Author's Accepted Manuscript

Modeling uncertainties in estimation of canopy LAI from hyperspectral remote sensing data—a Bayesian approach

Petri Varvia, Miina Rautiainen, Aku Seppänen



PII: S0022-4073(16)30759-2

DOI: http://dx.doi.org/10.1016/j.jqsrt.2017.01.029

Reference: JQSRT5576

To appear in: Journal of Quantitative Spectroscopy and Radiative Transfer

Received date: 11 November 2016 Revised date: 23 January 2017 Accepted date: 23 January 2017

Cite this article as: Petri Varvia, Miina Rautiainen and Aku Seppänen, Modeling uncertainties in estimation of canopy LAI from hyperspectral remote sensing data—a Bayesian approach, *Journal of Quantitative Spectroscopy and Radiative Transfer*, http://dx.doi.org/10.1016/j.jqsrt.2017.01.029

This is a PDF file of an unedited manuscript that has been accepted fo publication. As a service to our customers we are providing this early version o the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain

Modeling uncertainties in estimation of canopy LAI from hyperspectral remote sensing data – a Bayesian approach

Petri Varvia^a, Miina Rautiainen^{b,c}, Aku Seppänen^a

^aDepartment of Applied Physics, University of Eastern Finland ^bDepartment of Built Environment, School of Engineering, Aalto University ^c Department of Electronics and Nanoengineering, School of Electrical Engineering, Aalto University

Abstract

Hyperspectral remote sensing data carry information on the leaf area index (LAI) of forests, and thus in principle, LAI can be estimated based on the data by inverting a forest reflectance model. However, LAI is usually not the only unknown in a reflectance model; especially, the leaf spectral albedo and understory reflectance are also not known. If the uncertainties of these parameters are not accounted for, the inversion of a forest reflectance model can lead to biased estimates for LAI. In this paper, we study the effects of reflectance model uncertainties on LAI estimates, and further, investigate whether the LAI estimates could recover from these uncertainties with the aid of Bayesian inference. In the proposed approach, the unknown leaf albedo and understory reflectance are estimated simultaneously with LAI from hyperspectral remote sensing data. The feasibility of the approach is tested with numerical simulation studies. The results show that in the presence of unknown parameters, the Bayesian LAI estimates which account for the model uncertainties outperform the conventional estimates that are based on biased model parameters. Moreover, the results demonstrate that the Bayesian inference can also provide feasible measures for the uncertainty of the estimated LAI.

Keywords: leaf area index, spectral invariants, photon recollision probability, reflectance model, uncertainty quantification

1. Introduction

- New satellite missions with enhanced spectral reso-
- lution (e.g. Sentinel-2, EnMAP) will soon produce ex-
- tensive coverage of our planet. More efficient methods
- to handle and interpret environmental information from
- the large data volumes are urgently needed. So far, ap-
- plications of hyperspectral remote sensing (also known
- as imaging spectroscopy) have concentrated on moni-
- toring biochemical properties or functioning of vegeta-

ing also structural variables of forest canopies has not been widely demonstrated. In remote sensing of forest structure, hyperspectral data have mainly been used in the form of narrowband vegetation indices (VI), so that the information content of only a few spectral bands is used to estimate a structural characteristic of the canopy (e.g. [1, 2]). VI based approach also exhibit problems

tion. However, the added value of these data in estimat-

such as significant site-, species- and time specificity

(e.g. [3-5]), and do not account for the physical rela-

Preprint submitted to Elsevier

tionship between the forest structure and the observations.

Inversion of physically-based forest reflectance mod-22 els may offer a solution to using the full information 23 content, and not only selected bands, of hyperspectral data sets. The on-going growth in the availability of 25 hyperspectral remote sensing data sets has indeed inreased the use of physically-based modeling [6], and 27 new interpretations for links between canopy structure and detailed spectral features have been proposed (e.g. [7]). However, forest reflectance models usually con-30 tain many other unknown variables besides the variable 31 of primary interest; for example, forest background (or 32 understory reflectance) and leaf spectral properties vary 33 significantly even in the same biome. In addition, the effect of forest stuctural parameters, for example leaf 35 area index (LAI), on reflected radiation is usually nonlinear and saturates in very dense canopies. Combined, these two characteristics make the inversion of a forest reflectance model an under-determined and ill-posed problem [8, 9]. The complex nonlinear relationship between the leaf area index and the forest reflectance makes the estimation of LAI sensitive to uncertainties in the other model parameters. Thus, using fixed values 43 in the model inversion will most likely result in unreliable estimates of forest structure. A methodology which makes it possible to take into account the uncertainty in these variables is needed.

Bayesian inference (e.g. [10]) offers a coherent, yet 78 flexible framework for handling model uncertainties in 79 parameter estimation problems. In Bayesian approach, 80 uncertainties are modeled statistically. Also the parameters of primary interest (such as the LAI in the present 82 application) are modeled as random variables, allowing 83 the use of *a priori* information on the parameters. The 84

50

51

53

solution of a Bayesian inference problem is the posterior distribution, i.e., the conditional probability distribution of the unknown parameter given the measurement data. The Bayesian approach has been previously used in remote sensing of forest structural parameters, for example, from multispectral MODIS data by Zhang et al. [11]. In this paper, the prior information consisted of constraints for the model unknowns, i.e., the parameters were assumed to be uniformly distributed over feasible intervals. However, more feasible prior information on the statistics of the input parameters of reflectance models is often available. Moreover, studies on the effect of the parameter uncertainties in the LAI estimates and the feasibility of the Bayesian approach to recover from the errors caused by such uncertainties have not yet been reported.

The present work focuses on estimating LAI of forest canopies using hyperspectral data. A set of numerical simulations is carried out to study the effect of unknown reflectance model parameters to conventional LAI estimates which use fixed model parameters. Further, we study whether the LAI estimates could recover from errors caused by unknown reflectance model parameters, when a Bayesian approach is taken. In the Bayesian inference, informative, data-based prior models for the reflectance model parameters are written. In addition to evaluating Bayesian point estimates for LAI, the feasibility of Bayesian uncertainty estimates is investigated; in particular, we study how well the Bayesian credible intervals represent the uncertainty of the estimated LAI.

