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Improving ecological forecasts using model and data constraints

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GRADUATE SCHOOL OF ARTS AND SCIENCES

Dissertation

IMPROVING ECOLOGICAL FORECASTS USING MODEL AND DATA CONSTRAINTS

by

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B.S., University of Delaware, 2014

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Gentlemen, we have run out of money. Now, we must think.

—Winston Churchill

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IMPROVING ECOLOGICAL FORECASTS USING MODEL AND DATA CONSTRAINTS

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ABSTRACT

Terrestrial ecosystems are essential to human well-being, but their future remains highly uncertain, as evidenced by the huge disparities in model projections of the land carbon sink. The existence of these disparities despite the recent explosion of novel data streams, including the TRY plant traits database, the Landsat archive, and global eddy covariance tower networks, suggests that these data streams are not being utilized to their full potential by the terrestrial ecosystem modeling community. Therefore, the overarching objective of my dissertation is to identify how these various data streams can be used to improve the precision of model predictions by constraining model parameters.

In chapter 1, I use a hierarchical multivariate meta-analysis of the TRY database to assess the dependence of trait correlations on ecological scale and evaluate the utility of these correlations for constraining ecosystem model parameters. I find that global trait correlations are generally consistent within plant functional types, and leveraging the multivariate trait space is an effective way to constrain trait estimates for data-limited traits and plant functional types. My next two chapters assess the ability to measure traits using remote sensing by exploring the links between leaf traits and reflectance spectra. In chapter 2, I introduce a method for estimating traits from spectra via radiative transfer model inversion. I then use this approach to show that although the precise location, width, and quantity of spectral bands significantly affects trait retrieval accuracy, a wide range of sensor configurations are capable of providing trait information. In chapter 3, I apply this approach to a large database of leaf spectra to show that traits vary as much within as across species, and much more across species within a functional type than across functional types. Finally, in chapter 4, I synthesize the findings of the previous chapters to calibrate a vegetation model's representation of canopy radiative transfer against observed remotely-sensed surface reflectance. Although the calibration successfully constrained canopy structural parameters, I identify issues with model representations of wood and soil reflectance that inhibit its ability to accurately reproduce remote sensing observations.

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List of Abbreviations

AVIRIS	 Airborne visible / infrared imaging spectrometer
DBH	 Diameter at breast height
ED2	 Ecosystem Demography model, version 2
EDR	 Coupled PROSPECT-ED leaf-canopy radiative transfer model
\mathbf{FFT}	 NASA Forest Functional Types field campaign
J_{max}	 Maximum photosynthetic electron transport rate
LAI	 Leaf area index
LMA	 Leaf mass per unit area
MCMC	 Markov-Chain Monte Carlo
N_{area}	 Leaf nitrogen content per unit area
N_{mass}	 Leaf nitrogen content per unit mass
P_{area}	 Leaf phosphorus content per unit area
P_{mass}	 Leaf phosphorus content per unit mass
\mathbf{PFT}	 Plant functional type
PLSR	 Partial Least-Squares Regression
PROSPECT	 PROSPECT leaf radiative transfer model
Rd_{area}	 Leaf dark respiration on a leaf area basis
Rd_{mass}	 Leaf dark respiration on a leaf mass basis
RMSE	 Root mean square error
RTM	 Radiative transfer model
SLA	 Specific leaf area
$V_{c,max}$	 Maximum photosynthetic carboxylation rate

Chapter 1

Does the leaf economic spectrum hold within plant functional types? A Bayesian multivariate trait meta-analysis

1.1 Introduction

The diversity and dimensionality of the terrestrial biosphere is vast and complex, and therefore there has been a recurring debate in ecology about the utility of reductionist approaches for capturing this variability. In particular, the use of functional groups with common characteristics has been widely applied in biodiversity studies (Naeem and Wright, 2003) and is essential to the structure of many ecosystem models (Lavorel et al., 1997; Wullschleger et al., 2014). However, ecologists have long recognized the importance of individual variability and stochasticity in shaping ecosystems(Gleason, 1926; Bolnick et al., 2011; Rosindell et al., 2011; Clark, 2016), and the benefits of more finely-resolved representation of functional diversity for predictive ecology are supported by an increasing body of trait ecology literature(Mayfield et al., 2006; McMahon et al., 2011; Van Bodegom et al., 2012; Reichstein et al., 2014; Violle et al., 2014; Medlyn et al., 2015; Moran et al., 2016).

Plant functional traits can be used to link directly measurable features of individuals to their fitness within an ecosystem and, by extension, ecosystem performance as a whole (Violle et al., 2007). Recent syntheses of global trait databases have revealed that although the functional diversity across plant species is immense, this diversity

is constrained by allometries and trade-offs between plant strategies (Wright et al., 2004; Kattge et al., 2011; Klever and Minden, 2015; Díaz et al., 2016). One axis of trait covariation currently receiving attention is the 'leaf economic spectrum', which defines a trade-off between plant investment in productive but short-lived leaves versus less productive but sturdy and long-lived leaves (Wright et al., 2004; Shipley et al., 2006; Reich, 2014; Díaz et al., 2016) Leaf economic traits are well-correlated with individual plant productivity (Shipley et al., 2005; Niinemets, 2016a; Wu et al., 2016b), litter decomposition rates (Bakker et al., 2011; Hobbie, 2015), community composition (Burns, 2004; Cavender-Bares et al., 2004), and ecosystem function (Diaz et al., 2004; Musavi et al., 2015). The relative position of plant species along the leaf economic spectrum has been shown to be influenced by climate and soil conditions(Wright et al., 2004; Wright et al., 2005b; Cornwell and Ackerly, 2009; Ordoñez et al., 2009; Wigley et al., 2016). As a result, relationships between leaf economic traits and climate have been incorporated into ecosystem models to allow for continuous variation in plant function and environmental responses (Sakschewski et al., 2015; Verheijen et al., 2015b).

However, the use of among-trait and trait-environment correlations at the global scale, for both ecological inference and land surface modeling, has several important caveats. First, observed correlations at the global scale do not always hold at smaller scales (such as sites, species, and individuals). For example, some studies suggested consistent correlations across scales(Wright et al., 2004; Albert et al., 2010a; Asner et al., 2014) whereas others showed no or even opposite correlations(Albert et al., 2010b; Messier et al., 2010; Wright and Sutton-Grier, 2012; Feng and Dietze, 2013; Grubb et al., 2015; Wigley et al., 2016; Messier et al., 2017; Kichenin et al., 2013). Many mechanisms have been suggested for deviation from global trait relationships at smaller scales. Trade-offs between strategies may only be applicable when mul-

tiple competing strategies co-occur, and in cases where strong environmental filters allow only a narrow range of strategies, alternative processes can drive community assembly (Rosado and de Mattos, 2010; Rosado and de Mattos, 2017; Grime and Pierce, 2012). Different selective pressures dominate at different scales, particularly within versus across species (Albert et al., 2010b; Messier et al., 2010; Kichenin et al., 2013), and the large heterogeneity in the variance structures of traits suggests that different traits have contrasting sensitivity to these different pressures (Messier et al., 2016). Experimental evidence shows that species can alter different aspects of their leaf economy in a relatively uncoordinated fashion, even when the direction of univariate trait responses to environmental change is consistent (Wright and Sutton-Grier, 2012). Meanwhile, across different plant functional types, resource allocation patterns, for instance of nutrients to photosynthesis versus structure and defense, differ substantially, suggesting different investment strategies and varying relationships among traits (Ghimire et al., 2017). Second, among-trait correlations at any scale do not provide causal evidence for functional trade-offs or even similarity in response to external stimuli (Messier et al., 2016). Therefore, ascribing too much leverage to trait correlations can lead to an underestimation of plant functional diversity (Grubb, 2015). Third, plants maintain their fitness in a given environment through multiple independent strategies (corresponding to multiple mutually orthogonal axes of trait variability). As a consequence, changes in key leaf economic traits such as leaf nitrogen content and specific leaf area area may not affect other aspects of plant function, such as hydraulics (Li et al., 2015), overall plant carbon budget (Edwards et al., 2014), and dispersal (Westoby et al., 2002). Finally, modeling ecosystem function based on trait correlations is sampling from the hypothetical space of potential species and communities that could have evolved, rather than constraining models to forecast the actual vegetation we have today as the result of spatial separation and constraints on convergent evolution. Among other problems, this approach fails to account for the timescales required for adaptation as well as actual limitations of the physiology of different species and community assembly.

An alternative approach is to preserve existing PFT classifications (though potentially with finer taxonomic, functional, or spatial resolution, e.g. Boulangeat et al., 2012) while using statistical analyses to account for uncertainty and variability in the aggregated trait values. For example, the Predictive Ecosystem Analyzer (PEcAn, pecanproject.org), an ecosystem model-data informatics system, parameterizes PFTs using trait probability distributions from a Bayesian meta-analysis of plant trait data across many studies (Dietze et al., 2013; LeBauer et al., 2013). This approach explicitly separates the processes driving PFT-level differentiation from processes that drive finer-scale functional variability, and is useful for guiding future data collection and model refinement (Dietze et al., 2014). However, a univariate meta-analysis, like the one currently in PEcAn, is limited by its failure to account for trait correlations, therefore neglecting useful knowledge about relationships across PFTs and between traits. At the other extreme, existing regional and global scale analyses (e.g. Van Bodegom et al., 2012; Sakschewski et al., 2015) ignore variability within PFTs, often resulting in macroecological, evolutionary, and competitive trade-offs across PFTs being used to drive both acclimation and instantaneous responses within PFTs.

While the leaf economic spectrum has been investigated at the global scale, where it is robust, and at the site or plot scale, where deviations from it are common, it has received less attention at the intermediate scale of PFTs. Thus, this paper seeks to answer the following questions: First, to what extent does the leaf economic spectrum hold within vs. across plant functional types? Second, to what extent can the leaf economic spectrum and other patterns of trait covariance be leveraged to constrain trait estimates, particularly under data limitation? The answer to these question has implications for both functional ecology and ecosystem modelling. To evaluate these questions, we develop a hierarchical multivariate Bayesian model that explicitly accounts for across- and within-PFT variability in trait correlations. We then fit this model to a global database of foliar traits to estimate mean trait values and variancecovariance matrices for PFTs as defined in a major earth system model (Community Land Model, CLM, Oleson et al., 2013). We evaluate the ability of this model to reduce uncertainties in trait estimates and reproduce observed patterns of global trait variation compared to non-hierarchical multivariate and univariate models. Finally, we assess the generality and scale dependence of trait trade-offs by comparing covariance estimates globally and within each PFT.

1.2 Materials and methods

1.2.1 Trait data

Foliar trait data for this analysis comes from the TRY global traits database (Kattge et al. 2011). We focused our research on seven foliar traits: Leaf longevity (months), specific leaf area (SLA, m² kg⁻¹), leaf nitrogen content (N_{mass} , mg N g⁻¹ or N_{area} , g N m⁻²), leaf phosphorus content (P_{mass} , mg P g⁻¹ or P_{area} , g P m⁻²), leaf dark respiration at 25 °C ($R_{d,\text{mass}}$, μ mol g⁻¹ s⁻¹, or $R_{d,\text{area}}$, μ mol m⁻² s⁻¹), maximum Rubisco carboxylation rate at 25 °C ($V_{c,\text{max},\text{mass}}$, μ mol g⁻¹ s⁻¹, or $V_{c,\text{max},\text{area}}$, μ mol m⁻² s⁻¹), and maximum electron transport rate at 25 °C ($J_{\text{max},\text{mass}}$, μ mol g⁻¹ s⁻¹, or $J_{\text{max},\text{area}}$, μ mol m⁻² s⁻¹. For $V_{c,\text{max}}$, we only used values already reported in TRY as being at 25 °C. For R_d , we normalized the values to 25 °C based on reported leaf temperature values following the same methods as Atkin et al. (2015). For J_{max} , we normalized the values to 25 °C based on reported leaf temperature response function described in Kattge & Knorr (2007, Equation 1 therein). To avoid potential artifacts caused by different trait normalization, we performed analyses sep-

arately for both mass- and area-normalized traits (Osnas et al., 2013; Lloyd et al., 2013). We restricted our analysis to TRY data that have been quality-controlled and for which adequate species information was provided for functional type classification (see Kattge et al. 2011).

Although the light- and CO2-saturated photosynthetic rate (A_{max}) was an important trait in previous studies, we did not include it in our study for two reasons. First of all, data on raw photosynthetic rates are highly sensitive to measurement methodology and environmental conditions, which were generally inconsistent or unavailable in TRY. Second, A_{max} is not a good measure of photosynthetic capacity because it integrates over variability in many physiologically independent traits such as $V_{c,\text{max}}$, J_{max} , and stomatal conductance, and is therefore not used in vegetation models as a photosynthetic parameter (Ali et al., 2015).

Following past studies (Wright et al., 2004; Wright et al., 2005a; Onoda et al., 2011; Díaz et al., 2016), we log-transformed all trait values to correct for their strong right-skewness.

1.2.2 Plant functional types

Label	PFT	Number of species
BlETr	Broadleaf Evergreen Tropical	1229
BlETe	Broadleaf Evergreen Temperate	363
BlDTr	Broadleaf Deciduous Tropical	286
BlDTe	Broadleaf Deciduous Temperate	345
BlDBo	Broadleaf Deciduous Boreal	62
NlETe	Needleleaf Evergreen Temperate	130
NlEBo	Needleleaf Evergreen Boreal	30
NlD	Needleleaf Deciduous	19
ShE	Shrub Evergreen	1120
ShDTe	Shrub Deciduous Temperate	330
ShDBo	Shrub Deciduous Boreal	94

Table 1.1: Names, labels, and species counts for plant functional types (PFTs) used in this analysis.

Label	PFT	Number of species
C3GAr	C3 Grass Arctic	157
C3GTe	C3 Grass Temperate	624
C4G	C4 Grass	255

We assigned each species to a unique plant functional type (PFT) following the scheme in the Community Land Model (CLM4.5, Oleson et al., 2013); Table 1.1, Fig. 1.1. We obtained categorical data on growth form, leaf type, phenology, and photosynthetic pathway from the TRY database. Where species attributes disagreed between datasets (e.g., categorized as a shrub in one dataset but a tree in another), we assigned the attribute that was observed most frequently between the datasets (e.g., if five datasets say "shrub" but only one says "tree", we would classify it as a shrub). Where species lacked data on certain attributes, we assigned those attributes based on higher order phylogeny where appropriate (e.g., *Poaceae* family are usually grasses, *Larix spp.* are deciduous needleleaved trees) or otherwise omitted the species from our analyses. For biome specification, we collected all latitude and longitude data for each species, matched these data to 30 second (\sim 1 $\rm km^2)$ mean annual temperature (AMT, averaged 1970–2000) data from WorldClim-2 (Fick and Hijmans, 2017), calculated the mean AMT for all sites at which that species was observed, and then binned these species based on the following cutoffs: boreal/arctic ($AMT \leq 5^{\circ}C$), temperate $(AMT \leq 20^{\circ}C)$, and tropical $(AMT > 20^{\circ}C)$.

1.2.3 Multivariate analysis

Basic model description

In this study, we compared three different models representing different levels of complexity.

The simplest model was the 'univariate' model, in which each trait was modeled independently. For an observation $x_{i,t}$ of trait t and sample i:



Figure 1.1: Sample sizes for each trait-PFT pair. y axis is scaled logarithmically.

$$x_{i,t} \sim N(\mu_t, \sigma_t)$$

where N is the univariate normal (Gaussian) distribution with mean μ_t and standard deviation σ_t for trait t.

The second-simplest model was the 'multivariate' model, in which traits were modeled as samples from a multivariate distribution with a single mean vector and covariance matrix. For the observed vector of traits \mathbf{x}_i for sample *i*:

$$\mathbf{x_i} \sim mvN(\mu, \Sigma)$$

where mvN is the multivariate normal (Gaussian) distribution with mean vector μ and variance-covariance matrix Σ . We ran both of these models independently for each PFT as well as for the entire dataset (as if every observation belonged to the same PFT).

The most complex model was the 'hierarchical' model, in which observed trait values were drawn from a PFT-specific multivariate normal distribution describing within-PFT variation and whose parameters were themselves sampled from a global multivariate distribution describing the variation across PFTs. For the observed vector of traits $\mathbf{x}_{i,p}$ for sample *i* belonging to PFT *p*:

$$\mathbf{x}_{i,p} \sim mvN(\mu_p, \boldsymbol{\Sigma}_p)$$

 $\mu_p \sim mvN(\mu_g, \boldsymbol{\Sigma}_g)$

where μ_p and Σ_p are the mean vector and variance-covariance matrix describing variation within PFT p, and μ_g and Σ_g are the mean vector and variance-covariance matrix describing across-PFT (global) variation.

Model implementation

We fit the above models using a Gibbs sampling algorithm that leveraged known conjugate prior relationships for efficient exploration of the sampling space. For priors on all multivariate mean vectors (μ) , we used normal distributions:

$$P(\mu) \sim mvN(\mu_0, \Sigma_0)$$

This gives rise to the following expression for the posterior:

$$P(\mu \mid \mathbf{x}, \boldsymbol{\Sigma}, \mu_0, \boldsymbol{\Sigma}_0) \sim mvN(\mu^*, \boldsymbol{\Sigma}^*)$$
$$\boldsymbol{\Sigma}^* = (\boldsymbol{\Sigma}_0^{-1} + n\boldsymbol{\Sigma}^{-1})^{-1}$$
$$\mu^* = \mu_0\boldsymbol{\Sigma}_0^{-1} + \bar{\mathbf{x}}n\boldsymbol{\Sigma}^{-1}$$

where $\bar{\mathbf{x}}$ are the sample means of the data and n is the number of rows in the data.

For priors on all multivariate variance-covariance matrices, we used the Wishart distribution (W):

$$P(\mathbf{\Sigma}) \sim W(\nu_0, \mathbf{S}_0)$$

This gives rise to the following expression for the posterior:

$$P(\mathbf{\Sigma} \mid \mathbf{x}, \mu, \nu_0, \mathbf{\Sigma}_0) \sim (W(\nu^*, S^*))^{-1}$$

$$\nu^* = 1 + \nu_0 + n + m$$
$$\mathbf{x}^* = \mathbf{x} - \bar{\mu}$$

$$\mathbf{SS} = \mathbf{x}^{*T}\mathbf{x}^{*}$$
 $\mathbf{S}^{*} = (\mathbf{S}_{0} + \mathbf{SS})^{-1}$

where n is the number of rows and m is the number of columns in data matrix x (full derivation in Gelman et al., 2003).

The fundamentally multivariate nature of the sampling procedure described above makes it incapable of accommodating partially missing observations. Therefore, our algorithm also included imputation of partially missing data, which proceeded as follows: For a block of data \mathbf{x} containing missing observations in columns \mathbf{m} and present observations in columns \mathbf{p} , the missing values $\mathbf{x}[m]$ are drawn randomly from a conditional multivariate normal distribution at each iteration of the sampling algorithm:

$$\mathbf{x}'[m|p] \sim mvN(\mu', \Sigma')$$

$$\mu' = (\mathbf{x}'[p] - \mu'[p])(\boldsymbol{\Sigma}[p, p]^{-1}\boldsymbol{\Sigma}[p, m])$$
$$\boldsymbol{\Sigma}' = \boldsymbol{\Sigma}[m, m] - \boldsymbol{\Sigma}[m, p](\boldsymbol{\Sigma}[p, p]^{-1}\boldsymbol{\Sigma}[p, m])$$

For each model fit, we ran five parallel MCMC chains, continuing the sampling until the final result achieved convergence as determined by a Gelman-Rubin potential scale reduction statistic less than 1.1 (Gelman and Rubin, 1992). We implemented this sampling algorithm in an open source, publicly available R (version 3.4.3, R Core Team, 2017) package (http://github.com/ashiklom/mvtraits).

Analysis of results

To assess the impact of multivariate and hierarchical constraint on trait estimates, we compared the mean and 95% confidence intervals of trait estimates for each PFT from each model (Fig. 1.2). For reference, we also added the default parameter values of CLM 4.5 (Table 8.1 in Oleson et al., 2013) for SLA, N_{mass} , N_{area} , $V_{c,\text{max,mass}}$, and $V_{c,\text{max,area}}$ to Fig. 1.2. To convert CLM's reported C:N ratio to N_{mass} , we assumed a uniform leaf C fraction of 0.46. We then divided this calculated N_{mass} by the reported SLA to obtain N_{area} . We calculated $V_{c,\text{max,mass}}$ by multiplying the reported $V_{c,\text{max,area}}$ by the reported SLA.

To test the hypothesis that the multivariate and hierarchical models offer more value in terms of uncertainty constraint at smaller sample sizes, we calculated the relative uncertainty (α) as a function of the mean (μ) and upper ($q_{0.975}$) and lower ($q_{0.025}$) confidence limits of trait estimates.

$$\alpha = \frac{q_{0.975} - q_{0.025}}{\mu}$$

We then fit a generalized linear model relating relative uncertainty to sample size (n) for each of the model types (univariate, multivariate, and hierarchical; Fig. 1.3).

$$\log \alpha = b_0 + b_1 \log n$$

If all three models performed equally well at all sample sizes, their respective slope and intercept coefficients would be statistically indistinguishable. On the other hand, models that perform better should have lower intercept (b_0) coefficients, indicating generally lower uncertainty, and lower slope (b_1) coefficients, indicating a reduced sensitivity of uncertainty (α) to sample size (n).

