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# **Variability and Uncertainty Challenges in Scaling Imaging Spectroscopy Retrievals and Validations from Leaves Up to Vegetation Canopies**

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# **Abstract**

Imaging spectroscopy of vegetation requires methods for scaling and generalizing optical signals that are reflected, transmitted and emitted in the solar wavelength domain from single leaves and observed at the level of canopies by proximal sensing, airborne and satellite spectroradiometers. The upscaling embedded in imaging spectroscopy retrievals and validations of plant biochemical and structural traits is challenged by natural variability and measurement uncertainties. Sources of the leaf-to-canopy upscaling variability and uncertainties are reviewed with respect to: (1) implementation of retrieval algorithms and (2) their parameterization and validation of quantitative products through in situ field measurements. The challenges are outlined and discussed for empirical and physical leaf and canopy radiative transfer modelling components, considering both forward and inverse modes. Discussion on optical remote sensing validation schemes includes

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also description of a multiscale validation concept and its advantages. Impacts of intraspecific and interspecific variability on collected field and laboratory measurements of leaf biochemical traits and optical properties are demonstrated for selected plant species, and field measurement uncertainty sources are listed and discussed specifically for foliar pigments and canopy leaf area index. The review concludes with the main findings and suggestions as how to reduce uncertainties and include variability in scaling vegetation imaging spectroscopy signals and functional traits of single leaves up to observations of whole canopies.

#### **Keywords**

Quantitative remote sensing; Imaging spectroscopy; Retrieval of vegetation traits; Radiative transfer models; Inversion; Variability; Uncertainty; Scaling; Multiscale validation

## **1 Introduction**

Imaging spectroscopy, also known as hyperspectral remote sensing, measures the Earth surface radiance, as a function of the wavelength of the electromagnetic spectrum (from visible to long infrared), the illumination and observation geometry (Sun–object–sensor angularity) and temporal characteristics (acquisition date and revisit frequency) of a particular location represented by geographical coordinates and altitude (Malenovský et al. 2007; Schaepman et al. 2009). Consequently, the scale of an imaging spectroscopy observation is a function of the observation spatial, spectral and temporal extent and resolutions. It depends on spatial characteristics of an observed location, the observational geometry (radiance directions), spectral properties of sensed electromagnetic radiation and temporal specifications of a given data acquisition. Spatial scale of a remote sensing observation, given in the case of space-borne image data by the sensor instantaneous field of view (IFOV), might be due to physical and technical constrains different from the scale required by an observer or data user. For example, in imaging spectroscopy of vegetation one is often interested in biochemical traits of plants at the spatial resolution of single leaves, whereas the remotely sensed data represent whole canopies composed of several plant functional types. Consequently, the scaling techniques changing the size of a measurement unit and allowing us to decipher data acquired at one scale into informational content of another scale were established (Dungan 2001). Two general scaling approaches are being recognized: (1) upscaling: the bottom-up scaling of detailed information up to coarser (larger) units and (2) downscaling: the top-down scaling, which decomposes signals and information collected at broader scales into elementary constituents of smaller proportions (Marceau and Hay 1999). The general concept of scales in imaging spectroscopy of vegetation is further described by Gamon et al. (2019).

An initial error and uncertainty characterization of an imaging spectrometer was proposed by Schaepman et al. (2015). It has been later extended by Hueni et al. (2017) with an error traceability matrix covering several known error sources. The largest uncertainty in their error propagation scheme was assigned to the creation of vegetation products from a standardized reflectance image using an upscaling scheme. Sources of variability and uncertainty in the process of retrieving plant traits from imaging spectroscopy data

of vegetation canopies can be divided into the three broader clusters (Fig. 1): cluster I: sensor design, data acquisition and pre-processing (e.g., sensor calibrations, radiometric, geometrical and atmospheric data corrections; Hueni et al. 2013); cluster II: retrieval algorithm including parameterizations and simplifications imbedded in radiative transfer models (Knyazikhin et al. 2013); and cluster III: field data acquired in situ to constrain retrievals in the form of the prior knowledge and also to validate the retrieved remote sensing products (Mussche et al. 2001; Thimonier et al. 2010).

Assessment of uncertainties related to the acquisition and processing of imaging spectroscopy data requires detailed spectral and radiometric characterization of the sensor performance and operational set-up (including Sun–object–sensor illumination-viewing geometry, acquisition conditions in terms of actual atmospheric parameters including cloud cover) and specifications of the processing chain transforming raw image data to the radiance and reflectance products. Although the magnitudes of these uncertainties are instrument-specific, wavelength-dependent and vary in space and time, their sources are well known and can be quantified (Hueni et al. 2017). For instance, Bachmann et al. (2011) designed a full error propagation concept for airborne imaging spectroscopy data and also analysed the potential influences of spectral and radiometric calibration uncertainties on data products of the upcoming space-borne imaging spectroscopy mission EnMAP (Bachmann et al. 2015). The data quality assessment is part of good practices for many existing operational land-monitoring space-borne multispectral sensors, such as MODIS on Aqua and Terra (Vermote et al. 2002; Lyapustin et al. 2014), ETM+ on Landsat (Feng et al. 2012; Claverie et al. 2015; Vermote et al. 2016) or MSI on Sentinel-2 satellite platforms (Gascon et al. 2017; Gorroño et al. 2017). Due to a high similarity with hyperspectral remote sensing, these practices are adaptable and applicable also on imaging spectroradiometers.

Since cluster I in Fig. 1 (sensor design, data acquisition and pre-processing) does not contain any significant spectral–spatial scaling features, this review focuses on the identification of uncertainty and variability knowledge gaps taking place in the two remaining clusters related to: (1) empirical and physical upscaling retrieval approaches, including radiative transfer modelling (cluster II, Fig. 1) and (2) scaling of field measurements used for parameterization of retrieval algorithms and validation of imaging spectroscopy products (cluster III, Fig. 1). The specific objective is to outline challenges of natural variability and methodological uncertainty in spectral and spatial (geometrical) scaling of terrestrial vegetation optical properties (i.e. reflected, transmitted and emitted visible and infrared photon fluxes) from leaves up to canopies. Main attention is paid to retrievals and validation of biochemical and biophysical plant traits (e.g., content of foliar pigments or leaf area index—LAI) obtained from remote sensing imaging spectroscopy data at different spatial scales. Although the review discusses a concept of the multiscale ground air- and space-borne validation scheme, it does not present any quantitative meta-analyses nor error propagation computations, for which actual measurements acquired at several spatial scales simultaneously are required. Also, a temporal scaling of vegetation optical signals is not included, as this topic is extensive and requires a specific publication on its own.

