3.1 Introduction

Fossil energy use and land use change are the dominant drivers of the accelerating increase in atmospheric CO₂ concentration and the principal causes of global climate change (IPCC 2018; IPBES 2018). Many of the observed and projected impacts of rising CO₂ concentration and increased anthropogenic pressures on natural resources portend increasing risks to global terrestrial biomes, including direct impacts on biodiversity, yet the uncertainty surrounding the forecasting of biodiversity change, future climate, and the fate of terrestrial ecosystems by biodiversity and Earth system models (ESMs) is unacceptably high, hindering informed policy decisions at national and international levels (Jetz et al. 2007; Friedlingstein et al. 2014; Rice et al. 2018). As such, the impact of our changing climate and altered disturbance regimes on terrestrial ecosystems is a major focus of a number of disciplines, including the biodiversity, remote sensing (RS), and global change research communities.

Here we provide an overview of approaches to scale and map plant functional traits and diversity across landscapes with a focus on current approaches, leveraging on best practices provided by Schweiger (Chap. 15), benefits and issues with general techniques for linking and scaling traits and spectra, and other key considerations that need to be addressed when utilizing RS observations to infer plant functional traits across diverse landscapes.
3.1.1 Plant Traits and Functional Diversity

The importance of characterizing leaf and plant functional traits across scales is tied to the crucial role these traits play in mediating ecosystem structure, functioning, and resilience or response to perturbations (Lavorel and Garnier 2002; Reich et al. 2003; Wright et al. 2004; Reich 2014; Funk et al. 2017). The structural, biochemical, physiological, and phenological properties of plants regulate the growth and performance or fitness of plants and their ability to propagate or survive in diverse environments. As such, these traits are used to characterize the axes of variation that define broad plant functional types (PFTs), which in turn describe global vegetation patterns and properties (Ustin and Gamon 2010; Díaz et al. 2015), particularly in ESMs (Bonan et al. 2002; Wullschleger et al. 2014). Our focus here will be on leaf traits related to nutrition and defense that broadly fit within the concept of the leaf economics spectrum (LES, Wright et al. 2004), because these are most amendable to measurements using spectral methods. Other traits relating to reproductive strategies, hydraulics, physiology (though see Serbin et al. 2015), wood characteristics, etc. may be inferred from the traits described here, especially when combined with climate, soils, topography, or other data that generally are not directly detectable using RS.

Leaf nutritional properties and morphology are strong predictors of the photosynthetic capacity, plant growth, and biogeochemical cycling of terrestrial ecosystems (Aber and Melillo 1982; Green et al. 2003; Wright et al. 2004; Díaz et al. 2015). With respect to litter turnover and nutrient cycling, leaf traits that correspond to the distribution and magnitude of structural carbon and chemical compounds such as lignin and cellulose are used to infer the recalcitrant characteristics of canopy foliage (Madritch et al., Chap. 8). Capturing the spatial variation in these traits can therefore provide critical information on the nutrient cycling potential of ecosystems (Ollinger et al. 2002). On the other hand, leaf mass per area (LMA)—the ratio of a leaf’s dry mass to its surface area—and its reciprocal, specific leaf area (SLA), correspond to a fundamental trade-off of leaf construction costs versus light-harvesting potential (Niinemets 2007; Poorter et al. 2009). The amount of foliar nitrogen within a leaf, on a mass (N_{\text{mass}} \text{, } \%) or area (N_{\text{area}} \text{, g/m}^2) basis, strongly regulates the photosynthetic capacity of leaves given its fundamental role in the light-harvesting pigments of leaves (chlorophyll a and b) and photosynthetic machinery, namely, the enzyme RuBisCo (Field and Mooney 1986; Evans and Clarke 2018). Other traits, such as the concentration or content of water and accessory pigments, are important indicators of plant health and stress (Ustin et al. 2009). Moreover, the covariation of traits is also a primary focus of ecological and biodiversity research given strong trade-offs defining different leaf form and function (Díaz et al. 2015). For example, across the spectrum of plant functional diversity (Wright et al. 2004), foliar nitrogen and LMA form a key axis of variation that describes end-members between “cheap” thinner, low-LMA leaves with high leaf nitrogen, higher photosynthetic rates and faster turnover versus thick, expensive leaves with high LMA, low nitrogen, slower turnover, and longer leaf life spans. Other traits with strong
evidence for detection in the literature relate to plant allocation strategies (e.g., starch and sugar content) or defense compounds, such as phenolics (e.g., Asner et al. 2015; Kokaly and Skidmore 2015; Couture et al. 2016; Ely et al. 2019).

Despite the importance of characterizing leaf and plant functional traits across global biomes, the plasticity and high functional diversity of these traits makes this apparently simple goal extremely challenging (Reich et al. 1997; Wu et al. 2017; Osnas et al. 2018), and as such global coverage has been historically limited to specific biomes (Schimel et al. 2015). Leaf traits can vary strongly within and across species (Serbin et al. 2014; Osnas et al. 2018) and are strongly mediated by an array of biotic and abiotic factors (Díaz et al. 2015; Neyret et al. 2016; Butler et al. 2017). Within a canopy, for example, functional traits typically show high variation with average light condition and quality (Niinemets 2007; Neyret et al. 2016) where lower canopy leaves tend to be thinner and have lower photosynthetic rates and altered pigment pools to account for the lower light quality. Plant traits can also change across local resource gradients, including with variations in water, nutrient availability, and disturbance legacy (Singh et al. 2015; Butler et al. 2017; Enquist et al. 2017). Importantly, this pattern can be confounded by species composition, which is generally the strongest driver of trait variation.

RS has provided new avenues to explore trait variation at larger scales and continuously across landscapes (Fig. 3.1). For example, Dahlin et al. (2013) observed that leaf functional traits were more strongly mediated by plant community composition than environment across a water-limited Mediterranean ecosystem, explaining 46–61% of the variation on the landscape. Likewise, McNeil et al. (2008) found that 93% of variation in nutrient cycling in northern hardwood forests of the US Adirondacks could be explained by species identity. Yet the presence or absence of specific plant species is, in part, a consequence of habitat sorting processes and the adaptive mechanisms of plants that influence the environments in which they can persist, including their modification of traits in response to local conditions (Reich et al. 2003). Mapping species or communities to infer traits is impractical at anything other than the local scale due to the presence of more than 200,000 plant species on Earth. Dispersal and other stochastic processes also play a role. Across broad environmental gradients, traits display much larger variation, where climate, topography, and edaphic conditions drive changes in plant community composition and structure, which, in turn, drive the patterns of potential and realized plant traits in any one location (Díaz et al. 2015; Butler et al. 2017). Finally, factors such as convergent evolution may make some species spectrally similar, while phenology and phenotypic variation may make the same species look different across locations.

Temporal regulation of traits is a key factor driving changes in functional properties and the resulting functioning of the ecosystem. Seasonal changes in traits can be significant (e.g., Yang et al. 2016) and can strongly regulate vegetation functioning (e.g., Wong and Gamon 2015). Moreover, during the lifetime of a leaf, traits can change significantly (e.g., Wilson et al. 2001; Niinemets 2016), and in evergreen species, leaf age has been shown to be a strong covariate with functional trait values (e.g., Chavana-Bryant et al. 2017; Wu et al. 2017). Age-dependent and phenological changes in leaf traits can, in turn, have significant impacts on ecosystem functioning.
Given the role plant traits play in community assembly, characterizing the distribution, spatial patterns, and seasonality of traits is crucial for improved prediction of biodiversity change and ecosystem responses to global change. Numerous plant trait databases have been developed to store information on the variation in functional traits across space and time (e.g., Wright et al. 2004; Kattge et al. 2011; LeBauer et al. 2018) needed to inform biodiversity and ecological modeling research. However, repeated direct measurement of plant traits is logistically challenging, which limits the geographic and temporal coverage of trait variation in these databases. Moreover, capturing plant trait variation through time is critical, but currently lacking from most observations (but with notable exceptions, e.g., Stylinski et al. 2002; Yang et al. 2016) given a host of additional technical and monetary challenges. In particular, efforts to collect direct, repeat samples of functional traits in remote areas, such as high-latitude ecosystems and the remote tropics, can be severely hindered by access and other logistical considerations.