116

2. Materials and methods

s 2.1. Forest reflectance model

In this work, forest spectra (i.e. hyperspectral measurements) are modeled using the PARAS forest reflectance model [12] which is based on the concept of photon recollision probability. The PARAS model has the advantage of containing relatively few independent variables and performing well in boreal forests [12]. The bidirectional reflectance factor (BRF) of a forest, $r(\theta_1, \theta_2, \lambda)$, for a given solar zenith angle θ_1 , viewing zenith angle θ_2 , and wavelength λ , is modeled as: [12]

$$\begin{split} r(\theta_1, \theta_2, \lambda) &= \rho_g(\theta_1, \theta_2, \lambda) t_c(\theta_1) t_c(\theta_2) \\ &+ f(\theta_1, \theta_2, \lambda) i_c(\theta_1) \frac{\omega_L(\lambda) - p\omega_L(\lambda)}{1 - p\omega_L(\lambda)}, \end{split} \tag{1}$$

where ρ_g is the BRF of the understory layer, t_c is the tree canopy transmittance, $i_c=1-t_c$ the tree canopy interceptance, f the canopy upward scattering phase function and ω_L the leaf single scattering albedo. The photon recollision probability p is used in the model to describe the aggregated structure of forest canopies. It is the probability that a photon, after having survived an interaction with a canopy element, will interact with the canopy again.

The first term in Equation (1) describes the part of radiation that has penetrated the tree layer canopy and reflected upwards through the tree canopy after interacting with the understory layer. The second term models the radiation that has hit the tree canopy and scattered in the viewing angle. Even though the model ignores multiple interactions between the tree and understory layers, it has simulated reflectance factors similar to those obtained from satellite images [12]. If the model were to be used in snow conditions, i.e. with a highly reflecting background, modifications would be needed [13].

106

107

108

109

110

111

112

114

In this study, the following assumptions and approximations are made in parameterizing the PARAS model. We assume that LAI is related to the effective leaf area index (LAI_{eff}, commonly measured by e.g. the LAI-2000 Plant Canopy Analyzer) through a species-specific shoot clumping factor β so that LAI_{eff} = β LAI. Factor β , in turn, is related to the shoot silhouette-to-total-area ratio (STAR) as β = 4STAR.

The photon recollision probability p is approximated according to [14] as

$$p = 1 - \frac{1 - t_d}{\text{LAI}} = 1 - \frac{\beta(1 - t_d)}{\text{LAI}_{\text{eff}}},$$
 (2)

where t_d is the diffuse transmittance for the tree canopy layer. The canopy transmittance is modeled using Beer-Lambert's law as

$$t_c(\theta) = \exp\left(-\frac{\beta}{2} \frac{\text{LAI}_{\text{eff}}}{\cos \theta}\right),$$
 (3)

from which the diffuse canopy transmittance t_d in equation (2) is calculated following [13]:

$$t_d = 2 \int_0^{\frac{\pi}{2}} t_c(\theta) \cos(\theta) \sin(\theta) d\theta.$$
 (4)

The upward scattering phase function $f(\theta_1, \theta_2, \lambda)$ is approximated using the proportion of upward scattered radiation Q as [15]

$$f(\theta_1, \theta_2, \lambda) \approx Q = \frac{1}{2} + \frac{q}{2} \frac{1 - p\omega_L}{1 - pq\omega_L},$$
 (5)

where q in is a wavelength independent semi-empirical scattering asymmetry parameter. Parameter q describes the decrease in probability of the photon escaping the canopy with increasing scattering order, in other words, it models how photon escape probability decreases as the photon scatters deeper inside the canopy. Thus q is related to canopy density and increases with LAI (Table 2 in [15]).

2.1.1. Wavelength dependence

142

Leaf albedo ω_L and understory reflectance ρ_g are 175 143 wavelength dependent parameters. Thus, in the model, 176 144 ω_L and ρ_g are vectors of the same length as the satellitemeasured data vector. To reduce the number of un- 178 146 known variables in the inverse problem, we utilize known features of the vegetation spectra: The (green) 148 vegetation spectra have a typical shape which features 149 strong correlations between reflectance parameters cor-150 responding to certain wavelengths and discrete jumps 151 across other wavelength intervals. (For further discus-152 sion and references to experimental works on determin-153 ing the vegetation spectra, see Section 2.2.2). This en-154 ables the use of reduced order parametric representa-155 tions for ω_L and ρ_g . More specifically, we use cubic 156 monotone Hermite splines to represent the spectral vari-157 ables using 27 manually chosen node points that are 158 illustrated in Figure 1. The cubic monotone Hermite 159 spline is monotone between the node points and thus the 160 curve can change direction only on a node. By placing 161 the node points on the typical peaks and troughs of the 162 vegetation spectrum, with additional control nodes in between, the spline representation can follow the typical 179 164 shape of the spectrum with sufficient accuracy. Figure 180 165 1 also shows an example of how the spline representa-166 tion follows an original spectrum. Using the spline, the 182 167 variables ω_L and ρ_g are rewritten as

$$\omega_L = S(\lambda; \tilde{\lambda}, \tilde{\omega}_L), \tag{6}$$

$$\rho_{g} = S(\lambda; \tilde{\lambda}, \tilde{\rho}_{g}), \tag{7}$$

where $S(\cdot)$ is the spline function (piecewise polynomial), $\tilde{\lambda} \in \mathbb{R}^{27}$ is a vector consisting of wavelengths the corresponding to the spline nodes, and $\tilde{\omega}_L \in \mathbb{R}^{27}$ and the polynomial $\tilde{\rho}_g \in \mathbb{R}^{27}$, respectively, are the values of ω_L and ω_R at the node points $\tilde{\lambda}$. Because $\tilde{\lambda}$ is fixed, the spline ap-

proximations (6) and (7) are fully determined by $\tilde{\omega}_L$ and $\tilde{\rho}_g$, respectively. Thus, using the spline approximations, the low-dimensional vectors $\tilde{\omega}_L$ and $\tilde{\rho}_g$ are substituted for full-length ω_L and ρ_g as variables in the reflectance model.

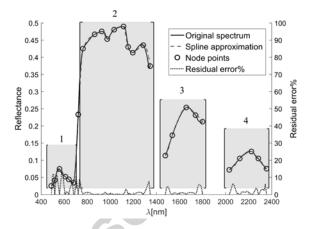


Figure 1: Spline approximation of a vegetation spectrum (synthetic understory reflectance) of 150 spectral bands, the original spectrum is shown with a solid line, the spline approximation with dashed line and the node points of the spline approximation with circles. The relative error between the approximation and the spectrum is shown with a dotted line. The figure also shows the division of the spectrum to correlated parts.