# **2 Upscaling in Retrievals of Vegetation Traits from Imaging Spectroscopy**

# **Data**

#### **2.1 Empirical Approaches Using Statistical Methods**

An operationally highly efficient upscaling approach is a direct statistical relationship established between ground measurements of plant traits and imaging spectroscopy observations. This method performs satisfactory for canopies with a vertically homogeneous architecture (e.g., moss and grass turfs, monocultural crops and plantations) that are, however, present less frequently in wild natural landscapes. Upscaling in heterogeneous vegetation canopies that are composed of multiple species, resulting in an irregular distribution of foliage and wood constituents in horizontal and vertical dimensions (e.g., bushlands and forests), requires a more rigorous sampling scheme. Significant investments of time and manpower are needed to collect a sufficient number of representative samples in order to establish a statistically robust regression model. Additionally, the samples must be collected within a short period, close to the time of remote sensing data acquisitions, to ensure the overall temporal consistency. Consequently, the number of samples is in reality often limited by available resources.

To overcome the complexity and high costs of sampling plants in their natural environments, measurements of small-size plant canopies can be for some cases conducted under controlled conditions in the laboratory or in experimental field trials. Such experiments are simpler and time-efficient, but they tend to be specific for a given site, time and plant functional type and consequently difficult to generalize. This approach was applied, for instance, in the study of Buddenbaum et al. (2012, 2015a, b), which investigated the effects of drought stress on young beech (*Fagus sylvatica*) trees under fully controlled irrigation regimes. Proximal hyperspectral images of the beech canopies were recorded once a week during the summer period, when half of the sample trees were cut off from water supply. Leaf reflectance and canopy spectral indices were combined with the partial least square regression (PLSR) (Wold et al. 2001) to upscale leaf chlorophyll and water content of individual leaves to image pixels of beech crowns. In another case study, Kanning et al. (2018) demonstrated the application of drone-based hyperspectral imagery for estimation of LAI and leaf chlorophyll content aiming to assess a potential yield of winter wheat (*Triticum aestivum*). Field measurements of LAI and leaf chlorophyll content were used to calibrate a local PLSR model based on spectral signatures extracted from wheat canopies growing under various N-fertilization levels. Direct transfer of an empirical retrieval method established in laboratory to imaging spectroscopy data acquired at different scales and locations has been demonstrated mostly for structurally simple canopies. For example, Malenovský et al. (2015) imposed a gradual water stress on three Antarctic moss species in laboratory-controlled environment. Laboratory measurements of moss traits and complementary spectroscopic measurements were used to train and optimize machine learning algorithms (support vector regressions) estimating chlorophyll content and effective leaf density of moss turfs as the quantitative stress indicators. Subsequent application of the machine learning models on drone-acquired imaging spectroscopy data of two Antarctic moss beds showed an acceptable accuracy of both estimated functional traits (Malenovský et al. 2017). To increase universality and applicability of the empirical upscaling schemes

to more complex canopies, various automatized field and laboratory high-throughput plant phenotyping systems combining a large number of multisensor (hyperspectral, chlorophyll fluorescence and thermal) imaging measurements of plants or even small trees have recently been developed (see review by Humplík et al. 2015). A high number of controlled environmental variables in plant phenotyping system allow researchers to build models that are more robust and potentially transferable to other plant types growing at different locations and conditions.

#### **2.2 Physically Based Approaches Using Radiative Transfer Models**

Mechanistic principals of spectral and spatial scaling effects can be studied with physically based radiative transfer models (RTMs). RTMs are computer algorithms that allow us to scale remotely sensed signals from detailed local to coarser regional and global scales based on our knowledge about light–object physical interactions (Liang 2004). The fundamental role of RTMs is to describe the structural, geometrical and optical effects that modulate remotely sensed signal at different scales. These models are particularly applicable for vegetation canopies, as they are able to simulate the complex nature of vegetation structures leading to specific effects when scaling from leaves to individual plants, fields and stands or whole ecosystems. Reflectance of single leaves is related to canopy hemispherical–directional reflectance function (HDRF) through the combination of structural (e.g., leaf angular distribution, leaf vertical and horizontal clumping and canopy cover causing spatially explicit self-shading effects), optical (reflectance and transmittance of leaves, branches and trunks) and geometrical (solar irradiation and sensor viewing geometries) properties of vegetation remote observations (Knipling 1970). Leaf optical properties simulated with leaf-level RTMs can be physically upscaled in the canopy-level RTMs.

**2.2.1 Leaf-Level RTMs—**The reflection and transmission of light incident on a leaf are determined by biophysical properties of its surface and the inner structures. The incoming photons penetrate deeper into the leaf and interact with its cellular, sub-cellular and intercellular structures, such as mesophyll cells, their organelles and intercellular air spaces. The optical properties of leaves, i.e. amount of absorbed and scattered (reflected and transmitted) light, are driven by the concentrations of light absorbing compounds (e.g., pigment pools, dry matter and water content) and by structural properties of leaves (e.g., thickness and arrangement of inner leaf surfaces). While the specific absorption coefficients of biochemical compounds and refractive index of inner leaf surfaces are usually retrieved from optical measurements, leaf structure can be reconstructed from, for instance, confocal microscopic images of leaf cross sections (Albrechtová et al. 2007). Leaf optical properties can be directly measured (Lukeš et al. 2017; Hovi et al. 2017) as well as modelled using leaf-level RTMs.

