SPECIAL FEATURE: REMOTE SENSING

Applied Vegetation Science IAVS

About the link between biodiversity and spectral variation

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Abstract

Aim: The spectral variability hypothesis (SVH) suggests a link between spectral variation and plant biodiversity. The underlying assumptions are that higher spectral variation in canopy reflectance (depending on scale) is caused by either (1) variation in habitats or linked vegetation types or plant communities with their specific optical community traits or (2) variation in the species themselves and their specific optical traits.

Methods: The SVH was examined in several empirical remote-sensing case studies, which often report some correlation between spectral variation and biodiversity-related variables (mostly plant species counts); however, the strength of the observed correlations varies between studies. In contrast, studies focussing on understanding the causal relationship between (plant) species counts and spectral variation remain scarce. Here, we discuss these causal relationships and support our perspectives through simulations and experimental data.

Results: We reveal that in many situations the spectral variation caused by species or functional traits is subtle in comparison to other factors such as seasonality and physiological status. Moreover, the degree of contrast in reflectance has little to do with the number but rather with the identity of the species or communities involved. Hence, spectral variability should not be expressed based on contrast but rather based on metrics expressing manifoldness. While we describe cases where a certain link between spectral variation and plant species diversity can be expected, we believe that as a scientific hypothesis (which suggests a general validity of this assumed relationship) the SVH is flawed and requires refinement.

Conclusions: To this end we call for more research examining the drivers of spectral variation in vegetation canopies and their link to plant species diversity and biodiversity in general. Such research will allow critically assessing under which conditions spectral variation is a useful indicator for biodiversity monitoring and how it could be integrated into monitoring networks.

KEYWORDS
biodiversity, monitoring, remote sensing, spectral variability hypothesis, vegetation

1 | INTRODUCTION

Biodiversity conservation has become a matter of international concern over the last decades. One challenge in the current efforts to conserve the remaining biodiversity is the development of a global biodiversity monitoring and early-warning system. This challenge is being addressed by the activities of, among others, the Group on Earth Observation's Biodiversity Observation Network (GEO BON) (Scholes et al., 2008; Walters & Scholes, 2017). A central task of GEO BON is to develop a set of essential biodiversity variables (EBV) that includes variables describing community composition, ecosystem structure, ecosystem function, genetic composition, species populations and species traits (Pereira et al., 2013). Given the global scale of the task, remote sensing (RS) is expected to make an important contribution to monitor some of these EBVs, particularly those describing species traits and ecosystem structure (Skidmore et al., 2015, 2021).

Besides this globally concerted effort to develop metrics and variables suitable for a global monitoring system, RS has also been invoked to describe and monitor local biodiversity patterns expressed for example by the number of plant species per unit area, also called (plant) species density or species count (Schmidtlein & Fassnacht, 2017). However, studies attempting to establish relationships between RS data and species counts are always of a correlative nature because it is not the taxonomic assignment but rather the traits of the species that affect the RS signal. Additionally, since RS of terrestrial biodiversity is mostly able to capture information about plant traits, most of the studies are uniquely addressing floristic diversity. This is a shortcoming because plant species diversity is not always a good proxy for the diversity of other taxonomic groups (Ritter et al., 2019).

Despite this, recent years have witnessed the emergence of several approaches to assess plant biodiversity via RS. In their review, Wang and Gamon (2019) differentiate between four approaches: (1) habitat mapping; (2) direct species mapping; (3) mapping functional diversity via functional plant traits; and (4) spectral diversity-based approaches. Here, we focus on the spectral diversity-based approaches and discuss conceptual and technical challenges related to the underlying spectral variability hypothesis (SVH) (Palmer et al., 2002). However, to provide some context, we briefly introduce the other approaches as well.

1. Habitat mapping — Inferring species counts from the mapping of habitats or linked vegetation types is a straightforward approach. It assumes that each type can be directly related to a number of species (e.g., Braun & Koch, 2016). For example, the approximate plant species numbers of particularly species-rich or species-poor forest or grassland types are often well known from field surveys. By mapping these types using RS (which essentially is the same task as creating a land-cover map with a quite detailed thematic differentiation) and optionally also considering spatial context (size of habitat patches, and composition of habitats), reasonable estimates of plant species numbers can be obtained. To obtain reliable results, profound knowledge of the plant species richness of the sampled habitats and their precise classification is required. The most important drawback is that this approach is based on categorical types. Hence gradients of species richness within a habitat or vegetation type are difficult to capture. Further, subtle degradations may be missed because only a categorical shift from one type to another would result in a change of the estimated species numbers (see also Schmidtlein & Sassin, 2004 and Feilhauer et al., 2020).

2. Direct species mapping — The feasibility to map individual plant species (particularly the classification of larger trees and shrubs or mono-specific stands) from RS data has been proven (e.g., review by Fassnacht et al., 2016). Particularly high spectral and spatial resolution data (e.g., airborne hyperspectral data or data from unmanned aerial systems) were found to accomplish this task with good accuracy (e.g., Modzelewska et al., 2021; Müllerová et al., 2017). However, the direct mapping of species over wider areas is typically limited by the trade-off between spatial resolution and coverage in most RS systems. Furthermore, the number of species that can be identified within a given data set may also be limited due to the lack of clear species-specific spectral signatures, or other characteristics (shape, texture) enabling distinguishing the species from their surroundings. Currently, most existing RS data sets seem to be unable to reliably separate more than 10–15 dominating species based on their optical traits as mirrored in the amount of target species typically considered (see Figure 3 in Fassnacht et al., 2016). However, given the fast development of methodical advances in the field of deep learning, these numbers may increase in the future, particularly if very high spatial resolution and/or time-series data are available (e.g., review by Kattenborn et al., 2021).

3. Mapping functional diversity — One approach to bypass current limitations of discriminating large numbers of plant species from RS data is to focus on plant functional types instead of individual species. This also takes into account the fact that the occurrence of such types can be of more direct relevance to ecosystem function. It is known that certain biochemical and structural plant traits have a clear effect on the reflected electromagnetic radiation (e.g., Jacquemoud et al., 2009; Kattenborn et al., 2019; Ollinger, 2010). Hence, the range and variation of these traits can be captured and mapped by RS data. Because areas with higher trait diversity tend to harbour more species (Biswas & Mallik, 2011), it is assumed that it is possible to indirectly quantify species counts based on the functional diversity patterns obtained by RS. The suitability of this approach has been demonstrated in a few case studies (e.g., Schweiger et al., 2018) but the verification across ecosystems is still missing. Furthermore, the mapping of trait diversity has a value in itself (and many applications) as functional traits are not only related to biodiversity but also to ecosystem functions and services, which ultimately constitute a conservation priority (Díaz & Cabido, 2001).

4. Spectral diversity-based approaches — Finally, the spectral variability hypothesis (SVH) suggests a more generic relationship between biodiversity and remotely sensed spectral information which can be used to estimate species counts or other biodiversity-related metrics from RS data. The SVH as originally suggested by Palmer et al. (2000, 2002) states that the biodiversity of a given area is positively related to the spectral variation of the same area captured by an RS image. The underlying assumption is that a higher spectral variation can be interpreted as a higher variation in (number of) habitats or linked vegetation types and hence a larger number of species (referred to as 'original SVH' hereafter). In the case of very fine spatial resolution, an increased spectral variation may also directly relate to a higher number of species with a higher diversity in the corresponding species-specific optical traits (hereafter, 'species SVH'). Both are closely related and sometimes difficult to untangle because optical community traits, which allow for differentiating habitats or vegetation types, can be traced back to optical species traits. It is hence rather a matter of scale which of both drives variation across pixels in a place. The intriguing simplicity of the SVH hypothesis may, however, suggest at first glance that this relationship can hold true across ecosystems and scales.