2.2. Bayesian inversion

Let us denote the vector of satellite measured bidirectional reflectances on the $N_{\lambda}=150$ spectral bands by $r \in \mathbb{R}^{150}$ and the vector of unknown variables by $x = \begin{bmatrix} \text{LAI}_{\text{eff}} & \tilde{\omega}_L^T & \tilde{\rho}_g^T & \beta \end{bmatrix}^T \in \mathbb{R}^{56}$. In the following, the problem of estimating the unknown model parameters x from the satellite measurements r is formulated as a problem of Bayesian inference. In a Bayesian setting, both the measurements r and the model unknowns x are modeled as random variables.

Let the parameters x have a prior probability density $\pi(x)$, which contains the available information on x before the reflectance measurements have been done. In

Bayesian inference, the prior density is then updated 221 with the information gained from the measurements by using the Bayes theorem

$$\pi(x|r) = \frac{\pi(r|x)\pi(x)}{\pi(r)} \propto \pi(r|x)\pi(x), \tag{8}$$

where $\pi(r|x)$ the likelihood function containing the information from the measurements, and $\pi(x|r)$ is the pos-196 terior density for the unknowns x, i.e., the conditional probability density of x given the measurements r. The $_{226}$ 198 posterior density $\pi(x|r)$ is the full solution of a Bayesian ₂₂₇ 199 inverse problem; Section 2.2.3 discusses the exploration 228 of the posterior density with an MCMC method, i.e., 229 201 finding useful point and spread estimates (such as pos-230 terior mean and credibility intervals) for x. The term $\frac{231}{231}$ 203 $\pi(r)$ in Eq. (8) can be thought of as a normalizing con-204 stant. 205

2.2.1. The likelihood function

207

208

209

210

211

212

213

215

219

The likelihood function $\pi(r|x)$ in theorem (8) is derived from the measurement model. Here, we model the measurements r as

$$r = h(x) + e, (9)$$

where h(x) is the PARAS model (1), including the approximations (2), (5), (6), and (7), and $e \in \mathbb{R}^{150}$ is an additive error term. The error e describes the discrepancy between the PARAS model output and the measured r and contains both the model error and the measurement noise.

In the case of the additive error model (9), the likelihood function $\pi(r|x)$ gets the form

$$\pi(r|x) = \pi_e(r - h(x)), \tag{10}$$

where $\pi_e(\cdot)$ is the density function of e. Here e is modeled as a multivariate normal distributed random variable with a zero mean and a covariance matrix Γ_e , and 249

hence, the likelihood function is

$$\pi(r|x) \propto \exp\left(-\frac{1}{2}(r - h(x))^T \Gamma_e^{-1}(r - h(x))\right).$$
 (11)

The error e is modeled as uncorrelated, with standard deviation of 10% of the data r in each band.

2.2.2. The prior density

The prior density $\pi(x)$ is a critical part of the Bayesian approach. In this work, separate prior densities for LAI_{eff}, $\tilde{\omega}_L$, $\tilde{\rho}_g$ and β are constructed. Uniform densities are used as priors for the scalar variables LAI_{eff} and β . For the spectral variables $\tilde{\omega}_L$ and $\tilde{\rho}_g$, Gaussian approximations are build based on empirical data that have been presented in the literature. The complete prior density $\pi(x)$ is finally formed by combining the variable-specific prior densities under the assumption of mutual statistical independence between LAI_{eff}, $\tilde{\omega}_L$, $\tilde{\rho}_g$ and β .

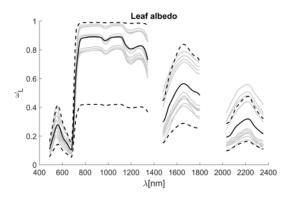
The effective LAI is by definition non-negative; also exceedingly large values of LAI are absent in a typical forest. As a prior distribution for LAI_{eff} we use a uniform distribution in the interval [0, 10]:

$$\pi(\text{LAI}_{\text{eff}}) = \begin{cases} \frac{1}{10}, & 0 \le \text{LAI}_{\text{eff}} \le 10\\ 0, & \text{otherwise.} \end{cases}$$
 (12)

Leaf albedo (ω_L) measurements for the three most common tree species in Finnish boreal forest (Scots pine, Norway spruce, and birch species) were reported by Lukeš *et al.* [16]. In our prior construction, the average of these species-specific albedos is used as the prior expected value for the node-point leaf albedo $\tilde{\omega}_L$, denoted with $\mu_{\tilde{\omega}_L}$. Peltoniemi *et al.* [17] presented reflectance measurements (BRF) of several common understory types. The average of these measurements is used as the prior expected value for node-point understory reflectance $\tilde{\rho}_g$, denoted with $\mu_{\tilde{\rho}_g}$. Note here that

234

the reported $\tilde{\omega}_L$ and $\tilde{\rho}_g$ are averaged only over the tree 284 species, not over the wavelength, and hence $\mu_{\tilde{\omega}_L}$ and $\mu_{\tilde{\rho}_g}$ 265 are vectors consisting of the average leaf albedos and 266 understory reflectances corresponding to 27 wavelengths 267 $\tilde{\lambda}$. For both $\tilde{\omega}_L$ and $\tilde{\rho}_g$ the prior standard deviation was 268 set to 20% of the expected value. This amount of variance was found to allow adequate range of possible $\tilde{\rho}_g$ 270 and $\tilde{\omega}_L$ values while still constraining the solution space 271 sufficiently. The prior expected value and 95% credisple intervals for ω_L and ρ_g are shown in Figure 2. The 273 figure also includes the spectral data [16, 17] used for 274 constructing the corresponding prior densities.



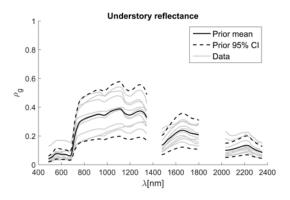


Figure 2: The expected values and 95% credible intervals for the prior densities of ω_L (top) and ρ_g (bottom), and the data used for constructing the priors.

The vegetation spectra have strong spectral correlation structure which is utilized in the prior. The model 288 for the correlation structure of both ω_L and ρ_g is written as follows: First, an uncorrelated Gaussian noise component is written to model the independent variations of the values of ω_L and ρ_g at the node points (i.e. elements of $\tilde{\omega}_L$ and $\tilde{\rho}_g$). Secondly, the measured band is divided into four non-overlapping parts (Figure 1), and the node points within each part are taken to be mutually strongly correlated. Thirdly, the background variation in the spectra is modeled with an additional correlation shared by all the nodes. The four parts in Figure 1 were chosen to reduce the correlation over the red edge between parts 1 & 2, and the water absorption bands between parts 2 & 3 and 3 & 4. This makes the prior fit better to different canopy and understory species compositions.