On the other hand, RS can provide the critical unifying observations to link in-situ measurements of plant traits to the larger spatial and temporal scales needed to improve our understanding of global functional and plant biodiversity (Fig. 3.1, Table 3.1). As such, a strong interest in the use of RS to characterize foliar functional traits and their diversity has emerged from three key areas: research in RS of leaf optical properties (Jacquemoud et al. 2009), the concept of the leaf

Fig. 3.1 There is a strong coupling between vegetation composition, structure and function, and the signatures observed by remote sensing instrumentation. Passive optical, thermal, and active sensing systems can be used to identify and map a range of phenomena, including minor to major variation in vegetation properties, health, and status across a landscape. Specifically, high spectral resolution imaging spectroscopy data can be used to infer functional traits of the vegetation through the measurement of canopy-scale optical properties which are driven by variation in leaf biochemistry and morphology, as well as overall canopy structure.
| Functional characterization | Trait | Example of functional role | Example Citations |
|-----------------------------|-------|-----------------------------|-------------------|
| PRIMARY                     | Foliar N (% dry mass or area based) | Critical to primary metabolism (e.g., Rubisco). | Johnson et al. (1994), Gastellu-Etchegorry et al. (1995), Mirik et al. (2005), Martin et al. (2008), Gil-Pérez et al. (2010), Gökkaya et al. (2015), Kalacska et al. (2015), Singh et al. (2015) |
|                             | Foliar P (% dry mass) | DNA, ATP synthesis | Mirik et al. (2015), Mutanga and Kumar (2007), Gil-Pérez et al. (2010), Asner et al. (2015) |
|                             | Sugar (% dry mass) | Carbon soiree | Asner and Martin (2015) |
|                             | Starch (% dry mass) | Storage compound, carbon reserve | Matson et al. (1994) |
|                             | Chlorophyll-total (ng g⁻¹) | Light-harvesting capability | Johnson et al. (1994), Zarco-Tejada et al., (2000a); Moorthy et al., (2008); Gil-Pérez et al. (2010), Zhang et al. (2008) |
|                             | Carotenoids (ng g⁻¹) | Light harvesting, antioxidants | Datt (1998), Zarco-Tejada et al. (2000a) |
|                             | Other pigments (e.g., anthocyanins; ng g⁻¹) | Photoprotection. NPQ | van den Berg and Perkins (2005) |
|                             | Water content (% fresh mass) | Plant water status | Gao and Goetz (1995), Gao (1996), Serrano et al., (2000), Asner et al. (2015) |
| PHYSICAL                    | Leaf mass per area (g m⁻²) | Measure of plant resource allocation strategies | Asner et al. (2015), Singh et al. (2015) |
|                             | Fiber (% dry mass) | Structure, decomposition | Mirik et al. (2005), Singh et al. (2015) |
|                             | Cellulose (% dry mass) | Structure, decomposition | Gastellu-Etchegorry et al. (1995), Thulin et al. (2014), Singh et al. (2015) |
|                             | Lignin (% dry mass) | Structure, decomposition | Singh et al. (2015) |
| METABOLISM                  | Vcmax (μmol m⁻² s⁻¹) | Rubisco-limited photosynthetic capacity | Serbin et al. (2015) |
|                             | Photochemical Reflectance Index (PRI) | Indicator of non-photochemical quenching (NPQ) and photosynthetic efficiency, xanthophyll cycle | Gamon et al. (1992), Asner et al. (2004) |
|                             | Fv/Fm | Photosynthetic capacity | Zarco-Tejada et al. (2000c) |
economics spectrum (Wright et al. 2004), and the development of global-scale foliar trait databases (Kattge et al. 2011). Within the signals observed by passive optical, thermal, and active sensing systems, such as light detection and ranging (lidar) platforms, is a whole host of underlying leaf chemical, physiological, and plant structure information that drives the spatial and temporal variation in RS observations (Ollinger 2011; Figs. 3.1, 3.2, and 3.3). As a result, RS provides the only truly practical approach to observing spatial and temporal variation in plant traits, canopy structure, ecosystem functioning, and biodiversity in absence of being able to map all species or communities everywhere (Schimel et al. 2015; Jetz et al. 2016). RS observations can provide the synoptic view of terrestrial ecosystems and capture changes on the landscape from disturbances and necessary temporal coverage via multiple repeat passes or targeted collection at specific phenological stages, yielding information needed to fill critical gaps in trait observations across global biomes (Cavender-Bares et al. 2017; Schimel et al., Chap. 19).

### Table 3.1 (continued)

| Functional characterization<sup>a</sup> | Trait | Example of functional role | Example Citations |
|----------------------------------------|-------|---------------------------|-------------------|
| Secondary                              | Bulk phenolics (% dry mass) | Stress responses | Asner et al. (2015) |
|                                        | Tannins (% dry mass) | Defenses, nutrient cycling, stress responses | Asner et al. (2015) |

<sup>a</sup>Categories of functional characterization are for organizational purposes only: Primary refers to compounds that are critical to photosynthetic metabolism; Physical refers to non-metabolic attributes that are also important indicators of photosynthetic activity and plant resource allocation; Metabolism refers to measurements used to describe rate limits on photosynthesis; and Secondary refers compounds that are not directly related to plant growth, but indirectly related to plant function through associations with nutrient cycling, decomposition, community dynamics, and stress responses.

#### 3.1.2 Historical Advances in Remote Sensing of Vegetation

Over the last four-plus decades, passive optical RS has been used as a key tool for characterizing and monitoring the composition, structure, and functioning of terrestrial ecosystems across space and time. For example, spectral vegetation indices (SVIs), such as the normalized difference vegetation index (NDVI), have been used to capture broad-scale plant seasonality or phenology and changes in composition, monitor plant pigmentation and stress, and track changes in productivity through time and in response to environmental change (e.g., Goward and Huemmrich 1992; Kasischke et al. 1993; Myneni and Williams 1994; Gamon et al. 1995; Ahl et al. 2006; Mand et al. 2010). Platforms, such as the Advanced Very High Resolution Radiometer (AVHRR), originally designed for atmospheric research, have been
leveraged to capture changes in plant “greenness” based on the ratio of red absorption in leaves (signal of pigmentation levels and change) to near-infrared reflectance (tied to internal cellular structure and water content) to monitor changes in plant vigor and change (e.g., Tucker et al. 2001; Zhou et al. 2001; Goetz et al. 2005; Goetz et al. 2006). With the advent of focused Earth-observing (EO) sensors, such as the Landsat constellation, the science and use of optical RS observations for monitoring plant properties and functioning increased substantially (e.g., Chen and Cihlar 1996; Turner et al. 1999; Townsend 2002; Jones et al. 2007; Sonnentag et al. 2007; Drolet et al. 2008; Foster et al. 2008; Peckham et al. 2008; Yilmaz et al. 2008). Since the earliest uses, optical RS observations from the leaf to suborbital to satellite EO platforms have been heavily leveraged in the plant sciences, RS, and biodiversity communities (e.g., Jacquemoud et al. 1995; Roberts et al. 2004; Ustin et al. 2004; Gitelson et al. 2006; Hilker et al. 2008; Pettorelli et al. 2016; Cavender-Bares et al. 2017).
3.1.3 Remote Sensing as a Tool for Scaling and Mapping Plant Traits

The use of leaf-level spectroscopy to understand plant functioning via biochemistry dates to the early twentieth century with papers describing light absorption and reflectance (Shull 1929; McNicholas 1931; Rabideau et al. 1946; Clark 1946; Krinov 1953). Billings and Morris (1951) made a direct linkage to differing ecological strategies of plants, in particular demonstrating that visible and near-infrared reflectance of species growing in different environments is directly linked to strategies associated with thermoregulation. Similarly, Gates et al. (1965) connected the interaction of light with leaves to internal leaf pigments and leaf structure (Fig. 3.2.) and how this relates to larger ecological processes.