The SVH has been extensively tested in case studies summarized for example in Rocchini et al. (2010), Schmidtlein and Fassnacht (2017) and Wang and Gammon (2019). The strength of the observed correlations between spectral variation and plant species counts (the most frequently applied biodiversity metric) varied strongly in these studies which raises doubts about the general validity of the SVH. Schmidtlein and Fassnacht (2017) pointed out several situations where the original SVH did not hold true and even found areas with the opposite relation, that is, increased plant species counts with lower spectral variation. These inverse relationships between spectral variation and plant species counts could be explained by the landscape composition of the region, proving that the original SVH does not hold true across all spatial scales and ecosystems. In this regard, earlier studies mention several more factors that potentially complicate the relationship between spectral variation and plant species counts, including for example seasonality, spatial resolution and the applied metrics to describe spectral variation (Rocchini et al., 2010, 2018; Schmidtlein & Fassnacht, 2017). Despite the controversy on the validity or applicability of the SVH, it still constitutes an intriguing idea, particularly due to its generic approach which in theory does not require a priori knowledge on the examined area. And even if it is clear by now that the SVH will not hold across all scales and ecosystems, it might still work well in selected environments and under certain pre-conditions (Schmidtlein & Fassnacht, 2017).

The aim of this study is to conceptually discuss and question causal relationships between spectral variation and species diversity (mainly plant species counts) considering the most important factors influencing spectral variation and hence this relationship. These factors include: (1) considered scale; (2) effects of reflectance changes over time; (3) effects of the method chosen to quantify spectral diversity; and (4) the weak link between habitat or ecosystem numbers and species counts. We support our perspectives by presenting examples including some data simulations and experimental data. With this, we seek to clearly point out the limitations of the SVH but at the same time also carve out the conditions under which spectral variation can make meaningful contributions to the RS-based monitoring of biodiversity.

The paper is structured as follows: we will first discuss scale-, phenology- and habitat-identity-related factors influencing the relationship between spectral diversity and plant species counts. Then we will briefly address some technical aspects related to the calculation of spectral-variation metrics and finally discuss and summarize our findings in a wider context.

2 | SCALE EFFECTS

With 'scale effects' we here refer to effects related to spatial extent (size of the study area) and spatial grain (pixel size, ground sampling distance or spatial resolution) of the spectral (RS) and biodiversity data. In ecology, the species–area relationship is one of the best-established concepts that describes the observation that the larger the extent of a given area is, the more species you can find in it (Rosenzweig, 1995). The exact relationship between species counts and area will depend on the characteristics of the ecosystem under analysis, its history and its surroundings. However, this relationship is always positive if the different-sized areas are nested. We can assume that the coarser the spatial grain of a given RS data set is at a given location, the more species are likely to occur within an individual pixel.

In contrast, we can assume that the coarser the spatial grain of the RS data is, the smaller is the overall spectral variation across all pixels of a given area. This is related to the general rule that aggregating fine-grain data will reduce extreme values (smoothing effect). In other words, RS data with fine spatial grain are more likely to differentiate among the spectral response of individual species, and capture land-cover types or individual objects with extreme spectral behaviour (e.g., at the landscape scale, a narrow bright dust road surrounded by dark forest; or a small dark pond in a bright savannah; and at fine scales, a bright white flower in front of darker green leaves). The coarser the pixels become, the more averaged out (i.e., smoothed) the reflectance values will be (Figure 1). Hence, for a given area, it can be assumed that any spectral-variation metric for a given area will decrease with pixel size (Figure 2). Furthermore, the coarser the grain of the RS data is, the fewer pixels are available for a given plot size to calculate the spectral-variation metric.