One of the most commonly used leaf RTMs is PROSPECT (Jacquemoud and Baret 1990). This model approximates the leaf inner structure by the *plate model* (Allen and Wette 1969, extended for non-compact leaves by Breece and Holmes 1971). The original PROSPECT model requires a relatively small number of input parameters (contents of chlorophylls a and  $b$ , dry matter and water content, and inner structural parameter  $N$ ), which makes it easy to

run in forward and also inverse directions. It was later extended to simulate the influence of leaf carotenoid (Féret et al. 2008) and anthocyanin contents (Féret et al. 2017). It was also incorporated into the FLUSPECT model, which reproduces the chlorophyll fluorescence emission of the photosystems I and II (Vilfan et al. 2016) and spectral manifestation of the photoprotective xanthophyll de-epoxidation cycle (Vilfan et al. 2018). Apart from PROSPECT, Dawson et al. (1998) developed the LIBERTY needle–leaf model to simulate the optical properties of needles, which are anatomically different from plate-like broad leaves. To account for differences in optical properties of the adaxial and abaxial leaf sides, Stuckens et al. (2009) developed the Dorsiventral leaf radiative transfer model (DLM). This model is able to reproduce optical differences between leaf sides based on few additional input parameters related to leaf inner structures.

As demonstrated in numerous studies, the inversion of leaf RTMs allows for non-invasive retrieval of the input model parameters (typically leaf biochemical properties) from measured leaf optical properties (Ustin et al. 2009). For example, Barry et al. (2009) inverted the PROSPECT model to estimate the chlorophyll content of Eucalyptus leaves measured with a spectroradiometer coupled with an integrating sphere. Their chlorophyll retrieval achieved the average root mean square errors (RMSE) of 5  $\mu$ g cm<sup>-2</sup> and 3  $\mu$ g cm<sup>-2</sup> for juvenile and adult leaves, respectively. Similarly, Malenovský et al. (2006) adjusted and inverted the PROSPECT model for the estimation of its inputs from the optical properties of Norway spruce needles. They minimized the prediction uncertainties in dry matter and water content by implementing the prior information of known inputs' dynamic ranges (i.e. minimal and maximal measured values) and achieved estimations with RMSE of 0.0019 g  $\text{cm}^{-2}$  and 0.0006 cm<sup>-2</sup>, respectively.

**2.2.2 Canopy-Level RTMs—A** large variety of canopy RTMs have been developed to scale the optical signatures of leaves up to canopy scales (Liang 2004). They can be categorized based on their approach for radiative transfer through vegetation canopies into six groups (Table 1): (1) turbid medium, (2) kernel-driven, (3) spectral invariants, (4) geometrical–optical, (5) discrete geometrical and voxel-based, and (6) Monte Carlo ray-tracing models. Each group has been designed for its specific purpose, which implies that they possess specific conceptual and computational assumptions with different levels of uncertainties. Table 1 summarizes the abilities of the RTM groups to represent canopy spatial and structural heterogeneities. It indicates their computational speed and some examples of the models. It is important to note that Table 1 does not present an exhaustive listing of all existing models. More extensive overview of canopy RTMs is available at, for instance, the Internet portal of the European Council Joint Research Centre [\(http://rami](http://rami-benchmark.jrc.ec.europa.eu/HTML/Home.php)[benchmark.jrc.ec.europa.eu/HTML/Home.php](http://rami-benchmark.jrc.ec.europa.eu/HTML/Home.php)), which presents a performance comparison of various RTMs carried out within the systematic radiative transfer model intercomparison (RAMI) exercise (Widlowski et al. 2007, 2013, 2015).

Quantitative assessment of forward modelling uncertainty can be conducted through the systematic sensitivity analysis, where the most accurate modelling solution, e.g., photon ray-tracing simulation applied on a detailed vegetation representation, is taken as a reference. The reference results are then compared to outcomes of simulations with a systematically varying input parameterization, more generalized assumptions or increased

levels of simplification. Apart from the direct comparison exercise, the global sensitivity analysis (GSA) can be performed to identify the most important inputs that modulate strongly the spectral outputs of RTMs (Verrelst and Rivera-Caicedo 2017). However, GSA is applicable only in case of a simple model with a limited number of input variables (e.g., SAIL; Verhoef 1984). As the theoretical uncertainty of RTMs increases with their increasing complexity, it can be reduced in complex models only by including available prior information. Consequently, the paradigm that the more detailed model is capable of producing more realistic and accurate simulations might not be true, if the uncertainty behind the model inputs (variables and a prior knowledge) is high. On the other hand, it is important to highlight that novel progressive techniques, such as close-range (ground-, tower- or drone-based) laser scanning (Schneider et al. 2014, 2019; Wallace et al. 2016; Janoutová et al. 2019) and proximal high-resolution imaging spectroscopy (Malenovský et al. 2015, 2017; Wyber et al. 2017), can satisfy the demands of complex RTMs for detailed unbiased inputs and prior information on plant structural, optical and biochemical properties.

A combination of leaf and canopy RTMs in an inverse mode has been frequently applied on imaging spectroscopy data to retrieve various model input parameters, i.e. leaf-level biochemical or canopy structural traits (Schlerf and Atzberger 2006; Homolová et al. 2013; Schneider et al. 2017; Verrelst et al. 2019). The two basic model inversion approaches are: (1) direct mathematical inversion (Laurent et al. 2013, 2014) and (2) indirect approach based on pre-simulated spectral look-up tables (Kimes et al. 2000). In the case of direct inversion, independent simulations are performed for each image pixel separately and model inputs of the most optimal radiative transfer solution are being sought. As the model inversion needs to be run multiple times, the method is not suitable for computationally intensive RTMs, but it allows each retrieval to be performed for different sets of model input parameters of simpler RTMs. This may increase the retrieval accuracy, especially if the site-specific prior information is included. In case of the indirect approach, all model runs are executed and stored in a pre-computed spectral database called *look-up table*. The best fit between the measured and simulated signal is then determined later using optimization or regression algorithms, such as minimization of the merit functions, artificial neural networks, genetic algorithms and many others. Since the inversion algorithms may differ in the retrieval accuracy, their appropriate selection is equally important to the selection of the suitable RTMs (Rivera et al. 2013). Selection of inappropriate model or incorrect set-up of the retrieval algorithm may result in an inversion ambiguity caused by the fact that the different combinations of model inputs result in identical spectral simulations. The ambiguity, also called a mathematically ill-posed problem, can be reduced or even removed by incorporating a prior knowledge on the simulated vegetation canopy (Combal et al. 2002).

