity

382 Most of the previously shown metrics are based on the distance among pixel
 383 values in a multidimensional spectral space. None of them considers the
 384 relative abundance of such pixel values in a neighbourhood.

385 By contrast, abundance-based metrics such as the Shannon entropy could
 386 output similar results despite a variable distance among pixel values. As an
 387 example, consider a 3x3 matrix of remotely sensed data:

$$\begin{pmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{d1} & x_{d2} & x_{d3} \end{pmatrix} \quad (2)$$

388 composed by the following values:

$$\begin{pmatrix} 10 & 13 & 15 \\ 18 & 20 & 23 \\ 19 & 21 & 22 \end{pmatrix} \quad (3)$$

389 then consider a different matrix:

$$\begin{pmatrix} 10 & 121 & 227 \\ 1 & 40 & 251 \\ 7 & 100 & 149 \end{pmatrix} \quad (4)$$

390 From a Shannon's entropy perspective, such matrices are equal in terms of
 391 heterogeneity. The Shannon's entropy is indeed based on the relative abun-
 392 dance (and richness) of a sample, and its value is 2.197 for both the matrices.

393 This value, equalling the natural logarithm of the number of classes (pixel
394 values), is also Shannon's maximum theoretical value given a 3x3 matrix,
395 due to the lack of identical numbers in the matrices. This example explicitly
396 shows that accounting for the distance among values and their relative abun-
397 dance is crucial to discriminate among areas in terms of measured (modeled)
398 heterogeneity.

399 One of the metrics accounting for both the abundance and the pairwise
400 spectral distance among pixels is the Rao's Q diversity index, as:

$$Q = \sum \sum d_{ij} \times p_i \times p_j \quad (5)$$

401 where d_{ij} = spectral distance among pixels i and j and p = proportion of
402 occupied area.

403 Hence, Rao's Q is capable of discriminating among the ecological diversity
404 of matrices 3 and 4, turning out to be 4.59 and 90.70, respectively. Appendix
405 1 provide an example spreadsheet to perform the calculation while the com-
406 plete R code is stored in the GitHub repository
407 <https://github.com/mattmar/spectralrao>.

408 We decided to make use of a case study to highlight the importance of
409 considering the distance among pixel values in remote sense ecological appli-
410 cation. The performance of Rao's Q index in describing landscape diversity
411 was tested in a complex agro-forestry landscape located in southern Portu-
412 gal. A test site with an area of about $10 \times 10 \text{ km}^2$ (centroid located at 38°
413 $39' 10.74'' \text{ N}$; $8^\circ 12' 52.30'' \text{ W}$) was selected to conduct the analysis. In this
414 area, a savanna-like ecosystem called montado occupies about 40% of the test
415 site, followed by traditional olive groves, pastures, vineyards, and irrigated
416 monocultures (e.g. corn fields). Montado is spatially characterized by the
417 variability of its tree density (e.g. Godinho et al. (2016)), and the gradient
418 between low and high tree density over space can lead to different structural
419 heterogeneity and habitat diversity.

420 Within the test site, polyculture under small farming context (e.g. veg-
421 etable gardens, orchards, and cereal crops) is an important feature of this
422 landscape by generating a high compositional and configurational spatial
423 heterogeneity (Figure 6). The main goal in using this case study is to demon-
424 strate the potential and effectiveness of the Rao's Q index in producing ac-
425 curately remote-sensing based maps of spatial diversity over such complex
426 landscape. For this study, a cloud-free Sentinel-2A (S2A) image acquired
427 on 8 of August 2016 was used to compute the NDVI at a 10 meters spatial
428 resolution. The S2A image download, as well as the atmospheric correction
429 (DOS method) were performed using the Semi-Automatic Classification plu-
430 gin (SCP) implemented in the QGIS software (QGIS Development Team ,
431 2016(@).