Based on these simple and known effects of scale on species counts and spectral-variation metrics, it can be deduced that if a relationship between spectral variation and species counts exists in a given region, the form of this relationship cannot be stable across scales, as seen also in the experimental work by Wang et al. (2018).
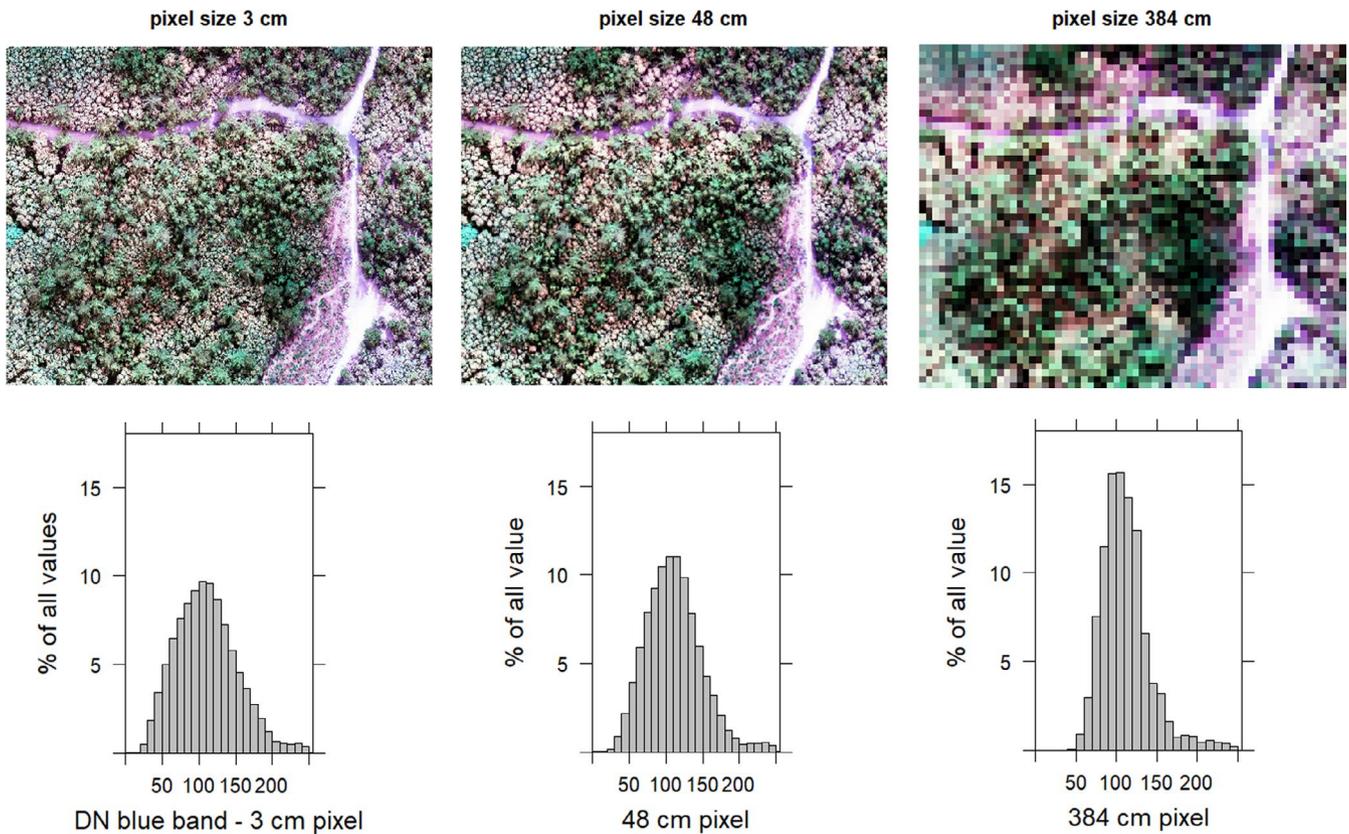
FIGURE 1 Scale effects on the distribution of spectral values. Depicted are histograms of digital number values of the blue band of an RGB-UAS (red–green–blue unmanned aerial system) image at different spatial grains (3-, 48- and 384-cm pixels). The UAS image shows a landscape with a mix of native shrubs, secondary natural forests, and plantation species in south-central Chile in the region of Maule (for exact location see Figure 2). The coarser the spatial resolution of the image, the less extreme the observed values are and the more intermediate values occur
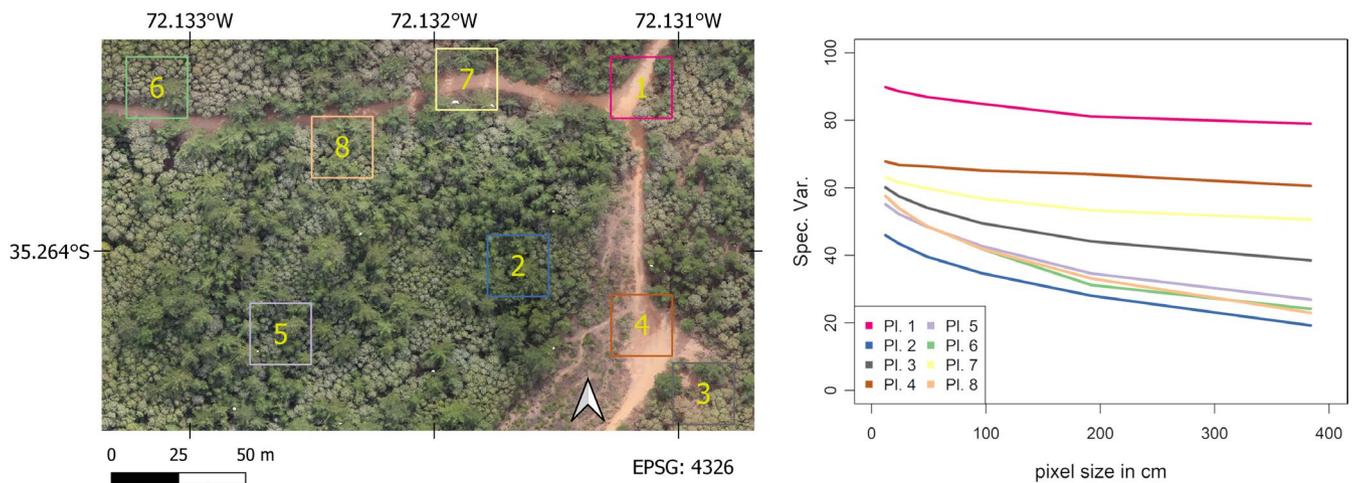

FIGURE 2 The right panel shows the development of spectral variation with changing pixel size (3 to 384 cm) for eight plots sized 630 m^2 within the area described briefly in Figure 1. The location of the plots is shown in the left panel. The spectral-variation measure for any plot is calculated based on the mean Euclidean distance of all pixels in the plot using the pixel values of the first two components of a Principal Components Analysis applied to the three bands of the red–green–blue imagery collected with the unmanned aerial system. The number of pixels used to calculate the spectral-variation measure decreases with increasing pixel size

A further important aspect related to the topic of scale refers to the visibility of plant individuals or stands, which are relevant to the species SVH. At fine grains, some individual species may be clearly identifiable in the RS data. However, rare species or species with small individuals might not show or be missed even at fine spatial grains. To provide a chance of capturing the contributions of the
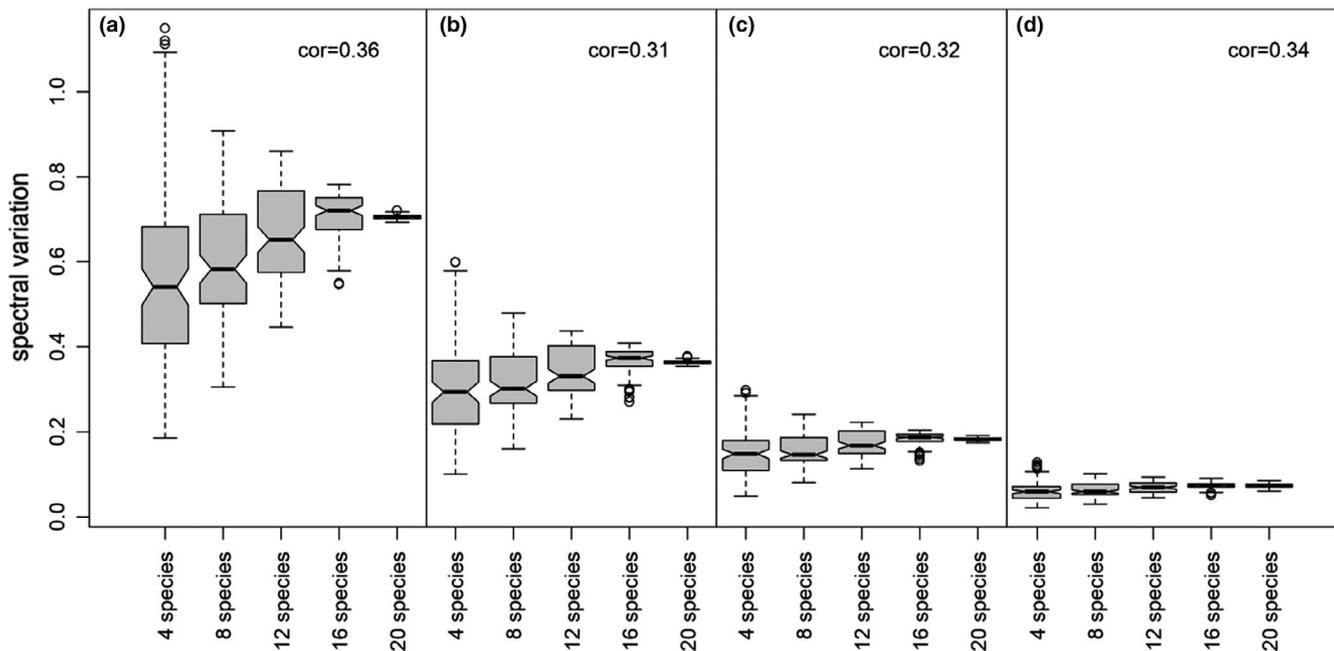
FIGURE 3 Degree of contrast-based spectral variation of simulated grassland plots. One hundred hyperspectral images were simulated, each at four spatial grains: from left to right, the original 100 × 100 pixels composed of spectra from 4, 8, 12, 16 and 20 species (a), then aggregated to 50 × 50 pixels (b), 25 × 25 pixels (c), and 10 × 10 pixels (d). Images were created by randomly filling up a 100 × 100 pixel array with spectra from 4–20 species. In total 21 species were available. Spectral variation was calculated in the same way as for Figure 2 (see Appendix S1 for more details). Indicated correlations are Spearman correlations between spectral variation and species counts
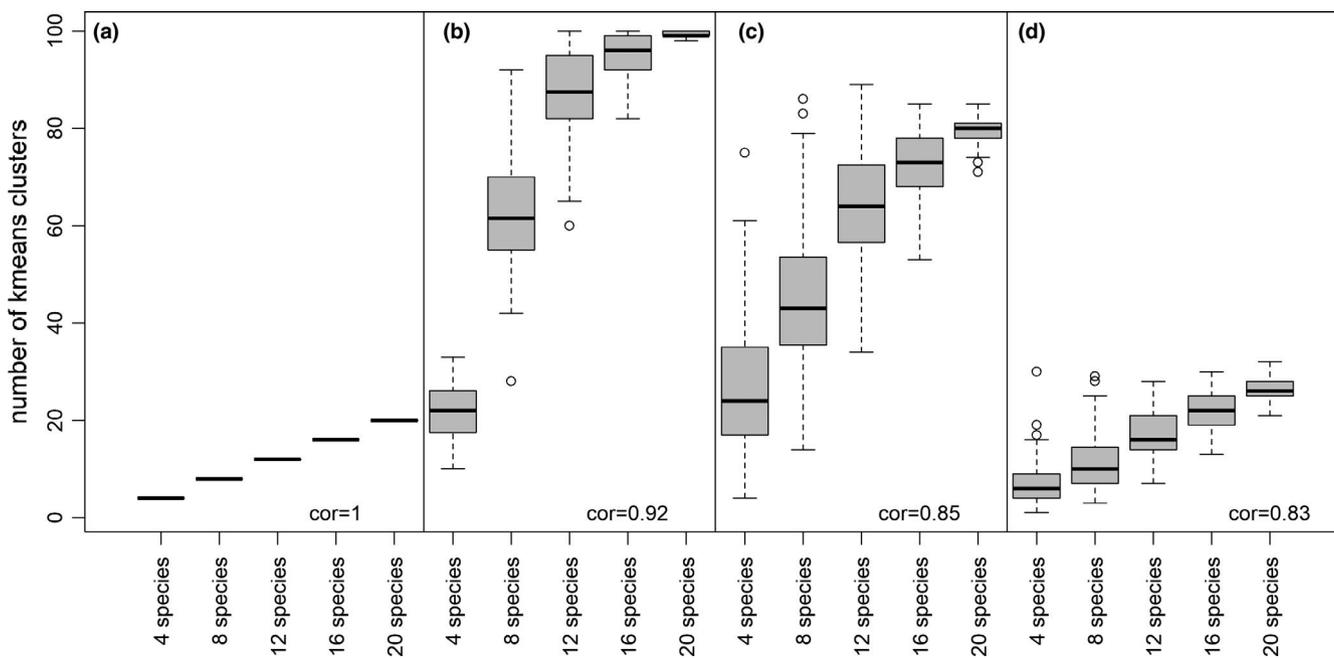

