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Advantages of retrieving pigment content [μg/cm^2] versus concentration [%] from canopy reflectance

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ABSTRACT

Photosynthesis is essential for life on earth as it, inter alia, influences the composition of the atmosphere and is the driving mechanism of primary production. Photosynthesis is particularly controlled by leaf pigments such as chlorophyll, carotenoids or anthocyanins. Incoming solar radiation is mainly captured by chlorophyll, whereas plant organs are also protected from excess radiation by carotenoids and anthocyanins. Current and upcoming optical earth observation sensors are sensitive to these radiative processes and thus feature a high potential for mapping the spatial and temporal variation of these photosynthetic pigments. In the context of remote sensing, leaf pigments are either quantified as leaf area-based content [μg/cm^2] or as leaf mass-based concentration [g/g or %]. However, these two metrics are fundamentally different, and until now there has been neither an in-depth discussion nor a consensus on which metric to choose. This is notable considering the amount of studies that do not explicitly differentiate between pigment content and concentration. We therefore seek to outline the differences between both metrics and thus show that the remote sensing of leaf pigment concentration [%] is unsubstantial. This is due to the fact that, firstly, pigment concentration is likely to primarily reflect variation in leaf mass per area and not pigments itself. Second, the radiative transfer in plant leaves is especially determined by the absolute content of pigments in a leaf and not its relative concentration to other leaf constituents. And third, as a ratio, pigment concentration is an ambiguous metric, which further complicates the quantification of leaf pigments at the canopy scale. Given these issues related to the use of chlorophyll concentration, we thus conclude that remote sensing of leaf pigments should be primarily performed on an area basis [μg/cm^2].

1. Introduction

Terrestrial plants are vital for the production of oxygen and organic matter through photosynthesis. Photosynthesis is primarily controlled by pigments, which are important links to assess plant stress, plant functioning, biological cycles, and biosphere-atmosphere interactions (Nelson and Yocum 2006; Blackburn, 2006; Kattenborn et al., 2018). Photosynthesis is performed by chlorophylls and carotenoids. Carotenoids, together with anthocyanins, protect chlorophylls and other plant material from photodamage (excess and UV radiation). Anthocyanins are further important indicators for pathogen defence (Lev-Yadun and Gould 2008, Zarco-Tejada et al., 2018).

These pigments primarily affect the radiative transfer in the visible spectrum, where solar radiation is highest (400–700 nm), whereas incident radiation that is not absorbed by the canopy or the ground is scattered. These scattered remnants constitute the basis for quantifying pigments such as chlorophylls, carotenoids, or anthocyanins using optical remote sensing observations (Tucker and Sellers, 1986; Jacquemoud et al., 1996; Blackburn, 2006; Kattenborn et al., 2017; Zarco-Tejada et al., 2018). Commonly, pigments are quantified using two different metrics - either as pigment content, i.e. pigment mass per leaf area [μg/cm^2] (hereafter referred as pigment$_{area}$) or as pigment concentration, i.e. pigment mass per leaf dry mass [g/g or %] (hereafter referred as pigment$_{mass}$). Note that the terms content and concentrations are often used interchangeably, while here we use content for per-area and concentration for per-mass. The choice of quantification method in remote sensing appears to be inconclusive, as both metrics are frequently referred to in the relevant literature (e.g. Jacquemoud et al., 1996; Zarco-Tejada et al., 2001; Asner and Martin, 2009; Jetz et al., 2016). Here, we argue that quantifying pigment$_{mass}$ with remote sensing is unsubstantial as 1) this measure does not explicitly reflect variation in pigments per se, but rather variation in leaf dry mass, 2)

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$pigment_{mass}$ is less accurately retrieved than $pigment_{area}$ using optical remote sensing and 3) it is more difficult to scale-up $pigment_{mass}$ to the canopy scale. We conclude that quantifying $pigments_{area}$ is more appropriate in remote sensing due to its explicit relation to radiative transfer, enhanced scalability and as it is a more direct expression of plant stress and functioning.