To assess the consistency of within- and across-PFT trait trade-offs, we looked at covariance estimates for each trait pair and, where these values were significantly different from zero (p < 0.05), we calculated the eigenvalues from the pairwise variancecovariance matrix for that trait pair and plotted the corresponding dominant eigenvectors centered on the mean estimates (Fig. 1.4). This figure provides a visual representation of relative positions of PFTs in trait space and both the direction and extent of within-PFT trait covariance, and is directly analogous to conceptual figures describing hierarchical trait variability across environmental gradients as presented in, for instance, (Cornwell and Ackerly, 2009) and (Albert et al., 2010b). Due to the small number of points used to estimate across-PFT covariance in the hierarchical model, none of the across-PFT covariances estimated in the hierarchical model were significantly different from zero (p < 0.05). For this reason, we compared within-PFT covariances as estimated by the hierarchical model with the covariances estimated by fitting a multivariate model to all of the data.

Besides the consistency in the direction of trait covariance globally and between different PFTs, we also investigated the strength and predictive power of these co-variances, which is represented by correlation coefficients (i.e. the pairwise covariance normalized to the variances of the component variables). To do this, we plotted the mean and 95% confidence interval of the pairwise trait correlation coefficients for the global estimate from the pooled multivariate model and PFT-level estimates from the hierarchical model (Fig. 1.5).

The R code and ancillary data for running these analyses is publicly available online via the Open Science Framework (OSF) at https://osf.io/w8y73/. The TRY data used for this analysis can be requested at http://try-db.org.

1.3 Results

1.3.1 Estimates of PFT-level means

In general, leaf trait estimates from the univariate, multivariate, and hierarchical models were similar (Fig. 1.2). Where we observed differences between models, the largest were between the univariate and multivariate models, while the additional constraint from the hierarchical model tended to have a minimal effect on trait estimates. Significant differences in trait estimates between univariate and multivariate



Figure 1.2: Mean and 95% confidence interval on best estimates of traits for each plant functional type from the univariate, multivariate, and hierarchical models. For leaf lifespan and SLA, results were not significantly different between the mass- and area-based models, so only results from the mass-based model are shown. For some PFT-trait combinations, where large error bars resulting from the relatively uninformative priors are substantially larger than the variability among means, the y axes are constrained to facilitate comparison.
models occurred even for traits with relatively large sample sizes, such as leaf nitrogen content.

Evergreen PFTs had by far the largest leaf lifespan, with the longest lifespan observed for temperate and boreal needleleaf evergreen species. Meanwhile, all of deciduous species had lifespans shorter than 7 months. Among deciduous species, lifespan was generally longer in warmer biomes than colder ones.

Across-PFT patterns in SLA and N_{mass} , P_{mass} , and $R_{d,\text{mass}}$ were similar. Temperate broadleaved deciduous trees and shrubs generally had among the highest values of these traits, while temperate evergreen trees and shrubs had generally among the lowest. However, none of these patterns were universal to all four traits. For example, tropical evergreen trees had relatively high N_{mass} and mean SLA and $R_{d,\text{mass}}$, but among the lowest P_{mass} . Similarly, temperate and boreal shrubs had higher N_{mass} and P_{mass} than any of the grasses, but comparable SLA.

Across-PFT patterns in N_{area} , P_{area} , and $R_{d,\text{area}}$ were different from their massnormalized counterparts. For example, tropical broadleaved evergreen and needleleaf evergreen trees had among the lowest N_{mass} and P_{mass} basis but among the highest N_{area} and P_{area} , while the opposite was true of deciduous temperate trees and shrubs. Species with N contents near the middle of the observed range did not shift as dramatically depending on type of normalization.

C3 grasses had both the highest $V_{c,\max,\max}$ and $V_{c,\max,\max}$. Compared to broadleaved trees, temperate needleleaved evergreen trees had lower $V_{c,\max,\max}$ but higher $V_{c,\max,\max}$. Among broadleaved trees, deciduous trees had higher $V_{c,\max,\max}$ and slightly higher $V_{c,\max,\max}$ than evergreen trees. Between the deciduous and evergreen tree PFTs, we observed no significant trend by climate zone.

C3 grasses and temperate needleleaved evergreen trees had the highest $J_{\text{max,area}}$, but temperate broadleaved deciduous trees had the highest $J_{\text{max,mass}}$. All of the shrub PFTs had the lowest $J_{\text{max,mass}}$ but average or above-average $J_{\text{max,area}}$, while the opposite was true of broadleaved tropical PFTs. Of the tree PFTs, needleleaved evergreen trees had the highest $J_{\text{max,area}}$ but the lowest $J_{\text{max,mass}}$.

A key application of this study was to provide data-driven parameter estimates for Earth System Models. To this end, we compared our mean parameter estimates with corresponding default parameters in CLM 4.5 (Oleson et al., 2013) (Fig. 1.2). Our mean estimates of SLA agreed with CLM's defaults (Oleson et al., 2013, Table 8.1 in) only for tropical broadleaved evergreen trees, and for all other PFTs, our estimates are significantly lower. For $N_{\rm mass}$, our estimates agreed reasonably well with CLM for every reen temperate trees, needleleaved trees, and C3 arctic grasses, and were substantially different for all other PFTs. Our $N_{\rm mass}$ estimates also varied much more across PFTs than CLM's parameters. For N_{area} , our estimates were significantly higher than CLM's for all PFTs, likely due to CLM's overestimates of SLA. Our estimates of $V_{c,\max_{max_{mass}}}$ were lower across all PFTs, with particularly large differences for tropical and temeprate broadleaf deciduous trees and evergreen shrubs, and temperate C3 grasses. Our estimates of $V_{c,\max,\text{area}}$ showed better agreement, though our values were still significantly lower for many PFTs. Like us, Kattge et al. (2009) also found that $V_{c,\max,\text{area}}$ was overestimated by Earth System models, but their estimates of $V_{c,\max,\text{area}}$ and N_{area} are generally slightly higher than ours.

We observed clear differences in the relative uncertainties of mean estimates with respect to sample size. All of the high-latitude PFTs consistently had among the largest error bars around their mean estimates relative to other PFTs, while the traits with the largest uncertainties were dark respiration, $V_{c,\max}$, and J_{\max} . For many of these trait-PFT combinations, the additional constraint from trait covariance provided by the multivariate and hierarchical models substantially reduced error bars, making it possible to compare estimates against those of other PFTs. Our analysis



Figure 1.3: Relative uncertainty in PFT-level trait estimates as a function of sample size for each model type. Lines represent linear models $(\log(y) = b_0 + b_1 \log(x))$ fit independently for each model type. In general, differences in estimate uncertainty between the univariate and multivariate models were minimal at large sample sizes but increasingly important at low sample sizes. However, differences in estimate uncertainty between the multivariate models were consistently negligible.

of the relationship between model type, sample size, and estimate relative uncertainty found that this covariance-based constraint from the multivariate model both reduced uncertainty overall (lower intercept) and reduced the sensitivity of estimate uncertainty to sample size (lower slope) compared to the univariate model (Fig. 1.3). However, this analysis revealed no consistent significant benefit from the hierarchical model.

1.3.2 Trait correlation patterns across- and within-PFTs

For all traits except leaf lifespan, pairwise trait correlations were generally consistent in direction both globally and within each PFT (Fig. 1-4). In particular, mass- and area-normalized traits were all positively correlated with each other and, respectively, positively and negatively correlated with SLA, both globally and within each PFT. The same was generally true of correlations of mass-based traits with leaf lifespan, but correlations of leaf lifespan with area-normalized traits were more variable. The correlation between N_{area} and leaf lifespan was positive globally and for evergreen shrubs, tropical broadleaved deciduous trees, temperate needleleaved evergreen trees but negative for temperate and boreal broadleaved deciduous trees and not significant for any other PFTs. Similarly, the correlation between P_{area} and leaf lifespan was positive globally but negative for evergreen shrubs and not significant for any other PFTs. The correlation between leaf lifespan and $R_{d,\text{area}}$ was significant and negative globally, but was not significant within any PFTs. The only significant correlations of leaf lifespan with $V_{c,\text{max,area}}$ and $J_{\text{max,area}}$ were negative for temperate broadleaved deciduous trees.

A large number of pairwise trait correlations were not significant. In some cases, this was driven by sample size (Fig. $1 \cdot 1$). For instance, needleleaved deciduous trees, the most undersampled PFT in our analysis, were often the only PFT for which a correlation was not statistically significant. In other cases, though, PFTs with smaller



Figure 1.4: Pairwise trait mean and covariance estimates for all data pooled globally (black) and for each PFT (colored). Covariance estimates not significantly different from zero (p < 0.05) are indicated by x symbols at the mean estimate. x and y axes vary on a log scale, reflecting the fact that the model was fit using the base 10 log of all traits. With the exception of leaf lifespan, pairwise covariances are consistent in direction but vary somewhat in magnitude between PFTs, and when comparing PFT-level and global estimates. However, many pairwise covariances are not statistically significant, particularly (but not always) for undersampled traits and PFTs.

sample sizes had significant pairwise correlations while PFTs with much larger sample sizes had none. For example, tropical broadleaved evergreen trees were relatively well-sampled for all traits, but none of their area-normalized traits were significantly correlated with leaf lifespan. In general, we observed fewer significant trait correlations among area-normalized traits than mass-normalized traits.

The strength of pairwise trait correlations varied substantially depending on scale, PFT, and trait (Fig. 1.5). The two pairwise trait correlations that exhibited the most consistent strength globally and within each PFT were the correlation between SLA and N_{area} , and between N_{mass} and P_{mass} . Correlation strength was often, but not always, related to sample size, with well-sampled PFTs exhibiting stronger correlations and undersampled PFTs exhibiting weaker correlations.

1.4 Discussion

1.4.1 Scale dependence of the leaf economic spectrum

The canonical leaf economic spectrum is defined by a negative correlation of between SLA and leaf lifespan, and a positive correlation of SLA with N_{mass} , P_{mass} , and photosynthesis and respiration rates (Wright et al., 2004). The first objective of this paper was to investigate the extent to which these relationships hold within and across PFTs. Our results indicate that the leaf economic spectrum generally still holds within PFTs, at least at the functional and phylogenetic scale of the current generation of Earth System Models. Within PFTs, correlations between SLA, N_{mass} , and P_{mass} were consistently positive, and correlations of these traits with leaf lifespan were generally negative (though, for many PFTs, correlations were not significantly different from zero). Although we did not include maximum photosynthesis rate $(A_{\text{max}}), V_{c,\text{max,mass}}$ and $J_{\text{max,mass}}$ generally exhibited the expected positive correlations with SLA and negative correlations with leaf lifespan, as did $R_{d,\text{mass}}$, though many



Figure 1.5: Mean and 95% CI on estimates of pairwise correlation coefficients for all data pooled globally (dark grey) and for each PFT (colored). For most PFT-trait pairs, correlations are mutually consistent in magnitude but vary in strength.

correlations were not significant, primarily due to sample size.

While the direction of relationships we observed was largely consistent across different PFTs, the strength of these correlations was more variable. For example, the correlations of SLA with N_{mass} and P_{mass} were generally weaker in needleleaved PFTs than in broadleaved PFTs. On the other hand, relationships of SLA and N_{area} were strongly negative for all PFTs (except the data-limited needleleaved deciduous trees), and temperate needleleaved species in particular had among the strongest SLA- N_{area} and SLA- P_{area} correlations of any PFT. Taken together with the finding that evergreen conifers are relatively unique in their consistently proportional allocation of N to cell walls and Rubisco (Onoda et al., 2017), our results support the idea that needleleaved species primarily adapt to environmental changes through structural changes (i.e. increasing or decreasing SLA) rather than through modulating foliar biochemistry (Robakowski et al., 2004).

We also found that the strength of the correlations of N with photosynthetic parameters $V_{c,\text{max}}$ and J_{max} -often used in ecosystem modeling to parameterize photosynthesis (Oleson et al., 2013; Rogers et al., 2017)-varied by plant functional type, whether the traits were normalized by mass or area. Although trait correlations are not necessarily indicative of allocation strategies, this result generally supports the findings of Ghimire et al. (2017) that N allocation strategies to photosynthesis vary widely by plant functional type. In particular, the correlations of N_{mass} with traits related to photosynthesis and respiration ($R_{d,\text{mass}}$, $V_{c,\text{max,mass}}$, and $J_{\text{max,mass}}$) were weaker for tropical evergreen broadleaved trees than for most other PFTs, but the correlation of these traits with P_{mass} was comparable or even slightly higher. This suggests that the productivity of tropical species is generally P-limited (Reich and Oleksyn, 2004; Ghimire et al., 2017), that N allocation strategies are more variable under N-poor than N-rich conditions (Ghimire et al., 2017), or more generally that photosynthetic parameters are affected more strongly by environmental covariates than leaf nitrogen contents (Ali et al., 2015). Meanwhile, our result that the N_{area} — $V_{c,\text{max,area}}$ correlation is generally weaker for needleleaved than broadleaved species was also found by Kattge et al. (2009), and supports the lower allocation of N to photosynthesis found by Ghimire et al. (2017). In light of this fact and considering that boreal forests, largely populated by needleleaf species, have the largest influence on global climate of any biome (Snyder et al., 2004; Bonan, 2008), we suggest that parameterization of needleleaf tree productivity based on foliar nitrogen content in Earth System Models be treated with caution.

Correlations of all traits with leaf lifespan were weaker (often to the point of becoming insignificant) within most PFTs than globally. This suggests that leaf economic relationships related to leaf lifespan are dominated by the fundamental differences between deciduous and evergreen PFTs, while the factors driving variability in leaf lifespan within PFTs are more complex and idiosyncratic (Reich et al., 2014; Wu et al., 2016a). That being said, much of this within-PFT variability is known to be driven by variations in shade responses, and a key limitation of our study is that we have no information about the relative canopy positions at which traits were collected (Lusk et al., 2008; Keenan and Niinemets, 2016a).

Across PFTs, the interaction between growth form and biome in PFT definitions (Table 1) confounds the interpretation of our results with respect to well established ecological and biogeographic patterns. For example, Poorter et al. (2009) found variation in SLA by growth form was, from highest to lowest, grasses, deciduous woody plants, evergreen woody plants, and succulents, while the pattern by biome was, again from highest to lowest, grassland, tundra, tropical forest, temperate forest, woodland, shrubland, and desert. We observed as expected that arctic grasses had lower mean SLA than temperate grasses, and that evergreen trees had lower SLA

than their deciduous counterparts. However, we observed by far the highest mean SLA values in temperate deciduous broadleaf trees, rather than in grass PFTs as expected. Similarly to Onoda et al. (2011), we found no consistent patterns in SLA with temperature: Among broadleaved evergreen PFTs, temperate species had lower SLA than tropical, but among broadleaved deciduous PFTs, temperate species had higher SLA than both tropical and boreal species. With respect to the expected decline in foliar N:P ratios with latitude (Reich and Oleksyn, 2004), we found that $N_{\rm mass}$ was generally higher in PFTs associated with colder biomes compared to warmer ones, but observed biome-related differences in $P_{\rm mass}$ only among deciduous broadleaved and needleleaved evergreen PFTs. Contrary to Atkin et al. (2015) , our results for both $R_{d,{\rm mass}}$ and $R_{d,{\rm area}}$ failed to show a trend with respect to biome. However, this comparison may not be entirely fair because our study design inherently averages over the extensive climatic variability within PFTs.

Finally, there has been some debate in the trait ecology community about the use of mass- or area-normalized traits in analyses of the leaf economic spectrum. Two studies (Osnas et al., 2013; Lloyd et al., 2013) independently concluded that leaf economic relationships among mass-based traits emerge inevitably out of variation in SLA and are therefore not ecologically meaningful. Responses to these criticisms have suggested that both mass- and area-based normalization have merit, as mass-based traits have a natural interpretation in terms of investment costs and allocation while area-based traits are important due to the fundamentally area-based nature of energy and gas fluxes through leaf surfaces (Westoby et al., 2013; Poorter et al., 2013). Our study suggests the latter, that investigation of trait correlations on both a mass- and area-basis can yield biologically and ecologically meaningful conclusions. For one, our discussion of differences in ecological strategies between broadleaved and needleaved species fundamentally depends on comparative analysis of mass- and area-normalized nutrient contents. Meanwhile, our discussion of tropical tree productivity with respect to foliar nutrient contents is generally supported by both mass- and area-normalized traits (i.e. the correlation between P and $V_{c,\max}$ is stronger than the correlation of Nand $V_{c,\max}$ for tropical species whether we use the mass- or area-normalized versions of these traits).

1.4.2 Covariance as constraint

The second objective of this paper was to investigate the ability of trait covariance to provide additional information that could be used to reduce uncertainties in trait estimates. In agreement with our expectations, our results show that accounting for trait covariance constrained the uncertainty around PFT-level trait means, particularly for trait-PFT combinations with low sample sizes (Fig. 1.2 and 1.3). Moreover, accounting for trait covariance occasionally also changed the position of trait mean estimates, even for PFT-trait combinations with relatively large sample sizes (e.g. $N_{\rm mass}$ for temperate broadleaved deciduous trees, Fig. 1.2). This result echoes Diaz et al. (2016) in demonstrating the importance of studying the multivariate trait space rather than individual traits. Such shifts suggest that the sampling of these traits in the TRY database is not representative, which is evident from looking at the relative sample sizes of different traits (Fig. 1.1; see also Kattge et al. 2011). These shifts also indicate that parameter estimates based on univariate trait data (e.g., LeBauer et al., 2013; Dietze et al., 2014; Butler et al., 2017) may not only be overestimating uncertainty, but may also be systematically biased. Although our results clearly show that many time- and labor-intensive traits, such as R_d , $V_{c,\max}$, and J_{\max} , still lack the observations to estimate covariance with other traits for certain PFTs, our results also show that the effective sample size of all traits is enhanced when covariance is taken into account. For example, field and remote sensing studies that estimate only certain traits like SLA and N_{mass} but not others (such as P_{mass} and $R_{d,\text{mass}}$) can leverage trait correlations to provide indirect constraint (Serbin et al., 2014; Singh et al., 2015; Musavi et al., 2015; Lepine et al., 2016). We therefore suggest that future observational campaigns consider trait covariance when deciding which traits to measure.

The additional benefit of hierarchical multivariate modeling in our study was limited, largely due to the relatively low number of points used to estimate that across-PFT covariance structure. Therefore, for parameterizing the current generation of ecosystem models using well-sampled traits, we suggest that simple multivariate models fit independently to each PFT are sufficient and that the additional conceptual challenges and computational overhead of hierarchical modeling are not required. However, for modeling work that requires larger numbers of PFTs (Boulangeat et al., 2012), and especially for models that are parameterized on the basis of individual species (e.g. Linkages, Post and Pastor, 2013), the benefits of hierarchical modeling may accumulate (Clark, 2016; Dietze et al., 2008; Cressie et al., 2009; Webb et al., 2010).

More generally, we foresee tremendous potential of multivariate and hierarchical modeling approaches to elucidating the role of functional traits in organismal and ecosystem function. Besides the many important foliar traits that we did not include (e.g. pigment contents, leaf hydraulic traits), our approach could readily be applied to other plant traits whose relationship to the leaf economic spectrum is less clear. One example is hydraulic traits: While stem and leaf hydraulic traits are correlated (Bartlett et al., 2016), a potential scaling between hydraulic and leaf economic traits is poorly understood (Reich, 2014; Li et al., 2015). Similarly, reexamining the relationships defining wood (Chave et al., 2009; Baraloto et al., 2010; Fortunel et al., 2012) and root (Kramer-Walter et al., 2016; Valverde-Barrantes and Blackwood, 2016) economic spectra, as well as their relationship to the foliar traits; would provide useful information on possible scale-dependence of plant growth and allocation strategies. We emphasize that the relative difficulty of measuring hydraulic and other non-foliar traits (e.g. Jansen et al., 2015) further increases the value of any technique that can fully leverage the information they provide. More generally, multivariate and hierarchical modeling has the potential to reveal functional trade-offs that are mutually confounding at different scales, thereby enhancing our understanding of processes driving functional diversity.

1.4.3 Conclusions

The tremendous functional diversity of plants continues to be a major challenge for functional ecology and ecosystem modeling. Functional diversity research fundamentally depends on dimensionality reduction through a search for meaningful pattern that can be exploited to take reasonable guesses at average behavior. The trait tradeoffs comprising the leaf economic spectrum are one such pattern. In this paper, we reaffirm the existence of the leaf economic spectrum both globally and, with some caveats, within plant functional types typically used in the current generation of Earth System Models. We also highlight how the strength of leaf economic relationships can be influenced by biotic and abiotic factors specific to certain PFTs. Finally, we show how patterns of trait covariance like the leaf economic spectrum can be leveraged to inform trait estimates, particularly at small sample sizes.