FIGURE 4 Manifoldness-based spectral variation of simulated grassland plots. One hundred hyperspectral images were simulated each at four spatial grains: from left to right, the original 100 × 100 pixels (a), then aggregated to 50 × 50 pixels (b), 25 × 25 pixels (c), and 10 × 10 pixels (d) and composed of spectra from 4, 8, 12, 16 and 20 species (100 images for each number of species). Images were created by randomly filling up a 100 × 100 pixel array with spectra from 4–20 species. In total 21 species were available. Spectral variation was calculated by first applying a K-means clustering with 100 clusters to a mosaic including all synthetic images (of a given grain); then the number of unique classes assigned by the unsupervised K-means classification was determined for each individual image

visible species in the framework of the species SVH, the spatial grain of the RS data should be adapted to the size of individuals or species stands occurring in a given ecosystem. For example, grasslands may require a notably finer spatial grain than forests to capture important patterns in spectral variation (see also section 3 *Phenology and other temporal effects*).

It follows that the choice of spatial scale for capturing species richness has severe consequences for SVH-based counts. Considering that even within the same vegetation type, the size of stands and individuals differs between species, it becomes clear that a single 'correct' or 'ideal' spatial scale for capturing species richness using RS does not exist. Further pitfalls are to be expected when several ecosystems are considered simultaneously.

Another example of how spatial grain influences the relationship between spectral variation and species counts is given in Figures 3 and 4. Here, the spectral variation of synthetic hyperspectral images of grasslands expressed with two different types of spectral-variation metrics is depicted in relation to the number of species and the spatial grain of the images. Each of the synthetic hyperspectral images was created by randomly filling up an array of 100×100 pixels in the x and y dimensions with species-specific spectral signatures. In total, we used 21 spectral signatures corresponding to 21 herb and grass species of Central Europe, thus reducing the real-world complexity by neglecting infra-specific variation. We created 100 of these images for each number of species tested (4, 8, 12, 16, 20, 21), with one species per pixel. Then we calculated two spectral-variation metrics for the original images with 100×100 pixels (Figures 3a,4a) as well as for the same images after they were spatially aggregated to 50×50 pixels, 25×25 pixels, and 10×10 pixels (Figures 3b–d,4b-d). The spatial aggregation was conducted with a simple calculation of means using the 'aggregate'-function of the raster package (Hijmans & van Etten, 2012) in R (R Core Team, 2013) (see Appendix S1 for more details). The first spectral-variation metric (SV_continuous) was calculated based on the mean Euclidean distance of all pixels in the plot using the pixel values of the first two components of Principal Components Analyses applied to the 85 bands of the synthetic hyperspectral images and calculated for a mosaic of the 500 synthetic images of a given aggregation level (see Supplementary material for more details). This metric captures the degree of contrast of the pixels. Following the species SVH, the higher the mean Euclidean distance is, the more species should be present. The second spectral-variation metric (SV_categorical) was derived from an unsupervised K-means clustering with 100 clusters applied to a mosaic of all synthetic images of a given spatial grain. We selected more clusters than species in order to allow for more clusters forming after aggregating pixels with the corresponding increase in reflectance types. In the original image, where each of the species corresponds to a single spectrum, the clustering stops after having derived the number of classes that fits the number of species. After the clustering, the number of unique classes to which the pixels of an individual synthetic image within the mosaic were assigned during the unsupervised K-means classification was determined. This metric captures the manifoldness of the pixels in the image. Following the species SVH, it is assumed that the more unique classes exist in the image, the more species are present. These simulations serve to make three important points: (i) in the results for the original images and SV_continuous metric, we can see that the median spectral variation increases from 4 to 20 species. However, at the same time, numerous (approximately 25%) of the simulated images (even those

composed of only four species) have higher spectral variation than the highest spectral variation observed for 20 species (Figure 3a). The number of K-means clusters in the SV_categorical metric necessarily matches the species numbers perfectly for the original images since no intraspecific spectral variation was considered (Figure 4a). (ii) Both metrics (expectedly) decrease with increasing level of aggregation of the pixels (coarser spatial grain). (iii) Differences in median spectral variation between images with differing numbers of species decreases with increasing level of aggregation (Figures 3a–d, 4b–d).