By the 1970s, work with spectrophotometers at the US Department of Agriculture (USDA) led to the use of spectral methods for constituent characterization—near-infrared spectroscopy (NIRS) to predict moisture, protein, fat, and carbohydrate content of feed (Norris and Hart 1965; Norris et al. 1976; Shenk et al. 1981; Davies 1998; Workman and Weyer 2012), generally using linear regression on dry samples. In the 1980s and 1990s, field and laboratory studies used these earlier spectrometer systems to develop relationships and approaches to link leaf optical properties and underlying biochemical and structural properties, including variations in leaf moisture condition (Hunt and Rock 1989). For example, Elvidge (1990) utilized

Fig. 3.3 High spectral resolution measurements of leaves and plant canopies enable the indirect, non-contact measurement of key structural and chemical absorption features that are associated with the physiological and biochemical properties of plants.
spectroscopy to describe optical properties of dried plant materials in the 0.4–2.5 micron range that enable detection of plant biochemistry from spectroscopy. Similarly, Curran (1989) summarized spectral features across this same spectral range that could be used in RS of plants, identifying not just the specific absorption features associated with pigments but also features related to harmonics and overtones related to molecular bonds of hydrogen (H) with carbon (C), nitrogen (N), and oxygen (O) in organic compounds (e.g., Fig. 3.3). In addition, by the late 1980s, researchers began to utilize novel, experimental airborne imaging spectrometer systems to map vegetation canopy chemistry in diverse landscapes. Using an early-generation NASA imaging spectrometer, the airborne imaging spectrometer (AIS, Vane and Goetz 1988), these studies illustrated the capacity to map landscape variation in foliar biochemical properties, including nitrogen and lignin (Peterson et al. 1988; Wessman et al. 1988; Wessman et al. 1989). AIS was the precursor to the Airborne Visible/Infrared Imaging Spectrometer (AVIRIS, Vane 1987). Following on this work, several others explored the impacts of leaf functional traits on reflectance properties of plant canopies and the ability to retrieve canopy chemistry, leveraging several important airborne campaigns including the Oregon Transect Ecosystem Research (OTTER) project and the Accelerated Canopy Chemistry Program (ACCP) (e.g., Card et al. 1988; Peterson et al. 1988; Matson et al. 1994; Bolster et al. 1996; Martin and Aber 1997).

These early studies became the basis for studies using imaging spectrometry to infer nutrient use and cycling in natural ecosystems (e.g., Martin and Aber 1997; Ollinger et al. 2002; Ollinger and Smith 2005). By the 1990s, the promise of spectroscopy for ecological characterization led to the increased use of handheld portable spectrometers in the field (e.g., instruments from Analytical Spectral Devices, GER, Spectra Vista Corporation, Spectral Evolution, Ocean Optics, LiCor, and PP Systems), as well as research that led to the use of narrowband SVIs for characterizing rapid changes in leaf function in response to the environment and leaf physiology (e.g., photochemical reflectance index, PRI, Gamon et al. 1992; Penuelas et al. 1995; Gamon et al. 1997). The review by Cotrozzi et al. (2018) provides a more detailed summary of the history of spectroscopy for plant studies, while Table 3.1 provides a summary of the key functional traits observable with spectroscopic RS approaches. As a consequence of studies at the leaf level and using early imaging spectrometers, a host of airborne sensor systems emerged, such as AVIRIS (Green et al. 1998), HyMap (Cocks et al. 1998), Airborne Prism Experiment (APEX, Schaepman et al. 2015), the Carnegie Airborne Observatory (CAO, Asner et al. 2012), AVIRIS-Next Generation (Miller et al. 2018; Thompson et al. 2018), and the US National Ecological Observatory Network (NEON) imaging spectrometer (Kampe et al. 2010) in the twenty-first century. The NASA prototype satellite EO-1 (Middleton et al. 2013) included the Hyperion sensor as an early test of the capacity to make hyperspectral measurements from space, leading to the development of a number of spaceborne missions planned for the early 2020s (Schimel et al., Chap. 19).
3.1.4 Key Considerations for the Use of Imaging Spectroscopy Data for Scaling and Mapping Plant Functional Traits

One of the chief challenges to effectively using imaging spectroscopy has been the acquisition of data of sufficient resolution, quality, and consistency for broad application in vegetation studies (Table 3.2). This necessitates measurements in the shortwave infrared (SWIR, 1100–2500 nm) in addition to the visible and near infrared (VNIR, 400–1100 nm). While VNIR wavelengths are most sensitive to pigments and overall canopy health, longer wavelengths are required to retrieve many biochemicals and LMA (Serbin et al. 2014; Kokaly and Skidmore 2015; Serbin et al. 2015; Singh et al. 2015). Spectral resolution is critical as well, with 10 nm band spacing and 10 nm full-width half maximum (FWHM) generally considered essential to identify traits detected based on narrow absorption features. Even finer resolution is required to detect spectral features that rely on narrow (<0.5 nm) atmospheric windows, such as solar-induced fluorescence (SIF, Yang et al. 2018). Other key considerations include sufficient signal-to-noise ratio (SNR) to identify important spectral features, accounting for both coherent and random noise related to detector sensitivity, dark current, and stray light. Additional sensor characteristics important to using imaging spectroscopy include spectral distortion. Most sensors are push-broom sensors, in which an image is constructed via the forward movement of the platform. Spatial samples are measured in the X-dimension (pixels) of the detector array and spectral wavelengths in the Y-dimension. Nonuniformity may arise due to differences in detectors in both dimensions, meaning that different detectors in the X-dimension see different central wavelengths (smile) and offsets in the Y-dimension lead to band-to-band misregistration (keystone). All of these effects can influence the ability to detect traits reliably within one scene or across multiple scenes using common algorithms. Full understanding of detector (and thus image) uniformity as well as the measurement point-spread function in 3-D (spatial X [detector X], spatial Y [platform movement], and spectral [detector Y]) is critical to accurate retrievals.

All RS data require some level of post-processing. Imaging spectroscopy is no different; prior to implementing algorithms for trait retrieval (Sect. 3.2.2), additional efforts must be undertaken to ensure consistent measurements in consistent units such that retrievals from imagery from multiple sources, dates, locations, etc. can be compared. Minimally, pixel measurements should be converted to radiances (w m\(^{-2}\) sr\(^{-1}\) nm\(^{-1}\)) based on laboratory calibrations and regular vicarious measurements of stable targets. With proper instrument characterization, keystone, smile, and other radiometric artifacts can be reduced. Subsequently, atmospheric corrections to convert radiance to reflectance (percent) are essential for cross-site studies. The approaches to atmospheric correction are numerous and tailored to particular environments, e.g., terrestrial vs. aquatic systems. Even within terrestrial applications, approaches differ among airborne data products (e.g., NASA’s AVIRIS-Classic and AVIRIS-NG sensors vs. NEON AOP) and do not necessarily yield consistent reflectance imagery. Finally, new approaches that take advantage of
Table 3.2 Traceability matrix for a global imaging spectroscopy mission for terrestrial ecosystem functioning and biogeochemical processes

| Science target                                                                 | Science objectives                                                                                                                                                                                                 | Functional characterization | Trait                                     | Spectral range and sampling | Other measurement characteristics                                                                 | Example citations                                                                 |
|--------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------|------------------------------------------|----------------------------|---------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------|
| Theme III: Marine and Terrestrial Ecosystems and Natural Resource Management  | New essential measurements of the biochemical, physiological and functional attributes of the Earth’s terrestrial vegetation                                                                                               | Primary biochemical content | Foliar N (% dry mass or area based)     | 450–2450 nm @ ≤15 nm                       | Seasonal cloud free measurement for ≤ 80% terrestrial vegetation areas. Radiometric range and sampling to capture range of vegetation signals from tropical to high latitude summers. Signals-to-Noise Ratio consistent with tropical to high latitude vegetation (e.g., red region, >500:1). At least three years of measurement to capture inter-annual variability and seasonally as robust baseline for ≥80 of the terrestrial ecosystems. | Johnson et al. (1994), Gastellu-Etchegorry et al. (1995), Mirik et al. (2005), Martin et al. (2008), Gil-Pérez et al. (2010), Gökkaya et al. (2015), Kalacska et al. (2015), Singh et al. (2015) |
|                                                                                   |                                                                                           | Foliar P (% dry mass)                                                                                                                             | 450–2450 nm @ ≤15 nm                                                   |                                                                           | Mirik et al. (2005), Mutangao and Kumar (2007), Gil-Pérez et al. (2010), Asner et al. (2015) |