Chapter 2

Quantifying the influences of spectral resolution on uncertainty in leaf trait estimates through a Bayeian approach to RTM inversion

2.1 Introduction

The terrestrial biosphere is fundamentally dependent on the interactions between plants and solar radiation through photosynthesis. Consequently, we can learn a lot about the structure and functioning of ecosystems by studying these interactions in detail, and over the last several decades our capability do so has expanded dramatically. Specifically, global scale remote sensing observations from satellites such as Landsat, MODIS, and AVHRR have been used to map and monitor vegetation productivity, distribution, and abundance at high temporal frequency (Loveland et al., 2000; Friedl et al., 2002; Hansen et al., 2010; Houborg et al., 2015). At the landscape scale, satellite and sub-orbital (airborne) platforms with high spatial (e.g. World-View, < 1 m) and/or spectral (e.g. AVIRIS Classic, 10 nm) resolution sensors have been able to quantify the spatial distribution of canopy structure, nutrient status, and species composition (Asner et al., 2015; Banskota et al., 2015; Singh et al., 2015). In addition, field spectrometers with the highest available spectral resolution have provided a fast and relatively simple method for characterizing and monitoring leaf physiology, biochemistry, and morphology (Serbin, 2012; Couture et al., 2013; Sullivan et al., 2013; Serbin et al., 2014; Zhao et al., 2014).

An important caveat of using spectral information to study vegetation is that the optical properties being measured are often not of primary interest. Rather, we are interested in physiologically or ecologically meaningful variables such as total biomass, photosynthetic efficiency, species composition, biomass, or biochemistry that drive observed spectral signatures of vegetation and which can be inferred from the optical properties. This connection is usually made empirically, either by simple regression with spectral vegetation indices (SVIs) (Fassnacht et al., 2015; Haboudane et al., 2002; Huete et al., 2002) or through more advanced statistical methods such as partial least squares regression (PLSR) (Couture et al., 2013; Serbin, 2012; Serbin et al., 2014; Singh et al., 2015) and wavelet transforms (Banskota et al., 2013; Blackburn and Ferwerda, 2008; Cheng et al., 2010). However, these approaches can have important limitations depending on the application. First, the empirical nature of these methods can result in sensor, site, and/or vegetation specific relationships, as evidenced by the substantial variability in coefficients and choice of wavelengths across studies (Croft et al., 2014; Huete et al., 2002; Knyazikhin et al., 1998; Leprieur et al., 1994; Liu et al., 2012; Myneni et al., 2002; Wessels et al., 2012). Second, empirical approaches are not a direct mechanistic relationship between spectra and plant properties and therefore do not provide the true connections between optical properties and variables of interest (Knyazikhin et al., 2012). As a result, extrapolating empirical approaches and relationships to larger regions or new locations can be challenging. Moreover, the indirect, derived data products that arise from such analyses may have a limited capacity to inform ecosystem models (Quaife et al., 2008), as they often introduce assumptions that conflict with the internal logic of the processes represented in these models.

In contrast, radiative transfer models (RTMs), which provide a more mechanistic

link between plant traits and spectral signatures, can be a useful alternative to empirical approaches. A variety of standalone RTMs exist from the leaf (Dawson et al., 1998; Feret et al., 2008; Ganapol et al., 1998) to canopy scales (Jacquemoud et al., 2009; Kuusk, 2001; Verhoef, 1984; Wang and Li, 2013). In addition, RTMs are often an important component of dynamic vegetation models, where they are used to calculate surface energy balance and light availability for photosynthesis (Medvigy et al., 2009a; Ni-Meister et al., 2010; Kobayashi et al., 2012). In this study, we focus on the leaf-level PROSPECT model (Jacquemoud and Baret, 1990; Feret et al., 2008), which has been extensively used in forward (simulation) mode to develop and test new remote sensing techniques (Croft et al., 2014; Féret et al., 2011; le Maire et al., 2004; Zarco-Tejada et al., 2013) as well as to estimate leaf traits from spectral observations via inversion (Atzberger and Richter, 2012; Feret et al., 2008; Jacquemoud et al., 1995; Jacquemoud et al., 2009; Li and Wang, 2013; Li and Wang, 2011; Zarco-Tejada et al., 2004). However, the commonly used approaches for RTM inversion—such as least-squares minimization and look-up tables—fail to directly quantify the uncertainties and account for the correlations among the resulting parameter estimates. The characterization of uncertainty is a fundamental requirement for drawing meaningful scientific conclusions from results and for assimilating results into statistical or mechanistic models (Cressie et al., 2009; Quaife et al., 2008).

Applying Bayesian statistics to RTM inversion activities provides a direct means to quantify the uncertainty and covariance of parameter estimates while combining multiple sources of information. The use of independent prior information has been a critical component of RTM inversion as a way to solve the otherwise underdetermined problem of estimating a large number of RTM parameters from a small number of observations(Combal et al., 2003; Lauvernet et al., 2008; Yao et al., 2008; Pinty et al., 2011; Laurent et al., 2014; Mousivand et al., 2015). While these studies either neglect parameter uncertainty or estimate it using computationally-efficient approximations (e.g. Gaussian posterior distributions), recent work has demonstrated the efficacy of fully-Bayesian Markov Chain Monte Carlo (MCMC) approaches for inversion of the PROSAIL canopy RTM using MODIS (and "MODIS-like") data(Zhang et al., 2005; Zhang et al., 2006; Zhang et al., 2009). However, to the authors' knowledge, such approaches have yet to be applied to hyperspectral data, neither at the canopy nor the leaf scales. A recent study by Lepine et al. (2016) further demonstrated that PLSR estimates of canopy nitrogen are less sensitive to spectral resolution than spatial resolution and sensor fidelity, but no comparable analyses has been attempted for other foliar constituents, nor, for that matter, using a physically-based RTM rather than an empirical regression. In this study, we examine the effects of measurement spectral characteristics on accuracy, uncertainty, and covariance of leaf traits estimated from spectral inversion of a leaf RTM. First, we demonstrate the applicability of a fully Bayesian approach to leaf RTM inversion and validate this approach using data from the NASA Forest Functional Types (FFT) database of field spectra (Serbin et al., 2014; Singh et al., 2015). Second, we simulate reflectance observations using the spectral response functions of ten common remote sensing platforms and test the accuracy and precision with which our inversion algorithm can retrieve parameters from these observations. Although such an experiment is highly idealized, it does provide insight on the absolute theoretical limits of RTM inversion by different remote sensing platforms and illustrates how subtle changes in spectral measurement characteristics can affect inversion results. More broadly, this work reiterates the power of a Bayesian framework for fully utilizing the vast archive of remote sensing and field spectral observations to enhance our understanding of ecosystem processes.

Table 2.1: Summary of PROSPECT 5 parameters. Ranges for Car, Cw, and Cm are based on the datasets used for their calibration (ANGERS for Cab and Car, LOPEX for Cw and Cm) as reported in Feret et al. (2008). The ranges for N and Cab are calculated from the LOPEX and ANGERS databases, respectively. Units for Cw and Cm are adjusted for readability (original units are g cm⁻²).

Parameter	Description	Unit	Range
Ν	Structural parameter; effective number of mesophyll layers	Unitless	1.09 to 3.00
Cab	Total chlorophyll (a and b) density	$\mu \mathrm{g cm^{-2}}$	0.78 to 106.72
Car	Total carotenoid density	$\mu \mathrm{g}\mathrm{cm}^{-2}$	0 to 25.3
Cw	Equivalent water thickness	$ m gcm^{-2}$	43 to 439
Cm	Leaf dry matter content per unit area	${ m gcm^{-2}}$	17 to 152

2.2 Methods

2.2.1 Inversion procedure

The PROSPECT 5 model simulates the full spectral reflectance and transmittance of a leaf over the 400–2500 nm range using five key parameters related to leaf structure and biochemistry (Feret et al., 2008). In the PROSPECT model, a leaf is treated as a set of N partially transparent flat plates, each with wavelength-dependent transmissivity $k\lambda$. Transmissivity $k\lambda$ is based on the linear combination of empirically calibrated specific absorption spectra for total chlorophyll (a and b), total carotenoids, water, and dry matter (e.g. cellulose, lignin, protein) multiplied by their respective quantities (given by the parameter values: Cab, Car, Cw, Cm) (Table 2.1).

The objective of RTM spectral inversion is to estimate the physical RTM parameters from the observed spectral information. This is accomplished through a statistical inversion, wherein we seek the set of parameters that minimizes the residual error between PROSPECT-modeled and measured reflectance. Our approach to the inversion of PROSPECT is distinct from previous studies (Combal et al., 2003; Feret et al., 2008; Féret et al., 2011; Li and Wang, 2011; Li and Wang, 2013) in two important ways. First, whereas many past studies use both reflectance and transmittance to estimate parameters, we use only reflectance. Reflectance is generally easier to measure than transmittance, which requires special instrumentation such as integrating spheres that often have inadequate designs and yield poor signal-to-noise ratios, especially in the longer wavelengths (i.e. > 2μ m). As well, inversion on reflectance data alone allows transmittance measurements as optional data for independent validation. Second, unlike past leaf-level PROSPECT inversion studies that only provide point estimates of parameters, we performed our analysis within a Bayesian framework that provides the joint probability distribution of the PROSPECT 5 parameters, $\theta = N, Cab, Car, Cw, Cm$, and the residual standard deviation, σ , as the output. The general mathematical statement of this posterior distribution is given as follows:

$$P(\theta, \sigma \mid X) \sim P(X \mid \theta, \sigma) P(\theta) P(\sigma)$$
$$P(X \mid \theta, \sigma) \sim Normal(PROSPECT5(\theta) \mid X, \sigma)$$

where $PROSPECT5(\theta)$ is the modeled reflectance given θ , and X is a vector of observed reflectance values. The residual error is assumed to be normally distributed with a mean of 0 and standard deviation of σ .

We set the prior distribution for N to a lognormal distribution shifted to have a minimum of 1, and parameterized based on a review of literature using the PROSPECT model (le Maire et al., 2004; Ferreira et al., 2013; Croft et al., 2014).We assigned the remaining parameters log-normal priors based on summary statistics and histograms from the LOPEX, ANGERS, HAWAII, and CALMIT spectral databases as reported by Feret et al. (2008) .The residual standard deviation σ was assigned an uninformative inverse gamma prior, which is conjugate with the normal distribution and therefore allows for computationally efficient Gibbs sampling.

We sampled the joint posterior distribution of the PROSPECT 5 parameters using the Metropolis-Hastings (MH) algorithm with adaptive block sampling (Haario et al., 2001). For this, we initialized each inversion using parameter values drawn at random from the prior distributions. For each inversion, we ran the algorithm five times (i.e. five independent chains) for 100,000 iterations each. At each iteration, the algorithm proposes a parameter vector, calculates the vector's likelihood based on the observations and the prior, and accepts or rejects the vector based on this likelihood. The proposal step performs a random draw from a multivariate normal distribution centered on the last accepted parameter vector. The covariance matrix for the multivariate normal proposal distribution was re-computed every 100 iterations as follows: (1) the univariate standard deviation of each parameter and the Pearson product-moment correlation matrix were computed; (2) the standard deviation vector was multiplied by the ratio of the acceptance rate in the last 100 samples to the target acceptance rate (set to 0.234, as per Haario et al. 2001); (3) the resulting standard deviation vector was converted to a diagonal matrix and multiplied to both sides of the correlation matrix to give a re-scaled covariance matrix. For each inversion, we determined MCMC convergence based on a value of the Gelman-Rubin multivariate potential scale reduction factor of less than 1.1 (Gelman & Rubin 1992, as implemented in the R coda package v.0.18–1 by Plummer et al.). For runs that did not converge, we repeated this process with a 20% smaller target acceptance rate for the adaptation step, which increases the size of the sampling space for each chain and therefore reduces the likelihood of getting trapped in local minima. Across the >10,000 inversions performed in this study, only five failed to converge (after five inversion attempts)—all for simulated CHRIS-Proba spectra (see Section 2.3)—and we excluded these data points from our analysis. We visually examined a random subset of the resulting trace plots and autocorrelograms and determined that a common burn-in period of 80,000 samples and a thinning interval of 20 was sufficient for an accurate and representative sample of the joint posterior distribution. After applying the burn-in and thinning filter, we calculated the mean, standard deviation, and 95% confidence intervals of the sampled parameter values.

With chains running in parallel, the inversion of one leaf spectrum with our specifications takes approximately 4 minutes (on one Intel Xeon X5570 CPU @ 2.93GHz), and running the entire set of over 10,000 inversions required for this paper took several days (running up to 16 inversions simultaneously on a high performance computing cluster). That being said, we anticipate that recoding of the algorithm from R to a compiled language will dramatically increase (>50x) the computational efficiency of our approach.

The inversion algorithm described above is available as an open-source, publiclyavailable R (R Core Team, 2017) package housed within the PEcAn ecoinformatics toolbox github.com/pecanproject/pecan/tree/master/modules/rtm (Dietze et al., 2013; LeBauer et al., 2013). This package allows users to simulate spectra using the PROSPECT family of radiative transfer models and apply our inversion algorithm to their own models and data. For more information, refer to the package vignette on the PEcAn tutorials page pecanproject.github.io/tutorials.html.

2.2.2 Validation

Data

We tested the ability of our inversion to accurately estimate leaf traits using data collected as part of the NASA Forest Functional Types (FFT) campaign (Deel et al., 2012; Serbin et al., 2014; Singh et al., 2015). This dataset consists of leaves collected from various positions within the canopy for 52 species from 13 sites across the Northeast and Midwest USA. An Analytical Spectral Devices (ASD) FieldSpec 3 Full Range (350 to 2500 nm) Spectroradiometer was used together with a leaf clip and internal calibrated light source to measure reflectance on the adaxial surface of 1348 unique leaves. For a subset of 765 of these leaves, the same instrument was used with an ASD integrating sphere setup to measure transmittance through the

leaf adaxial surface. Our database included both broadleaf and conifer species. For conifer measurements, we constructed edge-to-edge mats of needles larger than the spot size of the light source (Serbin, 2012; Singh et al., 2015). As detailed in Serbin (2012), we found minimal changes in reflectance/transmittance measurement up to a threshold of differing gaps between needles. These observations are henceforth referred to as "FFT measured reflectance and transmittance", respectively. In addition to spectral measurements, laboratory measurements of leaf dry mass per unit area (LMA) and equivalent water thickness (EWT) were available for 950 leaves. For further information on the sampling methodology, see Serbin et al. (2014).

During exploratory analysis, we observed that inversion results by leaf habit displayed some distinct differences and conifer species were consistently less accurate than results for broadleaved species, reflecting ecological differences in leaf structure that are not well represented by the PROSPECT model. Therefore, to better contextualize our results, we performed both validation steps for the entire data set and separately for broadleaved and conifer species. However, even within the conifer functional type, we found certain species and foliar morphologies showed much larger errors than others. These differences could be ecological in nature or an artifact related to the challenges of measuring full-range reflectance and transmittance of different types of conifer needles. To investigate whether these errors aligned with established ecological classifications, we grouped species based on their approximate succession ("early", "mid", or "late"), following the general classification scheme of Dietze & Moorcroft (2011), except that we grouped the "Northern" and "Southern Pine" functional types as "early conifer." Classification based on succession is useful for this study because it is indicative of plant shade tolerance (Dietze and Moorcroft, 2011), which is closely linked to leaf structure and biochemistry (Poorter et al., 2009).

We applied our inversion algorithm individually to each of the FFT measured

reflectance spectra (n = 1348), resulting in an estimate of the joint probability distribution of the PROSPECT 5 parameters for each leaf. We then generated a dataset of synthetic reflectance spectra ("FFT simulated reflectance") by using the middle 90% of these parameter estimates (n = 1040) as inputs to the PROSPECT 5 model. These synthetic reflectance spectra were used as data in the sensor simulation experiment (Section 2.3). We used real parameter estimates rather than random draws from a distribution to preserve their ecological ranges and covariances resulting from within-and between-species tradeoffs in traits such as those described for the leaf economics spectrum (Wright et al., 2004).

We then performed two different tests to evaluate the accuracy of these parameter estimates: (1) We compared the FFT simulated reflectance and transmittance to measured reflectance and transmittance, and (2) we directly compared the inversion estimates of PROSPECT 5 parameters Cw and Cm to measured values of EWT and LMA, respectively.

Reflectance and transmittance

A common way to validate model inversion is to run the model in forward mode using the estimated parameters as inputs and compare the output to the original data. For our study, we used the inversion estimates of the PROSPECT parameters as inputs to the PROSPECT model to predict reflectance and transmittance spectra, which we then compared to the observed reflectance and transmittance. Errors in spectral inversion can originate from multiple sources, including measurement error (both trait and spectra), failure of the PROSPECT model to fully capture leaf spectral features (i.e. model formulation error), and parameter identifiability issues in the inversion algorithm. To isolate algorithmic error, we first performed the validation on a set of synthetic reflectance and transmittance spectra (n = 1348). To investigate the remaining sources of error, we performed the same validation on FFT measured reflectance (n = 1348) and transmittance (n = 765) spectra. For both reflectance and transmittance, we calculated the mean and 90% and 95% confidence intervals on the absolute error (simulated – measured) at each wavelength. The overlap of the 95% confidence interval with 0 was used to judge statistical significance. To facilitate comparison with other RTM inversion studies (Feret et al., 2008; Di Vittorio, 2009a), we also computed the root mean square error (RMSE), bias (BIAS), and bias-corrected RMSE (SEPC) averaged across the visible (VIS, 400–800 nm) and near-infrared (NIR, 801–2500 nm) regions of the spectrum:

$$RMSE = \sqrt{\frac{\sum (x_i - x_0)^2}{n}}$$
$$BIAS = \frac{\sum x_i - x_0}{n}$$
$$SEPC = \frac{\sum (x_i - x_0 - BIAS)^2}{n}$$

where x_i is the simulated value (reflectance or transmittance), x_0 is the observed value, and n is the number of spectra considered.

Leaf water content and mass per area

For leaves that had paired measurements of reflectance and EWT and LMA (n = 950), we compared the mean inversion estimates for PROSPECT parameters Cw and Cm to measured values of EWT and LMA, respectively. For each, we compared the mean inversion estimate to the measured value via the RMSE, BIAS, and SEPC as above (with inversion estimate x and measurement xo) as well as relative RMSE (RMS%E) and the relative bias-corrected RMSE (CV):

$$RMS\%E = \sqrt{\frac{\sum \left(\frac{x_i - x_0}{x_0}\right)^2}{n}} \times 100\%$$

Table 2.2: Spectral, spatial, and temporal characteristics of remote sensing platforms and instruments considered in the sensor simulation experiment. Note that AVIRIS spatial resolution is dependent on aircraft altitude and instrument field of view.

Sensor	Number of Bands	Spectral range (nm)	Bandwidth (nm)	Spatial resolution (m)	Revisit time (days)
AVIRIS NG	416	380 to 2510	5	0.3 to 4.0	On-demand
AVIRIS Classic	216	400 to 2500	10	< 10 to 20	On-demand
CHRIS-Proba	62	410 to 1050	1.5 to 12	36	7 to 8
Hyperion	225	350 to 2500	10	30	16
Landsat 5 (TM)	6	450 to 2350	60 to 270	30	16
Landsat 7 $(ETM+)$	6	440 to 2350	60 to 280	30	16
Landsat 8 (OLI)	8	435 to 2295	20 to 185	30	16
MODIS	7	459 to 2155	20 to 50	250 to 500	1 to 2
VIIRS	10	402 to 2275	15 to 60	750	1 to 2
AVHRR	3	580 to 1640	100 to 275	1090	1

$$CV = \frac{SEPC}{x_0} \times 100\%$$

2.2.3 Sensor simulation experiment

Recent work has shown that PLSR estimates of foliar nitrogen content are less sensitive to spectral resolution than to other factors such as spatial resolution and sensor fidelity (Lepine et al., 2016). However, the PLSR approach implemented in that study was unable to quantify the uncertainty around the nitrogen estimates. We hypothesize that the spectral characteristics of most common remote sensing platforms are sufficient to accurately estimate the leaf biophysical parameters modeled by PROSPECT, but that the uncertainties in these parameters will increase with declining spectral resolution. To test this hypothesis, we transformed the FFT simulated reflectance spectra using the relative spectral response functions of 11 common remote sensing platforms (Table 2.2), and used our Bayesian inversion of PROSPECT 5 to retrieve the starting parameters from the transformed spectra. For input parameters, we used the inversion results from measured spectra, thereby capturing a large range of ecologically realistic values and preserving inherent covariances between parameters. To account for observation error, we simulated Gaussian random noise (with mean 0 and standard deviation 2.5×10^{-4}) smoothed with a Gaussian filter (kernel width 11) to account for inherent autocorrelation in hyperspectral measurements.

We then examined how two characteristics of the inversions varied between sensors: Relative bias (α) indicates how closely the mean parameter estimate (μ) matched the true value (p) and is a useful measure for describing the accuracy of the estimate's central tendency.

$$\alpha = \frac{\mu - p}{p}$$

Uncertainty (π) describes the width of the 95% confidence interval of the estimate (s) relative to the mean value, and is useful for ascertaining the precision with which the inversion is able to estimate a parameter.

$$\pi = \frac{s}{\mu}$$

We note that both statistics are normalized to facilitate inter-parameter comparison. Both metrics were computed for each parameter for each inversion and then averaged over all simulated spectra.

We recognize that this experiment does not fully capture all of the variability associated with inversion of real observations from these sensor systems given its failure to account for canopy structure, atmospheric effects, sun-sensor geometry, and sensor radiometric resolution. However, this experiment is capable of illustrating the ability to characterize uncertainty in inversion results and improves the confidence with which we can extract information from lower quality data sources. Moreover, this experiment sets a theoretical limit on the accuracy and precision of leaf trait retrieval from spectral RTM inversion, thereby contextualizing past RTM inversion results (Zhang et al., 2005; Zhang et al., 2006; Zhang et al., 2009; Zhang et al., 2012) and guiding future research in the field.