432 The NDVI was used as input data for Rao's Q index computation using
433 a window size of 3×3 pixels. The performance of the Rao's Q was compared
434 to the Shannon Entropy index (Shannon's H), which is one of the simplest,
435 and widely used, remote sensing-based diversity measures for landscape het-
436 erogeneity assessment (Rocchini et al., 2016). To investigate whether both
437 diversity indices differ between land cover types, one-way ANOVA tests were
438 performed. This approach was used for analysing the degree of dissimilarity
439 between Rao's Q and Shannon H index across two high complex land cover
440 types; i) montado, and ii) polyculture. To do so, a sample of 60 squares with
441 250×250 meters size was randomly selected over these two land cover types.
442 Each square represents a sample of 625 S2A NDVI pixels, thus corresponding
443 to a total of 37,500 pixels over the 60 squares. For the comparison between
444 both indices, the coefficient of variation (CV) was calculated for each $250 \times$
445 250 m squares. Regarding the Rao's Q performance, Figure 6 clearly points
446 to the significant improvements shown by Rao's Q index compared to the
447 Shannon H index in describing the spatial diversity. In particular, it can be
448 seen through the Figure 6, that Rao's Q index can highlight different gra-
449 dients of spatial diversity of montado areas, which present high tree density
450 variability (Figure 6), and thus high spatial heterogeneity. One-way ANOVA
451 tests revealed that both indices values were significantly different between
452 the two land cover types (montado: $F = 503.3$, $p < 0.001$; polyculture: $F =$
453 889.8 , $p < 0.001$). Overall, the obtained results demonstrate the capability of
454 Rao's Q index in producing accurate landscape diversity maps in a complex
455 landscape such as the Mediterranean agro-forestry systems.

456 7 Conclusion

457 In this paper, we showed several methods based on ecological β -diversity,
458 which can be investigated by remote sensing through the calculation of
459 ecosystem heterogeneity, to estimate the spatial variability of biodiversity.
460 When there is a wide range of heterogeneity, for example when the data
461 include homogeneous and heterogeneous zones, no single measure might cap-
462 ture all the different aspects of β -diversity (e.g. Baselga (2013)). That is why
463 we suggested in this manuscript multivariate and multidimensional methods
464 (e.g. multivariate statistics and multidimensional distance matrices) based
465 on the spectral signal and its variability over space to account for different
466 aspects of diversity, also including distance- and abundance-based methods
467 (e.g. the Rao's Q).

468 Biodiversity measured as species richness is often used for conservation
469 purposes, hence the importance of avoiding an under- or over-estimate has

470 been highlighted (Chiarucci et al., 2009). Furthermore, pairwise distance-
471 based methods might be profitably used to detect not only diversity hotspots
472 in an area but also the variation of biodiversity over space, and potentially
473 over time, once multitemporal sets of images are used.

474 In this paper we focused on optimising measures of β -diversity based on
475 remote sensing data. Such measures might be used to regress species diversity
476 against remotely sensed heterogeneity, based on new regression techniques
477 which maximise the possibility of predicting the zones in a study area, or at
478 larger spatial scales, of peculiar conservation value. As an example, shrink-
479 age regression, recently applied in biodiversity conservation (Authier et al.,
480 2017) could allow a direct focus on habitat modelling, which is one of the
481 major strengths of remote sensing (Gillespie et al., 2008). Moreover, such
482 analysis might be performed in a Bayesian framework allowing to i) model
483 multidimensional covariates with non-stationary variation over space (Ran-
484 dell et al., 2016), such as the bands of satellite images, and ii) model the
485 errors in the output and their variation over space (Rocchini et al., 2017).

486 As previously stated, the suggested methods for β -diversity estimation
487 from remote sensing are mainly based on distances, but they could be effec-
488 tively translated to relative abundance-based methods. As an example Roc-
489 chini et al. (2013) introduced the possibility of applying generalized entropy
490 theory to satellite images with one single formula representing a continuum
491 of diversity measures changing one parameter. One of the best examples
492 in this framework could be the use of Hill numbers, in which diversity is
493 expressed as:

$${}^qD = \left(\sum_{i=1}^S p_i^q \right)^{\frac{1}{1-q}} \quad (6)$$

494 where S = number of samples / pixels and p_i = relative abundance of a
495 species / spectral value. varying the parameter q , qD varies accordingly in
496 several diversity indices, e.g. for $q = 0$ qD is the simple number of species,
497 for $\lim(q) = 1$ qD equals Shannon's entropy, etc. (Hsieh et al., 2016).

498 Furthermore, connectivity analysis might also be taken into account (Moila-
499 nen et al., 2005, 2009). For instance, a remote sensing based connectivity
500 network among different sites, based on β -diversity measures, could be ap-
501 plied for the estimate of landscape connectivity and consequent genetic flow,
502 as demonstrated by Vernesi et al. (2012). It has also been shown that commu-
503 nity related biodiversity indicators are often missing from current monitoring
504 programmes (Vihervaara et al., 2017); thus methods such as remote sensing
505 based Rao's Q diversity applied for various ecosystems might improve other-
506 wise challenging monitoring of biological communities.