(continued)
| Science target | Science objectives | Functional characterization | Trait | Spectral range and sampling | Other measurement characteristics | Example citations |
|----------------|--------------------|----------------------------|-------|----------------------------|-----------------------------------|-------------------|
|                |                    |                            | Sugar (% dry mass) | 1500–2400 nm @ ≤15 nm |                                   | Asner and Martin (2015) |
|                |                    |                            | Starch (% dry mass) | 1500–2400 nm @ ≤15 nm |                                   | Matson et al. (1994) |
|                |                    |                            | Chlorophyll-total (mg g\(^{-1}\)) | 450–740 nm @ ≤10 nm |                                   | Johnson et al. (1994), Zarco-Tejada et al. (2000a), Gil-Perez et al. (2010), Zhang et al. (2008), Kalacska et al. (2015) |
|                |                    |                            | Carotenoids (mg g\(^{-1}\)) | 450–740 nm @ ≤10 nm |                                   | Datt (1998), Zarco-Tejada et al. (2000a) |
|                |                    |                            | Other pigments (e.g., anthocyanins; mg g\(^{-1}\)) | 980 nm ± 40, 1140 ± 50 @ ≤20 nm |                                   | van den Berg and Perkins (2005) |
|                |                    |                            | Water content (% fresh mass) | 1100–2400 nm @ ≤20 nm |                                   | Gao and Goetz (1995), Gao (1996), Thompson et al. (2015), Asner et al. (2016) |
|                |                    |                            | Leaf mass per area (g m\(^{-2}\)) | 1500–2400 nm @ ≤20 nm |                                   | Asner et al. (2015), Singh et al. (2015) |
|                |                    |                            | Fiber (% dry mass) | 1500–2400 nm @ ≤20 nm |                                   | Mirik et al. (2005), Singh et al. (2015) |
| Physical/structural content | Cellulose (% dry mass) | 1500–2400 nm @ ≤20 nm | Gastellu-Etchegorry et al. (1995), Thulin et al. (2014), Singh et al. (2015) |
|-----------------------------|------------------------|------------------------|-------------------------------------------------------------------|
|                             | Lignin (% dry mass)    | 1500–2400 nm @ ≤15 nm  | Johnson et al. (1994), Gastellu-Etchegorry et al. (2014), Thulin et al. (2014), Singh et al. (2015) |
| Metabolism                  | Vcmax (μmol m⁻² s⁻¹)   | 450–2450 nm @ ≤15 nm   | Serbin et al. (2015)                                              |
|                             | Photochemical Reflectance Index (PRI). | 450 to 650 nm @ ≤10 nm | Gamon et al. (1992), Asner et al. (2004) |
|                             |                        | 450 to 800 nm @ ≤20 nm |                                                                   |
|                             | Fraction of absorbed photosynthetically active radiation by chlororphyll, fAPARchl. |            |                                                                   |
| Secondary biochemical content | Bulk phoeolics (% dry mass) | 1100–2400 nm @ ≤10 nm | Asner et al. (2015)                                                |
|                             | Tannins (% dry mass)   | 1100–2400 nm @ 10 nm   | Asner et al. (2015)                                                |
| Required for atmospheric correction | Water vapor Cirrus clouds Aerosos | 980 nm ± 50, 1140 ± 50 @ ≤20 nm | Thompson et al. (2015), Gao et al. (1993) |
|                             |                        | 940 nm ± 30, 1140 ± 40 @ ≤20 nm |                                                                   |
|                             |                        | 450–1200 nm @ ≤20 nm   |                                                                   |
advances in computing capacities and newer optimal estimation (OE) approaches for radiative transfer retrieval of atmospheric parameters are poised to transform atmospheric correction in the 2020s (Thompson et al. 2018).

Following atmospheric correction, scene-dependent corrections are often required, including corrections for different illumination and reflectance due to sun-target-sensor geometry, i.e., the bidirectional reflectance distribution function (BRDF). Current methods to correct for across-track (and along-track) illumination variation account for differences in vegetation structure and density, either through continuous functions (Schläpfer et al. 2015; Weyermann et al. 2015) or using land-cover stratification (Jensen et al. 2018). However, BRDF corrections are also rapidly changing and likely will be improved by new OE methods. As well, methods requiring land-cover stratification are generally limited to local studies, whereas broad-scale implementation across biomes and through time will be most stable as long as scene-specific stratification is not required.

In addition to BRDF, corrections for topographic illumination are required (Singh et al. 2015). However, such corrections can result in poor performance for highly shaded slopes; they enhance noise on shaded slopes while suppressing signal on illuminated slopes. In addition, differential illumination may still remain in images due to multiple sensor artifacts as well as effects of vegetation structure (Knyazikhin et al. 2013). These effects can be effectively addressed using vector normalization (Feilhauer et al. 2010; Serbin et al. 2015) or continuum removal (e.g., Dahlén et al. 2013). Such approaches largely address structure-induced reflectance effects of broadleaf and graminoid canopies, with minor variances remaining in conifers. The residual effect of canopy structure on trait mapping largely relates to an inability to fully account for within-canopy scattering of diffuse radiation, especially in conifer forests.

Finally, when integrating data from multiple sources to map canopy traits, users must address wavelength calibrations. Different sensors may have different band centers, and these may change (on airborne devices) as they are recalibrated from time to time. This requires image resampling, which is data and processing intensive and—to be done precisely—requires good knowledge of spectral response functions or model recalibration to new wavelengths.

### 3.2 Linking Plant Functional Traits to Remote Sensing Signatures

All materials interact with light energy in different and characteristic ways. With respect to terrestrial ecosystems, spectroscopic RS leverages spectroradiometers, which measure the intensity of light energy reflected from or transmitted through leaves, plant canopies, or other materials (e.g., wood, soil, Fig. 3.3). The absorbing and scattering properties of the individual elements (e.g., leaves, twigs, stems) within the canopy or surface (soil) are defined by their physical and 3-D structure as well as chemical constituents or bonds (Figs. 3.2 and 3.3), which drives the vari-
ability observed in reflectance spectra (Figs. 3.1 and 3.4). Thus, the underlying variation in plant canopy structure, function, and leaf traits in turn drives the optical properties and spectral signatures detected by RS platforms (Ollinger 2011). As such, the capacity to infer plant health, status, stress, and leaf and plant functional traits with optical RS observations is tied to the physical principle that plant physiological properties, structure, and distribution of foliage within plant canopies are reflected in the RS signatures of leaves within a canopy (Curran 1989; Kokaly et al. 2009; Ollinger 2011).

3.2.1 Spectroscopy and Plant Functional Traits

With the advent of laboratory and field spectrometer instrumentation, the leaf to landscape-scale RS of vegetation traits and functional properties began in earnest in the early 1980s (Sect. 3.1.3). As stated in Sect. 3.1.4, there are a host of important
considerations with the use of leaf and imaging spectroscopy for scaling plant functional traits. In addition, the underlying drivers of vegetation optical properties are complex and numerous (Ustin et al. 2004; Ollinger 2011). For example, in the visible range (~0.4–0.75 microns) of the electromagnetic (EM) spectrum, the strong absorption of solar energy by photosynthetic pigments in healthy, green foliage dominates the optical properties of leaves (Ustin et al. 2009; Figs. 3.2. and 3.3). Importantly, knowledge of leaf pigment pools and fluxes provides key insight into plant photosynthesis, environmental stress, and overall vigor. As such a significant amount of research has focused on the retrieval of foliar primary and accessory pigments using spectroscopic and other RS measurements (e.g., Jacquemoud et al. 1996; Richardson et al. 2002; Sims and Gamon 2002; Ustin et al. 2009; Féret et al. 2017). Blackburn (2007) and Ustin et al. (2009) provide more detailed reviews on the use of spectroscopy to remotely sense pigments in higher plants.