The entire workflow for this paper is summarized in Figure 2.1. The data and R source code for performing all analyses in this study have been made publicly available



Figure $2 \cdot 1$: Workflow illustrating the steps in this study as well as the figures to which they correspond.

at github.com/ashiklom/sensor-manuscript.

2.3 Results

2.3.1 Validation

Reflectance and transmittance

For the inversion of synthetic spectra, we found no statistically significant (p < 0.05) spectral bias at any wavelength (not shown). As well, the observed differences between input and simulated output were one to two orders of magnitude smaller than corresponding errors in the inversion of measured spectra (Figure 2.2). These results collectively illustrate that our algorithm is unbiased and contributes minimally to errors in the inversion of measured spectra.

For the inversion of measured spectra, we observed substantial variability in the spectral bias across all analyzed leaves, resulting in statistically significant (p < 0.05) bias in only a few specific wavelength regions (Figure 2·2). For both broadleaf and needle-leaf conifer species, reflectance was typically overestimated between 1600 and 1900 nm and underestimated between 1000 and 1300 nm and between 2000 and 2500 nm. The errors in the 1600 to 1900 nm and 2000 to 2500 nm ranges covered more wavelengths and had larger magnitude for conifer species than broadleaved species. Broadleaved species also had a statistically significant reflectance overestimate in the 400 to 500 nm range and an underestimate at 1300 nm, while conifer species had a significant reflectance overestimate at 1300 nm.

For both measured and synthetic spectra, transmittance bias (BIAS = -0.0133) was, on average, greater in magnitude than reflectance bias (BIAS = 0.0018), with a mean positive bias for broadleaved species (BIAS = 0.0012) and a mean negative bias for conifer species (BIAS = -0.0346) (Figure 2·2, Table 2.3). However, the between-leaf variability in bias was also large and resulted in statistically significant bias in only a small number of specific spectral regions. For both broadleaved and conifer species, we observed a significant underestimate in transmittance in the chlorophyll a absorption 400 and 500 nm. Specifically for conifer species, we also observed underestimates in transmittance at the vegetation "red edge" around 700 nm and at a water absorption feature around 1900 nm.

Leaf water content and mass per area

Similar to the results of the spectral validation, the inversion estimates of Cw and Cm (compared to measured values of EWT and LMA, respectively) displayed higher accuracy for broadleaf ($CV_{Cw} = 18.8\%$, $CV_{Cm} = 24.5\%$) versus conifer species



Figure 2.2: Bias in FFT simulated reflectance (top) and transmittance (bottom) spectra compared to measurements over all leaves (left) and only hardwood (middle) and conifer (right) species. For a given wavelength, the solid black line is the mean bias, the dark grey bounded by the dotted line is the 90% confidence interval, the light grey region bounded by the dashed line is the 95% confidence interval, the red line highlights a bias of 0, and the red shaded regions highlight bias significant at the 95% confidence level.

Table 2.3: Reflectance (Refl.) and transmittance (Tran.) spectral validation error statistics aggregated across the visible (400–800 nm) and infrared (801–2500 nm) regions. Values from other studies are included for comparison.

		RMSE	Visible BIAS	SEPC	RMSE	Infrared BIAS	SEPC
Refl.	FFT All — Broadleaf — Conifer Feret et al. (2008): CALMIT — ANGERS — HAWAII Di Vittorio (2009)	$\begin{array}{c} 0.0083\\ 0.0063\\ 0.0101\\ 0.032\\ 0.019\\ 0.021\\ 0.0255\end{array}$	$\begin{array}{c} 0.0018\\ 0.0023\\ 0.0011\\ 0.010\\ 0.001\\ -0.008\\ 0.005 \end{array}$	$\begin{array}{c} 0.0071 \\ 0.0042 \\ 0.0090 \\ 0.028 \\ 0.019 \\ 0.020 \\ \end{array}$	$\begin{array}{c} 0.0098\\ 0.0064\\ 0.0127\\\\ 0.016\\ 0.036\\\end{array}$	-0.0020 -0.0009 -0.0035 	0.0061 0.0034 0.0064 0.014
Trans.	FFT All — Broadleaf — Conifer Feret et al. (2008): CALMIT — ANGERS — HAWAII Di Vittorio (2009)	$\begin{array}{c} 0.0404 \\ 0.0248 \\ 0.0553 \\ 0.029 \\ 0.018 \\ 0.022 \\ 0.0422 \end{array}$	$\begin{array}{c} -0.0133\\ 0.0012\\ -0.0346\\ -0.005\\ -0.005\\ 0.003\\ 0.0294\end{array}$	$\begin{array}{c} 0.0336\\ 0.0167\\ 0.0389\\ 0.025\\ 0.017\\ 0.020\\\end{array}$	$\begin{array}{c} 0.0551 \\ 0.0450 \\ 0.0661 \\ \\ 0.016 \\ 0.020 \\ \end{array}$	0.0040 0.0266 -0.0293 0.001 -0.003 	$\begin{array}{c} 0.0537\\ 0.0336\\ 0.0566\\\\ 0.015\\ 0.017\\\end{array}$

Table 2.4: Error statistics for the comparison of inversion estimates of PROSPECT parameters Cw and Cm and measured values of equivalent water thickness (EWT) and leaf dry mass per unit area (LMA), respectively. Values from other inversion studies are included for comparison.

		RMSE	BIAS	SEPC	CV	RMS%E
	FFT Broadleaf	17	5	16	18.8	21.64
	— Conifer	187	90	164	52.3	67.29
Cw / EWT	Feret et al. (2008): LOPEX	17	-3	17	15.2	
$(g m^{-2})$	- ANGERS $$	20	-1	20	17.1	
	Feret et al. $(2011): #3$	27				
	Li & Wang (2011)	12	5		20.10	
$\begin{array}{c} \mathrm{Cm} \ / \ \mathrm{LMA} \\ \mathrm{(g \ m^{-2})} \end{array}$	FFT Broadleaf	20	-18	9	24.5	43.75
	— Conifer	121	35	116	61.6	65.51
	Feret et al. (2008): LOPEX	34	21	27	51.0	
	- ANGERS $$	26	1	26	49.8	
	Feret et al. $(2011): #3$	31				
	Li & Wang (2011)	8	-7		13.75	



Figure 2.3: Modeled and observed equivalent water thickness $(g m^{-2})$ for both conifers and hardwoods (top), just hardwoods (bottom left), and just conifers (bottom right). Point colors indicate plant type (top) or successional stage (bottom). The dashed line represents a 1:1 fit.

 $(CV_{Cw} = 52.3\%, CV_{Cm} = 63.3\%)$ (Table 2.4). For the broadleaved species, our parameter estimates were within the range observed previously (Table 2.4). While the inversion estimates for conifer species show a lower performance compared to broadleaf trees, the error inversion results were primarily driven by a single plant functional type—early successional conifers, which consisted entirely of pine species (*Pinus* family). Notably, a few estimates for mid-successional conifer species displayed significant divergence with observations, but in general fell along the 1:1 relationship (Figures 2.3 and 2.4).



Figure 2.4: Modeled and observed leaf dry mass per unit area (g m⁻²) for both conifers and hardwoods (top), just hardwoods (bottom left), and just conifers (bottom right). Point colors indicate plant type (top) or successional stage (bottom). The dashed line represents a 1:1 fit.

	Uncertainty (π)					Relative bias (α)				
Sensor	Ν	Cab	Car	`Ćw	Cm	Ν	Cab	Car	`Ćw	Cm
ASD Field Spec	0.20	0.54	2.91	0.26	1.33	-0.001	0.05	0.08	0.01	-0.05
AVIRIS NĞ	0.87	2.36	12.78	1.12	5.81	-0.004	0.05	-0.03	0.004	-0.03
AVIRIS Classic	1.62	4.61	26.06	2.13	11.02	-0.04	0.06	-0.44	-0.01	-0.08
Hyperion	1.69	4.81	27.35	2.23	11.44	-0.04	0.05	-0.49	-0.02	-0.06
CHŘÍS-Proba	21.93	20.77	53.86	106.5	173.8	-0.71	-0.50	-2.52	2.41	87.84
Landsat 5	8.90	17.14	114.8	13.32	66.43	-1.53	-0.64	-5.16	-0.76	-0.89
Landsat 7	8.84	21.90	134.2	12.94	66.07	-1.52	0.55	-9.17	-0.77	-0.91
Landsat 8	4.31	12.23	118.5	11.05	27.99	-0.33	0.28	-3.02	-0.32	-0.005
MODIS	10.29	15.99	220.5	16.65	86.00	-1.20	0.07	-29.14	-1.88	5.43
VIIRS	2.49	13.24	174.4	4.75	18.23	-0.09	1.57	-18.06	-0.09	0.004
AVHRR	25.47	114.2	263.3	74.58	179.1	-0.26	-7.47	-39.04	-8.04	77.21

Table 2.5: Uncertainty and relative bias in parameter estimates from inversion of simulated spectra filtered through relative spectral response curves of different sensors.



Figure 2.5: Mean uncertainty (a) and relative bias (b) (as defined in section 2.3) of inversion estimates for each parameter and simulated sensor. Sensors are arranged along the x-axis in approximate order of increasing spectral resolution.

2.3.2 Sensor simulation experiment

Parameter error

Across all of the selected sensors, the highest PROSPECT 5 parameter inversion uncertainty and bias were observed for Car (Figure 2.5, Table 2.5). This can readily be explained by the Car specific absorption feature, which is both extremely narrow and overlaps substantially with that of Cab (not shown). On the other extreme, the most accurate and least uncertain retrieved parameter was N, which is related to the reflectivity of the leaf across the entire spectrum (Figure 2.5, Table 2.5). Despite relatively narrow absorption features, most simulated sensors were able to retrieve Cab with reasonably good accuracy, which is not surprising given the long history of monitoring vegetation pigmentation using various platforms. Similarly, all sensors except CHRIS-Proba and AVHRR retrieved Cw with low uncertainty and bias, reflecting the wide and strong absorption features of water in the NIR and SWIR (Figure 2.5, Table 2.5). The failure of CHRIS-Proba to retrieve Cw can be attributed to its inability to measure in this spectral range. The retrieval accuracy for Cm was much more sensor dependent, with good performance among the simulated hyperspectral sensors, VIIRS, and Landsat 8, followed by lower performance for simulated Landsat 5 and 7 and MODIS, and a poor result for the simulated Chris-PROBA and AVHRR data (Figure 2.5, Table 2.5). Although the specific absorption feature for Cm is very wide, the sensitivity of reflectance to Cm values is much lower than for other parameters and almost the entire feature can be masked or confounded by Cw (Figure S1). This suggests that Cm is very dependent on precise locations of certain bands and therefore explains the differences in the estimate accuracy of apparently similar sensors like Landsat 5, 7, and 8 (Table 2.2). More generally, the importance of precise band widths and locations is evidenced by the noticeably better performance of Landsat 8 compared to Landsat 5 and 7 for certain parameters (Figure 2.5, Table 2.5) despite



Figure 2.6: Example joint probability distribution for parameter inversion estimates of simulated spectra using the full spectra (red; top panels) and the relative spectral response functions of AVIRIS NG (cyan), Landsat 8 (dark blue), and MODIS (orange). Dotted lines indicate true parameter values. Note that the axis range of the top panels is substantially smaller than that of the bottom panels.

the subtle differences in the sensors' respective bandwidths (Table 2.2).

Parameter uncertainty and covariance

Figure 2.6 shows an example of processed inversion output based on the high spectral resolution field spectrometer data and the spectral response functions of AVIRIS NG, Landsat 8, and MODIS. All four plots are simulated from a single set of parameters, so differences in results are caused only by variations in spectral measurement characteristics.Out of these four sensors, the uncertainties increase with approximately

decreasing spectral resolution, with lowest uncertainties in the full spectra, secondlowest for AVIRIS NG, second highest for Landsat 8, and highest for MODIS. The shapes of parameter covariances are distinctly different between these sensors, reflecting differences in the ability of the inversion to distinguish between parameters based on the available information. Across all four sensors, we observe strong positive covariance between N and Cm, since these parameters influence wide regions of the reflectance spectrum in opposite ways. Similarly, we also observe a positive covariance between N and Cab, although the strength of this covariance is not equal across sensors. The remaining covariances are mostly specific to MODIS, whose band configuration increases the overlap between the associated parameters.

We find that inversion estimates for the field spectra are occasionally falsely overconfident. For instance, the true value of N and Cw is outside the 95% confidence limit of their estimated joint probability distribution at full, field spectrometer resolution. That being said, this is less of an issue for the other sensors, where the joint probability distribution encompasses the true value. This suggests that spectral resolution below 5 nm may not provide additional information content, particularly for the broad absorption features within leaves, because of the strong autocorrelation between adjacent wavelengths. More importantly, although the joint posterior probability distributions from Landsat 8 and MODIS appear wide, the resulting parameter values are constrained by an order of magnitude or more compared to the priors.

2.4 Discussion

In this manuscript, we reiterate the power of the Bayesian RTM inversion framework for using spectral data to characterize vegetation and monitor ecosystem dynamics. The use of a physically-based model to describe the interaction of light with different vegetation structural and biochemical components improves the extent to
which such an approach can be generalized across vegetation types and sub-orbital and spaceborne platforms compared to more empirical approaches. Moreover, this physically-based approach enables estimation of vegetation properties from sensors of varying spectral resolution, and our ability to quantify uncertainty in our estimates provides the versatility to assess the performance of various sensors for a range of applications.

Our inversion results are comparable to other studies (Feret et al., 2008; Féret et al., 2011; Li and Wang, 2011; Di Vittorio, 2009a). The results outperformed those of Feret et al. (2011) despite the fact that we performed the inversion on measured spectra and inverted all five PROSPECT parameters, whereas Feret et al. (2011) performed inversions on synthetic spectra and did not attempt to estimate the structure parameter N. As such, we suggest that our approach does not come at the cost of model performance, and, importantly, enables the use of a much wider range of spectral data to explore vegetation dynamics. Our method contrasts with some previous methods (e.g., Feret et al., 2008; Féret et al., 2011) that utilize both reflectance and transmittance observations to invert leaf models such as PROSPECT. These require the use of additional, expensive instruments, such as an integrating sphere, that typically introduce significant noise and potential errors in the measurements given their inadequate design across a range of leaf habits. In addition, our approach suggests the possibility to instead use leaf reflectance observations alone to scale canopy-scale RTMs by coupling measured reflectance with simulated transmittance.

Placed in the context of past inversion studies, our work reveals some continuing challenges in the use of PROSPECT to model leaf optical properties and provides some guidance for future RTM development. For instance, we noted issues with using PROSPECT to model reflectance and transmittance in the 400 to 500 nm range (Figure 2.2) that have also been reported in previous studies. Feret et al. (2008) observed a consistently negative transmittance bias and occasionally a positive or

negative reflectance bias. Similarly, Croft et al. (2013) report systematic underestimates of reflectance in this part of the spectrum. One possible source of bias is PROSPECT's simplified description of leaf structure (Jacquemoud and Baret, 1990) and failure to account for specular reflectance off the leaf surface (Grant, 1987). Another possible source of error is imprecise calibration of the leaf refractive index, which has a relatively strong wavelength dependence in the region of interest (400-500 nm) (Feret et al., 2008). Alternatively, this bias could be the result of the failure of the PROSPECT 5 model to properly represent the spectral properties of chlorophyll in leaves, potentially requiring additional calibration across a broader range of species and environments. The common specific absorption feature for chlorophyll a and b $(kCab(\lambda))$ in PROSPECT 5 used in this study is empirically calibrated to a single data set (ANGERS; Feret et al., 2008), and many studies have shown that this feature may need to be re-calibrated to the data at hand to obtain accurate inversion estimates, particularly for species dissimilar to those in the ANGERS data set (Malenovský et al., 2006; Moorthy et al., 2008; Zhang et al., 2008; Li and Wang, 2013). As well, PROSPECT 5 fails to distinguish between chlorophyll a and b, which have overlapping but distinctly different absorption signatures and whose ratios have been shown to be affected by environmental conditions (Blackburn, 2006; Di Vittorio and Biging, 2009; Di Vittorio, 2009a). Fortunately, it has been shown that not only can chlorophyll a and b be distinguished using imaging spectroscopy (Di Vittorio, 2009b), but that these differences can be incorporated into a RTM to improve its performance (Di Vittorio, 2009a).

Reflectance in the SWIR region (>1500 nm)—where we observed significant reflectance bias (Figure 2.2)—is influenced by three PROSPECT parameters: N, Cw, and Cm. All three parameters modulate reflectance in this spectral region monotonically: Reflectance increases with higher values of N and decreases with higher values of Cw and Cm. This means that it is unlikely that incorrect parameter trade-off within the algorithm (e.g. preferentially selecting Cw over Cm) could contribute to

within the algorithm (e.g. preferentially selecting Cw over Cm) could contribute to this error. Feret et al. (2008) also reported similar reflectance bias patterns for the ANGERS data set despite using a different inversion methodology. We hypothesize this bias is the result of PROSPECT's insufficient characterization of the specific absorption spectrum of leaf dry matter $(kCm(\lambda))$, since the absorption characteristics of water $(kCw(\lambda))$ are well known and N is not dependent on an absorption feature. This would also help explain the negative bias we observed between spectral inversion estimates of Cm and direct measurements of LMA (Figure 2.4, Table 2.4). Other studies have also reported a bias but the direction of this bias has not been consistent, with some studies showing negative bias across all their data (Li and Wang, 2011; Cheng et al., 2014) and others reporting a bias whose magnitude and direction is data-dependent (Feret et al., 2008). This may partially be explained by the simple treatment of non-pigment compounds in the current PROSPECT model, wherein protein, cellulose, hemicellulose, sugar, starch, and lignin are aggregated into a single parameter (Cm) (Fourty et al., 1996). As with chlorophyll, the absorption feature for Cm is empirically derived (Feret et al., 2008) and fails to represent variability in the relative abundance of the different components (Poorter et al., 2009). Fortunately, Wang et al. (2015) demonstrated that, with proper calibration, it is possible to use PROSPECT inversion to determine leaf protein as well as combined cellulose and lignin content. Furthermore, measurements of LMA are an aggregate of a number of constituents including chlorophyll, carotenoids, lipids, organic acids, phenolics, and vascular tissue (Poorter et al., 2009), which would positively bias the measurement compared to the spectral estimate. Finally, it is possible that strong positive covariance between N and Cm (Figure 2.6) caused by their significant spectral overlap interferes with accurate estimation of Cm. However, based on our finding that inversions of simulated spectra did not display this problem (Field spectra in Figure 2.5), we conclude the error is in fact driven more by model formulation than by parameter identifiability. We are aware of only one other study that attempted to estimate all five PROSPECT parameters (including the structure parameter, N) simultaneously: Li & Wang (2011) presented a novel algorithm for PROSPECT inversion that assigns a separate merit function to each parameter (rather than a single common merit function for all parameters) and demonstrated its improved performance over traditional approaches. However, although their new algorithm reduced error and bias in the LMA estimates, a negative bias comparable to the one we report still remained across all of their data sets.

Based on these results, we suggest that future PROSPECT development should aim for finer distinction in leaf chemical components. That being said, the introduction of additional parameters into a model must be approached with caution, as parameter precision and identifiability tend to decrease with model complexity. The ability of our Bayesian inversion to quantify parameter uncertainty and covariance makes it useful for nested model selection. An alternative approach to addressing the issue of empirically-calibrated absorption coefficients is to explicitly account for their uncertainty and covariance structures. Within our Bayesian framework, such uncertainties could be treated as observation errors and propagated to the uncertainty in parameter estimates. In subsequent work, we will explore such a calibration using coupled spectral-trait data from multiple available datasets.

The relatively large magnitude in our observed transmittance bias (compared to reflectance) is likely the result of using only reflectance as input in our inversion. A combined approach using measured reflectance and transmittance observations, collected on the same leaf samples, may have shown the variability distributed more evenly because the minimization of the residuals would have been more balanced between the two vectors of data. Ultimately, higher uncertainties in transmittance estimates compared to reflectance are a consequence of the inherent challenges in using integrating spheres to measure transmittance, especially the substantial noise in the SWIR regions. This is supported by the absence of significant systematic bias between measured and modeled transmittance across the overwhelming majority of the spectrum (Figure $2\cdot 2$). Moreover, although the confidence intervals on transmittance bias are as high as 25% at some wavelengths, averaging over all spectra and aggregating across the visible (400 to 800 nm) and infrared (801 to 2500 nm) regions leads to result similar to those reported in other field spectra inversion studies, even though these studies used both reflectance and transmittance as input. Although our overall transmittance RMSE values were two to three times higher than those reported by Feret et al. (2008), these errors are inflated by the inclusion of conifer species, for which reflectance is harder to measure reliably and the assumptions of the PROSPECT model are not satisfied (Jacquemoud and Baret, 1990; Di Vittorio, 2009a; Allen et al., 1969). As well, measurements of needle-leaf transmittance often result in considerable noise in longer wavelengths (SWIR, >2000 nm) given the physical challenges of making these measurements on needle-leaf species (and other leaf types), generally poor lamp performance as compared to other methods, and the much smaller transmission of light in these wavelengths (often resulting in signals below the precision of the instrument). As such we would expect higher reported error compared to other leaf morphologies. For example, in examining our broadleaf samples we observed that the statistics for transmittance are much closer to those reported by Feret et al. (2008), despite not including measured transmittance in the inversion. Our transmittance error statistics are also similar to those reported for conifers by Di Vittorio (2009a) who used transmittance information and a re-calibrated version of the LIBERTY leaf RTM (Table 3). Moreover, our reflectance statistics show error comparable to or lower than those reported in similar studies (Feret et al., 2008; Di Vittorio, 2009a).