2. Rationale

2.1. Pigment concentration primarily reflects leaf dry mass and not pigment variation itself

Put simply, $pigment_{mass}$ [%] is the ratio of $pigment_{area}$ [μg/cm^2] and the Leaf Dry Mass per Area [g/cm^2] (LMA):

$$pigment_{mass} = pigment_{area}/LMA \tag{1}$$

Leaf dry mass is composed of carbohydrates (hemi-cellulose, cellulose, starch), proteins, lignin and waxes, and it generally reflects differences in leaf lifespan resulting from adaptations to environmental factors (Grime et al., 1997, Wright et al. 2004, Díaz et al., 2016). As evinced using global trait databases, LMA has a higher variance than leaf traits related to photosynthesis, e.g. leaf nitrogen content [mg/cm^2] or photosynthetic capacity [μmol/m^2/s] (see Wright et al. 2004; Osnas et al., 2013; Lloyd et al., 2013). This is critical as leaf resource investments (e.g. LMA) and leaf traits relating to photosynthesis are largely independent of one another (Osnas et al., 2013; Llyod et al. 2013; Osnas et al., 2018) and accordingly the division by LMA actually dominates the actual variation of pigments content.

Here we demonstrate these relationships for leaf pigments using a dataset comprising LMA, $chlorophyll_{area}$, $carotenoid_{area}$, and $anthocyanin_{area}$ values from 45 herbaceous species retrieved in-situ (see supporting information for details). The coefficient of variation of LMA (38.4%) clearly exceeds that of $chlorophyll_{area}$ (24.8%), $carotenoid_{area}$ (15.0%), and $anthocyanin_{area}$ (26.1%). Correspondingly, a principal component analysis (Fig. 1) of LMA, $pigments_{area}$ and $pigments_{mass}$ reveals that $pigments_{mass}$ primarily reflect the LMA gradient (strong negative correlation). Gradients of $pigments_{area}$, in contrast, are largely orthogonal and thus uncorrelated with LMA. Thus, it can generally be expected that gradients of $pigments_{mass}$ predominantly mirror the variation in LMA, which in turn overshadows the actual variation of $pigments_{area}$.

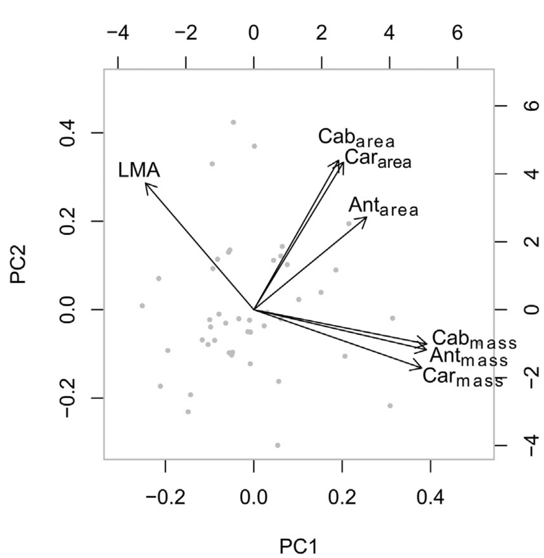

Fig. 1. Principal component transformation of LMA, $chlorophyll_{area}$, $carotenoid_{area}$, $anthocyanin_{area}$, $chlorophyll_{mass}$, $carotenoid_{mass}$, and $anthocyanin_{mass}$. $Pigments_{area}$ are largely independent from LMA, whereas $pigments_{mass}$ predominantly reflect the variation in LMA.

2.2. Remote sensing of pigment content outperforms pigment concentration retrievals

As reported by previous authors, the retrieval of leaf constituents is more accurate for absolute contents per area than for concentration per mass (Grossman et al., 1996; Jacquemoud et al., 1996; Oppelt and Mauser, 2004). This can be explained by the radiative transfer mechanisms: Leaf constituents affect the reflectance properties of a plant canopy through absorption and scattering, whereas these effects increase with increasing contents of the respective constituent (e.g. pigments). The spectral signal is therefore determined by the absolute content of the constituent (e.g. $pigments_{area}$) and not by its concentration relative to LMA. In other words, concentrations ($pigment_{mass}$) cannot represent the absolute amount of matter interacting with electromagnetic radiation (also see Jacquemoud et al., 1996). For this reason, pigments in radiative transfer models are parametrized by specific absorption coefficients on an area basis. $Pigment_{mass}$ is the ratio of $pigment_{area}$ to LMA, which further implies that remote sensing of $pigment_{mass}$ (e.g. through statistical models) ideally requires the simultaneous consideration of spectral features corresponding to both pigments (in the visible range) and LMA (in the short wave infrared range), as illustrated using empirical canopy reflectance data in Fig. 2. However, the retrieval of LMA using optical canopy reflectance is commonly challenging, as the respective spectral features are overshadowed by water absorption (Jacquemoud et al., 1996; Homolová et al., 2013). Moreover, and in contrast to visible and near infrared wavelengths, the short-wave infrared information is generally affected by lower signal-to-noise ratios, increased spectral shifts, and increased calibration uncertainties (Cocks et al., 1998; Bachmann et al., 2015). Uncertainties in the retrieval of LMA spectral features propagate into errors of $pigment_{mass}$ assessment. Thus, the retrieval of $pigments_{mass}$ is substantially impaired as it requires spectral information of the short wave infrared range (which is not always available) and the generally less accurate retrieval of the LMA variation. In contrast, the retrieval of $pigments_{area}$ only relies on spectral features in the visible range (Fig. 2a).