Within the near-infrared (NIR, ~0.8–1.2 microns) portion of the EM spectrum, optical signals are generally dominated by scattering from internal leaf structures, structural properties, water, and leaf epidermal layer (Figs. 3.2 and 3.3). In addition, strong leaf water absorption features in the NIR, centered on ~0.97 and 1.1 microns, are often used to remotely sense vegetation water content (e.g., Hunt and Rock 1989; Gao and Goetz 1995; Sims and Gamon 2003; Stimson et al. 2005; Colombo et al. 2008). Much of the early research into the use of spectroscopic RS focused on leaf and canopy water content retrieval given its importance in plant function and as an important indicator of moisture (Fig. 3.5) and other stress. In attached, fresh leaf material, water also dominates the spectral absorption features of the SWIR (1.3–2.5 micron) portion of the EM (Hunt and Rock 1989; Sims and Gamon 2003); as a result, spectral optical properties are strongly regulated by leaf and canopy water content in this region (Fig. 3.5). Along with water absorption, a number of other biochemical and structural trait absorption features exist in the SWIR wavelength region (Fig. 3.3), including cellulose, lignin, structural carbon, and nutrients and proteins (Curran 1989; Elvidge 1990; Kokaly et al. 2009; Ollinger 2011; Ely et al., 2019). Removal of water from leaf materials can sometimes enhance the detection of these absorption features (e.g., see Serbin et al. 2014 and references within; Fig. 3.5). However, at the canopy scale, a number of studies have demonstrated the capacity to retrieve these foliar biochemical properties in the SWIR region (e.g., Wessman et al. 1988; Martin and Aber 1997; Townsend et al. 2003; Kokaly et al. 2009; Asner et al. 2015; Singh et al. 2015), perhaps because of the increased signal due to multiple scattering within canopies (Baret et al. 1994).

In addition to the underlying leaf biochemical and structural characteristics, leaf orientation, display, and distribution in a canopy are also strong drivers of plant optical properties (Ollinger, 2011; Fig. 3.4). Decreasing the leaf area of a canopy generally results in a higher reflectance signal from elements deeper within the canopy, including twigs, branches, stems, and soil/litter layer (Asner 1998; Asner et al. 2000; Ollinger 2011). Canopies with flat, horizontal leaves tend to have higher NIR reflectance than those with more erect, vertical leaves, depending on the sun-sensor geometry. Leaf anatomy and average leaf angle vary widely across species
Fig. 3.5. Together, leaf optical properties and canopy architecture regulate the remote sensing signatures observed in remote sensing data. In addition, changes in leaf internal biochemistry or structure (i.e., functional traits) as a result of biotic or abiotic factors can change these signatures over space and time. For example, a prolonged drought can cause changes in leaf internal water content and potentially a redistribution of internal pigmentation. We can simulate the potential changes in optical signatures associated with a drought using a leaf and canopy-scale radiative transfer models (RTM), in this case PROSPECT-5b (Féret JB et al. 2008) and SAIL (Verhoef and Bach 2007), to illustrate the changes in leaf and canopy spectra over the course of a low, moderate, and high drought event. Here we modified pigment and water content from low to high for a range of canopies, as represented by different LAIs, and for canopy-scale reflectance, we incorporated the sensor characteristics of AVIRIS-classic (Green et al. 1998) to illustrate what the canopy reflectance might look like from that sensor. (For illustration purposes only)
(Falster and Westoby 2003), with consequences for interpreting optical RS signatures (Ollinger 2011). Thus, when considering the use of RS approaches for mapping leaf traits, careful consideration of vegetation structure, collection characteristics, and sensor design is important.

Phenology, leaf seasonality, and leaf age are also important drivers of optical properties for a number of reasons. First, leaf traits can change significantly over the lifetime of a leaf (e.g., Wilson et al. 2001; Niinemets 2016; Chavana-Bryant et al. 2017; Wu et al. 2017), and the corresponding leaf optical properties will change in concert (Yang et al. 2016). Average leaf angle distribution can also change with leaf age or seasonally from younger, recently expanded leaves to fully expanded (Raabe et al. 2015), which can have significant impacts on canopy reflectance (Huemmrich 2013). Finally, atmospheric, insect, or other stressors typically change the chemical makeup of leaves and so their optical properties (e.g., Couture et al. 2013; Ainsworth et al. 2014; Cotrozzi et al. 2018).

### 3.2.2 Approaches for Linking Traits and Spectral Signatures

Despite the promise and utility of spectroscopy for the retrieval and mapping of plant traits across space and time, there has not been consensus or standardization of approaches and algorithm development in the RS and biodiversity communities. This is not entirely unexpected given the complexity of connecting traits and RS observations across the various scales of interest, from leaves to individual trees, communities, and landscapes (Schweiger, Chap. 15). In addition, early approaches (e.g., Peterson et al. 1988) were often later deemed inappropriate and often replaced by other techniques (e.g., Grossman et al. 1996). Access to more powerful, improved, and cheaper computing resources has also allowed for the exploration of more complex statistical and machine-learning approaches (see Schweiger, Chap. 15).

Two primary approaches have been utilized to link RS observations to functional traits—empirical, statistically based techniques and radiative transfer modeling (RTM; see also Meireles et al., Chap. 7; Ustin, Chap. 14).

#### 3.2.2.1 Empirical Scaling Approaches

With respect to empirical techniques, the use of SVIs was one of the earliest methods to explore the capacity to link a range of plant functional traits to vegetation spectra. Typically, with this approach a single SVI is linked with a trait of interest, such as leaf pigments or water content, to develop a simple statistical relationship between the trait of interest and corresponding variation in optical properties (e.g., Sims and Gamon 2003; Gitelson 2004; Colombo et al. 2008; Feret et al. 2011). The derived model is then used to estimate trait values for new leaves using only spectral measurements. This approach typically assumes the researcher has an *a priori* understanding of the links between the trait and resulting variation in the electromagnetic
An alternative approach is to explore the spectra and trait space to identify new or previously unknown SVIs that maximize the correspondence between optical properties and traits of interest (e.g., Inoue et al. 2008), akin to a data mining exercise. A challenge of this approach can be interpretation of the selected SVIs, where the resulting vegetation indices may not contain wavelengths with known absorption features relating to the trait of interest. The same general approach can also leverage multiple SVIs, provided the research avoids highly correlated portions of the spectrum (Grossman et al., 1996), to attempt to capture how variation in the trait of interest is reflected in various portions of the EM spectrum to other sites and plant species. However, a limitation to the use of SVIs has been the ability to generalize across broad canopy architectures, species, and environments due to the often site-specific modeling results or potential signal saturation issues with some SVIs (Shabanov et al. 2005; Glenn et al. 2008).

Continuous spectral wavelet transforms have been used to reduce the dimensionality of spectral data prior to developing simple statistical models (e.g., Blackburn and Ferwerda 2008). Wavelets are functions that are used to decompose a full, complex signal into simpler component sub-signals. When used with spectral data, the full reflectance signature can be decomposed in a way that allows the resulting wavelet coefficients assigned to each sub-signal to be related to concentrations of chemical constituents or other traits of interest, through standard statistical modeling approaches (e.g., linear regression). Previous studies have explored the use of wavelet methods to retrieve a host of functional traits, including pigments, water, and nitrogen content (e.g., Blackburn and Ferwerda 2008; Cheng et al. 2011; Li et al. 2018; Wang et al. 2018). Continuum removal together with band-depth analysis (Kokaly and Clark 1999) has also been utilized as a means to retrieve the chemical composition of leaves. In this approach, continuum removal lines are fit through the absorption features of interest based on those regions not in the areas of interest, then the original spectra are divided by corresponding values of the continuum removal line. The band centers can then be found by finding the minimum of the continuum-removed spectra. Normalization of the band centers is often used to standardize the values across samples. These data are then used to develop models to predict functional traits at the leaf and canopy scales, including foliar nitrogen and recalcitrant properties, such as the amount of lignin and cellulose (Kokaly et al. 2009).