Retrievals of vegetation traits via inversion of RTMs have been successfully applied at different spatial scales ranging from individual tree crowns and canopies of forest stands and crops up to global ecosystems. For example, Jay et al. (2016) achieved a high accuracy when retrieving leaf traits from close-range hyperspectral images of five tree species using the PROSPECT leaf model coupled with the COSINE close-range model accounting for specular reflection at leaf surface and local leaf orientation. Malenovský et al. (2013) used adjusted PROSPECT implemented in the discrete anisotropic radiative transfer (DART) model to retrieve leaf chlorophyll content per crown of a Norway spruce (*Picea abies*) forest

stand. They generated a RTMs *look-up table* in order to design a new chlorophyllsensitive and LAI-insensitive optical index, which applied to airborne imaging spectroscopy data showed similar retrieval RMSE of 2.42  $\mu$ g cm<sup>-2</sup> as an artificial neural network retrieval. Atzberger and Richter (2012) used the PROSPECT-SAIL model for inversion of crops traits from simulated Sentinel-2 satellite spectral observations. To reduce inversion ambiguity, they introduced object-based retrieval that takes into account also spatial information of several adjacent pixels. This way, they reduced the RMSE of LAI retrieval from 1.46 to  $0.54$  m<sup>2</sup> m<sup>-2</sup>. Strictly speaking, Sentinel-2 MSI as well as MODIS sensors on the Terra and Aqua satellites are not imaging spectroradiometers, but multispectral sensors. Still, MODIS products of LAI and the fraction of absorbed photosynthetically active radiation (Myneni et al. 2002) provide good examples of global vegetation traits produced operationally using canopy radiative transfer solutions that can be retrieved also from upcoming space-borne spectroscopy images.

Validation of vegetation traits retrieved from optical remotely sensed data is an essential part of the estimation process indicating its fidelity. Deviations of remote sensing products from hypothetically true values obtained through collection of ground measurements indicate the physical uncertainties (see Sect. 3), whereas uncertainties that cannot be assessed through a direct comparison with reference values are called theoretical uncertainties. The uncertainties provide the additional complementary information about potentially oversimplified parameterization, inappropriate assumptions or imperfect optimization of RTMs and retrieval algorithms. The theoretical uncertainties can be computed in the form of: (1) spectral residuals or standard deviations, when an ensemble of multiple optimal solutions is retrieved (Rivera et al. 2013) or (2) as a likelihood of values estimated in frame of statistical fuzzy approaches such as Bayesian methods (Cooper and Herskovits 1992). Several powerful retrieval methods originating from the field of Bayesian nonparametric statistic, as, for instance, the family of Gaussian processes regression (GPR; Camps-Valls et al. 2016), can deliver high accuracies and at the same time uncertainty intervals of their predictions (Verrelst et al. 2012). The uncertainty intervals indicate how confident the model is in a per-pixel prediction relative to what it has been presented during its training phase. Uncertainty can be used to mask out areas where the actual estimates exceeded the acceptable threshold of 20%, as proposed by the Global Climate Observing System (GCOS 2011). Additionally, it can be used to check transferability of locally trained models through spatial and temporal scales. As an example, Verrelst et al. (2013) trained and successfully validated a GPR model to estimate the total leaf chlorophyll content, which was based on locally selected training pixels of the space-borne image acquired with the CHRIS/PROBA mission of ESA over agricultural fields at Barrax region in Spain. The trained GPR model was then applied to an airborne imagery of a higher spatial resolution, acquired with a CASI imaging spectroradiometer. Per-pixel uncertainties obtained for selected pixels of both datasets indicated a potentially good transferability of the GPR model in case of selected agricultural crops, but they also revealed a failure of the model to retrieve reliably leaf chlorophyll content across the whole airborne image. This validation identified regions where more training data were required to improve robustness and accuracy of the GPR retrieval. More details about the imaging spectroscopy methods for retrieval vegetation traits can be found in Verrelst et al. (2019).

# **3 Upscaling of Ground Measurements for Validation of Imaging Spectroscopy Products**

#### **3.1 Remote Sensing Validation Schemes**

Remote sensing products retrieved empirically or physically from imaging spectroscopy data need to be accompanied with a proper validation indicating of their reliability and fidelity. It is important to note that collections of data for validation purposes as well as for parameterization of the empirical and the physical model-based retrievals are affected by the same sampling and upscaling issues. Validation can be understood as a process of analytical comparison with reference data measured usually in situ, which is presumed to represent the true target value (Justice et al. 2000). Validation can be, in a broader sense, considered as a combination of several activities, including comparison with: (1) precise fiducial reference measurements (when a few but very precise measurements are available), (2) other in situ reference measurements (when more but less precise measurements are available), (3) other satellite products, (4) outputs of models and (5) results from monitoring tools assessing spatial and temporal consistency. The term truth should be used with care, while keeping in mind that any ground or laboratory measurement is at best an unbiased traceable representation of the true value with an associated uncertainty (Hueni et al. 2017). The uncertainty is a combination of measurement precision (i.e. the closeness of two or more measurements represented by numbers of given digits) and *accuracy* (i.e. the closeness of a measured value to a standard of known value). Final ground-truth measurement uncertainties are specific to applied measurement protocols, where a sensor ground sampling distance and swath determine the number and spatial extent of field measurements and a vegetation type and traits under investigation determine the most appropriate sampling scheme, instrumentation and data processing. The first step towards a representative number of samples is creation of an appropriately sized elementary sampling unit (ESU). The ESU scheme is a well-established concept for indirect optical measurements of LAI and leaf inclination distribution of agricultural crops and also forest canopies (Weiss et al. 2004; Baret et al. 2005; Morisette et al. 2006). Still, different sampling and measurement strategies are used for LAI measurement than for quantification of leaf pigments, but also for low and homogenous crops than for tall and heterogeneous forest stands (Weiss et al. 2004). Being carried out by tree climbers (Schlerf et al. 2010), shotguns (Féret and Asner 2011), pole pruners (Singh et al. 2015), line launchers (Collis and Harris 1973) or crossbows (Wang et al. 2016), this sampling might be conducted in a less representative way. Singh et al. (2015) measured several leaf traits in mixed forest stands from the lower, middle and upper crown parts and compared different foliage sampling weighting schemes with the remote sensing signal. Based on the results, they used the foliar biomass per species derived from diameter–biomass relationships to scale foliar traits up to the canopy of each test plot. Despite practical difficulties to trace the field and laboratory measurement uncertainties, direct validation using ground *truth* is regarded as a fundamental effort for assessing fidelity of airborne and space-borne vegetation products.