The associated prior correlation matrix R is thus

$$R = \kappa_{\text{ind.}} \frac{I}{27 \times 27} + \kappa_{\text{part}} R_{\text{part}} + \kappa_{\text{all}} \frac{1}{27 \times 27},$$

s.t. $\kappa_{\text{ind.}} + \kappa_{\text{part}} + \kappa_{\text{all}} = 1,$ (13)

where $\kappa_{\text{ind.}}$ is the strength coefficient of uncorrelatedness, κ_{part} is the strength coefficient of correlation within the four band parts shown in Figure 1, κ_{all} is the strength coefficient of background correlation, I is identity matrix, $\mathbf{1}$ is a matrix consisting of ones, sizes of the matrices are denoted under the symbols, and finally

$$R_{\text{part}} = \begin{bmatrix} \mathbf{1} & 0 & 0 & 0 & 0 \\ 0 & I & 0 & 0 & 0 \\ 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 & 0 & \mathbf{1} \end{bmatrix}. \tag{14}$$

In this study we use the values $\kappa_{\text{ind.}} = 0.3$, $\kappa_{\text{part}} = 0.4$, $\kappa_{\text{all}} = 0.3$.

Using the correlation matrix R, the prior covariance

matrices for $\tilde{\omega}_L$ and $\tilde{\rho}_g$ are then respectively

$$\Gamma_{\tilde{\omega}_I} = S_{\tilde{\omega}_I} R S_{\tilde{\omega}_L} \tag{15}$$

$$\Gamma_{\tilde{\rho}_g} = S_{\tilde{\rho}_g} R S_{\tilde{\rho}_g}, \tag{16}$$

where $S_{\tilde{\omega}_L}$ and $S_{\tilde{\rho}_g}$ are diagonal matrices that contain the prior standard deviations of $\tilde{\omega}_L$ and $\tilde{\rho}_g$ on their main diagonal. With the expected values and the covariance matrices, the Gaussian prior densities for $\tilde{\omega}_L$ and $\tilde{\rho}_g$, 316 constrained to the range [0, 1], are

$$\pi(\tilde{\omega}_L) \propto \begin{cases} \exp\left(-\frac{1}{2}(\tilde{\omega}_L - \mu_{\tilde{\omega}_L})^T \Gamma_{\tilde{\omega}_L}^{-1}(\tilde{\omega}_L - \mu_{\tilde{\omega}_L})\right), & 0 \leq \tilde{\omega}_L \leq 1 \\ 0, & \text{otherwise,} \end{cases}$$

(17)

$$\pi(\tilde{\rho}_g) \propto \begin{cases} \exp\left(-\frac{1}{2}(\tilde{\rho}_g - \mu_{\tilde{\rho}_g})^T \Gamma_{\tilde{\rho}_g}^{-1}(\tilde{\rho}_g - \mu_{\tilde{\rho}_g})\right), & 0 \leq \tilde{\rho}_g \leq 1^{322} \\ 0, & \text{otherwise.} \end{cases}$$

(18)

Due to the monotonicity of the chosen spline representations (6) and (7), constraining only the node points to the physically possible range [0, 1] is sufficient to keep the spectral variables ω_L and ρ_g in that range everywhere.

295

297

298

299

300

302

303

304

305

306

307

308

309

The shoot clumping parameter β for the coniferous species varies between 0.4 and 0.6 [18]. For broadleaved species, $\beta = 1$ by definition. Defining β for mixed canopies is problematic. For the sake of practicality it is assumed that there is an effective canopywide β that describes the average shoot clumping effect. We take this to be the weighted average of species-specific β 's. For β we use a uniform prior on the interval [0.4, 1]

$$\pi(\beta) = \begin{cases} \frac{5}{3}, & 0.4 \le \beta \le 1\\ 0, & \text{otherwise.} \end{cases}$$
 (19) 338

It would be possible to model also the correlations 340 between the variables LAI_{eff}, β , $\tilde{\omega}_L$ and $\tilde{\rho}_g$. However, 341

quantified information on these correlations is scarce. Therefore it is approximated that these variables are mutually independent. With this approximation, the resulting prior density for x is

$$\pi(x) = \pi(\text{LAI}_{\text{eff}})\pi(\tilde{\omega}_L)\pi(\tilde{\rho}_g)\pi(\beta). \tag{20}$$

2.2.3. The posterior density and estimates

Substitution of equations (11) and (20) to the Bayes' theorem (8) gives out the posterior density $\pi(x|r)$. The posterior density is used for computing point and interval estimates for the variables x. In this study, the posterior mean is used as the point estimate for x. As an interval estimate, 95% credible intervals are computed. A 95% credible interval for variable $x_i \in \mathbb{R}$ is an interval [a,b] that satisfies

$$\int_{a}^{b} \pi(x_{i}|r)dx_{i} = 0.95,$$
(21)

where $\pi(x_i|r)$ is the posterior marginal density of the variable x_i . Note that here x_i is a single element of the parameter vector x, such as the effective LAI or leaf albedo on a single band. Equation (21) has no unique solution: in this study the interval is chosen such that the probability mass below and above the interval [a, b] is equal.

Computation of the posterior mean and credible intervals requires integration over the posterior density. This can be accomplished numerically using for example Markov chain Monte Carlo (MCMC) methods (e.g. [19]). In MCMC methods, a random walk is used to draw samples from the underlying distribution and these samples are then used to approximate statistics of the distribution.

As the MCMC method, we use the delayed rejection adaptive Metropolis (DRAM) algorithm [20]. The DRAM algorithm is formulated as follows. Denote a

374

380

381

Gaussian proposal distribution by $q(y; \lambda, C)$, where μ is 368 342 the expected value and C is the covariance matrix. This $_{369}$ distribution is used to generate the next proposed state 370 344 in the random walk.