This example is highly simplified by assuming an approximately equal cover and a random distribution of each species in each image and by assuming that each species individual has exactly the same spectral signature. Nevertheless, the example illustrates a key weakness of spectral-variation metrics capturing the degree of contrast in the visible to shortwave–infrared region (SV_continuous): even if only four species are present, the spectral variation can be very high (higher than the variation of 20 species) in case the amplitudes of the reflectance values of these four species differ a lot.

This problem is closely related to the fact that healthy plant species' spectral signatures all follow a similar typical reflectance curve and hence the overall spectral variation is limited from the start. If even under such simplified and 'close-to-perfect' conditions, the link between spectral variation and plant species counts (within a single ecosystem type) is weak (Spearman correlation of 0.35 in the original data with 100×100 pixels for SV_continuous), it is very unlikely that it will improve under natural conditions with notably increased complexity in species' vertical and horizontal arrangements. On the other hand, the spectral-variation metric based on K-means clustering (SV_categorical) which imitates the spectral-species concept (e.g., Féret & Asner, 2014) will in theory result in a perfect relation between the number of species and the number of clusters if there is just one species per pixel and species feature a unique spectral signature. Although these preconditions are unrealistic, the experiment still prooves that the species SVH concept may have its applications if metrics capturing the manifoldness of the pixels in the image are applied.

3 | PHENOLOGY AND OTHER TEMPORAL EFFECTS

The majority of Earth's ecosystems is influenced by daily, seasonal and stochastic dynamics in terms of environmental conditions. Physiological processes such as photosynthetic activity are strongly coupled with these dynamics, and in turn vegetated surfaces also show daily, seasonal or random variation in the related optical traits that shape the electromagnetic signal captured by RS sensors. Species may have more unique spectral signatures at one time but less pronounced differences at another time, meaning that the species SVH will lead to varying results over time. Corresponding processes may affect the original SVH as well. For example, meadow types may be well distinguishable before mowing but loose this separability afterwards.

3.1 | Daily variation

Simple examples of daily variation are changes in leaf orientation to reduce or increase the amount of captured incoming radiation and to thereby regulate evapotranspiration (Chávez et al., 2014). Regular daily variation may be considered less problematic for most polar-orbiting satellite systems with fixed fly-over times. However, there might be related changes in spectral variation in airborne data and in longer time series in the case of orbit shifts of polar-orbiting satellites. For example, vegetation in (semi-)arid regions may adapt its leaf orientation in rather short time periods (Chávez et al., 2014) and a shift in overflight time of one hour as for example reported for Landsat 5 (Zhang & Roy, 2016) may result in notably different spectral signatures and hence spectral variation even though no true change in plant species counts has occurred.

3.2 | Seasonal variation

Seasonal variation is quite well predictable but still poses problems with respect to the SVH because it may be responsible for a notable share of the overall spectral variation at a given location, even if focussing only on the main vegetation period. Furthermore, in many types of ecosystems, e.g., dryland, grassland and savanna ecosystems as well as in forests' understorey layers, the development of annual herbs and grasses and short-lived species, as well as flowering events and leaf phenology are important. They can lead to a high degree of variation in important optical traits such as leaf area index (LAI), leaf-angle distribution and pigments (colours) (e.g., Landmann et al., 2015; Qi et al., 2014; Spanner et al., 1990). The large influence of flowering events on the spectral signal has been discussed for example in Schiefer et al. (2021).

Figure 5 shows an example of the seasonal variation in spectral signatures of a few common grass and herb species of Central Europe. The spectra were collected during an outdoor cultivation experiment (see Appendix S1). We can see that some of the grassland species strongly differ in their spectral behaviour depending on the phenological state in which their spectral signature is captured.

If we relate this phenological behaviour of herbs and grasses to the species SVH, it becomes clear that all typically used continuous spectral-variation measures would be notably influenced by this phenomenon (corresponding effects on the original SVH can also be assumed). In Figure 5 we can also see that the similarity of the spectra of the six species varies a lot over the year. While at the beginning of the vegetation season (31 May) the six species have widely varying optical traits and corresponding diverse
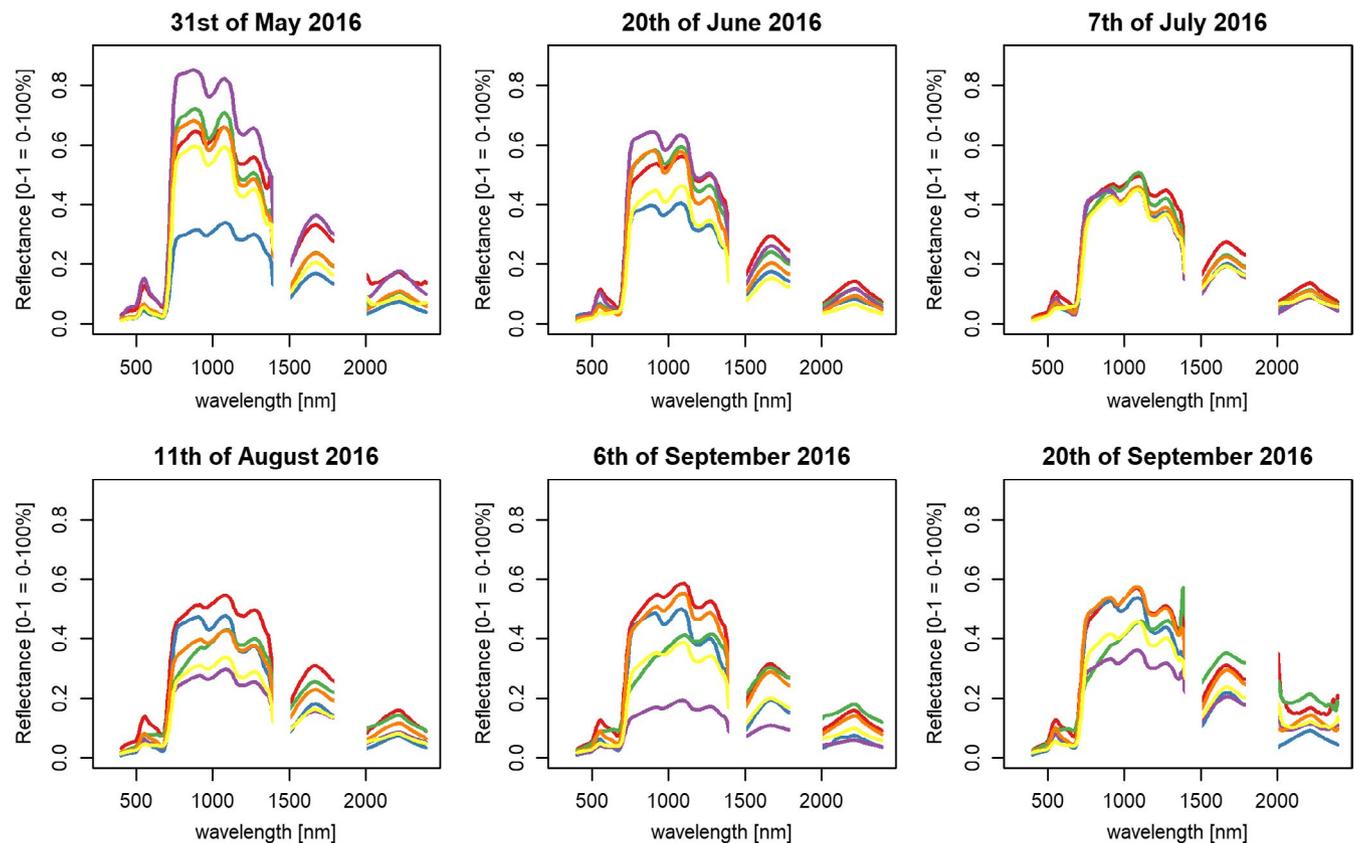