Over the last two decades, several globally produced vegetation products were derived from time series of medium-resolution satellite sensors such as SPOT/Vegetation (Baret et al. 2007), MODIS (Myneni et al. 2002) or MERIS (Bacour et al. 2006) and significant

efforts have been spent in their validation and assessment of their spatial and temporal consistency. The field validation ground-truth data have been for a variety of vegetation types obtained through dedicated field campaigns coordinated locally or internationally within operational science data networks. One of the largest international networks that operate worldwide is FLUXNET [\(www.fluxnet.fluxdata.org;](http://www.fluxnet.fluxdata.org/) Baldocchi et al. 2001). FLUXNET data have been used to validate gross primary production (GPP), LAI, fraction of absorbed photosynthetically active radiation (FPAR) and albedo products of MODIS (Turner et al. 2006). Extensive regional validation campaigns were conducted, for instance, by the Big-Foot project for validation of MODIS vegetation products (Cohen and Justice 1999), the VALERI project for validation of the European Space Agency (ESA) instruments such as MERIS (Baret et al. 2005) or through a series of ESA coordinated campaigns such as SEN2FLEX and SEN3EXP for validation of Sentinel-based products. Although these satellite sensors are multispectral, their validation schemes are adjustable and transferable to upcoming hyperspectral space missions, such as the Italian national mission PRISMA (Amato et al. 2013) or the German national mission EnMAP (Guanter et al. 2015).

The importance of data quality control and uncertainty quantification has been addressed in the Quality Assurance Framework for Earth Observation (QA4EO 2009) created by the Committee on Earth Observation Satellites (CEOS), requesting that all datasets and derived products contain a fully traceable indicator of their quality. Consequently, the Land Product Validation (LPV; [http://lpvs.gsfc.nasa.gov\)](http://lpvs.gsfc.nasa.gov) subgroup of CEOS developed a framework for intercomparison and validation of global land products, such as LAI, FPAR and fraction of vegetation cover (fCover). LPV released the community established best practices and guidelines, which adopted a hierarchical approach with four validation stages (Fernandes et al. 2014). In the first stage, product accuracy is assessed from a small  $( $30$ ) set of selected$ locations and time periods by comparison with ground-truth or other suitable reference data. In the second stage, the same validation is carried out for a significant set of locations and times, and spatial and temporal consistency is evaluated globally. In the third stage, the product uncertainties and their structure are quantified in a statistically robust way over multiple locations and times globally. The last fourth stage includes systematic and regular updates of the third stage results to match releases of new products, new versions or simply to monitor the performances of the product as long as the satellite time series expands. LPV is searching for supersites with fully characterized land surfaces and vegetation types, which is a prerequisite for their parameterization in 3D radiative transfer models. These sites will serve as test beds for in situ sampling strategies and product algorithm intercomparisons. The LPV activities also resulted in an On Line Interactive Validation Exercise platform (OLIVE; <http://calvalportal.ceos.org/web/olive>; Weiss et al. 2014) hosted by ESA. OLIVE permits the validation of global LAI, FPAR and fCover products within the two ensembles of sites: (1) 445 BELMANIP2 sites (Baret et al. 2006), containing selected sites of existing sensor networks (FLUXNET, AERONET, VALERI and BigFoot), and (2) 113 DIRECT sites (Garrigues et al. 2008a, b). The OLIVE platform has a potential to be extended towards biophysical products derived from newer medium-spatial resolution satellite data, e.g., from the OLCI sensor onboard of Sentinel-3. However, validation of vegetation products with a higher spatial resolution and inclusion of new products (e.g., leaf chlorophyll content)

would require significant changes in the OLIVE validation reference data structures and procedures.

Validation of vegetation products that are not delivered by any satellite platform on the operational basis (e.g., leaf chlorophyll, carotenoid and water content) are less internationally coordinated and their global validation datasets are rare (e.g., Croft et al. in review). ESA funded in 2018 the Fiducial Reference Measurements for Vegetation (FRM4VEG) project [\(https://frm4veg.org/](https://frm4veg.org/)), aiming to establishing protocols required for traceable in situ measurements of vegetation-related parameters for validation of Copernicus products from multispectral sensors of Sentinel-2, Sentinel-3 and PROBA-V. The fiducial reference measurements should ensure units' traceability in validation schemes that are independent from retrieval procedures and accompanied by an uncertainty budget. The standardized ground truth is planned to be measured for remote sensing products as surface reflectance, FPAR and canopy chlorophyll content.

#### **3.2 Multiscale Validation Approach**

Since the validation data must be collected within a time frame, for which the validated variable remains unchanged, the ground-*truth* datasets are often limited in size due to resource restrictions and time constraints. As it is hard to collect a representative number of ground measurements in few days after the data acquisition, a validation of global remote sensing products with a limited number of sampling points might be unreliable. One possible way to improve the validation process is to apply a multiscale (multilayer) validation approach. The multiscale validation incorporates local-to-regional high-spatial resolution airborne or satellite data, as an upscaling intermediate layer that is placed between field measurements and a medium-to-low-spatial resolution space-borne product (see Fig. 2). This scheme offers an opportunity to split the validation into two consecutive steps. In the first step, pixels of an airborne high-resolution map are compared and validated against the corresponding truth of field measurements. In the second step, the airborne vegetation product is enlarged by new clusters of high-resolution pixels and compared to values of corresponding medium-to-low-resolution satellite pixels. The first validation step may take advantage of the very high spatial resolution  $(< 1 \text{ m})$ allowing to extract from the field sampling locations, e.g., ESU or sampled tree crowns, only those pixels that are not contaminated by unwanted landscape elements (e.g., bare soil or other surrounding vegetation types (Kükenbrink et al. 2019). Within the second step, one may identify and include a higher number of suitable corresponding validation pixel clusters from airborne and space-borne products, which may potentially increase the representativeness of validation. Additionally, spatial aggregation of high-resolution airborne pixels reassembles spectral information of a low-resolution satellite data more precisely than an integration of spatially limited ground measurements. Practical application of the multiscale validation, however, requires fulfilling of several technical conditions. First, to allow the quantitative assessment, all compared variables must be collected simultaneously, i.e. during the same vegetation growth stage, and have to be expressed in the same physical units, preferably in accordance with the International Systems of Units (SI). Second, all datasets must be spatially co-registered within the same geographical projection system and precisely geocoded with an acceptable positional error (smaller than