- 1. Initialization: Choose a point $x^{(0)}$ to be the start $x^{(0)}$ state of the random walk and choose an initial proposal covariance matrix C.
- 2. Metropolis step, do for each iteration *i*:

347

349

350

351

353

354

356

358

360

361

362

364

366

367

- (a) Sample a candidate $y^{(i)}$ from the proposal distribution $q(y; x^{(i-1)}, C)$ (the Gaussian proposal distribution is now centered on the previous state $x^{(i-1)}$).
- (b) Calculate acceptance ratio:

$$\alpha_1 = \frac{\pi(y^{(i)}|r)}{\pi(x^{(i-1)}|r)}.$$

- (c) Accept the new candidate $y^{(i)}$ with probability $\min\{1, \alpha_1\}$. If accepted, set $x^{(i)} = y^{(i)}$.
- 3. Delayed rejection step, do if the candidate $y^{(i)}$ was rejected:
 - (a) Sample a new candidate $\eta^{(i)}$ from the second level proposal distribution $q(\eta; x^{(i-1)}, \gamma C)$, where γ is a scaling factor.
 - (b) Calculate

$$\alpha_{12} = \frac{\pi(\eta^{(i)}|r)}{\pi(y^{(i)}|r)}$$

(c) Calculate the second level acceptance ratio:

$$\alpha_2 = \frac{\pi(y^{(i)}|r)q(\eta^{(i)};y^{(i)},C)(1-\alpha_{12})}{\pi(x^{(i-1)}|r)q(\eta^{(i)};x^{(i-1)},C)(1-\alpha_1)}.$$

- (d) Accept the new candidate $\eta^{(i)}$ with probability min{1, α_2 }. If accepted, set $x^{(i)} = \eta^{(i)}$, otherwise keep the previous state and set $x^{(i)} = 395$ $x^{(i-1)}$.
- 4. Adaptation, do every kth iteration: Compute a new 397 proposal covariance $C = sCov(x^{(0)}, ..., x^{(i)}) + s \in I$, 398 where $Cov(x^{(0)}, ..., x^{(i)})$ is the sample covariance 399

of the states $x^{(0)}, \ldots, x^{(i)}$, s is a scale parameter, I is an identity matrix and ϵ is a small positive constant. The $s \in I$ term ensures that the new proposal covariance is nonsingular.

5. Run until i = N + B, where N is the desired number of samples and B is the length of the burn-in period. Discard the first B states $x^{(0)}, \ldots, x^{(B)}$.

If the steps 3 and 4 are omitted from the above algorithm, it reduces to the standard Metropolis algorithm. The delayed rejection and adaptation steps make the algorithm more efficient than the standard Metropolis and make the method more robust against poorly chosen initial proposal covariance.

In this paper, a total of N = 600000 Monte Carlo samples are computed using 12 parallel random walks of 50000 samples each. The length of the burn-in period is chosen to be 5000 samples. In the delayed rejection step of the DRAM algorithm, covariance scaling factor of $\gamma = 0.1$ is used. The adaptation step in DRAM is done after every k = 200 iterations, with parameters $\epsilon = 10^{-5}$ and $s = 2.4/\sqrt{56}$.

2.3. Simulation studies

In this study, the effect of unknown reflectance model parameters on the LAI estimates is investigated using synthetic hyperspectral remote sensing (i.e. forest spectral) data. Synthetic data is used for the sake of validation: while the parameters LAI, β , ω_L and ρ_g are laborious to measure on field, the simulation studies allow for comparison of the estimates with the true values. However, care must be taken in analyzing the results, because when using simulated data, not all model inaccuracies are accounted for.

2.3.1. Simulated stands

400

419

420

421

423

A total of 500 random synthetic boreal forest stands 426 401 were generated and the forest reflectance was simulated 427 402 using the PARAS model. The simulated spectra consist 428 403 of 150 spectral bands emulating the EO-1 Hyperion in- 429 404 strument. First, the dominant tree species (pine, spruce 430 or broadleaved) was chosen with uniform probability. 431 406 The proportion of the dominant species in the species 432 407 mixture was sampled uniformly from the interval 50%- 433 408 100%; the remainder was then randomly divided be- 434 409 tween the two minority species. The composition of the 435 410 understory layer was then sampled to roughly emulate 436 411 the typical species composition of a Finnish boreal for-412 est with the chosen dominant tree species, that is, the understory of broadleaved stands contains mostly grasses 438 414 and some dwarf shrubs, spruce dominated stands have 439 415 mosses and bilberry, and pine stands have mosses, lin- 440 416 gonberry, heather and lichens. Ranges of the understory 441 417 components are presented in Table 1.

Table 1: Understory composition of the simulated forest stands.

Table 1. Officerstory composition of the simulated forest stands.							
Species	Pine	Spruce	Broadleaved	444			
Mosses	0 - 50%	40 – 100%	0 – 30%	445			
Bilberry	n/a	0 - 50%	0 – 30%	446			
Lingonberry	0 - 100%	n/a	n/a	447			
Heather	0 - 100%	n/a	n/a	448			
Lichens	0 - 100%	n/a	n/a	449			
Grasses	n/a	n/a	30 - 100%	450			
Soil	0 – 10%	0 - 10%	0 - 10%	430			

The leaf area index was chosen randomly from the $_{453}$ uniform distribution $\mathcal{U}(0,5)$. The leaf albedo ω_L and $_{454}$ understory reflectance ρ_g were formed as a linear combination of the experimental values presented in [16] $_{456}$ and [17], respectively, according to the sampled species $_{457}$ fractions of both the tree layer and the understory. Fi-

nally, the shoot clumping factor was sampled based on the tree species combination, with deciduous tree fraction contributing $\beta = 1$, spruce $\beta \sim \mathcal{N}(0.5, 0.05^2)$ and pine $\beta \sim \mathcal{N}(0.6, 0.05^2)$.

After all the input parameters were sampled, the PARAS model was used to simulate the forest reflectance. Gaussian random noise with standard deviation of 10% of the reflectance on each band was added to the modelled reflectance. The variance of this simulated radiometric noise was somewhat higher than in most real instruments to compensate for the lack of systematic errors in the simulated data.

2.3.2. Maximum likelihood estimates

The conventional approach to model based estimation of LAI_{eff} is to invert the reflectance model corresponding to parameters ω_L , ρ_g and β that are fixed to some *a priori* defined values. We studied the tolerance of such LAI_{eff} estimate to misspecification of the parameters ω_L , ρ_g and β . More specifically, we considered conventional maximum likelihood (ML) estimates, obtained by maximizing the likelihood function (11) with respect to LAI_{eff}.

For each of the 500 study stands, the ML estimate was computed using two choices of parameters ω_L , ρ_g and β : 1) In the first ML estimate, the true parameter values in the corresponding study stand were used. This choice is of course unrealistic, since these parameters are practically always unknown. 2) In the second set of ML estimates, parameters ω_L , ρ_g and β were fixed to their average values over the ensemble of simulated study stand test, i.e., to their population means. The latter estimate can be considered as a solution corresponding to the best realistically available approximation for the parameter values, and is expected to exhibit estima-

tion error that is caused by the misspecification of the parameters. 492

The one-dimensional optimization problem (maxi- 493 mizing (11) with respect to LAI_{eff}) was solved by brute 494 force to 0.1% accuracy, to ensure that the resulting es- 495 timate was the global maximum (due to the nonlinear- 496 ity, the likelihood has multiple local maxima in some 497 cases). For computational reasons, the range of LAI_{eff} 498 was constrained to [0, 10].