Through our sensor experiment, we explicitly demonstrate the tradeoffs between spectral information content and parameter uncertainty and identifiability. With increasingly coarse spectral resolution, we observed not only wider parameter confidence intervals indicating higher uncertainty but also tighter covariance structures indicating a reduced ability to distinguish between parameters (Figure 2.6). This comparison approach can be used to guide future enhancements of radiative transfer models by quantitatively showing whether a model of a given complexity is warranted given data of a particular quality. For example, in our simulation experiment, all the full-range hyperspectral sensors were capable of accurately estimating chlorophyll and carotenoids, but the ability of multispectral sensors to do so was dramatically lower (Figure 2.5, Table 2.5). We therefore can conclude that the use of PROSPECT 5 is warranted when performing inversion of hyperspectral data, but PROSPECT 4 (which does not distinguish between pigments) may be preferable for multispectral data. A similar framework can be used to determine the utility of increasingly complex future versions of PROSPECT that further differentiate leaf biochemical and structural components.

Importantly, the results of our sensor simulation experiment are highly idealized due to their failure to consider canopy structure, atmospheric effects, sun-sensor geometry, and sensor radiometric and spatial characteristics. However, a similar Bayesian inversion framework has been shown to work on MODIS data for the related coupled leaf-canopy RTM PROSAIL (Zhang et al., 2005; Zhang et al., 2006; Zhang et al., 2009; Zhang et al., 2012) and we believe the framework can be readily applied to other RTMs that address many of the limitations of our study. In future work, we will explore Bayesian spectral inversion of the coupled leaf-canopy RTM responsible for energy balance calculations in the ED2 ecosystem model (Medvigy et al., 2009a) on atmospherically corrected and orthorectified AVIRIS imagery, which will be an important milestone in bringing together the remote sensing and ecological modeling communities. In the long run, our framework could also be extended to the inversion of coupled canopy-atmosphere models using a combination of meteorological and spectral data from Earth Observation satellites, leveraging the relative advantages of each platform to generate unified time series of ecologically meaningful parameters with unprecedented spatial and temporal resolution.

2.5 Conclusions

This study introduces a novel application of Bayesian spectral inversion to the PROSPECT 5 leaf RTM that explicitly takes into account uncertainty and correlation in parameter estimates. Validation of our algorithm on a coupled leaf spectral-trait database revealed accuracy comparable to previous inversion algorithms despite only using reflectance observations and the default PROSPECT model (i.e. no additional refinement of the specific absorption features). By simulating reflectance measurements with the spectral characteristics of different remote sensing platforms, we were able to quantify the relationship between spectral resolution and parameter uncertainty. Although our simulated observations are highly idealized, we believe the resulting patterns in retrieved parameter accuracy and precision are representative of the advantages and limitations of the spectral configurations of different sensors for remote sensing of vegetation. Our work reinforces the notion that Bayesian spectral inversion provides a powerful and versatile framework for future RTM development and single-and multi-instrumental remote sensing of vegetation, and we encourage members of the remote sensing community to apply and build upon the tools we have developed.

Chapter 3

Leaf optical properties shed light on foliar trait variability at individual to global scales

3.1 Introduction

A key objective of present-day ecosystem ecology is to develop a predictive understanding of how terrestrial ecosystems will respond to rapid and widespread enviromental changes defining the Anthropocene. Plant functional traits serve as bellwethers of many aspects of plant ecophysiology, and understanding how traits respond to biotic and abiotic forcings has become a top priority in terrestrial ecology. As I discussed in Chapter 1, global trait databases are useful for evaluating theories about plant ecological strategies and can be used to constrain parameters of dynamic vegetation models.

However, there are fundamental limits on the ecological questions that can be answered using static trait databases. For one, such databases are spatially and phylogenetically incomplete, often in domains most critical to the global climate system such as boreal and tropical forests (Jetz et al., 2016). More importantly, because these databases generally do not contain observations collected on the same individuals through time, they are limited in their ability to inform us about direct dynamic responses of plant function to environmental changes. These changes are perhaps most pronounced in deciduous plants, whose leaves within a single season undergo a full life cycle accompanied by dramatic changes in pigment concentrations (Yang et al., 2016), morphology (Poorter et al., 2009), and productivity (Parent et al., 2010). Such intra-specific and intra-individual changes also occur in evergreen plants. For instance, in tropical evergreen broadleaf trees, leaf biochemistry and productivity varies significantly with leaf and plant age (Kitajima et al., 1997; Kitajima et al., 2013; Chavana-Bryant et al., 2016; Wu et al., 2016a). Similarly, conifer needles undergo morphological and biochemical changes over the course of their lifetime that reflect shifting priorities in terms of ecological strategy (Kuusk et al., 2017). Besides these developmental changes, plant traits also respond to biotic and abiotic stressors, including drought (Sun et al., 2018; Buchner et al., 2017; Bayat et al., 2016), heat (Chapin and Shaver, 1996; Serbin, 2012), elevated CO_2 (Medlyn et al., 2015; Lindroth, 2010), insect infestation (Di Vittorio and Biging, 2009; Marti et al., 2012), and pathogens (Horst et al., 2009).

Understanding the contributions of these many different drivers of plant trait variability necessarily requires large sample sizes over a wide range of conditions. Meanwhile, observing responses directly requires measurements through time. Traditional methods for assessing traits are ill-suited to this task because they are generally labor intensive and often require destructive sampling. As I discussed in Chapter 2, spectral measurements of plant tissues are capable of providing a fast and non-destructive assessment of plant traits. Leaf reflectance spectra have been widely used to study plant functional traits, both to elucidate patterns of natural variability (Cavender-Bares et al., 2017; Asner et al., 2015) and for assessing trait responses to stress (Serbin et al., 2014; Bayat et al., 2016; Sun et al., 2018). Furthermore, by clarifying the relationships between plant optical properties and traits, studies using leaf spectra are essential to the remote mapping and monitoring of traits (Schneider et al., 2017; Schimel et al., 2013; Schimel et al., 2015; Jetz et al., 2016).

Although, a variety of traits have been estimated empirically from spectra, the contribution of those traits to actual reflectance is not always clear. Some of the traits estimated empirically, such as $V_{c,\max}$ and $J_{c,\max}$, are not actually properties of plants but rather model parameters inferred from measurements of plant activity, so they by definition cannot influence plant reflectance. Similarly, elemental concentrations and ratios (particularly leaf N) are among the most common targets of spectroscopy, but these elements are present in plants primarily in larger molecules. However, the fact that these "invisible" traits can be accurately estimated from spectra indicates that they are often correlated related to other actually "visible" traits, but the exact nature of these correlations is still not well understood. In this study, I focus on six foliar traits (hereafter known as "optical" traits) that do contribute directly to leaf reflectance, and which are themselves relevant to plant function (Figure 3.1): (1)Leaf mesophyll structure, expressed as the effective number of leaf mesophyll layers, provides a physical mechanism for leaf adaptation to light independent of biochemical changes in photosynthetic machinery (Ivanov et al., 2016; Schollert et al., 2017). (2) Leaf chlorophyll content (the sum of chlorophyll a and b) drives the amount of photosynthetically active radiation absorbed by leaves and is therefore closely related to plant photosynthesis (Croft et al., 2017). Chlorophyll absorbs strongly in the visible range, particularly in the blue and red regions, where absorbance is >90%. (3) Leaf carotenoid pigments are related to the xanthophyll cycle, a key mechanism for preventing plant photooxidiative stress under drought, heat stress, and high light (Ruban et al., 2007). Carotenoid pigments absorb light most strongly in blue, to a lesser extent, green wavelengths. (4) Leaf anthocyanin pigments have a somewhat poorly understood role in plant physiology, but generally seem to enhance leaf tolerance to a wide range of stressors including drought, ultraviolet radiation, heavy metals, and photooxidation (Gould, 2004). Anthocyanins absorb most strongly in green and, to a lesser extent, blue wavelengths. (5) Leaf water content is closely related to leaf health and productivity, and is useful as an indicator of overall plant water status (Peñuelas et al., 1994; Kramer and Boyer, 1995; Cheng et al., 2011; Chavana-Bryant et al., 2016). Water is the mean factor driving leaf absorbance in shortwave infrared wavelengths (>1300 nm), and has particularly deep absorption features around 1450, 1950,

lengths (>1300 nm), and has particularly deep absorption features around 1450, 1950, and 2500 nm. (6) Finally, leaf dry mass per area is indicative of a wide variety of plant functional characteristics (Poorter et al., 2009) and is a key parameter in determining plant ecological strategy (Wright et al., 2004; Reich, 2014). Although exact molecular composition varies substantially across species and individuals, leaf dry mass is generally dominated by minerals, organic acids, structural and nonstructural carbohydrates, phenolics, proteins, lignin, and lipids (Poorter et al., 2009). Collectively, these molecules have an absorption peak in very blue wavelengths, negligible absorption in the visible and near-infrared, and gradually increasing absorption across the shortwave infrared region.

The six traits described above are used by the PROSPECT leaf radiative transfer model to simulate leaf reflectance and transmittance (Jacquemoud and Baret, 1990; Feret et al., 2008; Féret et al., 2017). PROSPECT has been used extensively for the simulation of leaf and, (combined with canopy models) canopy reflectance, as well as for estimation of leaf spectral characteristics through spectral inversion (Chapter 2, Jacquemoud et al., 2009). Unlike empirical approaches for estimating leaf properties from spectra, including spectral indices (le Maire et al., 2004; Féret et al., 2011) and partial least squares regression (PLSR) (Serbin et al., 2011), PROSPECT aims to provide a causal understanding of leaf optical properties. This means that, by design, PROSPECT intends to be generic across all species and conditions, and, more importantly, makes it a useful tool for applications where the links between leaf properties and spectra are important, such as modeling leaf absorbance for photosynthesis



Figure 3.1: (Top) Example reflectance spectra of *Acer rubrum* leaves. (Bottom) Normalized absorption coefficients for optical traits in this study.

and for improving representations of energy balance in terrestrial biosphere models. However, the extent of PROSPECT's generality has not been well tested, with most PROSPECT studies focusing on a relatively small set of species that are fairly similar to those used for PROSPECT's original calibration (Feret et al., 2008; Féret et al., 2011; Féret et al., 2017; Li and Wang, 2011; Wang et al., 2015a).

The above discussion culminates in the following three questions: First, how well can leaf optical traits be estimated from PROSPECT inversion over a wide range of species and experimental designs? Second, how do leaf optical traits vary across a variety of environmental conditions and species? Specifically, how is intraspecific variability in optical traits related to various growing conditions including local climate, canopy light environment, and exposure to pathogens? As well, how well can interspecific variability in traits be explained by species attributes frequently used for grouping species into functional types (e.g. plant growth form, photosynthetic pathway, phenological habit)? Third, how are leaf optical traits related to other leaf traits not directly estimable from PROSPECT inversion? To address these questions, I applied my PROSPECT inversion methodology (Chapter 2) to a large database of leaf spectra and traits collected in a variety of natural and experimental settings.

3.2 Methods

3.2.1 Data

Data from this project were assembled from 22 projects on leaf spectra and related foliar traits (Table 3.1). Most of these datasets are available in the ECOSIS spectral library (https://ecosis.org/), with the following exceptions: Data from Barnes et al. (2017) are hosted in a publicly-available Open Science Framework repository described in the manuscript. Data for Di Vittorio (2009), Wu et al. (2016), and Yang et al. (2016) were provided directly by the authors. Finally, data from both NGEE

Table 3.1: Project information

Short name	Long name	Samples	Species	Sites
ACCP ANGERS Barnes 2017	Accelerated Canopy Chemistry Program (ACCP) Angers, France spectra from INRA Barnes et al. 2017. Beyond greenness: Detecting	$850 \\ 274 \\ 86$	$\begin{array}{c} 46\\37\\1\end{array}$	$5 \\ 1 \\ 1$
	temporal changes in photosynthetic capacity with			
Cali. Eco. Traits	hyperspectral reflectance data. PLoS ONE. Fresh Leaf Spectra to Estimate Leaf Traits for California	261	16	34
Cedar Creek Biodiv.	Ecosystems 2014 Cedar Creek ESR Grassland Biodiversity	780	17	1
	Experiment: Leaf-level Contact Data: Trait Predictions			
Corn var.	Spectral Characterization of Multiple Corn Varieties:	288	1	1
Di Vittorio 2009 Hawaii 2000 LOPEX Milkweed stress	West Madison Agricultural Station 2014 Di Vittorio 2009 Hawaii 2000 vegetation species spectra Leaf Optical Properties Experiment (1993) Common Milkweed Leaf Responses to Water Stress and Elevated Temperature	$504 \\ 588 \\ 66 \\ 735$	$\begin{array}{c}2\\56\\45\\1\end{array}$	$\begin{array}{c}3\\48\\1\\1\end{array}$
Missoula TS	Missoula Montana lodgepole pine & big sagebrush time	100	2	4
NASA FFT NASA HyspIRI NGEE Arctic	series NASA Forest Functional Types (FFT) NASA HyspIRI field campaign Next Generation Ecosystem Experiment (NGEE) - Arctic	$1369 \\ 1704 \\ 614$		$ \begin{array}{c} 130 \\ 12 \\ 3 \end{array} $
NGEE Tropics	Tropics	700	20	1
Pepper K/N	Fresh and Dry Pepper Leaf Spectra with Associated Potassium and Nitrogen Measurements	119	1	1
PVY solanum	Varietal Discrimination and Detection of PVY in	761	1	1
Santa Monica Mtns. Soybean aphid	Solanum tuberosum: Hawaii 2014 Santa Monica Mountains vegetation species spectra Productivity and Characterization of Soybean Foliar	$353 \\ 1131$	$\begin{array}{c} 24 \\ 1 \end{array}$	$\begin{array}{c} 1 \\ 1 \end{array}$
Spectral variation	Traits Under Aphid Pressure Spectral Variation Between Leaf-level and Canopy-level Measurements	16	1	1
Wu 2016 Yang 2016	Wu et al. 2016 New Phytologist canopy traits study Yang et al. 2016 Remote Sensing of Environment	$\begin{array}{c} 160 \\ 497 \end{array}$	$\begin{array}{c} 17 \\ 3 \end{array}$	$\frac{1}{2}$

projets and the HyspIRI campaign were provided by Shawn Serbin. Collectively, these data are comprised of nearly 12,000 observations from 346 species, and span a wide geographic (Figure 3.2) and climatic range (Figure 3.3).

3.2.2 Trait estimation via PROSPECT inversion

The PROSPECT leaf radiative transfer model (Jacquemoud and Baret, 1990; Jacquemoud et al., 2009; Feret et al., 2008; Féret et al., 2017) simulates leaf reflectance and transmittance for 400 to 2500 nm wavelengths at 1 nm increments as a function of leaf morphological and biochemical characteristics. In this chapter, I compared the



Figure 3.2: Collection locations of spectra used in this analysis, colored by project name.



Figure 3.3: Collection locations of spectra used in this analysis in climate space. Climate data are from WorldClim (Fick and Hijmans, 2017).

performance of four different versions of PROSPECT, each of which uses a different combination of leaf traits: PROSPECT 4 uses total chlorophyll content per area $(\mu g \ cm^{-2})$, leaf water content per area $(g \ m^{-2})$, and leaf dry matter content per area $(g \ m^{-2})$ (Feret et al., 2008). PROSPECT 5 extends PROSPECT 4 with a parameter for total carotenoid content per area $(\mu g \ cm^{-2})$ (Feret et al., 2008). PROSPECT 5B adds an additional parameter for total "senescent brown pigment" content (arbitrary units) (Jacquemoud et al., 2009). Finally, PROSPECT D adds an additional parameter for total anthocynanin content per area $(\mu g \ cm^{-2})$ (Féret et al., 2017). The absorption coefficients for PROSPECT-D aligned with example leaf reflectance spectra are shown in Figure 3.1.

To estimate traits from leaf spectra, I generally followed the Bayesian RTM inversion approach of (Shiklomanov et al., 2016), except that I replaced the Metropolis-Hastings algorithm with a more efficient Differential Evolution algorithm with "snooker" update as implemented in the BayesianTools R package (Hartig et al., 2017). Forward simulations and Bayesian inversion of PROSPECT are implemented in the R package PEcAnRTM (Shiklomanov et al., 2016), which is open source and freely available at https://github.com/pecanproject/pecan/modules/rtm. Where leaf spectra extended beyond the 400 to 2500 nm wavelength range of the PROSPECT model. I used only the observations from 400 to 2500 nm. Where leaf spectra were sampled at a spectral resolution coarser than 1 nm or did not include all wavelengths simulated by PROSPECT, I subset the PROSPECT output in the likelihood function to match the observations. Where leaf spectra were sampled at a finer spectral resolution than 1 nm, or where wavelengths did not align at 1 nm intervals, I used cubic spline interpolation (default method in the base R function spline) to align the spectra with PROSPECT output. Where leaf spectra were provided as "pseudo-absorbance" $(1 - \log_{10}(R))$, I added the corresponding transformation to the PROSPECT output

in the likelihood calculation.

3.2.3 Analysis

To validate PROSPECT inversions, I compared trait estimates from PROSPECT inversion with direct measurements of the corresponding traits, where these traits were available. To explore project- and plant functional type-specific biases in the inversion, I fit robust linear regressions (via iterated re-weighted least squares, as implemented in the rlm function in the MASS R package) to investigate the ability of trait estimates from spectra to predict the measured traits (Figure 3.4).

To investigate the effects of experimental treatments and environmental conditions, I fit a linear fixed effects model for each optical trait and each treatment, with an additional fixed effect for species if multiple species were present in that treatment. To investigate the role of intraspecific variability in climate, I subset the data to species that were present at least 10 different sites and fit a fixed-effects model to each optical trait as a function of species, annual mean temperature, and annual precipitation. I then present the direction of each fixed effect coefficient and whether the coefficient was significant (Figure 3.9).

One study in this dataset—Yang et al. (2016)—explicitly looked at the seasonal trajectories of leaf reflectance, allowing me the chance to investigate the phenology of leaf optical traits (Figure 3.10).

To investigate the correlations among leaf optical traits, I performed a principal components analysis on the pairwise correlation matrix of all inversion estimates (Figure 3.11). To investigate the correlations between optical traits and other traits measured directly, I calculated the pairwise non-missing correlations (R function cor with option use = pairwise.complete.obs) and plotted the resulting correlation coefficients using the corrplot package. I performed this analysis for both individual observations and species means, where a trait was observed for at least 3 individuals

or species, respectively.

I performed all analyses using R version 3.5 (R Core Team, 2017). The data and code for performing these analyses are open source and freely available at https://github.com/ashiklom/rspecan.

3.3 Results

3.3.1 Estimating traits via PROSPECT inversion

Across most projects and traits, the four different PROSPECT versions performed similarly in terms of their ability to retrieve traits (Figure 3.4). For all versions of PROSPECT, leaf water content was consistently the most accurate trait retrieved, while retrievals of other traits were highly project-specific. For several projects spanning a large range of species (Cali. Eco. Traits, NASA FFT, and NASA HyspIRI), moving from chlorophyll as the only pigment (PROSPECT 4) to chlorophyll and carotenoids (PROSPECT 5/5B) drastically reduced inversion accuracy of dry matter contents, but this accuracy was restored by the further addition of anthocyanins and modification of the refractive index in PROSPECT D (Figure 3.4). Because PROSPECT-D also retrieves anthocyanin content and generally performed as well or better than other versions, it was the version selected for subsequent analyses.

Inversion accuracy varied significantly by project and growth form (Figures 3.4, 3.5, and 3.6). In terms of regression R^2 , inversion accuracy was highest for broadleaved trees, lower for herbs and needleleaved trees, and lowest for grasses. However, there was substantial project-specific variability in accuracy between these groups. For example, both water and LMA retrievals from the California Ecosystem Traits dataset were consistently much worse than for other datasets for both broadleaved and needleleaved trees, while the LOPEX and ANGERS datasets (against which PROSPECT is calibrated) performed very well for all traits for broadleaved trees, herbs, and grasses.



Figure 3·4: Validation of PROSPECT against observed trait values, by project and PROSPECT version. Y-axis represents R^2 values for robust linear regression.



Figure 3.5: Validation of PROSPECT-D against observed trait values. Grey lines indicate 95% confidence intervals around trait estimates. Solid, colored lines are robust regressions fit to the data by project and functional type. The solid black line is a regression fit to all of the data for a given functional type. The dashed black line is a 1 to 1 fit.



Figure 3.6: Regression-based validation of trait retrieval using Bayesian PROSPECT-D inversion. Each bar represents the R^2 value of a robust linear regression of observed trait value as a function of inversion estimate for a particular species (including additive and multiplicative bias correction). Colors indicate species functional type, as determined by the interaction of growth form and leaf morphology.