In addition to the empirical SVI approach, as discussed in Schweiger (Chap. 15), partial least-squares regression (PLSR) modeling has been used extensively in the development of spectra-trait models for measuring, scaling, and mapping plant functional traits (e.g., Ollinger et al. 2002; Townsend et al. 2003; Asner and Martin 2008; Martin et al. 2008; Dahlin et al. 2013; Singh et al. 2015; Ely et al. 2019). A key attribute of PLSR is the capacity to utilize the entire measured portion of the EM spectrum as predictors (i.e., X matrix) without requiring a priori selection of wavelengths or SVIs (Wold et al. 1984; Geladi and Kowalski 1986; Wold et al. 2001). PLSR avoids collinearity (i.e., spectral autocorrelation across wavelengths) in the predictor variables (i.e., reflectance wavelengths), even if predictors exceed
the number of observations (Geladi and Kowalski 1986; Wold et al. 2001; Carrascal et al. 2009). This is done through singular value decomposition (SVD), which reduces the X matrix down to relatively few non-correlated latent components. While PLSR was originally used in chemometrics, the features and benefits of PLSR also fit well within the goals of connecting spectral signatures to leaf functional traits. PLSR leverages the fact that different portions of the EM spectrum change in concert with various nutritional, structural, and morphological properties of leaves and canopies—in other words, leveraging the known covariance between variations in leaf optical properties and leaf traits (Ollinger 2011). Importantly, PLSR also allows for univariate or multivariate modeling where multiple predictands (i.e., Y matrix) can be modeled simultaneously with the same spectral matrix to account for the covariance between X and Y but also among the various Y (response) variables (Wold et al. 1984; Geladi and Kowalski 1986; Wold et al. 2001). Wolter et al. (2008) review of the use of PLSR in RS research, and Carrascal et al. (2009) summarize its use in ecology, as well as key features of PLSR.

Several approaches and implementations of PLSR have been used within the overarching “plant trait mapping” paradigm, including various spectral transformations and the use of prescreening of wavelengths or down-selection of suitable of pixels (e.g., Townsend et al. 2003; Feilhauer et al. 2010; Schweiger, Chap. 15; Asner et al. 2015). In a typical PLSR implementation (e.g., Fig. 3.6), foliar samples are first collected from vegetation canopies and processed to obtain the functional traits of interest. For leaf-scale algorithms, the optical properties of the leaves are typically measured in situ or within a small window (2–4 hours) prior to further

Fig. 3.6. A simple example illustrating how leaf functional traits and optical properties (e.g. reflectance) are combined in an empirical partial least-squares regression (PLSR) modeling approach to develop spectra-trait algorithms. The input traits and reflectance spectra are combined and used to train and test a PLSR model, using either cross-validation and/or independent validation (e.g., Serbin et al. 2014), and the resulting model can then be applied to other spectral measurements to estimate the traits of interest.
processing. Leaf and/or image spectra for the pixel containing the plots or sample locations are then linked with these functional trait measurements to develop the PLSR algorithm. Typically, for models utilizing imaging spectroscopy data, plot-scale estimates of traits are derived using measurements of basal area, leaf area by species, or other means to produce a weighted average of each trait by dominant species within given ground area (e.g., McNeil et al. 2008; Singh et al. 2015). The algorithm is evaluated using internal validation during model development (e.g., cross-validation) and/or using a set of training and validation data to build and test the model predictive capacity across a range of similar samples and optical properties. Some approaches utilize additional steps to characterize the uncertainties associated with the sample collection, measurements, and other issues (e.g., instrument noise) in the PLSR modeling step. For example, Serbin et al. (2014) and Singh et al. (2015) introduced a novel PLSR approach that can account for uncertainty in the prediction of trait values, which has later been used by other groups (Asner et al. 2015). Image-scale algorithms are often used to derive functional trait maps (e.g., Fig. 3.7) to explore the spatial and/or temporal patterns of traits across the landscapes of interest (e.g., Ollinger et al. 2002; McNeil et al. 2008).

Fig. 3.7. Much like developing a leaf-scale PLSR model for estimating leaf functional traits, such as leaf nitrogen concentration (Fig. 3.6), we can also utilize high spectral resolution imaging spectroscopy data, such as that from NASA AVIRIS to build models applicable at the canopy to landscape scales (e.g., Dahlin et al. 2013; Singh et al. 2015). Here we show a simple illustration of the linkage between functional traits scaled to the canopy, for example based on a weighted average of the dominant species in the plot, connected with the reflectance signature of these canopies. Once linked, we can develop PLSR algorithms conceptually similar to that of leaves resulting in canopy-scale spectra-trait models capable of mapping functional traits across the broader landscape.
While the PLSR approach produces algorithms that “weight” wavelengths by their importance in the prediction (Wold et al. 2001) of the functional traits of interest (e.g., Serbin et al. 2014), some researchers have also explored modifications to the standard PLSR approach that provide additional reductions in data dimensionality. For example, Li et al. (2008) coupled PLSR with a genetic algorithm (GA) approach to select a smaller subset of wavelengths to use in the final PLSR model for predicting leaf water content, measured as equivalent water thickness (EWT). DuBois et al. (2018) combined the SVI and PLSR approach by using all two-band AVIRIS wavelength combinations to model the relationship between spectral reflectance and ecosystem carbon fluxes across a water-limited environment. To date, the spectra-trait PLSR modeling approach has shown the capacity to characterize the widest array of leaf functional traits using the optical properties of plants across a broad range of species and ecosystems (e.g., Dahlin et al. 2013; Asner et al. 2014; Asner et al. 2015; Serbin et al. 2015; Singh et al. 2015; Couture et al. 2016).

Similar to the PLSR approach, researchers have leveraged various machine-learning approaches to connect RS observations to functional traits (e.g., Féret et al. 2018). Schweiger (Chap. 15) describes two commonly used machine-learning approaches in RS; several other approaches have also been used to model trait variation as a function of spectral measurements. More recently, Gaussian processes regression (GPR) has been recommended as superior to other machine-learning approaches for trait mapping from imaging spectroscopy data (Verrelst et al. 2012; Verrelst et al. 2016). GPR is a nonlinear nonparametric probabilistic approach similar to kernel ridge regression that directly generates uncertainty (or confidence) levels for the prediction (Wang et al. 2019). This is in contrast to PLSR uncertainties, generally assessed through permutation (Singh et al. 2015; Serbin et al. 2015). PLSR and GPR yield very similar results, both in terms of absolute trait predictions and relative scaling of uncertainties (Wang et al. 2019). PLSR is much more computationally efficient, and results are readily interpretable in terms of wavelength quantitative contribution to prediction (see Fig. 3.1 in Schimel et al., Chap. 19), whereas GPR only identifies relatively important wavelengths.

The challenge with most machine-learning approaches is that some level of data reduction is required for optimal performance. Standard approaches, such as principle component analysis (PCA) or minimum noise fraction (MNF) transformations, may reduce data dimensionality. However, features important to trait estimation may be buried in lower principle components, as high contrast variation (albedo, greenness, water content) dominate scene properties. In contrast, PLSR rotates the data into latent vectors optimized to the empirical dependent variables, which generally yields strong models for calibration data but can lead to poor model performance when confronted with new data that differ considerably from the model-building data sets.

### 3.2.2.2 Radiative Transfer Models and Scaling Functional Traits

An alternative to statistical, field-based, and empirical approaches for connecting leaf and canopy optical properties with plant functional traits, RTMs can be used either at the leaf and canopy scales to directly retrieve leaf traits (e.g., Colombo
et al. 2008; Darvishzadeh et al. 2008; Feret et al. 2011; Banskota et al. 2015; Shiklomanov et al. 2016) or in hybrid approaches where statistical algorithms are developed based on RTM simulations (e.g., Asner et al. 2011). RTMs encapsulate our best mechanistic understanding of the coordination among leaf properties, canopy structure, and resulting spectral signatures at the leaf and canopy scales, but abstracted to operate with different degrees of complexity and assumptions (Bacour et al. 2002; Nilson et al. 2003; Kobayashi and Iwabuchi 2008; See also Morsdorf et al., Chap. 4; Ustin and Jacquemoud, Chap. 14).