2.3.3. Bayesian estimates and reference methods

468

469

470

471

472

473

474

475

476

477

478

479

480

481

482

483

484

485

486

Next, the capability of the Bayesian approach to $_{501}$ tackle to problem of unknown model parameters ω_L , ρ_g $_{502}$ and β was studied. In the Bayesian inference, LAI_{eff}, $_{503}$ ω_L , ρ_g and β were simultaneously estimated from the $_{504}$ reflection data, as described in Section 2.2.

The Bayesian estimates were compared with two reference methods: 1) The ML estimates of LAI_{eff} corresponding to parameters ω_L , ρ_g and β fixed to their population means (see Section 2.3.2), and 2) empirical linear regression with a narrow-band vegetation index (VI).

We compared our new Bayesian approach with a typical empirical vegetation index using two narrow spectral bands. As there are a wide range of spectral indices in applied in hyperspectral remote sensing of vegetation, we selected the simple ratio water index (SRWI) which has recently been reported as the best performing index for estimating LAI_{eff} in our biome of interest, i.e. the boreal forests [2]. The SRWI is defined as

$$SRWI = \frac{r_{854}}{r_{1235}}. (22)$$

To construct the the empirical regression model, first, a 518 separate set of 100 random stands were simulated and 519 the SRWI was calculated for each stand. Ordinary lin- 520 ear regression was then performed between LAI_{eff} and 521

SRWI in the training set. The regression model was then used to estimate LAI $_{\rm eff}$ for each of the 500 study stands.

We note that as the empirical VI regression estimate does not rely on a reflectance model, it does not require specifying the model parameters ω_L , ρ_g and β . However, the uncertainty of these parameters does have an implicit effect on the accuracy of the VI regression based LAI_{eff} estimates: variation of these parameters in the training set obfuscates the correlation between the spectral reflectance data r and LAI_{eff}.

2.3.4. Effect of prior model on Bayesian estimate

We also studied the effect of the prior model on the Bayesian estimate. Hence, in addition to computing the Bayesian estimate corresponding to data based, informative prior models described in Section 2.2, the Bayesian estimate was also computed using uniform priors for all the parameters. The uniform priors simply constrain LAI_{eff} to the range [0, 10], ω_L and ρ_g to the range [0, 1] and β to [0.4, 1]. This estimate corresponds to one introduced by Zhang *et al.* [11].

3. Results and discussion

3.1. Sensitivity of the maximum likelihood estimate to model uncertainties

The results of studing the sensitivity of the ML estimate to model uncertainties is illustrated in Figure 3. When the true values of ω_L , ρ_g and β are used in the reflectance model, the estimated LAI_{eff} are very close to their true values in almost every study stand (Figure 3, left). Only a few significantly erroneous estimates are present – those estimates probably correspond to large realizations of observation noise. Moreover, the scatter

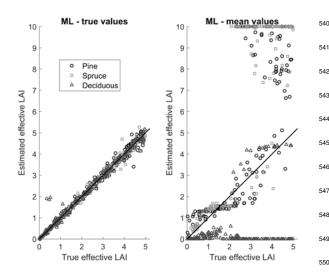


Figure 3: Estimated LAI_{eff} vs. true LAI_{eff} ML estimates corresponding to models with correct values of ω_L , ρ_g and β (left) and their population mean values (right). Pine dominated stands are marked with circles, spruce dominated with squares and deciduous with triangles.

plot shows a slight increase of the estimation error with increasing LAI_{eff}; this is caused by saturation of the forest reflectance: with the increase of LAI, the sensitivity of the reflectance measurements to a change in LAI decreases.

The ML estimates corresponding to the reflectance model with misspecified parameters ω_L , ρ_g and β (Figure 3, right) feature large errors. In particular, ML estimates are zero for several cases where the canopy is dense in reality, and on the other hand, several ML estimates are equal to 10 in cases where the true value of LAI_{eff} is between 2 and 5. In total, 28% of the ML estimates are above the maximum simulated LAI value of 558 559. We note that accumulation of the ML estimates to 569 values 0 and 10 is a result of bounding these estimates to the interval [0, 10] – without these constraints, many 561 of the estimates would be even more biased.

The root mean square errors (RMSE) and biases of 563

the two ML estimates are shown in Table 2. The comparison of the errors confirms the observation made based on Figure 3: the use of the approximate choices of parameters ω_L , ρ_g and β leads, on average, to large errors in the LAI_{eff} estimates.

The results demonstrate that ML estimates are highly intolerant to misspecification of parameters in the reflectance model. This intolerance is associated with ill-posedness of the inverse problem spanned by the reflectance model – small/moderate errors in the data or model can cause large errors in the estimates. Hence, although only ML estimates were considered in this study, caution should be taken in the interpretation of any model based LAI estimate which does not take into account the uncertainty of the model parameters.

Table 2: RMSE, relative RMSE and bias of effective LAI estimates for the Bayesian posterior mean estimates, the reference empirical VI regression and maximum likelihood estimates.

	RMSE	RMSE%	bias
ML estimate			
- correct model	0.19	7.81	0.0013
- approximate model	3.41	137.78	0.91
Posterior mean			
- informative prior	0.61	24.62	-0.0002
- uniform prior	1.14	45.88	-0.17
VI regression	1.10	44.36	0.11

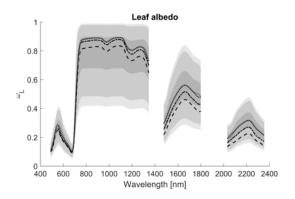
3.2. Performance of the Bayesian estimates

In this section, we discuss the performance of the Bayesian estimate with informative, data based priors. First, the full Bayesian solutions – including not only the point estimates but also credible intervals of the model unknowns – are illustrated with two example cases: one with low LAI (Section 3.2.1) and one with high LAI (Section 3.2.2). Comparison between the Bayesian estimates and the reference methods is

made. Finally, the performance of these estimates is 575 rated based on the statistics of the results correspond- 576 ing to the set of 500 study stands (Section 3.2.3). 577

3.2.1. Example 1: low LAI case

The first example stand is a spruce dominated stand with a low leaf area index of LAI_{eff} = 0.42. The spectra of ω_L and ρ_g (the 'simulated true values') are depicted in Figure 4. The figure also illustrates the the prior marginal densities of ω_L and ρ_g , and the (fixed) spectra of ω_L and ρ_g used in the ML estimate of LAI_{eff} (see Section 2.3.1) for comparison.