The full pairs plot (Figure 3.5) reveals that regression R^2 is insufficient for capturing all of the patterns in the validation. In several cases (e.g. water and LMA retrieval for conifers from the NASA FFT dataset, or carotenoid retrievals from the soybean aphid dataset), there is a saturation effect, whereby accuracy is good at lower trait values but declines as trait values increase. In other cases, there is a significant additive and/or multiplicative bias in retrievals — for instance, in the retrieval of chlorophyll and carotenoid contents from herbs.

3.3.2 Drivers of variability in leaf optical traits

Across all optical traits, roughly half of variability was explained by species identity (Figure 3.7). The variance across species means was largely idiosyncratic to species, with only up to 25% of variance explainable by species attributes (Figure 3.8). The most important explanatory attribute was leaf phenology (deciduous vs. evergreen), with occasional significant effects for leaf type (broad vs. needle), growth form (woody vs. herbaceous), and mycorrhizal association (arbuscular or non-arbuscular).

Leaf optical traits responded significantly to a range of natural and experimental stressors (Figure 3.9). Across the entire dataset, intraspecific variability in optical traits was weakly but, in some cases, significantly related to climate, with the strongest effects being declines in mesophyll structure and dry matter content with increasing temperature. Canopy light environment (i.e. whether a leaf was sunlit or shaded) also had a significant effect on most traits, at least for species on which a comparison was possible. Specifically, shaded leaves showed higher chlorophyll and anthocyanin concentrations and reduced mesophyll structure and water and dry matter contents.

Based on leaf reflectance measurements of *Populus deltoides* (eastern cottonwood) at the University of Arizona by Barnes et al. (2017), seasonal variations in vapor pressure deficit—but not leaf temperature—had significant negative effects on all



Figure 3.7: Fraction of variance in each optical trait explained by species identity, based on analysis of variance on least-squares linear regression.



Figure 3.8: Fraction of across-species variance in each optical trait (i.e. species means) explained by species attributes, based on analysis of variance on least-squares linear regression. A star (*) indicates attribute effects significant at the 90% confidence interval. Attributes are as follows: myco_is_am — Mycorrhizal fungi association (arbuscular or other such as ectomycorrhizal or ericoid); nitrogen_fixer — whether the species is a Nitrogen fixer; growth_form — tree, shrub, herb, or grass; ps_type — photosynthetic pathway (C3 or C4); leaf_type — leaf morphology (broadleaved or needleleaved); phenology — whether the species is deciduous or evergreen.



Figure 3.9: Effects of different sources of intraspecific variability on traits estimated via PROSPECT inversion. Each value is the fixed effect slope on the corresponding trait normalized to zero mean and unit variance, as estimated from a linear fixed-effects model. Color brightness indicates degree of statistical significance (90 or 95% confidence level), and color hues indicate effect direction (positive or negative).

traits, with the strongest effects on chlorophyll and anthocyanin contents. Similarly, warming and drought experiments on Asclepias syriaca (common milkweed) had strong and significant effects on almost all optical traits, with both treatments leading to significant decreases in leaf water content and effective number of mesophyll layers and increases in pigments and dry matter content concentrations (Couture, 2015). Leaf optical traits also responded significantly to chemical and biotic stressors. Based on data from Di Vittorio (2009), needles of *Pinus ponderosa* and *Pinus jeffreyi* from the northern Sierra Nevada mountains experienced reductions in all traits, but most strongly in pigment and dry matter contents, when afflicted with winter fleck (patchy mortality of needle epidermal cells, usually triggered by exposure to harsh winter weather), sucking and scale insect, and especially ozone damage. As well, spectral inversion revealed small but statistically significant declines across all optical traits except anthocyanins in *Solanum tuberosum* (potato) plants infected with potato virus Y (Couture, 2014). On the other hand, treatment of *Glycine max* (soybean) with aphids resulted in a small but significant increase in pigment concentrations, with the strongest effect observed at medium-level treatment (Singh, 2013).

Where such measurements were available, leaf optical traits exhibited a strong phenological signal (Figure 3.10). All optical traits showed a peak in late July / early August, followed by a decline into the fall, with the sharpest declines for pigments and water content and less precipitous declines for dry matter and mesophyll structure. Furthermore, the effective number of leaf mesophyll layers, and to a lesser extent, leaf dry matter content in shade leaves, appeared to increase in the late fall. With the exception of anthocyanin content, all traits for shaded leaves were higher and experienced a greater seasonal variability than sunlit leaves.



Figure 3.10: Optical trait estimates through a season for *Quercus rubra* (red oak) at Martha's Vineyard, MA by Yang et al. (2016). Colors indicate sunlit vs. shaded leaves. Line is a LOESS best fit with shaded standard error.



Figure 3.11: Principal components analysis of optical trait correlation matrix. (Left) Cumulative fraction of variance explained by each principal component. (Center, Right) Principal component scores and vectors for each optical trait for components 1 and 2 (center) and 2 and 3 (right).

3.3.3 Trait correlations

Optical traits estimated by PROSPECT are not mutually independent, but rather have some structure to their covariance (Figure 3.11). The first principal component, which explains roughly 50% of the variability, is defined by increases in all leaf traits and can be interpreted as overall leaf size and tissue density. The second principal component, which explains an additional 20% of the variability, is characterized by an approximate trade-off between structural traits (mesophyll structure and dry matter content) and physiological traits (chlorophyll, carotenoid, and water contents). The third principal component, which explains a further 15% of the variability, is dominated by a trade-off in water and anthocyanin concentrations.

Covariance of optical traits with six area-normalized traits—leaf nitrogen, carbon, cellulose, and lignin contents, $V_{c,\max}$, and J_{\max} —was strongly species specific, but, in



Figure 3.12: Intra-specific pairwise correlations of optical traits with direct measurements of area-based leaf N, C, cellulose, lignin, $V_{c,\max}$, and J_{\max} . Colors indicate plant functional type. Species are displayed along the y axis, and are sorted within each facet from highest to lowest average correlation across all traits. Analysis was performed only for species with at least 10 pairwise observations of each trait.

many cases, significant (Figure 3.12). In general, for any given species, most of the estimated optical traits exhibited similar correlations with the directly measured trait. For instance, for Glycine (*Glycine max*, GLMA4), all optical traits were positively correlated with leaf N, C, cellulose, and lignin, whereas for milkweed (*Asclepias syriaca*, ASSY), all of these correlations were negligible. Leaf nitrogen correlated best for the largest number of species with leaf chlorophyll and, to a slightly lesser extent, with dry matter content. Leaf carbon and lignin were most consistently correlated with leaf dry matter content, while correlations with cellulose were more idiosyncratic. $V_{c,\max}$ and J_{\max} were strongly positively correlated with all traits for *Populus deltoides* (PODE3), but completely uncorrelated for milkweed (ASSY). Correlations between optical and other traits were generally strongest for broadleaf trees, somewhat weaker for needleleaved trees, and weakest for herbs and grasses. Although this was also the general pattern in the validation, exploratory analyses (not shown) do not find any consistent relationship between trait retrieval accuracy (represented by validation R^2) and intraspecific correlation.

Among species means, almost all area-based traits were at least weakly positively correlated with each other (Figure 3.13). Among optical traits, the strongest correlations were among the three pigments, and of leaf water and dry matter contents. Spectrally-estimated leaf mesophyll structure and dry matter content correlated strongly with traits related to structure, namely C, cellulose, and lignin contents. Leaf N was most strongly correlated with dry matter and water contents and leaf mesophyll structure, and only weakly correlated with chlorophyll and carotenoid contents.

# meso	0.38	0.1	0.37	0.36	0.34	0.35	0.63	0.6	0.57	0.39	0.06	
	Chl.	0.67	0.53	0.39	0.2	0.16	0.08	0.36	0.24	0.29	0.16	- 0.8
		Car.	0.6	0.5	0.48	0.18	0.09	0.26	0.22	0.14	0.07	- 0.6
			Anth.	0.38	0.46			0.48	0.46	0.34	0.3	- 0.4
				Water	0.54	0.36	0.54	0.34	0.48	0.37	-0.07	- 0.2
					Dry matter	0.4	0.69	0.63	0.59	0.53	0.24	
			•			N	0.67	0.34	0.49	0.89	0.25	- 0
							С	0.7	0.88	0.36	0.63	0.2
								cellulose	0.77	0.31	0.28	0.4
									lignin	0.19	0.7	0.6
										protein	0.14	0.8
				•							starch	

Figure 3.13: Pairwise correlations among species means for PROSPECT inversion estimates and other, directly-measured areanormalized traits. In lower diagonal, circle color and size indicate correlation direction and strength, respectively. Values in upper diagonal are correlation coefficients, colored by direction and strength.

3.4 Discussion

3.4.1 Estimating traits through PROSPECT inversion

Establishing general, species- and site-independent relationships between leaf functional traits and optical properties is challenging. My results suggest that Bayesian PROSPECT inversion is a promising technique for achieving this objective. Averaged across the entire dataset, spectral estimates of traits were able to capture 50 to 75% of the variability in the true values of the traits (Figure 3.4). In addition, spectral trait estimates were able to not only identify but also ascribe a physiological mechanism to intra-specific variability associated with long-term acclimation and acute stress responses in both natural and experimental settings (Figure 3.9). By comparing retrieval accuracy across different versions, my results also reaffirm the value of recent improvements to PROSPECT. In particular, the successive additions of carotenoid (Feret et al., 2008) and anthocyanin (Féret et al., 2017) pigments significantly increased accuracy of chlorophyll retrievals in the phenological dataset of Yang et al. (2016) (Figures 3.5 and 3.4), which points to the importance of modeling non-photosynthetic pigments in leaves sampled early or late in the growing season.

That being said, the large scale validation demonstrated here reveals enduring challenges and development opportunities for modeling leaf optical properties and retrieving leaf traits from spectra. The particularly poor inversion accuracy for grasses (Figures 3.5 and 3.6) suggests that the biochemistry and morphology of grasses do not fit the assumptions of PROSPECT. Perhaps lower-hanging fruit is investigation of places where inversion estimates did well at capturing variability in traits, but were additively or multiplicatively biased. For example, estimates of chlorophyll and carotenoid content in herbs from two dramatically different environments and species (greenhouse-grown soybean and tundra vegetation) showed virtually the same multiplicative bias and accuracy (Figure 3.5). One possible culprit for this bias is the

chlorophyll a-b ratio, which varies within and across species (Kura-Hotta et al., 1987; Kitajima and Hogan, 2003) but is fixed in the current version of PROSPECT. Fortunately, a recently released update to PROSPECT succeeded in modeling chlorophyll aand b independently (Zhang et al., 2017). This advance continues an ongoing positive trend in improving the detail with which PROSPECT models leaf optical properties.

One conclusion of Chapter 2 was that the use of physically-based absorption coefficients, such as that for leaf water content, is important for accurate trait retrievals using physically-based radiative transfer models. Results from the wider range of species and projects in this chapter challenge this notion. Retrievals of leaf water content and total chlorophyll concentration had comparable overall R^2 values (Figure 3.4). However, leaf water content retrievals exhibited clear and significant projectspecific biases, especially at high values (Figure 3.5) Meanwhile, chlorophyll content retrieval was more consistently accurate across its entire range, even for needleleaved species (in the Di Vittorio dataset) (Figure 3.5) that poorly fit the parallel-plane assumptions of the PROSPECT model (Allen et al., 1969; Jacquemoud and Baret, 1990) and, more importantly, despite the fact that the chlorophyll absorption coefficients for PROSPECT are calibrated only against the ANGERS dataset, which does not have any conifers (Feret et al., 2008; Féret et al., 2017). Project-specific calibration has been shown to further improve the results of PROSPECT inversion (Li and Wang, 2013), which suggests that re-calibration of PROSPECT absorption coefficients against a wider range of species and environmental conditions (such as those used here) could lead to significant improvements in PROSPECT performance. Ongoing efforts to curate and make publicly available spectral observations, such as the ECOSIS project (ecosis.org), significantly aid such efforts.

3.4.2 Variation in optical traits

Optical traits showed substantial variability both within and across species. The extent of intra-specific variability in optical traits was substantial—from 30% for leaf structure and dry matter content to nearly 50% for pigment concentrations (Figure 3·7)—and fell comfortably in the range of intraspecific trait variability reported in other studies for similar traits (Messier et al., 2010; Albert et al., 2010a). Following the definition of McGill et al. (2006) that a useful "trait" is one that varies more across than within species, all six of the traits examined in this study technically qualify as "traits", but pigment concentrations only barely. In addition, the interspecific variability is poorly explained by species attributes typically used to define plant functional types (e.g. for dynamic vegetation models)—taken together, speciesspecific attributes were able to explain at most around 30% of interspecific variability (Figure 3·8). This result adds to the emerging body of literature on the limited ability of discrete plant functional types with fixed traits to effectively capture variability in plant and ecosystem function (Bodegom et al., 2011; van Bodegom et al., 2014; Verheijen et al., 2015a; Clark, 2016).

Some of the intraspecific variability in optical traits was not random, but rather suggested a systematic plastic response to biotic and abiotic stressors (Figures 3.9and 3.10). For example, the observed increase in leaf dry matter content with decreasing temperature and increasing precipitation both agree with the meta-analysis of leaf mass per area by Poorter et al. (2009). On the other hand, the absence of significant trends in pigment and water contents with respect to site temperature are likely because these traits respond more rapidly to environmental conditions, which is supported by their relatively higher fraction of intra-specific variability (Figure 3.7). This idea is further supported by the fact that pigment concentrations, but not leaf structure or dry matter content, responded significantly to within-season temperature fluctuations in the Barnes et al. (2017) dataset and to aphid pressure in the soybean aphid dataset (Figure 3.9). This positive response of chlorophyll concentration to aphid pressure is surprising. Alves et al. (2015) found significant effects of aphid infestation on soybean near-infrared reflectance and NDVI but no effect of on chlorophyll content. Meanwhile, Luo et al. (2012) found that wheat aphid infestation increased wheat leaf reflectance across the visible and near-infrared range, consistent with reduced pigment concentrations. This result is unlikely to be caused by inaccurate PROSPECT estimates of pigment concentrations because inversion accuracy of both chlorophyll and carotenoids for this dataset was among the highest in this study (Figures 3.4 and 3.5).

I observed statistically significant differences in leaf morphology and biochemistry between sunlit and shaded leaves. Chlorophyll content was significantly higher in shade leaves compared to sun leaves, which supports established theory that allocation of resources to light absorption relative to other photosynthetic functions (e.g. carbon fixation) increases with decreasing irradiance (Hikosaka and Terashima, 1995). At the same time, the reduced leaf dry matter content and mesophyll structure in shade leaves agrees with established understanding of the relationship between leaf mass per area and irradiance (Poorter et al., 2009). However, the lack of a significant shade effect on carotenoid content and the positive effect on anthocyanins are surprising, given the current understanding of the photoprotective role of these pigments (Young, 1991; Steyn et al., 2002). One explanation for the lack of a shade effect on carotenoids is that the response is non-linear, as has been shown in treatments with more finely varied light levels (Sonobe et al., 2017). An alternative, simpler explanation may be inaccuracy in retrievals related to the relative coarseness with which pigments are currently treated by PROSPECT (as discussed above).

Another source of intraspecific variability in optical traits explored in this study
was phenology (Figure 3.10). PROSPECT inversion was able to successfully capture the phenological progression of chlorophyll and carotenoid contents as they increase early in the growing season and decline in the fall (Yang et al., 2014; Yang et al., 2016). However, the results for leaf mass per area disagreed with the direct measurements in several important ways. First, contrary to direct observations at this site (Yang et al., 2016) and to expectations based on literature survey (Poorter et al., 2009), my estimates for leaf mass per area were consistently lower in sunlit than shaded leaves. Second, while direct observations show that leaf mass per area generally increases early in the growing season up to leaf maturity and then remains effectively constant until leaf abscission in the fall (Yang et al., 2014; Yang et al., 2016), my results show a decline in leaf mass per area in the late growing season for all leaves followed by a slight increase at the end of the growing season for sunlit leaves. The most likely explanation for this is inaccuracy in trait estimation, as evidenced by the extremely poor validation results for leaf mass per area for the phenological dataset (Figures 3.4and 3.5).

Finally, optical traits revealed signatures of acute stress from insects, pathogens, and extreme environmental conditions. In many cases, these effects agreed well with physiological expectations. For instance, the significant negative effects of winter fleck, sucking and scale insects, and especially ozone damage on pine needles reported here match the earlier results of Di Vittorio (2009) for this dataset as well as the broader literature consensus on the damaging effects of ozone on plant physiology (Lindroth, 2010). The same can be said for the adverse effects of Potato Virus Y on potato plants (Scholthof et al., 2011). However, in several cases, the direction of these effects was counterintuitive. Milkweed plants grown under elevated temperature and periodic drought stress (Couture, 2015) showed the expected decline in leaf water content (Peñuelas et al., 1994; Kramer and Boyer, 1995; Cheng et al., 2011), but showed a significant increase in pigment concentrations. The higher concentrations of carotenoids under drought stress and anthocyanins under elevated temperature could reasonably be explained as photoprotective adaptations (Young, 1991; Steyn et al., 2002; Gould, 2004). The increased chlorophyll content is harder to explain, but similar increases in chlorophyll in drought stressed plants have been reported (Vilfan et al., 2016). One possibility is that, because the chlorophyll is estimated on a leaf area basis, a reduction in leaf size and structure associated with declining water content could lead to an increase in apparent chlorophyll concentration, even if the mass-based concentration was constant or even slightly declined. Regardless, the demonstrated ability of this study to not only detect but to analyze the physiological mechanisms of stress reinforces the value of leaf spectroscopy in both natural and agronomic settings.

3.4.3 Patterns of trait correlation

Optical traits vary non-randomly not only in response to environmental conditions and stress, but also with each other and with other "invisible" traits. In Chapter 1, I found that the leaf economic spectrum—broadly, a multidimensional axis of trait variability defining a trade-off between productivity and resilience—generally held within plant functional types as well. The findings in this chapter suggest that the leaf economic spectrum applies to variability among optical traits as well, as the second principal component of optical trait variability was characterized by a tradeoff between productivity-related traits (pigments and water content) and structural traits (dry matter and mesophyll structure) (Figure 3·11). Both the explanatory power of the first two principal components (around 70%) and their interpretation correspond remarkably well to a global analysis of species means from TRY (Díaz et al., 2016). Meanwhile, the third principal component of optical trait variability can be interpreted as an axis of stress, which can lead to reductions in leaf water content (Peñuelas et al., 1994; Kramer and Boyer, 1995; Cheng et al., 2011) and can promote higher investment in anthocyanins for their protective properties (Gould, 2004). This is partially supported by my analysis of experimental treatments, water and anthocyanin contents did exhibit opposite responses to shade and warming (and to potato virus, though not significantly for anthocyanins) (Figure 3.9).

The signature of the leaf economic spectrum was less clear among species means. An economic trade-off between investment in pigments and structural molecules would imply negative correlations between these groups of traits, but my results show that at the species level, pigments are weakly positively correlated with structural traits (Figure 3·13). Meanwhile, optical traits related to structure, as well as leaf water content, were strongly positively correlated with leaf C, cellulose, and lignin. One explanation for these differences in correlations between pigments and structural molecules is that the former show relatively more plasticity whereas the latter are more phylogenetically conserved. This is supported by the analysis of variance performed in this study (Figure 3·7), as well as broader literature review of variability in leaf structure (Poorter et al., 2009; Onoda et al., 2017). In addition, the modest positive interspecific correlation of leaf N with both structural molecules and pigments agrees with the large interspecific variability in leaf N allocation to structural and photosynthetic molecules (Onoda et al., 2017).

Another key objective of this study was to investigate the ability of optical traits to predict other physiologically relevant traits that cannot be observed directly from spectra. In many cases, multiple optical traits were significantly positively correlated with area-based leaf N, C, cellulose, lignin, $V_{c,\max}$, and J_{\max} , which is not surprising given the extensive literature on empirical estimation of these traits from field and airborne spectroscopy (Serbin et al., 2011; Serbin et al., 2014; Asner et al., 2015; Cavender-Bares et al., 2017) as well as the coordination between these traits in plant physiology and ecological strategy (Kitajima and Hogan, 2003; Onoda et al., 2017; Croft et al., 2017). However, these correlations varied significantly between species, including for species within the same functional type (Figure 3.12). In part, this may be due to the unbalanced sampling in this analysis; specifically, some species were sampled across a much wider range of conditions than others (particularly those grown under different experimental treatments), and correlations are likely to be more consistent where plants experience extreme conditions that lead to overall declines in leaf condition. Patterns of trait covariance are also modulated by a number of environmental factors, such as dominant sources of limitation (e.g. light, water, or nutrients) (Borgy et al., 2017) or strength of competitive effects (Kunstler et al., 2015) (see discussion in Chapter 1), which vary substantially across this dataset. As such, identifying more precisely the drivers of variability in intraspecific trait correlations is an important future direction for this research.