the data ground sampling distance). Only then can any of the evaluated variables from any location and of any scale be mutually compared. Besides the quantitative accuracy assessment, a spatial consistency of estimated vegetation traits can be assessed from a pattern comparison of the airborne and satellite products. It may reveal the existence of the product spatial inhomogeneity and local anomalies due to insufficiencies in spectral, radiometric, geometrical and atmospheric calibrations and corrections. For instance, a wide field of view of airborne spectroradiometers causes a strong reflectance angular anisotropy, known as the bidirectional reflectance distribution function (BRDF) effect (Weyermann et al. 2014). Since this effect is less prominent in images of orbiting space sensors, one can investigate its impact by comparing both products, preferably accompanied with ground truth collected across the whole airborne image swaths.

The potential use and advantages of the multiscale validation scheme has been outlined and demonstrated by Baret et al. (2006) in the case of upscaling the information collected within the standardized ESU to: (1) high-spatial resolution and (2) medium-spatial resolution space-borne observations. Although several multiscale experimental validation campaigns were designed in the similar fashion, e.g., SEN2FLEX (Delegido et al. 2010; Corbari et al. 2013), SEN3EXP (Sobrino et al. 2012) or recently FLEXSense 2018 (Rascher et al. personal communication), the multiscale concept has not been, to our best knowledge, implemented as a standard validation component of any operationally produced global vegetation remote sensing product. Nonetheless, the concept is expected to receive more attention with an increasing affordability and availability of the very high-spatial resolution imaging spectroscopy data produced by manned and recently also unmanned airborne system (UAS) platforms (e.g., Lucieer et al. 2014; Juszak et al. 2017). In particular, UAS platforms might be of a high interest in this sense. They are offering data acquisitions with an unprecedent high detail due to short ground sampling distances and can be deployed multiple times over the same area on demand, which increases representatives and reduces potential errors in their quantitative measurements. Additionally, several studies have demonstrated that UAS is able to provide detailed measurements of vegetation canopy biochemical as well as structural parameters (Zarco-Tejada et al. 2012; Wallace et al. 2016; Malenovský et al. 2017).

#### **3.3 Natural Variability and Measurement Uncertainty in Upscaling Validation Schemes**

Uncertainty behind in situ measurements of a validation field data is related to the intrinsic natural variability of vegetation parameters in space and time, and to the nature of a measurement method. To illustrate this concept, Fig. 3 shows a hypothetical example of a remote sensing uncertainty assessment demonstrated on five virtual validation sites/ scenarios (VS). The measurement and the estimation uncertainties, driven by actual precisions and accuracies, are presented as a purple ellipse. In all cases, the ground-truth measurement uncertainty is expected to be smaller than the uncertainty of a corresponding estimate. Hence, the measurement uncertainty is given by an ellipse minor axis and the uncertainty of an estimate is given by its major axis. Horizontal black arrows are showing a real within-site natural variability of a given parameter, while grey zones illustrate a variability captured in validation measurements collected at given VS. Dashed line indicates the one-to-one line, i.e. the expected best fit between measured and estimated values.

When interpreting individual cases shown in Fig. 3, VS1 represents a slightly inaccurate (underestimated) retrieval with a high precision (the retrieval uncertainty interval is small). It is representative for a given site (the within-site variability equals the validation data variability); however, it captures only a small part of the total parameter natural variability. VS2 represents a very accurate but less precise retrieval (the retrieval uncertainty interval is larger than for VS1), which is covering a significant part of a total natural variability; however, it is non-representative for the site. (The within-site variability is larger than the actual variability of validation dataset.) VS3 represents a validation case similar to VS1 (i.e. of a high precision and representative for a given location), but with a low accuracy due to the retrieval overestimation. VS4 is also significantly inaccurate (an underestimated retrieval) and, moreover, most imprecise out of all presented cases (the retrieval uncertainty is the largest); however, it is representative for a given site and covers a significant part of the natural variability. Finally, VS5 represents an ideal scenario, which has a high accuracy without any bias and an acceptable precision. Additionally, VS5 is fully representative for the sampled site and captures a large portion of the existing natural variability. The most accurate, and subsequently successful, validation results should contain cases similar to VS5 that would be ideally distributed across the entire natural variability of a retrieved vegetation parameter (as shown in Fig. 3).

**3.3.1 Origins and Impact of Natural Vegetation Variability—**Natural variability of vegetation parameters is determined by variations in environmental conditions as light, nutrients and water availability, but also by plant species composition, i.e. species biodiversity. Additionally, an important contribution to the overall variability of leaf-level plant traits, such as specific leaf area, leaf nitrogen, chlorophyll and water content and others, is the intraspecific variability within the single species. While the interspecific variability, i.e. variations between different species, typically explains about 50–90% of the total leaf trait variability (Albert et al. 2010; de Bello et al. 2011), about 20–30% can be explained by the intraspecific variability (Auger and Shipley 2013). Figure 4a shows the interspecific variability in four leaf biochemical traits, serving as inputs into the leaf radiative transfer model PROSPECT (Jacquemoud and Baret 1990), measured for upper-canopy sunlit branches sampled from nine common central European tree species. This graph also illustrates the importance of the sample set representativeness relying on the actual sample size. While the sample collections for spruce and beech species are sufficiently large to capture existing variability of their leaf traits, the size of the remaining leaf sample sets is insufficient  $(n \t 12)$  and subsequently diminishing the true natural variability, which is expected to be between 10 and 80 µg of chlorophyll  $a +$  $b$  per cm<sup>2</sup> of the leaf area. Some tree species exhibit a significant variability in leaf traits within the individuals as an adaptation to canopy light gradients (Niinemets 2010). This is especially prominent in leaves exposed to direct sunlight (sunlit leaves), which contain higher levels of dry matter and photo-protective pigments in comparison with their shaded counterparts (Lichtenthaler et al. 2007). A good example is a shade-tolerant Norway spruce that demonstrates a large variability in leaf traits. Figure 4b shows that except the needle water content, which was found to be independent from the age of leaves, all other investigated traits of sunlit and shaded needles respond to the combination of needle age cohorts with a varying availability of direct and diffuse solar radiation.