FIGURE 5 Field-collected spectra of six species plotted for different timepoints in the year. Water absorption bands at 1400–1500 nm and 1800–2000 nm were excluded. Different colours represent the different species in this case (red = *Calamagrostis epigejos*; orange = *Geum urbanum*; blue = *Nardus stricta*; green = *Agrostis capillaris*; violet = *Aegopodium podagraria*; yellow = *Festuca ovina*). For explanations of the methodology to create the spectral curves, see Appendix S1

spectra, they have a very comparable spectral behaviour at the peak of the vegetation period (7 July). Assuming an equal fractional cover of the six species for which a continuous spectral-variation (SV_continuous) measure would be derived, the variation measure will change dramatically while the plant species number remains the same. Other spectral-variation metrics based on unsupervised clustering (SV_categorical) may be less influenced, but flowering and co-occurrence of the same species in different phenological stages (e.g., in areas with strong environmental gradients) might also affect the captured manifoldness (as for example represented by the number of classes identified by an unsupervised clustering algorithm in a given area).

Another example for SV_continuous is given in Figure 6. Here it can again be seen that the spectral variation hardly serves as indicator for differing numbers of species. More importantly, it is also apparent that depending on which species were selected in one of the fixed amounts of species examined, the spectral variation can drastically vary over the course of a year. While this is a simplified example, it can still be assumed that the corresponding effects will be visible in real data sets and might be even more complex due to higher intermixture of species canopies. In addition, it should be considered that phenology is only one driver of intraspecific variation in optical traits and hence spectral variation. The health status, growth form due to adaptations to the abiotic and biotic environment and stress events are examples for additional intraspecific variation in optical traits that are likely to occur, particularly when focussing on larger spatial extents.

3.3 | Unpredictable variation

Apart from phenological and daily sources of variation some impacts are more difficult to predict. Such impacts embrace temporary stresses and disturbances including for example droughts in forests (e.g., Asner & Alencar, 2010), mowing of grassland or laying down of plants after rainfall and wind (Feilhauer & Schmidtlein, 2011). Such non-regular variation caused by disturbance or sudden weather conditions is difficult to take into account. An extreme temporal example occurs in arid and semi-arid ecosystems where most of the species are hidden for most of the time, becoming visible only after rare and irregular rainfall events. Similar dynamics may also exist in wetlands where the occurrence of vegetation as well as the optical signal observed by RS data may fluctuate seasonally with the water table which in turn may relate to varying precipitation patterns. Similarly, precipitation-induced rapid vegetation developments can also be observed in other ecosystems and might be hard to describe with spectral-variation measures, particularly if RS data acquisitions are available at a limited temporal resolution.

In summary, seasonal and other temporal differences in optical traits can make up for a notable portion of the overall spectral variation in certain ecosystems and hence have a direct effect on both the original and the species SVH. A relationship between spectral variation and plant species counts (or an alternative biodiversity

metric) found in one part of the year may not exist in another (see also Schmidtlein & Fassnacht, 2017). Hence, establishing a stable link between spectral variation and biodiversity (at least in terms of plant species counts) seems highly challenging in ecosystems with a pronounced temporal dynamic. To use spectral variation as a proxy variable for biodiversity, identifying suitable time windows or including the temporal dimension into the applied spectral-variation measure may hence be important prerequisites. Studies based on repeated RS measurements throughout the season coupled with repeated in-situ sampling of vegetation could help to better understand the influence of phenological changes and other temporal effects. From RS data alone, it is difficult to disentangle the seasonal variation of optical traits of the same species from the seasonal exchange in different species' presence or detectability, and from other unpredictable variation introduced by abiotic and biotic drivers.

4 | HABITAT TYPE MATTERS AT LEAST AS MUCH AS HABITAT NUMBERS

An example for why habitat type (or vegetation type) matters at least as much as habitat numbers are Central European calcareous grasslands. These are very species-rich habitats, but at the spatial resolution of common satellite sensors their spectral variation is low. The area marked in green in Figure 7 shows such a calcareous grassland, the Garchinger Heide, near Munich. This area of 27 ha contains more than 240 species (Bayerisches Landesamt für Umwelt, 2020). However, when visually and numerically (Table 1) comparing the spectral variation within this area (polygon 1 in Figure 7) with the spectral variation of areas of the same size in the surrounding intensively used agricultural landscape (polygons 2–7 in Figure 7), it is obvious that, at the spatial resolution of a Sentinel-2 satellite image, most of the other areas have (in some cases notably) higher spectral variation, despite having a far lower number of species.