507 With this manuscript we hope to stimulate discussion on the available
508 methods for estimating β -diversity from remotely sensed imagery by propos-
509 ing innovative techniques grounded on ecological theory.

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514 Authors' contribution statement

515 All authors contributed to the development and writing of the manuscript.

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- 773 Figures

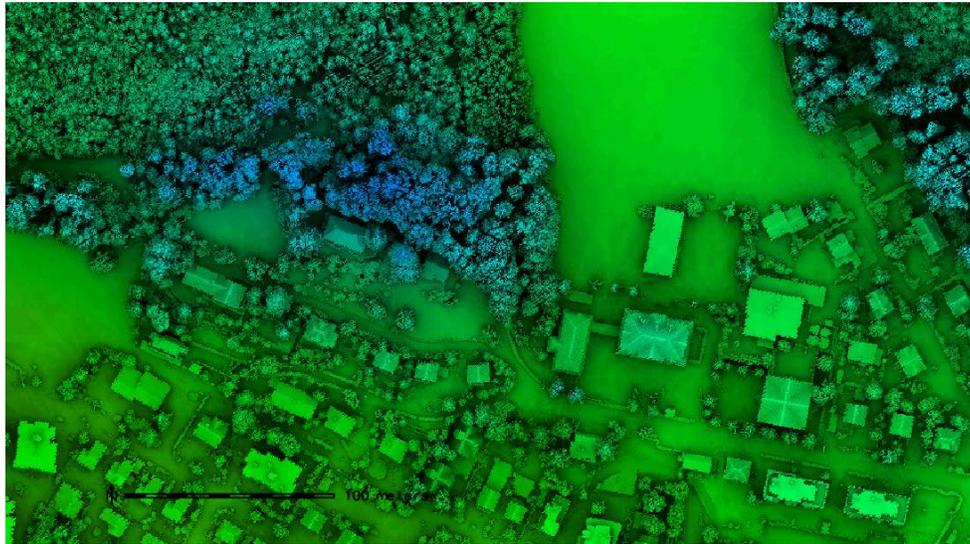


Figure 1: An example of how to couple information on compositional properties of the landscape by optical data together with structural (3D) properties by laser scanning LiDAR data.

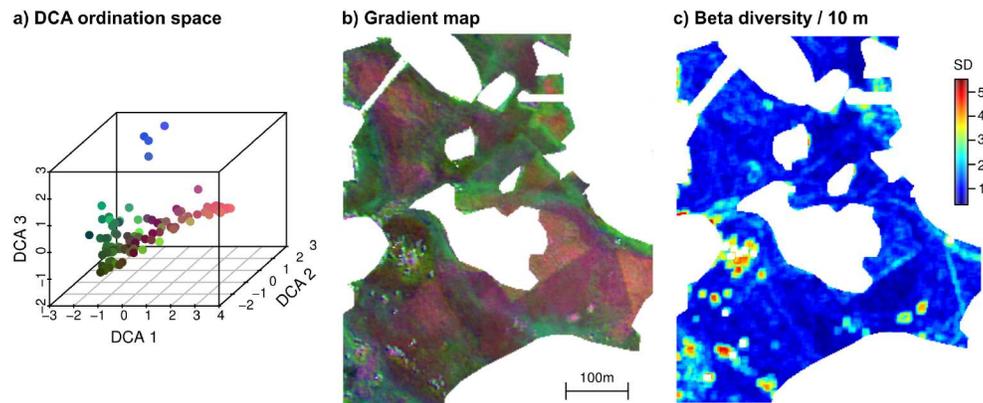


Figure 2: β -diversity assessment with a combination of ordination techniques and remote sensing. a) Three dimensional DCA ordination space of $n=100$ vegetation plots sampled in raised bogs, fens, transition mires and *Molinia* meadows in the alpine foothills of Southern Germany. An inter-plot distance of 4 SD corresponds to a full species turnover. b) Maps of the ordination axes resulting from a spatial prediction based on canopy reflectance. Each pixel has a predicted position in the ordination space that is indicated by its color. The color scheme corresponds to a). The map has a spatial resolution of 2 m x 2 m, which is in line with the sampled plot size. c) Cumulative change rates along the three DCA axes in a 5 x 5 pixel neighborhood. A high change rate indicates a high beta diversity.