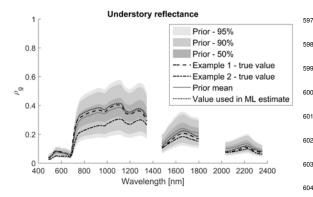


Figure 4: Prior marginal densities and prior expected values of leaf albedo and understory reflectance. The figure also contains the true values of ω_L and ρ_g of the examples 1 and 2, and the assumed values of ω_L and ρ_g used in computing the ML estimates.

The results of Example 1 are illustrated in Figure 5. The top image of Figure 5 represents the Bayesian estimates for the effective LAI corresponding to the informative priors; the posterior mean estimate is marked with a circle, and the 95% credible interval is shaded with gray. The true simulated value of the effective LAI is marked in the figure with a cross.

The Bayesian posterior mean estimate for LAI_{eff} is 0.74, and hence, somewhat overestimates the true value LAI_{eff}=0.42. On the other hand, the 95% (posterior) credible interval is [0.41, 1.07], i.e., the true value 0.42 lays inside this interval. It is notable that in this example case the 95% credible interval is significantly narrower than the *a priori* range [0, 10] for LAI_{eff}.

Posterior marginals for the leaf albedo ω_L and understory reflectance ρ_g as function of wavelength are illustrated in the center and bottom of Figure 5 respectively. In the case of low LAI the posterior 95% CI covers the true value of ω_L throughout the range (Figure 5, center). However, the posterior of ω_L is wide, nearly as wide as the prior density in some wavelengths, implying high uncertainty for the estimated values of ω_L . This is an expected outcome: In the case of low LAI, the reflecting surface area of the leaves is small, and the contribution of ω_L to the reflectance measurements is relatively low, i.e., the sensitivity of the measurements to ω_L is low, and consequently, ω_L remains uncertain after the inference from the data.

The posterior density of ρ_g (Figure 5, bottom), on the other hand, is rather narrow. This is again an expected result: In the case of low LAI, the understory has a large effect on the measured reflectance, and in contrary to ω_L , the measurements are sensitive to ρ_g .

The ML estimate for the effective LAI is marked in Figure 5 (top) with symbol ' \triangle '. In the case of low LAI,

656

the ML estimate for LAI_{eff} is 0.66. Thus, the ML es- 644 610 timate is relatively close to the true value (0.42), even 645 slightly more accurate than the Bayesian posterior mean 646 612 estimate. We note that in this example case, the true 647 613 spectra of ω_L and ρ_g were relatively close to the corre-614 sponding values assumed when computing the ML, and 649 615 hence, the effect of uncertainties of this parameters in 650 616 the LAI_{eff} estimates is minor. 617

The VI regression estimate is marked in Figure 5 652 618 (top) with symbol 'V'. In the low LAI case, the VI 653 619 regression estimate equals to 1.70, and is thus clearly 654 620 worse than the model-based estimates.

3.2.2. Example 2: high LAI case 622

621

In Example 2, LAI_{eff} was 4.87 and the stand was 658 dominated by pine. The results of this example case 659 624 are shown in the Figure 6. The Bayesian CM estimate 660 625 equals to 4.56, and is thus rather close to the true value. In this case the posterior density of LAI_{eff} (Figure 6, 662 627 top), is significantly wider than in Example 1 (Figure 5, top), implying that on high LAI stands, the estimate 664 629 for LAI_{eff} has larger uncertainty. This stems from the $_{665}$ 630 saturation of the forest reflectance mentioned in Section 6666 3.1: when the canopy gets very dense, the sensitivity 667 632 of the reflectance measurements to a change in canopy 668 LAI gets low. Note also that in both example cases, the 634 posterior density of LAIeff is skewed to the left; this is 635 another indication of the higher uncertainty of the large 636 LAI values caused by the saturation effect. 637

The posterior marginals for the leaf albedo ω_L and 671 understory reflectance ρ_g in Example 2 are shown in the 672 639 center and bottom of Figure 6, respectively. In this case, 673 640 the posterior density of ω_L is very narrow, indicating a 674 high credibility for the estimated ω_L . On the other hand, 675 642 the posterior density of ρ_g is wide in Example 2, indicating high posterior uncertainty of ρ_g . These are again an intuitive results: While in the low LAI case, the sensitivity of reflectance measurements to ω_L is poor, leading to high posterior uncertainty of ω_L , in the high LAI case, the measured forest reflectance results nearly entirely from canopy scattering, with almost no understory contribution, leading to high credibility of the estimated ω_L and high uncertainty of ρ_g .

In Example 2, the ML estimate for LAI_{eff} ('\(\Delta' \) in Figure 6, top) was 8.44, which is a heavily overestimated value. This error is again related to the saturation of the forest reflectance with high LAI. It is notable, that the ML estimate for LAI_{eff} is poor even though the the error in the variable ω_L behind the ML estimate is rather low (Figure 4). However, there is significant error in ρ_g and some error in β (β = 0.71 in the ML estimate vs. true value of 0.65).

In this example case, the VI regression estimate (represented by '♥' in Figure 6, top) was 4.07, i.e., slightly closer to the true value than in Example 1. This, however, does not mean that the VI regression estimates get generally better when LAI increases; in contrast, the set of simulations in the next section demonstrate that the overall accuracy of the VI regression estimates decreases with the increase of LAI.

3.2.3. Performance of the estimates over a set of 500 study stands

The performance of the Bayesian posterior mean estimates and the VI regression estimates is illustrated in Figure 7, showing a scatter plot of the estimated LAI_{eff} versus the true value of LAIeff corresponding to each estimation method.