Differences in leaf biochemistry and inner leaf structure are imprinted in leaf optical properties, i.e. leaf reflectance, transmittance and absorbance (Kokaly et al. 2009), which consequently vary among and within species (Lukeš et al. 2013; Noda et al. 2013; Atherton et al. 2017). Despite identical environmental conditions and similar leaf biochemical properties, the optical properties of the two broadleaf species displayed in Fig. 5, narrowleafed ash (Fraxinus angustifolia) and silver poplar (Populus alba), exhibit a different spectral behaviour when comparing the adaxial (upper) and the abaxial (bottom) leaf sides. When considering only the adaxial optical properties, both species are comparable, but the abaxial reflectance of poplar is significantly higher due to the layer of a white scurfy down (i.e. trichomes). This example demonstrates that differences in leaf adaxial and abaxial optical properties, which alternate the canopy reflectance, represent yet another upscaling uncertainty that is seldom considered during ground-truth field sampling (Stuckens et al. 2009). This leaf morphological adaptation is of a high importance for plants that are changing the actual leaf angularity in order to protect themselves from adverse environmental conditions of excessive solar irradiation intensity, as, for instance, olive trees (Olea europaea).

It is beyond the capabilities of this review to address the full range of variations in plant traits and their spectral properties. Nonetheless, the following suggestions, recommending how to proceed towards better understanding and inclusion of the vegetation-related variability, can be outlined:

- **•** First, combining data from multiple studies and field measurement campaigns into large and open-access databases would help scientists to reveal the true size of natural variability in plant traits and spectral properties. It would subsequently become possible to incorporate a large volume of data they contain in remote sensing scaling studies. Several initiatives of such a kind already exist. For instance, the global data-base of plant traits TRY [\(https://www.try-db.org](https://www.try-db.org), Kattge et al. 2011) has recently been used to derive global maps of specific leaf area, leaf dry matter content, leaf nitrogen, phosphorus concentrations and leaf nitrogen-to-phosphorus ratio (Moreno-Martínez et al. 2018). Field spectroscopy measurements have already been shared for a few years through online spectral databases such as SpecNet [\(https://specnet.info/](https://specnet.info/), Gamon et al. 2006), EcoSIS [\(https://ecosis.org/\)](https://ecosis.org/) and Specchio [\(http://specchio.ch](http://specchio.ch), Hueni et al. 2009). Shared databases, however, require fully standardized protocols for measurements of field traits and optical properties to be compatible.
- **•** Second, a possible way to address large-scale variability in vegetation imaging spectroscopy is to organize multiscale and multidisciplinary measurements campaigns that involve several research teams conducting concurrent field measurements at multiple sites simultaneously with drone-, air- and spaceborne imaging spectroscopy acquisitions. Good examples of such joint efforts are multiscale field/flight campaigns supported by ESA in the context of validation of current operational Sentinel missions (e.g., SEN2FLEX in 2005 and SEN3EXP campaign in 2009) and in preparation of the upcoming missions

as the FLEX Earth Explorer (e.g., HYFLEX in 2012 or FLEXSense campaign in 2018).

**•** Third, an additional way to better capture plant trait and spectral variability in the physically based retrieval scaling schemes is to improve representation of distinct vegetation functional types in existing RTMs. For example, a genuine architectural and structural representation of heterogenous forest canopies can be efficiently reconstructed from terrestrial laser scans of individual trees or sparse stands (Calders et al. 2015; Schneider et al. 2019). Such a semi-automatic approach allows us to separate non-photosynthetic and photosynthetic tree parts as well as sun- and shade-adapted leaves and adapt accordingly in RTMs vertical distribution of photosynthetic foliar pigment inputs, specifically chlorophylls and carotenoids (e.g., Janoutová et al. 2019).

**3.3.2 Sources of Field Data Measurement Uncertainty—**Most prominent sources of uncertainty in field vegetation measurements are related to sampling methods and to data measurement and post-processing protocols, including technical capabilities of instrumentation. The existing sampling schemes for validation of remote sensing product are outlined in Sects. 3.1 and 3.2. As indicated before, sampling approaches are expected to capture the natural variability of vegetation parameters within an area of interest, but in practice they are limited by available time and resources (manpower and technical equipment). Random sampling methods, which require a minimum prior knowledge on the parameter variability space, assume that collected samples are spatially independent. At the same time, practical constraints and failures in designing the truly random sampling scheme are often enforcing a compromise between a statistically optimal and an experimentally feasible sampling. Therefore, the random sampling methods are less suitable for species rich canopies, where omitting some important species due to the recombination of randomness results in an undersampling (Baraloto et al. 2010). Although no versatile field sampling scheme has been established yet, several attempts were made to standardize sampling schemes and protocols for certain vegetation traits, e.g., the already mentioned VALERI scheme developed for validation of space-borne LAI estimates (Baret et al. 2005).