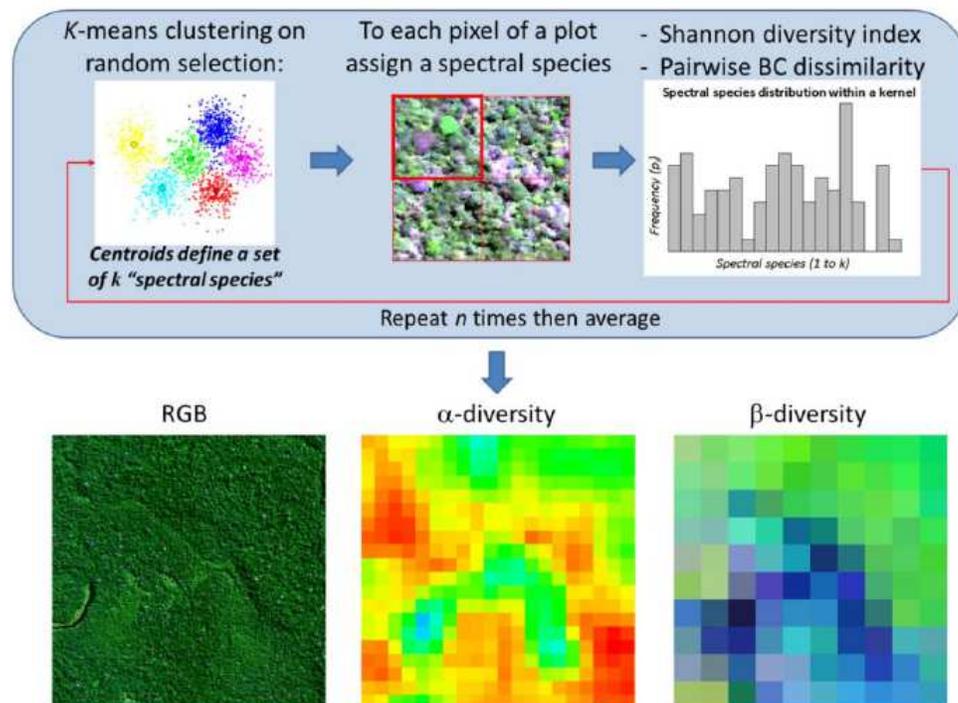


Figure 3: Spectral species can be identified in a hyper- or multi-spectral image by spatial clustering method and their distribution can be mapped. Such maps can further be used to apply local-based heterogeneity measurements (α -diversity) as well as iterative distance based methods to build β -diversity maps. Reproduced from Féret and Asner (2014a).

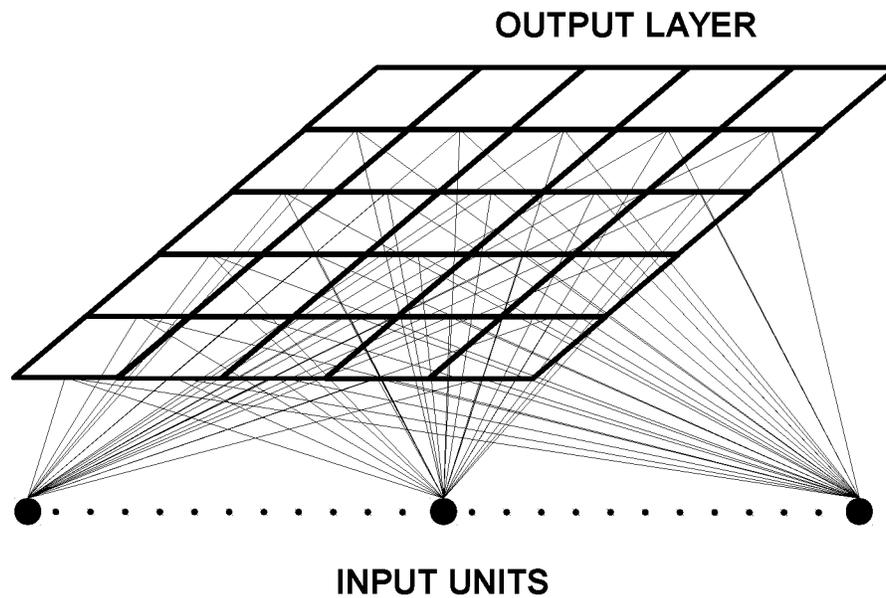


Figure 4: A self-organising feature map can be built starting from an input layer, e.g. the presence absence of a tree species or of a peculiar spectral value) which is connected to every unit in the output layer by a weighted connection. The self organising feature map uses unsupervised learning to map the location of field sites within the output space on the basis of their relative similarity in species or spectral composition. [Redrawn](#) from Foody and Cutler (2003).