3.5 Conclusions

This study is, to my knowledge, the first of its kind in synthesizing reflectance measurements from a wide collection of species and measurement conditions under a single common methodology. For one, it provides a valuable contribution to remote sensing methodology by demonstrating the capabilities and limitations of trait retrieval via inversion of various versions of PROSPECT. It is particularly novel in revealing that PROSPECT is able to detect and ascribe physiological meaning to plant responses to environmental conditions and acute stressors. More generally, this study contributes to the growing body of literature evaluating the drivers of variability in plant functional traits and reinforces the importance of intraspecific variability in plant function. Ultimately, this study showcases the value of leaf spectroscopy for ecology and agriculture.

Chapter 4

Cutting out the middle man: Calibrating and validating a dynamic vegetation model using remotely sensed surface reflectance

4.1 Introduction

My previous chapters have shown that models have much to gain, both in terms of direct parameter constraint from trait observations and from new process representations that emerge from trait ecology more broadly. However, there are limits on the extent to which traits alone can improve models. For one, even after examining a broad range of inter- and intraspecific factors, large fractions of variability in plant function remain unexplained. Moreover, vegetation models are simplified abstractions of reality, with many processes omitted or represented by simplistic empirical equations with little-to-no physical basis and therefore no directly measurable trait that can serve as a parameter constraint. In these cases, models can only be calibrated via their emergent predictions of state variables.

Many previous efforts have used various data streams calibrate or constrain dynamic vegetation model parameters and states. Among these data streams, remote sensing is particularly promising due to its consistent measurement methodology and largely uninterrupted global coverage. Data products derived from remote sensing observations have been effectively used to constrain, among others, phenology (Knorr et al., 2010; Viskari et al., 2015), absorbed photosynthetically-active radiation (Peylin et al., 2016; Schürmann et al., 2016), and primary productivity (MacBean et al., 2018).

However, there are issues with using derived remote sensing products to calibrate ecosystem models. Relationships of surface reflectance variables (such as vegetation indices) with characteristics of vegetation structure and function estimated by models are complex. For example, the assumption of a simple linear relationship between the normalized difference vegetation index and absorbed photosynthetically-active radiation (e.g. Peylin et al. 2016) has long been shown to be sensitive to variability in soil and leaf optical properties (Myneni and Williams, 1994), and is known to vary across spatial scales and sensor configurations (Fensholt et al., 2004). A related issue is that subtle but significant differences in the ways vegetation variables are defined, by both models and data products, can significantly affect the interpretation of remotely sensed data (Carlson and Ripley, 1997). Furthermore, uncertainties in derived remote sensing data products are often poorly quantified but known to be significant, to the extent that some studies advise against working with individual pixel values in favor of averaging across adjacent pixels (thereby dramatically reducing the spatial resolution) to achieve reasonable accuracy (Yang et al., 2006; Wang et al., 2004). Although these issues could be partially alleviated by robust, pixel-level uncertainty estimates for remote sensing data products, such estimates are generally not widely available for most data products. Collectively, these issues, combined with differences in sensor configuration and design, result in large differences in estimates of surface characteristics across different remote sensing instruments that lead directly to different estimates of carbon storage and flux (Liu et al., 2018).

One way to overcome the limitations of derived remote sensing data products while still leveraging the capabilities of remote sensing is to work directly with the observed surface reflectance. In the context of dynamic vegetation modeling, this can be accomplished by coupling these models with leaf and canopy radiative transfer models that simulate surface reflectance as a function of known surface characteristics (Quaife et al., 2008). Such an approach takes advantage of the fact that surface reflectance contains valuable information about vegetation structure and function without relying on the independent retrieval of these characteristics from reflectance data alone, which is often an ill-posed problem (Combal et al., 2003; Lewis and Disney, 2007). Moreover, besides enabling assimilation of remotely sensed data, training models to accurately simulate surface reflectance is essential to properly quantifying and testing hypotheses related to vegetation-climate interactions and feedbacks. For instance, the net climate effect of ongoing changes in Arctic vegetation composition depends on the balance of opposing radiative (lower albedo) and latent (increased transpiration) energy feedbacks (Swann et al., 2010), so forecasting this effect requires accurate models of canopy energy transfer. More fundamentally, light availability is a key control of photosynthesis and therefore has immediate, direct consequences for individual plant function (Hikosaka and Terashima, 1995; Robakowski et al., 2004; Niinemets, 2016b; Keenan and Niinemets, 2016b) as well as longer-term, indirect consequences for competition and ecological succession (Niinemets and Valladares, 2006; Kitajima et al., 2013; Falster et al., 2017).

Recognition of the importance of these processes has led to the development of vegetation models with explicit representations of canopy radiative transfer. The most accurate canopy radiative transfer models capture both vertical and horizontal heterogeneity with very high spatial resolution (Widlowski et al., 2007). However, such models are usually too computationally intensive for dynamic vegetation models, which employ various approximations based on simplifying assumptions to make the problem more tractable (Fisher et al., 2017). One common approach is the "two-

stream approximation", which simplifies the problem of directional scattering within a medium by modeling the hemispherical integral of fluxes rather than individual, directional components. In the context of radiative transfer in plant canopies, many different two-stream formulations have been developed, of which I highlight two: One formulation was developed by Kubelka and Munk (1931) and later adapted to vegetation canopies by Allen, Gayle, and Richardson (1970) and further refined by Suits (1971), Verhoef (1985), and others. This theory forms the foundation of the SAIL canopy radiative transfer model (Verhoef, 1984) and its derivatives (e.g. 4SAIL Verhoef et al., 2007), which have been used extensively in the remote sensing community for modeling and retrieving vegetation characteristics from spectral data (Jacquemoud et al., 2009). Another was developed by Meador and Weaver (1980) for atmospheric radiative transfer, and was subsequently adapted to canopy radiative transfer by Dickinson (1983) and refined by Sellers (1985). Due to its theoretical simplicity and low computational demand, this is the approach commonly used to represent radiative transfer in ecosystem models, including the Community Land Model (CLM, Oleson et al., 2013) and the Ecosystem Demography model (ED, Moorcroft et al., 2001; Medvigy et al., 2009b). The version of this scheme used in ED2 (and derivative models) is fairly unique in its explicit representation of multiple canopy layers, which allows ED2 to simulate competition for light, a key component of modeling vegetation demographics (Fisher et al., 2017). However, compared to physiological processes, the structure and parameterization of canopy radiative transfer schemes in demographic models has received relatively little attention. When canopy radiative transfer has been considered, it was shown to be important to a wide range of physiological and demographic processes. For example, using a modified version of the ED model, Fisher et al. (2010) showed that excessive light absorption by the top cohort resulted in unrealistically excessive growth of canopy trees at the expense of understory trees. Similarly, an analysis by Viskari et al. (in revision) demonstrated that the Ecosystem Demography (ED2) model's predictions of ecosystem energy budget, productivity, and composition are highly sensitive to the parameterization of the model's representation of canopy radiative transfer. Understanding and improving representations of canopy radiative transfer in dynamic vegetation models is therefore critical to accurate projections of the fate of the terrestrial biosphere.

Building on the work of Viskari et al., the objective of this chapter is to develop and demonstrate the calibration and validation of the ED2 model using remotely sensed surface reflectance. First, I link the canopy radiative transfer model in ED2 with the PROSPECT leaf radiative transfer model to allow ED to predict full-range, hyperspectral surface reflectance at each time step. Second, I calibrate this coupled leaf-canopy radiative transfer model at a number of sites in the US Midwest and Northeast where coincident plot vegetation survey data and observations of the NASA Airborne Visible/InfraRed Imaging Spectrometer (AVIRIS) are available.

4.2 Methods

4.2.1 Model description

The Ecosystem Demography version 2 (ED2) model simulates plot-level vegetation dynamics and biogeochemistry (Moorcroft et al., 2001; Medvigy et al., 2009b). By grouping individuals of similar size, structure, and composition together into cohorts, ED2 is capable of modeling patch-level competition in a computationally efficient manner.

Relevant to this work, ED2 includes a multi-layer canopy radiative transfer model that is a generalization of the two-stream solution of Sellers (1985). In its default configuration, the ED2 radiative transfer model solves for the overall hemispherical (i.e. diffuse) canopy albedo in two spectral "bands"—visible and near-infrared—as a function of each cohort's leaf area index and PFT-specific parameters for leaf and wood reflectance and transmittance, canopy clumping factor, and leaf orientation factor. The equations used are mostly adapted from the Community Land Model(Oleson et al., 2013), but a summary of key features is as follows:

The direct radiation flux is modeled as an exponential attenuation curve through the canopy based on each layer's transmissivity (τ_r) , which in turn is a function of the total area index (TAI) of the canopy layer and the inverse optical depth (μ_r) :

$$\tau_r = e^{-\frac{TAI}{\mu_r}} \tag{4.1}$$

The total area index (TAI) is the sum of the wood area index (WAI) and the effective leaf area index, with the latter calculated as the product of the true leaf area index (LAI) and the clumping factor (c, defined on the interval <math>(0, 1) where 0 is a "black hole"—all leaf mass concentrated in a single point—and 1 is a homogenous closed canopy):

$$TAI = cLAI + WAI \tag{4.2}$$

The true leaf area index for each PFT is calcluated in two stages: First, the total leaf biomass is calculated from the diameter at breast height via an exponential allometric equation parameterized for each PFT. Second, the leaf biomass is converted to leaf area index through the PFT-specific specific leaf area (SLA).

The optical depth is calculated based on the projected area (p) and the solar zenith angle (θ) :

$$\mu_r = \frac{\cos\theta}{p} \tag{4.3}$$

The projected area (p) is a function of the leaf orientation factor (f):

$$\phi_1 = 0.5 - f(0.633 + 0.33f) \tag{4.4}$$

$$\phi_2 = 0.877(1 - 2\phi_1) \tag{4.5}$$

$$p = \phi_1 + \phi_2 \cos\theta \tag{4.6}$$

The diffuse radiation flux is more complicated because light is scattered internally within canopy layers. Unlike the Community Land Model, which solves only for sunlit and shaded leaves, ED2 calculates the full canopy radiation profile by parameterizing the two-stream equations for each layer (as well as soil and atmosphere boundary conditions) and then using a linear system solver to solve for the radiation profile. For each layer, leaf and wood forward scattering (ω_+) are just the sums of their respective reflectance (r) and transmittance (t) values:

$$\omega_{+} = r + t \tag{4.7}$$

Leaf and wood backscatter (ω_{-}) are a function of their respective reflectance and transmittance values as well as the leaf orientation factor (f):

$$\omega_{-} = \frac{r+t+0.25(r-t)(1+f)^2}{2(r+t)}$$
(4.8)

Overall scatter (ι) and backscatter (β) of all elements in a canopy layer is modeled as the average of leaf and wood scatter, weighted by their respective area indices:

$$w_l = \frac{LAI}{LAI + WAI} \tag{4.9}$$

$$w_w = \frac{WAI}{LAI + WAI} \tag{4.10}$$

$$\iota = w_l \omega_{+,l} + w_w \omega_{+,w} \tag{4.11}$$

$$\beta = w_l \omega_{-,l} + w_w \omega_{-,w} \tag{4.12}$$

The inverse optical depth for diffuse radiation (μ_f) is calculated from the coefficients ϕ_1 and ϕ_2 (see equations 4.4 and 4.5):

$$\mu_f = \frac{1 - \phi_1 \ln \left(1 + \frac{\phi_2}{\phi_1 \phi_2}\right)}{\phi_2} \tag{4.13}$$

Note that μ_f simplifies to 1 when orientation factor is 0 (random, spherical distribution of leaf angles). Collectively, these coefficients are used to calculate the optical depth for diffuse radiation (τ_f):

$$\epsilon = 1 - 2\beta \tag{4.14}$$

$$\lambda = \frac{\sqrt{(1 - \epsilon\iota)(1 - \iota)}}{\mu_f} \tag{4.15}$$

$$\tau_f = e^{\lambda TAI} \tag{4.16}$$

The remaining coefficients are described in the Community Land Model manual (Oleson et al., 2013).

By default, ED takes as parameters PFT-specific leaf and wood reflectance and transmittance values with one value each for the visible and near-infrared spectral regions. For this analysis, I first modified ED to take an arbitrary number of leaf and wood reflectance transmittance values. From there on, I simulated leaf reflectance and transmittance using the PROSPECT 5 leaf RTM (see Chapters 2 and 3). For soil and wood reflectance, I used means of the corresponding spectra from Asner (1998), resampled to 1 nm resolution. The final coupled PROSPECT-ED canopy radiative transfer model (hereafter known as "EDR") has 10 parameters for each PFT: 5 parameters for PROSPECT (number of mesophyll layers, and area-based chlorophyll, carotenoid, water, and dry matter contents), specific leaf area, base and exponent for the leaf allometry, and clumping and orientation factors.

4.2.2 Sensitivity analysis

To provide a basis for understanding the behavior of EDR, I performed a one-attime sensitivity analysis to explore how its reflectance predictions vary with each leaf optical and canopy structural parameter. To assess the mathematical foundation of the EDR canopy model (i.e. the Sellers two-stream scheme) without the confounding influence of multiple cohorts, I first performed this sensitivity analysis on a simulated plot containing only a single mature tree cohort. For comparison, I also included simulations using the 4SAIL canopy radiative transfer model. The 4SAIL model simulates four reflectance "streams"—diffuse (hemispherical) and direct (directional) reflectance for both diffuse and direct incident radiation— but because EDR only simulates diffuse reflectance and its input is dominated by direct radiation (at least on sunny days, which are necessary for satellite and high-altitude airborne data), I used the "directional-hemispherical" output for all comparisons. For its representation of leaf angle distribution, 4SAIL uses an ellipsoidal model that takes as input the mean leaf inclination angle (θ), which is related to EDR's leaf orientation factor (f) by:

$$\cos\theta = \frac{1+f}{2} \tag{4.17}$$

Unlike EDR, 4SAIL does not account for canopy clumping. (4SAIL does have a "hot spot" parameter to account for strong bi-directional reflectance effects from structurally heterogeneous canopies, but this parameter only affects the bi-directional reflectance, which was not used in this analysis).

To investigate the way EDR models interactions between canopy layers, I also performed a similar sensitivity analysis on a simulated plot with two cohorts—a dominant early successional cohort and a sub-dominant mid-successional cohort. I examined the sensitivity of total canopy reflectance to the optical properties of both the dominant and sub-dominant cohort, and looked at how this sensitivity was affected by clumping in the upper cohort.

4.2.3 Model calibration

For model calibration, I selected 47 sites from the NASA Forest Functional Types (FFT) field campaign that contained plot-level inventory data (stem density, species identity, and DBH) coincident with observations of the NASA Airborne Visible/Infrared Imaging Spectrometer (AVIRIS). These sites are mostly located in the United States Upper Midwest with several sites also in upstate New York and western Maryland, and include stands dominated by either evergreen or deciduous trees and spanning a wide range of structures, from dense groups of saplings (bottom right) to sparse groups of large trees (top left) (Figure $4 \cdot 1$). Based on ED's PFT definitions, these sites contained a total of five different temperate plant functional types: Early successional hardwood, northern mid-successional hardwood, late successional hardwood, northern pine, and late successional conifer.

I calibrated EDR using the same general Bayesian inversion as in Chapter 3. The inversion fit all sites simultaneously, such that at every MCMC iteration, the algorithm proposed a set of all parameter values for each PFT and simulated spectra for each site based on its observed composition and structure. Because of unrealistic



Figure 4.1: Sites selected for analysis, in "stand structure" (*main figure*) and geographic (*inset*) space. Colors indicate the fraction of the stand that is made up of evergreen PFTs.

values in the shortwave infrared spectral region in the AVIRIS observations, likely caused by faulty atmospheric correction, I only calibrated the model with observations from 400 to 1300 nm. In addition, I changed the fixed variance model used in Chapters 2 and 3 to a two-parameter heteroskedastic variance model ($\sigma = a + bX$) to account for the fact that both model and observation errors are typically proportional to reflectance values. To generate the initial history state files required by EDR, I ran ED2 itself for one day in midsummer (July 1), starting from vegetation initial conditions based on observed composition and structure.

For priors on the five PROSPECT parameters and specific leaf area, I performed a hierarchical multivariate analysis (see Chapter 1) on PROSPECT parameters estimated from chapter 3 and, where available, direct measurements of specific leaf area. For priors on the leaf biomass allometry parameters, I fit a multivariate normal distribution to allometry coefficients from Jenkins et al. (2003, 2004) using the **PEcAn.allometry** package. For the clumping factor, I used a uniform prior across its full range (0 to 1), and for the leaf orientation factor, I used a weakly informative re-scaled beta distribution centered on 0.5.

To alleviate issues with strong collinearity between the two allometry coefficients and the specific leaf area, I decided to remove the allometry exponent coefficient (but not the intercept) from the calibration by fixing it at its prior mean for each plant functional type. Doing so dramatically improved the stability of the inversion algorithm and the accuracy of the results.

I evaluated the performance of the calibrated model by comparing the posterior credible intervals of modeled spectra against the AVIRIS observations at each site. To assess the role of model structure in predictive error, I also included predictions using the 4SAIL model parameterized with the posterior means from the EDR calibration (except for clumping factor, which is absent from 4SAIL). In addition, I compared



Figure 4.2: Sensitivity of EDR and 4SAIL predicted canopy reflectance to leaf optical traits. For all figures, leaf area index is fixed at 4.88. EDR simulations are for a single-cohort canopy (Early Hardwood) with clumping factor 0.09 and orientation factor 0.06. 4SAIL predictions are for directional-hemispherical reflectance.

model predictions of leaf area index (which depend on parameters calibrated in the model) against field observations.

4.3 Results

4.3.1 Sensitivity analysis

The general character of the sensitivities of EDR and 4SAIL to leaf optical properties is similar, but the magnitudes of these sensitivites are different (Figure 4.2). EDR consistently shows significantly higher reflectance across most of the spectrum than 4SAIL. Sensitivity to leaf mesophyll structure is lower in EDR than 4SAIL, while sensitivity for chlorophyll and water contents is comparable. Sensitivity to leaf dry mass per area is comparable for both models in the shortwave infrared, but significantly higher for 4SAIL in the near infrared.

EDR and 4SAIL show different responses to leaf area index (Figure 4.3). Although both models predict declines in reflectance with increasing leaf area in the visible and shortwave infrared range, 4SAIL also predicts a decline in the near infrared while EDR predicts an increase. Furthermore, 4SAIL predicts more reflectance sensitivity at low leaf area indices and saturation of reflectance around 4, while EDR shows a more gradual decline in sensitivity, particularly in the near-infrared range. An important caveat to these results is that, particularly at low leaf area index, they are strongly dependent on the value of the background soil reflectance. To match the EDR default (see Methods), 4SAIL was configured with a relatively bright soil reflectance (i.e. a fairly dry soil), which explains the decline in near-infrared reflectance as leaf area increases. When the soil background is dark, SAIL shows increasing nearinfrared reflectance with increasing leaf area (but saturating to the same value as the contribution of the soil background becomes negligible at high leaf area).

Similarly to leaf area, EDR and 4SAIL agree on the directionality leaf orientation effects on reflectance (declining reflectance with increasingly vertical leaves), but differ in their sensitivities, with EDR having a much lower sensitivity to changing leaf angles. Finally, sensitivity of EDR to canopy clumping is nearly identical to that of leaf area index, which makes sense given the interaction between these terms in defining canopy transmissivity (Equations 4.1 and 4.2).

Compared to 4SAIL, EDR consistently overpredicts canopy reflectance across the entire spectrum (Figures 4.2, 4.3, and 4.4). A significant part of this bias can be explained by the inclusion of wood reflectance in EDR, but a persistent positive



Figure 4.3: Sensitivity of EDR and 4SAIL predicted canopy reflectance to leaf area index (top) and leaf orientation factor (middle). (Bottom) Sensitivity of EDR predicted canopy reflectance and clumping factor, with dashed line indicating 4SAIL predictions for the same leaf area index, PROSPECT parameters, and approximately equivalent soil background. Configuration is the same as in Figure 4.2.



Figure 4·4: Comparison of predicted canopy reflectance by 4SAIL (directional-hemispherical) and EDR with and without wood reflectance included.

bias remains across most of the spectrum even after setting wood reflectance to zero (Figure 4.4).

EDR canopy reflectance is highly sensitive to the properties of the tallest cohort, and shows virtually no sensitivity to the optical properties of lower cohorts (Figure 4.5). Clumping (or reduced LAI) allow more light to penetrate the canopy and therefore increases the sensitivity of canopy reflectance to the properties of lower layers, but this sensitivity is effect is still significantly muted compared to the top canopy.

4.3.2 Model calibration

Model calibration substantially improved the precision of almost all parameter estimates, even when prior distributions were strongly informative (Figure 4.6). In most cases, the posterior distribution fell within the prior, but there were a few notable exceptions. Specifically, northern pines had significantly higher calibration estimates of chlorophyll content and leaf mass per area and significantly lower estimates of the orientation factor (though the prior on the latter was not based on data). Late hardwoods also had orientation factor estimates much lower than the prior, and also had significantly lower estimates of leaf mesophyll structure.

The ability of EDR to reproduce observed spectra at every site was strongly site-dependent (Figure 4.7). At a majority of the sites, EDR systematically overpredicted reflectance in the visible range (Figure 4.8), while errors in the near-infrared region were more variable. As shown in the sensitivity analysis, this consistent overprediction of visible reflectance is likely driven by wood reflectance (Figure 4.4). 4SAIL also showed a lot of site-to-site variability in its performance, but generally performed better in the visible range than EDR.