At the leaf scale, RTMs were generally spawned from earlier work that identified the relationships between fresh and dried leaf reflectance and a range of foliar traits, including pigments, water content, nitrogen, dry matter, cellulose, and lignin. The realization that leaf optical properties were fundamentally tied to the concentration and distribution of leaf traits led to the development of models that could closely mimic the spectral patterns across the shortwave spectral region (0.4–2.5 microns) based on select leaf properties, such as chlorophyll and water content, as well as structural variables. By far the most widely and commonly used leaf-level RTM is the PROSPECT model (Jacquemoud and Baret 1990; Feret et al. 2008), which simulates leaf directional-hemispherical reflectance (R) and transmittance (T), allowing for the calculation of leaf absorption (1-R+T) based on leaf biochemical and morphological properties, primary and accessory pigments, water content, LMA, or dry matter content, brown material, and an approximation of the thickness of the internal leaf mesophyll layer (Féret et al. 2008; Féret et al. 2017). PROSPECT then simulates leaf optical properties based on a generalized plate model describing leaves as a stack of N homogenous absorbing layers that are calculated based on the values of input leaf traits and their corresponding spectral absorption coefficient. Other prominent leaf models include the Leaf Incorporating Biochemistry Exhibiting Reflectance and Transmittance Yields (LIBERTY) model (Dawson et al. 1998) and LEAFMOD (Ganapol et al. 1998). In particular, LIBERTY is notable given its original application focusing on improving the modeling of needle-leaf evergreen conifer species and their leaf optical properties based on several leaf traits, similar to PROSPECT, but also including foliar lignin and nitrogen content.

Moving to the canopy scale, RTMs are far more numerous with a wide variety of complexities, assumptions, and requirements (Verhoef and Bach 2007; Widlowski et al. 2015; Kuusk 2018). Most canopy RTMs leverage leaf-scale models, such as PROSPECT, to provide the leaf optical properties (i.e., leaf single-scattering albedo) needed to simulate canopy directional-hemispherical reflectance across select wavelengths, simulated spectral bands, or specific SVIs. Generally, the soil boundary layer is either prescribed or simulated using a simple model of soil BRDF (e.g., Hapke model, Verhoef and Bach 2007), and stem or woody material reflectance and transmittance (when used) is prescribed. Canopy RTMs can be separated into two main classes, homogenous and heterogenous models. Homogenous models assume the canopy to be horizontally unlimited and treated as a turbid medium of sufficiently large number of phytoelements (leaves, stems, other materials). For example, the Ross–Nilson model of plate medium (Ross 1981) assumes these elements to be composed of small bi-Lambertian “plates” described by their reflectance and transmittance properties with a specific leaf angle distribution (LAD). Leaves are
small compared to the full canopy medium, with no self-shading, and transmittance is a function of optical properties and leaf area index (LAI). Additional canopy parameters were added, including the hot-spot and canopy clumping to describe sun-sensor illumination effects and the inhomogeneity of the canopy elements (Kuusk 2018). Early SAIL models also fall into this classification (e.g., Verhoef 1984). On the other hand, heterogenous canopy RTM models, including 3-D models, address the fact that vegetation canopies are heterogenous (e.g., gaps between crowns, spatial structure, differing canopy architectures) but range widely in their complexity and implementations. These models provide enhanced detail in the modeling of vegetation canopies but are necessarily more complex. Often these models require additional information to model vegetation “scenes,” which can include information on tree crown shape, stem location, and other properties (e.g., hot spot, clumping) in addition to leaf optical properties, sun-sensor geometry, and LAI. These models range from 3-D Monte Carlo ray-tracing models, such as FLIGHT (North 1996) and FLiES (Kobayashi and Iwabuchi 2008), to analytical and hybrid approaches using a variety of canopy structure schemes including geometric optical (GO) representation of individual plants where tree placement follows a statistical distribution and leaf and stem scattering elements are homogenously distributed (e.g., Kuusk and Nilson 2000; Nilson et al. 2003). For example, multiple stream, including four-stream, two-layer models often utilize simplifying assumptions, to model canopies as homogenous and continuous (i.e., “slab canopies”), but which are composed of a large number of small scattering elements (leaves, sometimes leaves and stems) with arbitrary inclination angles (e.g., 4SAIL2, Verhoef and Bach 2007). The scattering elements and the soil can be prescribed with specific optical properties using observed data or based on a leaf RTM, such as PROSPECT (Jacquemoud et al. 2009). In addition, some models can divide complex scenes into smaller cells to perform the radiative transfer calculations (e.g., DART, Gastellu-Etchegorry et al. 2015) where the level of simulation detail is based on the size of the cells and the degree of detail built into the model scene components. See the review by Kuusk (2018) for more details regarding canopy RTMs and their design, diversity, assumptions, and approaches.

The use of RTMs allows for the estimation of leaf and canopy traits using simulated canopy reflectance, without some of the limitations or challenges of empirical approaches (3.3.1), such as the requirement of field sampling, scaling leaf traits to the canopy, and other issues such as the timing of field and imagery collections. Furthermore, RTMs can provide a more mechanistic connection between traits and reflectance allowing for potentially broader application than empirical approaches in areas were ground sampling may be sparse (e.g., remote regions such as the Arctic or the tropics). In addition, RTMs provide the opportunity to prototype inversion approaches across a range of remote sensing platforms and evaluate the trade-offs between different sensor designs, spectral resolutions, and temporal coverage (Shiklomanov et al. 2016), enabling the development of cross-platform retrieval algorithms.

Depending on the application, and RTM complexity, inversion can be conducted at the pixel or larger patch scales (i.e., collections of relatively homogenous areas of
vegetation) to characterize spatial and temporal patterns in plant functional (e.g., pigments) and structural (e.g., LAI) properties. In RTM inversion, the leaf-scale model is often the focus, where the goal is to invert the canopy and leaf models jointly to extract estimated foliar traits based on observed canopy reflectance (e.g., Colombo et al. 2008). Many other studies have focused on retrieving canopy-scale parameters, such as LAI (e.g., Darvishzadeh et al. 2008; Banskota et al. 2015). Early approaches leveraged RTM inversions that focused on numerical optimization techniques to minimize the difference between modeled and observed reflectance across similar wavelengths (e.g., Jacquemoud et al. 1995). Other methods have utilized look-up table (LUT) inversion (e.g., Weiss et al. 2000) where a range of simulated canopy reflectance patterns are generated in advanced by varying leaf and canopy inputs across predetermined values. These simulated spectra are then compared to observations where either a single or select number of closely matching modeled spectra, and their associated inputs, are selected as the solution to the inversion. Bayesian RTM inversion methods have also been utilized (e.g., Shiklomanov et al. 2016) as a means to retrieve leaf and canopy properties as joint posterior probability distributions through iterative sampling of the input parameter space. The use of RTMs ranges from retrieval of vegetation functional and structural traits to the characterization of landscape functional diversity (Kattenborn et al. 2017; Kattenborn et al. 2019).

3.3 Important Considerations, Caveats, and Future Opportunities

3.3.1 Field Sampling and Scaling Considerations

There are several important considerations and best practices when developing algorithms for the remote estimation of plant traits (see Schweiger, Chap. 15). We will only briefly touch on these here. A key first step is to consider the scope of the research and area of interest, focusing specifically on considerations such as local climate conditions, terrain, vegetation, and canopy access. Specifically, the spatial locations, site, and canopy access (e.g., is it possible to reach canopy foliage?); vegetation composition and canopy architecture; timing of collection; and methods for sample retrieval are key to identify prior to field campaigns in order to maximize the utility of the field samples for conversion of RS signatures to accurate trait maps. Furthermore, it may be important to consider what approach may be best to characterize the vegetation canopy architecture and/or composition to facilitate scaling of each trait to the pixel or plot scale (e.g., using basal area, LAI). This may strongly depend on the dominant vegetation types, where more open canopies may require a different approach to a closed canopy, or on the spatial resolution of the imagery. Observational data range is a primary consideration (see Schweiger, Chap. 15), and sample locations should be chosen to cover the range of canopy types and vegetation communities that will fall within the RS observations. The timing of the field
sampling should be as close to the RS collection date as possible, as an optimal approach, but at least be selected to match the phenological stage of the vegetation during the imagery collection, if leveraging sample campaigns in following year(s).