The example of the Garchinger Heide relates to the issue of (rare) species-rich habitats that has been already discussed in one of the earliest works on the SVH (Palmer et al., 2002). In the example of the Garchinger Heide, a small habitat with a comparably homogeneous spectral signature contains a high number of plant species. Including or excluding this habitat type from a given area will have a tremendous effect on the plant species count but hardly any effect on the spectral variation. This is a major flaw of the original SVH and strong assumptions have to be made to still enable a general validity of the concept: it is valid to assume that if an additional habitat is added to a given area, the spectral variation of the area will increase, along with the species count (at least it will not diminish). However, comparing for example two areas A and B in which A has two and B has three habitats, B will only have more species than A in the case that B includes all the habitats that are also occurring in A. If this is not the case, it is easily possible that area A has two species-rich habitats and area B has three species-poor habitats and hence, area A could harbour more species than area B while B might still have a higher spectral variation. This problem persists independently
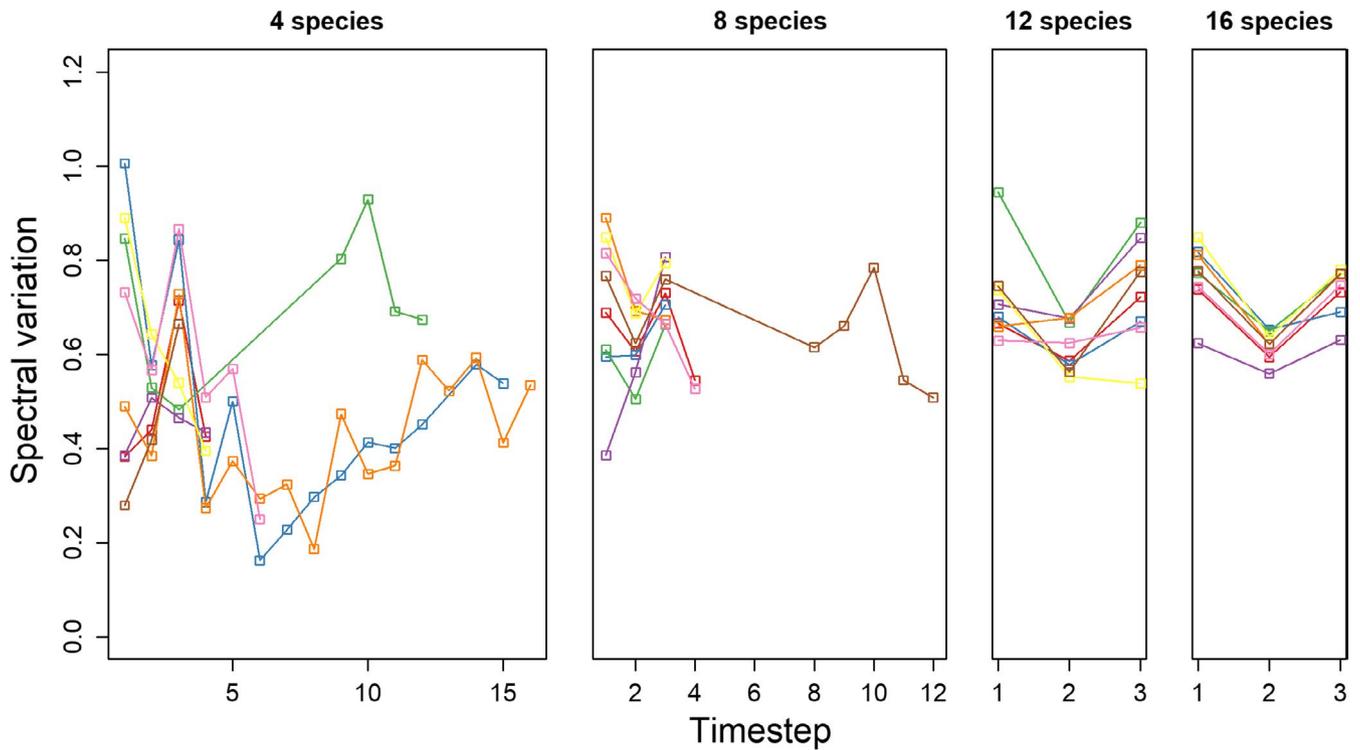
FIGURE 6 Changes of degree of contrast-based spectral variation during the vegetation period (SV_continuous). In the panels, each colour indicates one random composition of species and the line indicates how the spectral-variation value for this composition changes over time. The 'pixels' of each species of the synthetic images were filled with the corresponding field-measured spectra from the corresponding time step. For better visual interpretation we only plotted 8 of the 100 random compositions of 4, 8, 12 and 16 species summarized in Figure 3. Since not for all species spectra were measured at each timepoint, we only plot spectral-variation values of time points where spectra were available for each of the respective species. As can be seen, the higher the number of species is, the less likely it is, that spectra were measured for all species. This is why for 12 and 16 species only spectral-variation values for the first three time steps were available

from the applied type of spectral-variation metric (SV_continuous or SV_categorical).

Following the species SVH, spectral variation would be used to characterize biodiversity patterns only within a single patch (habitat) such as the Garchinger Heide; however, what might be problematic is that there is patchy structure within that area as well. Hence, it would quickly become hard to decide at which scale a between-site approach finishes and at which scale a within-site approach starts. Nevertheless, we can assume that the more we zoom into patches, the more relevance gains the 'species SVH'. The predictive power of the latter has been discussed above and is summarized in Figures 3 and 4.

A further related problem is that habitats that may appear spectrally very similar in the RS data due to shared canopy-dominating species, may still differ widely in species counts. A related example from Central Europe is the various European beech (*Fagus sylvatica*)-dominated forest communities which range from species-poor (Luzulo-Fagetum beech forests) to species-rich (Cephalanthero-Fagetum beech forests) forests. The biodiversity of those habitats is dominated by the herb layer which is hardly visible below the dense canopies of the beech forests and hence cannot be captured by RS.

5 | SPECTRAL-VARIATION METRICS

5.1 | Technical considerations

5.1.1 | Choice of the spectrum/spectral regions — radiometric resolution

Spectral-variation (SV_continuous) metrics calculated based on the variation of the reflectance values of the wavebands in the RS image are affected by the spectral coverage of the bands as well as the radiometric resolution of the bands and sun-sensor geometry (Schaepman-Strub et al., 2006). While differences in radiometric resolution of different sensors can be accounted for by using standardized data or physical units (e.g., surface reflectance values), differing numbers and widths of wavebands are harder to address. Hence, the same metric calculated for different satellite sensors may have notably different meanings and capture different processes leading to the observed spectral variation. This might be a problem with respect to the SVH, especially if data from different sensors are compared and SV_continuous metrics are used.
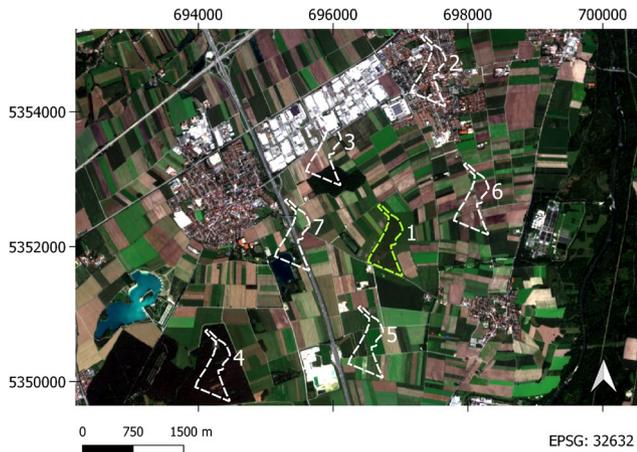
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FIGURE 7 The 'Gachinger Heide' near Munich, Germany (marked in green with id = 1), a species-rich calcareous grassland embedded in a landscape of intensive agriculture. The spectral diversity of this grassland is compared to other landscape elements of the same size (marked in white with id = 2–7). Area #1 contains many more species than the other areas although only one habitat type is included in this patch. Its spectral variation is accordingly low (Table 1)

TABLE 1 Overview of spectral diversity values calculated with a spectral variation (SV_continuous) metric for landscape patches shown in Figure 7

Landscape element id (Figure 7)	Spectral variation[a]
1 – Species-rich calcareous grassland	319
2 – Urban area	2041
3 – Agricultural/urban interface	1544
4 – Forest	595
5 – Agriculture	1778
6 – Agriculture (bare)	1022
7 – Agriculture/forest/road/water	1557

[a]Mean Euclidean distance of all Sentinel-2 pixels within the polygons calculated from the first two Principal Components Analysis (PCA) components of the Sentinel-2 raster stack. PCA components were calculated based on digital numbers of the L1C product of Sentinel-2 (nominal value range between 0 and 10000).

5.1.2 | High contrast land surfaces will increase spectral variation

Areas with particularly high or low reflectance values in some wavebands (e.g., bare-soil areas, rocks, sealed surfaces etc.) will have a notable influence on any spectral-variation measure capturing the degree of spectral contrast (SV_continuous). So far, no clear indications were made how this should be considered in the framework of the SVH. An obvious solution could be to exclude all non-vegetated areas by applying a vegetation mask before calculating the spectral-variation metrics. While this is feasible for very fine-grain RS data, it might already become challenging for intermediate spatial resolution

data sets including Sentinel-2 and Landsat which typically contain a large number of mixed pixels. Furthermore, scarcely vegetated patches can also contribute to species numbers. For example, in harsh environments such as coastal dune ecosystems, many focal species are small and occur in a very fine mosaic pattern of bare sand and vegetation (e.g., Ewald et al., 2020). Such areas may face the risk of being masked even though making a notable contribution to the species numbers. This problem may be less prominent for SV_categorical metrics but depending on the number of non-vegetated surface types present in an area, it might still cause some additional unwanted variability.