The ability of EDR to reproduce observed leaf area index was also strongly sitedependent, with some of the accuracy explained by the functional type of the tallest



Figure 4.5: Sensitivity of EDR canopy reflectance to leaf water content of top (*left*) and bottom (*right*) cohorts within a multi-cohort canopy, when the top canopy is closed (*top*) and highly clumped (*bottom*). Top and bottom cohorts are, respectively, Early and North Mid Hardwood with DBH 40 and 30, LAI 2.4 and 1.3, and equal stem density. Clumping factors for closed and clumped canopies are 0.9 and 0.3, respectively.



Figure 4.6: Summary statistics for model calibration parameter prior and posterior distributions.



Figure 4.7: Comparison between AVIRIS observations (black), posterior credible intervals on EDR predicted spectra (green), and posterior mean predictions using 4SAIL (red, dashed) for each site used in the calibration.



Figure 4.8: Same as Figure 4.7, but zoomed into the visible (<750 nm) spectral region.



Figure 4.9: Predictions of leaf area index by EDR, compared to observed values. Colors indicate the plant functional type of the tallest cohort at each site.

cohort (Figure 4.9). In general, EDR tended to over-predict leaf area index for coniferdominated stands and under-predict for hardwood-dominated stands. For mid- and late-hardwood-dominated stands in particular, EDR predicted substantial variability in leaf area index that was not present in the observations.

Mismatch between EDR predictions and AVIRIS reflectance were likely caused by a number of factors related to site composition and structure (Figures 4.8 and 4.10). In some sites, the mismatch was most likely due to a mismatch in leaf area index, such as BI02, BI03, and MN06. Notably, at BI02 and BI03 (and several other sites), EDR and 4SAIL show opposite biases—EDR over-predicts visible reflectance but successfully captures the near-infrared reflectance, while 4SAIL does the opposite (Figure 4.7). This can be linked to the two models' different responses to leaf area index revealed in the sensitivity analysis (Figure 4.3).

Where late hardwood trees were relatively abundant near the top of the canopy (Figure 4.10), EDR often over-predicted reflectance in the red (sites BH03, BH05, BH10, and BI01; Figure 4.8) even though the LAI retrieval was reasonably accurate. This was likely related to the low inversion estimate of late hardwood clumping factor (Figure 4.6), which tends to emphasize the much redder wood and soil background (Figure 4.3). However, some other late hardwood-dominated sites showed good performance for both spectra and leaf area index, such as NC17, NC22, and OF04 (Figure 4.7). Similarly, the high clumping factor estimate for late conifer trees (Figure 4.6) was compensated over-predicted leaf area index (driven by increases in the leaf biomass allometry coefficient; Figure 4.9), as in sites OF01, SF01, and SF04. More generally, EDR tended to perform best in mature stands comfortably dominated by early or mid hardwoods or northern pines.



+ Early_Hardwood + North_Mid_Hardwood + Late_Hardwood + Northern_Pine + Late_Conifer

Figure 4.10: Vertical profile of cumulative leaf area index and composition at each site in this analysis. Vertical black lines indicate the mean \pm 1 standard deviation of the observed leaf area index. Sites are arranged in the same order as Figures 4.7 and 4.8.

4.4 Discussion

The accurate simulation of canopy radiative transfer is key to a number of ecosystem processes, including photosynthesis, soil respiration, and hydrology. For its representation of radiative transfer, ED2 uses a modified version of the two-stream model of Sellers (1983) as implemented in the Community Land Model (Oleson et al., 2013) but adapted for multiple canopies. My comparison of this model against 4SAIL, a two-stream model with a long history of use in the remote sensing community (Jacquemoud et al., 2009), reveals some important differences in behavior, even independent of its multi-cohort nature. One key limitation is the representation of wood reflectance. In EDR, as in the Community Land Model, the backscatter of a layer is the average of leaf and wood reflectance weighted by their respective area indices. Although wood is an important scattering element at low LAI, it has widely been shown to have negligible contributions to canopy reflectance in mature dense stands, and where its contribution is significant, it is typically in the near infrared rather than the visible spectral range (Asner, 1998; Malenovsky et al., 2008; Verrelst et al., 2010). Therefore, the strong sensitivity of EDR to wood reflectance for a closed canopy (Figure 4.4) is unrealistic, and was likely a major reason for its persistent visible bias compared to both 4SAIL-predicted and AVIRIS-observed canopy reflectance even after calibration (Figure 4.8). I suggest that a more accurate but still conceptually simple (and computationally light) approach to capturing wood reflectance is to model it as part of the background soil layer rather than the scattering leaf layer.

I did not examine the ability of EDR to reproduce observed canopy reflectance in the absence of wood reflectance, though this is a logical next step. However, based on the fact that 4SAIL generally did well at predicting visible reflectance (Figure 4.8) and that EDR predicted significantly brighter canopies than 4SAIL even after the wood reflectance correction (Figure 4.4), there seem to be additional structural erbut different magnitudes of EDR and 4SAIL sensitivity to leaf optical properties and orientation suggest that other aspects of canopy structure are driving differences between these models (and, presumably, differences with observations as well). Part of the mismatch between EDR predictions and observations (Figures 4.7 and 4.8) is the result of the soil background, which was set to a constant, relatively bright value across all sites, but is known to vary significantly with soil moisture, understory vegetation, and litter cover. Future work could better leverage existing models of soil reflectance (e.g. Hapke, 1981; Hapke and Wells, 1981) to better capture differences in soil background across sites and measurement conditions. That being said, the effects of different soil background are generally most pronounced at sites with low leaf area and/or high clumping, and should become less important as leaf area increases. The fact that EDR continues to monotonically increase its canopy brightness with increasing leaf area despite starting from a relatively bright soil background (Figure 4.3; note that 4SAIL does not show this behavior) points to potential issues with the way EDR handles its boundary conditions. Fortunately, alternative efficient representations are available in the literature. For example, Pinty et al. (2004, 2006) define a one-dimensional, turbid-medium radiation scheme that calculates the contribution of soil reflectance separately for direct and diffuse radiation, and which has a more sophisticated treatment of bi-directional reflectance effects, which are currently lacking in EDR. Similarly, 4SAIL also offers a more sophisticated treatment of bi-directional reflectance effects.

A key feature of EDR design is its representation of multiple co-existing plant cohorts competing for light within a single patch. As mentioned in the introduction, a previously-identified limitation of representing multiple canopy layers in a two-stream scheme is that the top cohort absorbs a disproportionate fraction of the light at the expense of marginally lower cohorts (Fisher et al., 2010). This effect was present in my results as well. In a closed canopy (high clumping factor), major changes in the leaf optical properties of lower cohorts had a minimal effect on overall canopy reflectance, and the effect was still muted in a highly clumped canopy (low clumping factor; Figure 4.5). This problem may be further exacerbated by the over-prediction of total canopy reflectance discussed above, as this further reduces the absorbed radiation available to all canopies (but especially understory ones) for photosynthesis. One solution to this is the use of a finite crown area model (Dietze et al., 2008); unlike the implementation of canopy clumping discussed in this work, which effectively "thins" a layer but still does not provide the understory with any direct radiation, a finite crown area model introduces true gaps into the canopy, which can significantly stimulate understory growth. An example implementation of this concept is the "perfect plasticity approach" (Weng et al., 2015) where trees above a certain height threshold share direct sunlight and compete for a fixed amount of horizontal space within the overstory. A useful avenue for development and parameterization of these models is comparison to more sophisticated and realistic three-dimensional representations of radiative transfer (e.g. Widlowski et al., 2007), which are themselves too computationally demanding to be coupled to ecosystem models, but from which empirical distributions and response functions could be derived and against which the behavior of simpler models could be evaluated.

A significant body of remote sensing literature argues that the inversion of coupled leaf-canopy radiative transfer models is ill-posed because of the collinearity of structure and biochemistry effects on canopy reflectance (e.g. Combal et al., 2003; Lewis and Disney, 2007). Even with tight prior constraint on leaf optical properties from a large meta-analysis, I saw evidence of significant trade-offs between parameters. In particular, in this analysis, three parameters influenced canopy reflectance in virtually identical ways through modulating the (effective) leaf area index: specific leaf area, leaf biomass allometry, and clumping factor. This collinearity resulted in frequent mismatches between observed and modeled leaf area index despite high accuracy in modeled reflectance spectra (Figures 4.10 and 4.7). Additional measurements of poorly constrained but highly influential structural parameters should help alleviate this problem. Fortunately, these structural metrics are often effectively retrieved from LiDAR observations from terrestrial (Eitel et al., 2016), airborne (Antonarakis et al., 2014), and satellite platforms (Coyle et al., 2015).

Finally, despite many challenges related to canopy radiative transfer modeling, surface reflectance is nevertheless a promising approach for benchmarking and performing data assimilation on ecosystem model outputs. Remote sensing observations are unrivaled in their spatial completeness and extent, notably extending to regions like the tropics and high latitudes that are relatively undersampled but have a disproportionate impact on the global climate system (Schimel et al., 2015) and/or global biodiversity (Jetz et al., 2016). At the same time, satellite time series provide multi-decadal records with relatively high temporal frequency, which have tremendous utility for calibrating model projections of past ecological dynamics (Kennedy et al., 2014; Pasquarella et al., 2016). Used in combination with other emerging data sources, including global trait databases and eddy covariance measurements, remote sensing can be a transformative force in ecosystem ecology.

4.5 Conclusions

The objective of this study was to calibrate the canopy radiative transfer scheme inside the ED2 dynamic vegetation model by comparing its predictions of surface reflectance against airborne imaging spectroscopy data. The calibration successfully constrained the posterior distributions of model parameters related to canopy structure (leaf angle, canopy clumping, and leaf area index) for five plant functional types characteristic of temperate forests of the northeastern United States. However, comparisons of predicted spectra post-calibration against observations reveal widespread biases. This suggests that there are structural issues with the ED2 radiative transfer model that inhibit its ability to accurately predict surface optical properties. Sensitivity analyses, along with comparison against an alternative canopy radiative transfer model more commonly used by the remote sensing community (4SAIL), shed additional light on the problem and provides avenues for future exploration and model improvement. One issue was unrealistically high sensitivity to wood reflectance, which could be addressed by calibration of parameters related to wood area index (such as wood allometries) or, if that fails, alternative representations of the contribution of wood reflectance to canopy reflectance. That being said, wood reflectance alone was insufficient to explain bias in predicted spectra. We suggest that this error is likely related to soil reflectance, but additional sensitivity analyses (for instance, by varying soil reflectance in simulations with dense, closed canopies) are required to confirm this. Ultimately, this work demonstrates the utility of using surface reflectance predictions to evaluate model representations of canopy radiative transfer, and thus contributes to the rapidly expanding body of literature on applications of remote sensing to dynamic vegetation modeling.

Chapter 5 Conclusions

The value of terrestrial ecosystems to human well-being, both direct and indirect, is difficult to overestimate. The same can be said about the complexity of terrestrial ecosystems, which has been a major obstacle to forecasting ecosystem responses to human and natural pressures. Fortunately, our ability to observe terrestrial ecosystems, and to perform sophisticated analyses and simulations using these observations, has never been greater, and only continue to improve thanks to both technological improvements and changing attitudes about data sharing. The overarching objective of my dissertation was to explore novel ways that observations could be used in the context of simulation modeling of the terrestrial biosphere. In particular, my work focused on improving data constraint on model parameters, especially through near-surface, airborne, and satellite remote sensing. The results of this work provide many opportunities for data-driven model improvement, both direct (through better parameterizations of leaf and canopy processes) and indirect (through insights about scales and drivers of ecological variability).

My first chapter focused on covariance patterns among leaf traits related to leaf morphology and photosynthetic metabolism through a multivariate meta-analysis of a global traits database. Previous work has shown that, at the global scale, variability in these traits was constrained by a trade-off between faster growth rates and higher recalcitrance (a.k.a. the "leaf economic spectrum") (Wright et al., 2004; Díaz et al., 2016), but that these trade-offs were often absent within species and communities (Albert et al., 2010b; Messier et al., 2010; Wright and Sutton-Grier, 2012). My work investigated whether the leaf economic spectrum scale was present between these two extremes, at the scale of plant functional types used by the current generation of dynamic global vegetation models. My key result was that, in general, leaf economic relationships were present within plant functional types, though the strength of these relationships varied. Moreover, as a result of the strong correlation patterns among traits, I was able to generate much more precise estimates of plant functional type means (which can be used as vegetation model parameters) than using standard multivariate methods, particularly for data-limited trait-functional type combinations. Future work should extend this meta-analysis to additional traits—particularly root traits, which are highly consequential to plant function but are generally much more data limited—and to alternative (and optionally larger) plant functional type definitions.

The idea that that additional measurements of readily observable traits can be used to inform traits that are much harder to observe is an exciting prospect for remote sensing, which has the capability to provide huge volumes of trait data at relatively low cost and effort. This was the motivation behind my second chapter, which aimed to develop a consistent, physically-based methodology for estimating leaf traits from proximal or remote measurements of optical properties. In this study, I introduced an approach for estimating leaf traits and their uncertainties via Bayesian inversion of a leaf radiative transfer model. I then applied this approach to simulated spectra to explore the relationship between the spectral bands of remote sensing instruments and the accuracy and precision with which those instruments could retrieve known leaf traits. I found that while trait estimates from hyperspectral instruments were consistently and significantly more precise instruments than estimates from multispectral instruments, all sensor configurations were able to estimate at least some of the traits with greater precision than an uninformative prior distribution. Notably, coarser resolution instruments struggled to distinguish traits with overlapping spectral features (such as chlorophylls and carotenoids), but the Bayesian methodology

was able to accommodate this through the joint posterior distributions, which were significantly constrained even when the marginal distributions were not. This work comes with several important caveats, all of which could be readily addressed in future analyses. First of all, I only considered spectral resolution, and did not consider other critical aspects of sensor and mission design, such as radiometric resolution, signal-to-noise ratio, spatial resolution, revisit frequency, and directional sampling. Second, I only evaluated the ability of these instruments to retrieve leaf traits from leaf spectra, whereas real retrievals are significantly complicated by canopy structure (see Chapter 4), atmospheric contamination, and sun-sensor geometry, among others. That being said, the value of this computational "sensor experiment" is to emphasize the importance of careful band selection, as I show that even small changes to band width and location can have significant consequences for retrieval of vegetation properties. More generally, this study demonstrates how modeling the observed remote sensing signal as a function of vegetation features allows information from multiple different platforms to be used synergistically.

Whereas chapter 2 was focused on sensor design and remote sensing methodology, chapter 3 delved into the ecophysiology of leaf spectra. First, this study investigated how well a state-of-the-art leaf radiative transfer model (PROSPECT) was able to related leaf traits and spectra across a wide range of species and measurement conditions. In general, leaf radiative transfer model inversion successfully captured 50 to 75% of the variability in leaf traits, though retrieval accuracy varied significantly by plant functional type and project due to a combination of highly variable measurement techniques and physiological or morphological differences between plant functional
types. Second, this study quantified the drivers of variability in leaf traits estimated from leaf spectra. I found that traits varied approximately equally within and across species, with morphological and structural traits showing less plasticity compared to traits related to photosynthesis and hydraulics. Species also defied characterization into plant functional types—attempting to do so captured at most roughly one-third of interspecific variability. Finally, this study assessed the extent of correlation between leaf traits directly estimable from leaf spectra and other traits that, so far, can only be measured directly. I found evidence of the leaf economic spectrum (see Chapter 1) in leaf optical traits as well, both within and across species, but many intraspecific trait correlations were strongly species-dependent. Future work could expand on this study in several ways. For one, the causes of the substantial variability in leaf trait retrieval accuracy need to be investigated in more detail, paying special attention paid to details about the measurement methodology (such as the use of leaf clips vs. integrating spheres, contact vs. proximal measurements). In addition, important questions remain about the sources of intraspecific variability in leaf traits. Namely, how much of this variability is between individuals of the same species as opposed to between leaves on the same tree? How do traits on the same leaf vary over the course of a season, or even of a single day? Similarly, how quickly and how much do leaf traits change in response to acute or prolonged stress? Fortunately, because leaf spectra are rapid and non-destructive, they are particularly well equipped to explore these and related questions, and future studies of plant ecophysiology would benefit significantly from adding leaf spectra to their measurement protocols.

My fourth and final research chapter advances beyond the leaf scale to the canopy scale. Canopy radiative transfer modeling has long been an essential tool for interpreting remote sensing signals (Verhoef, 1984; Jacquemoud et al., 2009). At the same time, canopy radiative transfer models (albeit of a different lineage) have been an essential component of dynamic vegetation models, where they are needed to determine light absorption for photosynthesis and to model surface energy balance (Dickinson, 1983; Sellers, 1985; Oleson et al., 2013). This chapter sought to unify these two schools of thought by first training a vegetation model's (Ecosystem Demography model, or ED2) own canopy radiative transfer scheme to predict full-range hyperspectral surface reflectance, and consequently calibrating and validating the model against airborne imaging spectroscopy measurements. Applying the same general Bayesian inversion approach used in chapters 2 and 3 to the canopy radiative transfer model, I was able to significantly constrain model parameters related to canopy structure compared to their uninformative priors. However, the resulting predicted spectra often departed significantly from both observations and predictions using a radiative transfer model commonly used in the remote sensing community. These analyses suggest that, at the very least, the calibration omitted important parameters related to wood and soil properties, and more likely that the canopy radiative transfer model has underlying structural errors that inhibit its ability to accurately simulate remotely sensed canopy reflectance. Additional work, primarily in the form of sensitivity analyses, is needed to more precisely diagnose the sources of model error and provide a road map for model improvement.

Overall, there are several major lessons to be learned from my dissertation research. The first lesson is that, at least in terms of traits, plants are frustratingly idiosyncratic, which poses problems for both vegetation modeling and remote sensing. As chapter 3 showed, individuals from the same species are often just as, if not more different from each other than from individuals of other species. Moreover, both chapters 1 and 3 show that variability among species from the same functional type can be greater than the variability between functional types. Models with fixed parameters for plant functional types therefore average over a tremendous amount of variability, and cannot represent the types of functional responses to stress or changing conditions observed in the various studies in chapter 3. The same can be said of satellite remote sensing, which is forced to condense complex stands of highly heterogeneous individuals into a single pixel with an average reflectance spectrum. Given comparable inter- and intra-specific variability in optical traits (and therefore spectra), it is hard not to be pessimistic about the ability of multispectral satellites to detect any but the most severe of stresses in heterospecific stands.

Another challenge, long known to the remote sensing community and reaffirmed in this dissertation, is the complexity of physically modeling vegetation optical properties, even when the traits are known. My second and third chapters show that we have an incomplete understanding (or at least, incomplete models) of vegetation-light interactions even at the leaf level, as evidenced by species-specific biases and large fractions of unexplained variability in trait retrieval. Some of these issues are due to differences in measurement approaches, and more work needs to be done to provide concrete recommendations regarding techniques for accurately and consistently measuring leaf spectra. However, systematic differences in trait estimation even within the same dataset point to issues with model calibration and structure. The large variability in both traits and trait correlations across species points to a need to continue to push leaf radiative transfer models to explicitly distinguish between multiple classes of molecules (e.g. separate chlorophyll a and b; model lignin, cellulose, and starch separately rather than collectively as "dry matter content"), and, in the process, to depend less on empirically calibrated absorption coefficients. Although increasing the level of detail in this way can lead to problems with equifinality, my dissertation has consistently demonstrated that Bayesian methods are well-suited for both acknowledging equifinality when it exists (through strong correlations in the joint posterior distribution) and for resolving it when independent prior information is available. As my fourth chapter shows, radiative transfer modeling becomes even more challenging at the canopy level, where the complexities of modeling individual leaves are compounded by leaf arrangement and orientation, contributions from wood and soil, and strong directional effects of both incident and outgoing radiation. Canopy radiative transfer models that do a reasonably good job of capturing these effects while remaining computationally tractable exist in the remote sensing literature (Verhoef, 1984; Pinty et al., 2006), and have been successfully coupled with ecosystem models in the past (Quaife et al., 2008). However, my work suggests that the canopy radiative transfer models popular in the ecosystem modeling community (Dickinson, 1983; Sellers, 1985) may be less well suited for modeling remote sensing signals, likely due to their failure to account for the directionality of canopy reflectance. Future work should dive more deeply into the structure underlying these respective canopy radiative transfer models to find ways in which the latter can learn from the former.

More generally, the final lesson of my dissertation is the importance of synergies and synthesis to improving ecological forecasting. No single observation method is capable of providing a picture of an ecosystem sufficiently complete to improve every aspect of an ecological forecast. However, synergies between multiple observations each providing incremental constraint on a different component of the ecosystem—can lead to much more important improvements. For example, my fourth dissertation chapter applied the multivariate meta-analysis from chapter 1 to the results from chapter 3 to generate strongly informative multivariate priors on leaf optical properties, without which the retrieval of canopy structural parameters would have been hopelessly ill-posed. This example demonstrates not only the power of combining similar observations at multiple scales (leaf traits estimated from leaf spectra and airborne imaging spectroscopy, not to mention the survey data that provided the composition of each site), but also the utility of process-based models as scaffolds for doing so. Significant progress in ecological forecasting will almost certainly require the development of many more synergies like these, and has the necessary positive externality of promoting collaboration across different disciplines.

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CURRICULUM VITAE