A number of different methods have been used to collect plant functional traits to link with RS imagery (e.g., Wang et al. 2019). Common approaches for the collection of canopy leaf samples include the use of slingshot, pruning pole, and shotgun (Lausch et al., Chap. 13), but also include line-launcher and air cannon (e.g., Serbin et al. 2014); simpler tools and hand shears are often used for accessible, shorter canopies. Regardless of the sample collection approach, harvested leaves should be reasonably intact and minimally damaged in order to avoid any issues with changes in leaf chemistry from physical damage or stress. In addition, leaves should be immediately measured for leaf optical properties and fresh mass, if these are of interest, then stored in humidified and sealed bags and placed in a cool, dark place prior to transport for further processing. Processing should then be completed within 2–4 hours of sampling—though a much shorter time between sample and measurement or different sample storage and handling (e.g., flash freezing in liquid nitrogen) may be needed for specific biochemical traits. Typically top-of-canopy, sunlit samples have been the main focus; however, more recent work has also begun to focus on collection of canopy and subcanopy samples (e.g., Serbin et al. 2014; Singh et al. 2015). This provides the ability to evaluate the depth in the canopy needed to link traits with image, which may vary by vegetation type or LAI.

### 3.3.2 Evaluating Functional Trait Maps and the Need to Quantify Uncertainties

Maps of plant functional traits are useful for a wide variety of applications. From an ecological perspective, maps of plant traits across broad biotic and abiotic gradients can be used to explore the drivers of plant trait variation in relation to climate, soils, and vegetation types (e.g., McNeil et al. 2008). Modeling activities can leverage these trait maps as either inputs for model parameterization across space and time (Ollinger and Smith 2005) or to evaluate prognostic plant trait predictions. However, to maximize the utility of functional trait maps a detailed understanding of the their uncertainties across space and time is required.

In the earliest functional trait mapping work, predictive model uncertainties were limited to the “goodness of fit” and overall model root mean square error (RMSE) statistics provided by the modeling approach (e.g., Wessman et al. 1988; Martin and Aber 1997; Townsend et al. 2003). While this information is helpful to understand the accuracy of the model fit, that level of accuracy assessment is insufficient for characterizing the uncertainty of the trait maps themselves. Mapping efforts should instead provide an accounting of the trait measurement, scaling, and algorithm uncertainties and provide this information in the resulting trait map data products. However, detailed error propagation is not trivial, particularly with respect to empirical modeling approaches, and is an ongoing and active area of research in the RS
sciences and not discussed in detail here. On the other hand, efforts to provide product uncertainties do exist. Serbin et al. (2014) and Singh et al. (2015) illustrate how to incorporate data and modeling uncertainties at the leaf and canopy scales in the mapping of plant functional traits. This approach captures the uncertainties stemming from the leaf-level estimation of traits (Serbin et al. 2014) and the modeling of plot-level spectra and trait values (Singh et al. 2015) using a similar PLSR and uncertainty analysis approach. The result is an ensemble of PLSR models to apply to new RS data providing mean and error metrics for every pixel in the image. However, even approaches such as these fail to incorporate and propagate the uncertainties stemming from the atmospheric correction workflow given the challenge of extracting the information needed to enable this on a pixel-by-pixel or even a scene-by-scene basis. Future work will be required to focus on capturing this information and providing it to the end-user who conducts the trait mapping efforts.

Uncertainty in RTM approaches have generally been derived based on inversion approaches applied to imagery. For example, as described in Sect. 3.2.2.2, a commonly used approach to the inversion of RTM simulations for the RS of functional traits is the use of LUTs. Some LUT approaches provide results based on the “best fit” of the model inversion results to the RS observations. However, this only provides an assessment of error where field measurements can be used to evaluate the retrieved values. Given the challenge of equipotentiality in RTM approaches, later efforts have used an ensemble of best fit results to provide a mean and distribution of values that provide a good fit of modeled reflectance to observed (e.g., Weiss et al. 2000; Banskota et al. 2015). Using this approach allows for the description of pixel-level uncertainty based on the best fit ensembles; however, these need to be combined with an accuracy assessment to get a true uncertainty of the functional trait retrievals. More recent approaches have leveraged Bayesian inversion approaches that provide output that is not a point estimate for each parameter but rather the joint probability distribution that includes estimates of parameter uncertainties and covariance structure (Shiklomanov et al. 2016). Regardless of the approach, the key is that the derived products provide a reasonable assessment of trait uncertainty across the spatial and temporal domain (where appropriate).

3.3.3 Current and Future Opportunities in the Use of Remote Sensing to Characterize Functional Traits and Biodiversity

The ability to map foliar functional traits from imaging spectroscopy greatly expands the potential for understanding patterns of vegetation function and functional diversity both locally and broadly across biomes, especially in comparison to the challenges of fully characterizing spatial and temporal (across seasons and between years) variation using field data (e.g., the TRY database). With forthcoming spaceborne sensors (see Schimel et al., Chap. 19) and continental-scale experiments...
like the US National Ecological Observatory Network (NEON), we are able to test relationships among traits and characterize functional diversity at unprecedented scales. For example, NEON is collecting imaging spectroscopy data at 1 m resolution and waveform lidar data almost annually for 30 years at 81 10 km × 10 km sites covering 20 biomes defined for the USA. With the addition of lidar, which enables measuring traits such as plant area index, canopy height, canopy volume, and aboveground biomass (of forests), a broad suite of traits can be leveraged to test relationships that have been published in the literature (e.g., the leaf economics spectrum) and are generally tested now at global scales using extensive—but still not comprehensive—databases such as TRY. With spaceborne imaging, phenological variation in traits (e.g., Yang et al. 2016) can be further explored. For example, preliminary mapping of key functional traits across all NEON biomes in the USA shows the leaf economics spectrum relationship between LMA and nitrogen for forest and grassland ecosystems east of the US Rocky Mountains (Fig. 3.8.) in comparison to the data set used for the original LES studies, GLOPNET (Global Plant Trait Network, Wright et al. 2004; Reich et al. 2007). Importantly, the use of data from RS platforms, such as NEON, AVIRIS, and upcoming spaceborne sensors (see Schimel et al., Chap. 19), enables the filling of critical research gaps and global coverage in remote regions, as suggested by Jetz et al. (2016) and Schimel et al. (2015). The relationship does not differ significantly from published relationships but does suggest a breadth of the relationship as well as outliers for a number of observations many orders of magnitude higher than is possible from field databases. Field databases are still required for basic science studies, as well as inventory, calibration, and validation, but RS offers new possibilities for baseline characterization of Earth’s functional diversity and thus testing new hypotheses about the drivers of such variation, using the range of traits detectable from RS (Tables 3.1 and 3.2).

Fig. 3.8. LMA versus nitrogen for NEON for GLOPNET observations (black dots, truncated to observations with LMA <600) vs. pixel predictions derived for NEON sites east of the US Rocky Mountains (color gradient). Color gradient is density of pixel observations based on 333,500 pixel values randomly extracted from 447 flight NEON flight lines in 18 sites across 6 biomes.
Furthermore, coupling of spectral and functional trait databases (e.g., ecosis.org) will facilitate more rapid development and testing of new functional algorithms or the expansion of the scope of inference of existing models. In addition, the inclusion of high spectral resolution sensors on unmanned aerial systems (UASs, Shiklomanov et al. 2019) provides the opportunity to leverage similar scaling approaches as presented in this chapter with UAS observations to provide unprecedented temporal coverage and targeted spatial sampling that can be used to understand ecosystem in new detail or aid in the scaling from the plant to grid cell. In all, functional trait maps from imaging spectroscopy will supplement data and approaches presented by Butler et al. (2017) or Moreno-Martínez et al. (2018) for broad-scale trait characterization.

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