5.2 | Discrete vs continuous data

The above discussions have demonstrated advantages of SV_categorical over SV_continuous metrics. The continuous approach is the one proposed originally by Palmer et al. (2000) who emphasize continuity in the spatial analysis as a major advantage of the SVH. The SV_categorical approach is closely related to the spectral-species approach originally suggested by Féret and Asner (2014), where class numbers (typically obtained by a spectral clustering approach) are considered proxies of species numbers (thus relating to the 'species SVH'). Recently, this approach has been scaled up to wider spatial extents and to a higher level of biological organization (e.g., vegetation types or habitats) (Rocchini et al., 2021). The approach has some obvious advantages: (1) consistency over time may increase as even if the optical traits of plant species change over the year, the land-cover patches or landscape elements may be more persistent (e.g., a broad-leaved forest stand may look very different in a satellite scene acquired in summer and winter but may be detectable as a spectrally homogeneous spatial unit/patch in both scenes); (2) spectrally extreme pixels or land-cover types will not have unproportionally large influence on the spectral-variation metric but will rather represent individual discrete classes amongst a plethora of other classes; and (3) the approach is essentially summarizing the continuous spectral values into spatial objects that represent landscape elements or individual species and hence mirror the core assumption of the original SVH or species SVH better. Schmidtlein and Fassnacht (2017) reported persistently higher correlations between species counts and an SV_categorical metric compared to an SV_continuous metric based on Euclidean distances calculated in the spectral feature space of several MODIS bands, but the approach could still not remove the problems of individual habitats with very high (or very low) species numbers discussed in section 4 *Habitat type matters at least as much as habitat numbers*.

6 | FINAL REMARKS

Most of the issues related to the SVH as described in this study pose challenges not only to the SVH but also to other commonly applied RS-based biodiversity assessments outlined in section 1 *Introduction*.

A commonly claimed advantage of RS-based biodiversity monitoring is that repeated and standardized measurements are possible with comparably little effort which enables capturing temporal changes. This is an important requirement for any monitoring. As discussed in this study, establishing a direct and universally valid link between the RS signal and biodiversity information collected in the field is extremely challenging due to the nature of optical RS which does not allow to address the different biodiversity facets equally. Instead of focussing on taxonomic or phylogenetic differences (as typically focused on in field surveys), RS and particularly the spectral-variation approach relies on optical traits that are driven by functional and morphological differences between the species (such as the architecture of leaves and branches, size, width and colour of the leaves, size and colour of inflorescences, etc.). In case a species shows high and spatially differentiated variation in morphology during the life cycle or due to plasticity or disease or pests or disturbance (Feilhauer & Schmidtlein, 2011), it can falsely increase or lower the spectral variation and hence the species number predictions.

One question that could be raised, however, is whether searching for this generalized direct link between biodiversity and RS data is useful in the first place. Most RS-based approaches attempt to identify the link between biodiversity and RS signal in the spatial rather than temporal dimension. This is in direct contradiction to the proclaimed most important property of RS data, that is, the option for repeated acquisitions and monitoring over time. Most ecologists and biodiversity experts agree that detailed biodiversity surveys on the ground are the most reliable way to correctly assess biodiversity of a given region. One could assume that once the current biodiversity of a given area is inventoried and well understood (and the best way to do so is going to the field), the main task would be to monitor whether the biodiversity at this location is changing or remaining constant within a certain level of expected natural fluctuations. RS might be a suitable technology for addressing such task, with spectral variation being a key variable.

Adapting to this scenario, the central task of RS would lay in the change detection aspect, that is, in the identification of changes in the spectral and structural properties of the ecosystem rather than describing or mapping the ecosystem/biodiversity state. This type of RS-based monitoring is theoretically possible without support of any field data by simply comparing the current (spectral/structural) state of an area against an expected state derived from earlier observations. It is important that this comparison must occur on multiple spatial and temporal scales to account for the natural dynamics of a given ecosystem (which may widely differ, for example a fire may not have a notable effect on biodiversity in a savanna but may make a huge difference in a temperate ecosystem, natural succession cycles may be fast in one area and very slow in another, etc.). Spectral variation measured at multiple spatial grains and for various extents (window sizes) could be, amongst others, an efficient metric contributing to such a 'real' monitoring scheme.

In this study, we pointed out issues that question a universal, causal direct link between spectral variation and species counts. The reflective properties and hence the spectral variation of a given area in an RS data set is affected by numerous factors including the landscape composition, spatial grain of the data, the acquisition time and corresponding sun-sensor geometry and the methodical approach to calculate the spectral variation. In some ecosystems, the spatial non-stationarity in the link between spectral variation and species numbers introduced by these factors is likely to be an insurmountable obstacle. Based on the points raised here and considering the results from earlier studies (e.g., Schmidtlein & Fassnacht, 2017) we recommend to carefully revise under which condition a link between spectral variation and biodiversity can be assumed. As demonstrated in this study, simple simulation experiments can support this task and are an efficient means to identify conceptual weaknesses of some aspects of the SVH and to compare different methodical approaches to calculate spectral variation. Making valuable field-collected biodiversity data openly available and testing the links between biodiversity and spectral variations in a more systematic way using multiple metrics and approaches could further contribute to an improved understanding of the link between spectral variation and biodiversity.

The need for a more systematic testing of the links between biodiversity and spectral variations applies not only in the context of SVH but also with respect to other RS-based approaches to map and monitor biodiversity as it is likely that the factors influencing spectral variation discussed here do not apply solely for the SVH but also for other commonly discussed approaches to estimate (spatial) biodiversity patterns from RS data. We hence recommend that future studies should focus more on efficiently capturing changes in landscapes over time (and hence a potential change of biodiversity) rather than solely on the direct mapping of biodiversity patterns across space. The latter can be achieved with field surveys at much higher quality but might nevertheless benefit from an indirect integration of RS data. RS data can for example guide and improve the sampling design of biodiversity surveys by providing a pre-stratification of the study area, which also was the original motivation for developing the SVH (Palmer et al., 2002). Similar approaches have successfully been applied in forest inventories for decades and have proven to increase their efficiency.

AUTHOR CONTRIBUTIONS

All authors contributed to the development of the main messages communicated in the study. Fabian Fassnacht wrote the manuscript with contributions of all authors, and conducted the data analyses. All authors discussed the results and commented on the manuscript.

DATA AVAILABILITY STATEMENT

The spectra used in this study for data simulations are available at https://ecosis.org/package/canopy-reflectance-plant-functional-gradient-ifgg-kit (https://doi.org/10.21232/krt4-6x67). The corresponding R-codes can be found at: https://github.com/fabianfassnacht/SVH. UAV images used in Figures 1 and 2 can be made available upon request. Sentinel-2 data used in Figure 7 are freely available for example on ESA's data hub and can be found with the image ID: S2B_MSIL1C_20190830T102029_N0208_R065_T32UPU_20190830T130621.

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SUPPORTING INFORMATION

Additional supporting information may be found in the online version of the article at the publisher's website.

Appendix S1. Approach to create synthetic images from field spectrometer measurements