2.3. Pigment concentration is generally an inconclusive proxy with impaired scalability

Being a relative concentration, $pigment_{mass}$ is generally an inconclusive metric: high $pigment_{mass}$ can result from either high $pigment_{area}$ and intermediate LMA or intermediate $pigment_{area}$ and low LMA. It is therefore possible for two leaves or plant canopies to have equivalent $pigment_{mass}$, but differ greatly in $pigment_{area}$ and LMA. Accordingly, $pigment_{mass}$ does not explicitly indicate if a plant canopy actually has low pigment content, e.g. due to stress or its inherent plant functional properties (compare Fig. 3).

This ambiguity similarly limits the scalability to the canopy level, which is pigment content per canopy surface area [g/m^2] (hereafter referred as $pigment_{canopy}$). $Pigment_{canopy}$ relates to the absolute photosynthesis of a vegetated area and is thus directly relevant for assessing productivity or atmosphere-biosphere interactions (De Pury and Farquhar, 1997; Peng et al., 2011). Here, we seek to demonstrate the limited scalability of $pigment_{mass}$ using a straightforward approach, i.e. upscaling leaf constituents to the canopy scale by incorporating Leaf Area Index [m^2/m^2] (LAI). LAI is a proxy for the total foliage area within the canopy area and can be retrieved from remote sensing data with acceptable accuracy (Zarco-Tejada et al., 2001; Myneni et al., 2002; Schlerf et al., 2005). In case of $pigment_{area}$, upscaling to $pigment_{canopy}$ merely requires a multiplication with LAI (Eq. (2)). In contrast, scaling $pigment_{mass}$ to $pigment_{canopy}$ requires prior knowledge on the absolute foliage mass in the entire canopy surface area, i.e. the product of LAI and the LMA (Eq. (3)).

$$pigment_{canopy} = pigment_{area} \cdot LAI \tag{2}$$

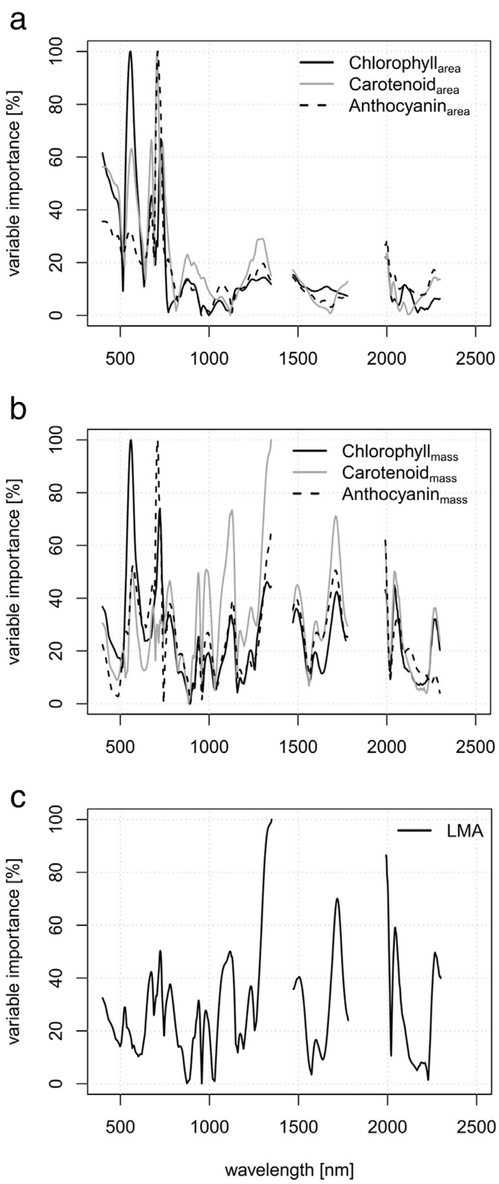

Fig. 2. Scaled variable importance of partial least square regression models for the retrieval of pigments$_{area}$ (a), pigments$_{mass}$ (b) and LMA (c) based on 2270 canopy spectra of 45 herbaceous species (see supplementary information for details). The variable importance demonstrates that pigment$_{mass}$ retrieval relies on VIS and SWIR information (pigments and LMA), whereas the retrieval of pigment$_{area}$ solely relies on VIS information.