Several systematic and non-systematic measurement uncertainties of eco-physiologically important vegetation parameters can be reduced only by establishing standardized measurement and data post-processing protocols (Pérez-Harguindeguy et al. 2013) and by using the state-of-the-art, accurate and well-calibrated instrumentation. For example, the uncertainty of optical hand-held devices for quick determination of leaf pigment contents, which are frequently used to validate remote sensing products for crops and broadleaf canopies, is significantly impacted by errors in instrument calibration (Cerovic et al. 2012; Parry et al. 2014). Another example is the determination of canopy or a single-tree crown LAI, which is conducted with several indirect optical methods (Bréda 2003; Jonckheere et al. 2004). LAI measurements by means of hemispherical photography were found to be accurate for short-stature crops (Garrigues et al. 2008a, b), but still challenging in forest canopies, where additional effects of woody elements, foliage clumping and the corresponding appropriate camera exposure settings have to be considered (Zhang et al. 2005; Macfarlane et al. 2007; Thimonier et al. 2010; Liu et al. 2015). Some studies reported

disagreement in forest LAI measurements between digital hemispherical photography and other optical indirect instruments, such as the widely used LiCor Plant Canopy Analyser or AcuPAR, especially in dense canopies with a higher LAI (Mussche et al. 2001; Thimonier et al. 2010; Eckrich et al. 2013). The foliage clumping has a pronounced effect on computation of the total LAI (LAIt), especially in coniferous forest stands (Chen et al. 1997). It can enhance the final LAIt uncertainty, if being underrated or, respectively, overrated, especially in forests where trunks are part of its computation. Bao et al. (2018) showed that exclusion of trunks in a spruce (Picea crassifolia) forest led to a reduction in the average LAIt by 19.6% and 8.9%, depending on applied clumping estimation method. Hence, the clumping correction coefficient counts for an additional and important error source of LAI measurements that require a standardized measurement protocol.

# **4 Conclusions**

Empirical retrievals of vegetation traits from imaging spectroscopy data use direct upscaling approaches, such as statistical regressions established between ground and remotely sensed measurements. Due to their simplicity, they require few inputs and consequently have fewer sources of potential uncertainties. More recent machine learning statistical methods (e.g., Gaussian Processes Regression) can additionally produce assessments of the theoretical uncertainty intervals in the form of the performance likelihood computed during their training phase. However, these methods are tightly linked to the conditions and spatial relations for which they were trained. Hence, their transferability to other locations and applicability on other type of imaging spectroscopy data can potentially result in unacceptable retrieval accuracy. The physically based retrievals that involve radiative transfer simulations of photon interactions with vegetation are in principle more versatile and transferable across scales and space, but inclusion of sophisticated and complex radiative transfer models brings a higher demand on number of input parameters. Field and laboratory measurements, which are collected to satisfy this demand, introduce additional sources of potential uncertainties (i.e. imprecisions and inaccuracies) that have to be quantified and if possible reduced.

The upscaling validation schemes of imaging spectroscopy vegetation products share with the retrieval processes several sources of natural variability and measurement uncertainties, especially those related to field data collections. The magnitude of uncertainty triggered by a number of measured upscaling inputs can be reduced by developing and sharing standardized measurement protocols that use novel and more accurate measurement techniques (e.g., a laser scanning of vegetation structural features). The measurements must be conducted with precise and accurate instrumentation, in which calibrations are refereed to international standards. Additionally, the multiscale ground air- and space-borne validation schemes, carried out within a cooperative international validation campaigns, would increase robustness of vegetation remote sensing products by facilitating direct identification of actual estimation inaccuracies and by collecting sufficient amount of data for a comprehensive computation of imaging spectroscopy error propagation.

Unlike the measurement uncertainty, it is unfeasible and undesirable to diminish the natural variability in plant functional traits. The existing variability must be properly characterized

and included in model parameterization and product validation efforts. Regrettably, field measurements often suffer from insufficient sampling designs, resulting in an inadequate cover of the traits' variability. Here, fast technological advancements in high-throughput measurement techniques (as, for instance, rapid repetitive observations from unmanned airborne systems) and an open-access sharing of the plant spectral and functional trait databases can assist scientists with increasing representativeness of groundtruth data for upscaling imaging spectroscopy retrievals and validations from leaves to vegetation canopies.

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## **Fig. 1.**

Sources of variability and uncertainty encumbering imaging spectroscopy of vegetation originating from: I. sensor design, remote sensing data acquisition and pre-processing, II. design of algorithms retrieving quantitative vegetation traits using empirical and radiative transfer modelling (RTM) and III. parameterization of retrievals and validation of their accuracy using field data



# **Fig. 2.**

Schematic description of a multiscale upscaling strategy for validation of remotely sensed vegetation traits using the three scale levels: (1) ground measurements collected within elementary sampling units (ESU) or from individual trees (i.e. crown samples), (2) clusters of canopy pixels or individual tree crowns (i.e. crown pixels) from a very high-spatial resolution airborne imagery and (3) space-borne pixels of a lower spatial resolution corresponding to pixel clusters of ESU or tree crowns



### **Fig. 3.**

Theoretical validation of imaging spectroscopy retrieval estimates for five virtual validation sites (VS; modified according to ESA-ESTEC FLEX Bridge Study Final Report, 2016)

Malenovský et al. Page 28



### **Fig. 4.**

Interspecific (**a**) and intraspecific (**b**) species variability of four foliar biochemical traits: chlorophyll  $a + b$  (green), total carotenoids (red;  $\times$  5), dry matter (grey) and water content (blue). Data were collected at the FLUXNET sites in the Czech Republic (McGloin et al. 2018): Norway spruce site Bílý K íž (49°30′07.55″N, 18°32′2,74″; 2016), European beech site Štítná nad Vlá í (49°02′09.51″N, 17°58′1,64″; 2013) and mixed floodplain forest site Lanžhot (48°40′53.57″N, 16°56′46.79″; 2015). Leaf traits are expressed per hemisurface leaf area (i.e. half of the total leaf area). Horizontal line of each box indicates the median, the bottom and top edges of the box indicate the 25th and 75th percentiles, respectively, and the whiskers extend to 1.5 times of the interquartile range. Numbers in brackets indicate number of collected leaf samples (n)



### **Fig. 5.**

Differences in two-sided leaf optical properties, i.e. reflectance (bottom signatures) and transmittance (upper signatures), measured at adaxial side (blue) and abaxial side (green) of two broadleaved species (Fraxinus angustifolia and Populus alba) sampled at Lanžhot mixed floodplain forest stands (Czech Republic; 48°40′53.57″N, 16°56′46.79″E; 2015)

# **Table 1**

# **Characteristics of canopy-level radiative transfer models (RTMs) and their spatial error sources**