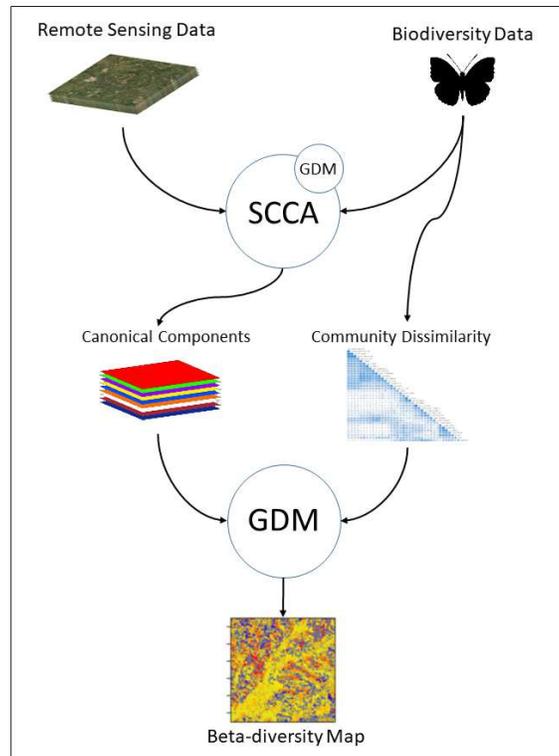


Figure 5: An example of the Sparse Generalized Dissimilarity Model (SGDM) approach. Remote sensing data and biodiversity data in the field can be coupled by Sparse Canonical Correlation Analysis to produce canonical components and a community dissimilarity matrix, which are then used to build a Generalized Dissimilarity Model to finally derived a β -diversity map.

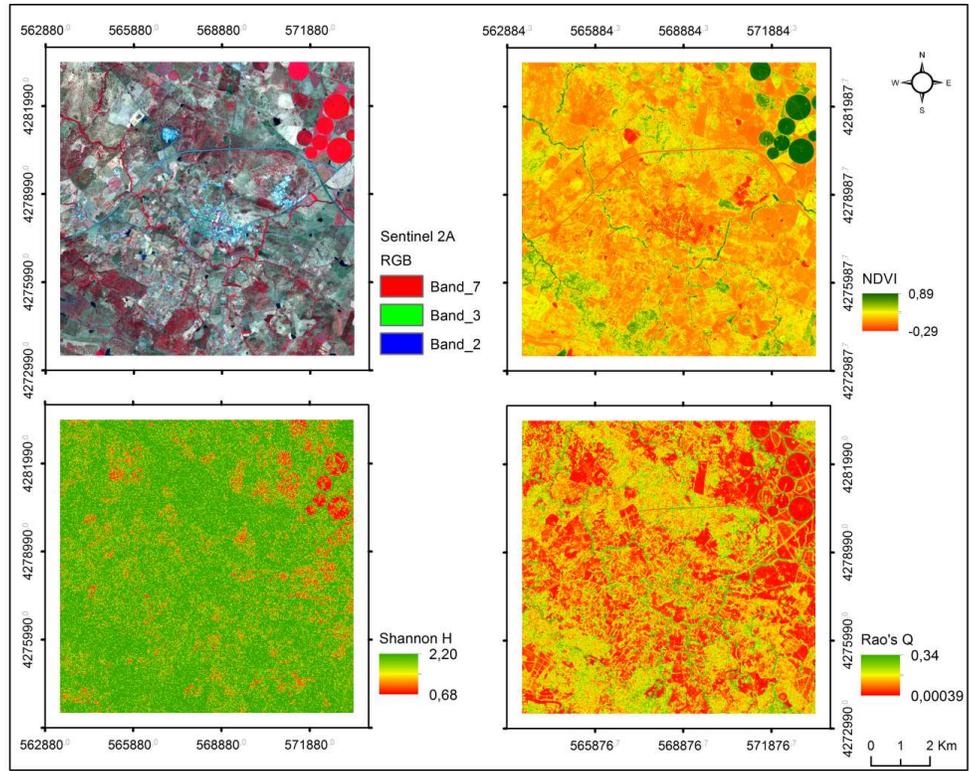


Figure 6: Upper panels: Sentinel-2A scene (8 August 2016) and derived NDVI for the agro-forestry systems test site located in southern Portugal. Lower panels: results from Shannon's H and Rao's Q indices computation. Shannon index tends to overestimate the landscape diversity when compared to the Rao's Q index.