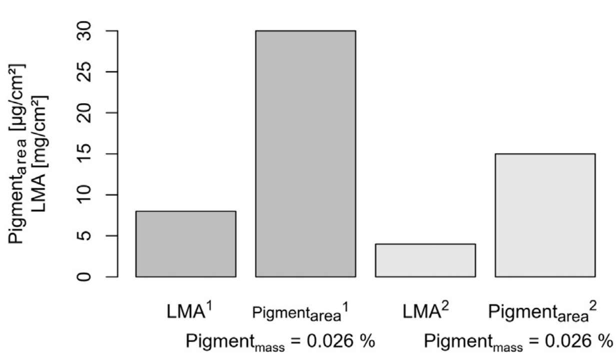

Fig. 3. Scheme demonstrating equal pigment concentration despite varying pigment contents and LMA of two samples (1, 2).

$$pigment_{canopy} = pigment_{mass} \bullet LAI \bullet LMA \quad (3)$$

However, as described in section 2, the quantification of LMA requires SWIR information and is generally limited using canopy reflectance (compare Homolová et al., 2013). Thus, scaling pigment$_{mass}$ to the canopy requires additional information on the dry weight of the foliage (LMA) and may be negatively affected by error propagation of the LMA estimates.

3. Discussion and concluding remarks

For monitoring vegetation photosynthesis and physiological status, from the above arguments, we strongly advocate a focus on pigment content per area, rather than pigment mass concentration. Most studies currently reporting on pigment$_{mass}$ (see supplementary information Table S-2) do so without a precise justification on why they quantify pigments as concentration. We assume that the frequent use of pigment$_{mass}$ may primarily be adopted from plant ecology, where leaf nutrients (e.g. nitrogen or phosphorus) are frequently quantified on a mass basis rather than an area basis (see Wright et al. 2004 or Díaz et al., 2016). A primary reason for this might be that leaf nutrients are commonly measured from plant powder (see e.g. Cornelissen et al., 2003), so normalizing the extracted constituent is trivial on a mass basis. However, as indicated above and by Osnas et al. (2013), Lloyd et al. (2013) and Osnas et al. (2018), normalizing traits describing photosynthetic functions on a mass basis introduces severe statistical and conceptual issues, as the variance in leaf resource investments is naturally higher than the variance of photosynthetic traits, and leaf resource investments are largely independent of photosynthetic functions. The second reason why many studies assessed pigment concentration may stem from a plant function perspective, where one might argue that there is a motivation to map pigments$_{mass}$ using remote sensing, as the latter possibly indicates the photosynthetic return per unit of invested dry matter (compare Westoby et al., 2013). Following this logic, all things being equal, a plant with low LMA receives higher photosynthetic returns per unit invested dry matter, than a plant with high LMA. However, the fact that LMA is highly correlated with leaf lifespan implies that the eventual return per unit invested LMA greatly depends on the time span in which the leaf performs photosynthesis. Accordingly, pigment$_{mass}$ at a given point in time does not explicitly reveal the photosynthetic return per unit invested leaf dry matter.

Literature reviewed during the preparation of this manuscript revealed that with regard to pigment quantification the terms content and concentration are frequently used interchangeably (in approximately a third of studies assessed here, see supplementary information). Future studies should explicitly state what metric is being used and why, with per-leaf area-content of pigment as the standard. Moreover, some authors even compare their results for pigment concentration retrieval with results obtained for pigment content, and vice-versa. Yet, as highlighted above, pigment content and concentration are not directly comparable.

Based on the outlined rationale, we conclude that the quantification of plant pigments using remote sensing and canopy reflectance should be performed on an area basis rather than a mass basis. We assume that these rationales also apply for the remote sensing of leaf nitrogen, as pigments and nitrogen are generally highly correlated in leaves.

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Appendix A. Supplementary information

Supplementary data to this article can be found online at https://doi.org/10.1016/j.rse.2019.05.014.

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