Generally, the Bayesian posterior mean estimates us-

In the entire range [0, 5] of LAI_{eff}, these estimates pos-713 sess only small/moderate errors, except for a few out- 714 679 liers (Figure 7, top left). Especially, in some dense pine 715 680 dominated stands the LAI_{eff} is largely overestimated, 716 and in a few deciduous stands the LAIeff is underesti-682 mated. Overall, the error increases with increasing LAI 683 - as expected, due to saturation effect discussed above. 684 The comparison of the scatter plots of the Bayesian 685 estimates in Figure 7 (top left) and the ML estimates in 719 686 Figure 3 shows that the Bayesian estimates are not as 720 687 accurate as the ML estimates corresponding to models 721 688 with correct parameters ω_L , ρ_g and β (Figure 3, left). 722 689 However, the Bayesian estimates clearly outperform the 723 690 ML estimates corresponding to parameters ω_L , ρ_g and β fixed to their population means (Figure 3, right). This 725 692 observation is verified by the statistics of the estimates 726 693 shown in Table 2: The RMSE of the Bayesian estimate 727 694 is larger than the RMSE of the ML estimate with the 728 695 correct parameters but significantly smaller than that of the ML estimate with the approximate parameters. The 730 697 bias is, in fact, smaller than either of the ML estimates. 731 698 The results support the feasibility of the Bayesian ap- 732 699 proach to inversion of the reflectance model: Although 733 700 the accuracy of the estimates decreases from the ideal 734 case where the parameters are known, the Bayesian esti- 735 702

ing the informative prior yield quite reliable estimates: 712

677

703

704

705

706

707

708

710

The scatter plot of the VI regression estimates is 739 drawn in Figure 7 (top right). This plot shows signif- 740 icantly larger variation from the true LAI_{eff} than the 741 Bayesian CM estimates corresponding the informative 742 prior, and in the small values of LAI_{eff} (especially for 743 0 \leq LAI_{eff} \leq 1), the VI regression estimates clearly 744

mates tolerate the uncertainties of the reflectance model 736

significantly better than ML estimates using approxi- 737

mate values for the parameters.

feature a large positive bias. Table 2 reveals that the VI regression estimates are clearly less reliable than the Bayesian posterior mean estimates using the informative prior, but more accurate than the ML estimates using approximate parameters.

3.3. Effect of prior model and uncertainty quantification

The scatter plot of the Bayesian posterior mean estimate using the uniform prior is shown in Figure 7 (bottom). This plot and the statistics in Table 2 indicate that the accuracy of this estimate is in the same level as the accuracy of the VI regression estimate, i.e., the Bayesian estimates using the uniform prior are clearly more erroneous than those corresponding to the informative prior. Especially the overestimation of LAI_{eff} in dense pine dominated stands and the underestimation of LAI_{eff} in deciduous stands is significantly larger when uniform prior is used. This result suggests that the construction of the informative prior models for the parameters ω_L and ρ_g is advantageous over simply constraining these parameters.

Table 3 shows the RMSE% and the bias for the estimates of LAI_{eff}, ω_L , ρ_g and β based on Bayesian approach. The results are represented for both Bayesian estimates: those corresponding to uniform priors and those with the informative priors.

In cases of both prior models, the RMSEs of LAI_{eff} and ω_L have little variation with respect to the majority species. For ρ_g the RMSE and bias of spruce-dominated stands are significantly better, which results from the fact that the expected true ρ_g of spruce-dominated stands is closest to the prior mean for ρ_g . The direction of the bias for the pine and deciduous stands

points towards the prior mean. Another notable aspect 779 745 is the relatively large overestimation of β on the spruce 780 stands, which goes hand in hand with the overestimation 781 747 of LAI_{eff} on spruce-dominated stands. The results of the $_{782}$ table indicate that when using the informative prior, the 783 estimation accuracy is generally fairly good. When us-784 750 ing the uniform prior, the performance is consistently 785 751 752

In addition to evaluating the point estimates, we also 787 investigated the feasibility of the Bayesian estimates to 788 quantify the (posterior) uncertainty of the model un- 789 knowns. For this purpose, we computed the coverage 790 percentages of 95% credible intervals (CI%) for LAI_{eff}, 791 ω_L, ρ_g and β ; this statistic is defined as the percentage of 792 stands on which the true parameter value lies within the 793 computed 95% credible interval (Equation (21)). The 794 ideal value of the CI% would be 95%.

When using the informative priors, CI% of the effective LAI for the whole set of stands is 82.40%, which indicates a slight underestimation of the uncertainty of LAI_{eff}. For the other parameters, the CI% is close to 797 95%, indicating that the approach gives a very good 798 measure for the uncertainty of the estimated parame- 799 ters. When using the uniform prior models for the pa-800 rameters, CI%s are generally poorer. Especially, CI% 801 of LAI_{eff} is only 59.20%, which indicates a large underestimation of the estimate uncertainty.

3.4. General discussion

753

754

755

756

757

758

760

761

762

763

765

766

767

768

770

771

773

774

775

777

In this study, cubic monotonic Hermite splines were 806 used to enforce smoothness on the spectral variables ω_L 807 and ρ_g and to implement dimension reduction. This representation has the strength that informative priors for 809 the spectral variables can be constructed in a straight- 810 forward way, if expected value and variance of those

variables is known at the node points. This is a clear advantage compared to some other possible low dimensional representations such as those based on principal components.

Overall, our results (Tables 2 and 3) support the use of informative prior models of the parameters ω_L and ρ_g in the Bayesian inference based on the reflectance model. The results show clearly the smallest estimation errors for LAI_{eff} when the informative prior models are used. Moreover, Bayesian approach with the informative prior models provides at least somewhat feasible means for quantifying the estimate uncertainties, yet the uncertainty of the LAIeff was slightly underestimated in this numerical study. The informative prior formulation could be possibly further improved by including additional auxiliary information, for example seasonality, forest inventory data and spatial correlation.

4. Conclusions

Estimation of canopy LAI from hyperspectral imagery can be done via inversion of a forest reflectance model. Forest reflectance models, however, contain many other unknown, confounding variables in addition to LAI. In this paper, we investigated the effects of the model uncertainties on LAI estimates. Moreover, we studied whether the LAI estimates could be recovered from the errors caused by the model uncertainties by taking a Bayesian approach to forest reflectance model inversion. Moreover, we studied whether the Bayesian approach could be used of quantification of the estimate uncertainties.

The proposed approach was evaluated using realistic simulated data representing boreal forests. The performance of the Bayesian estimates was superior to the ref-

853

erence estimates in RMSE and bias. The results also 845 812 show, that if parameters other than LAI are fixed to 846 their best-guess value, the estimates based on inverting 847 814 the reflectance model are often vastly erroneous. We 815 also tested the effect of prior model formulation for the 816 model unknowns; i.e., the informative prior formulation 817 was compared with simple uniform prior formulation. 818 With the informative priors the Bayesian estimates pro-819 duced significantly smaller estimation errors and better 820 estimates for the parameter uncertainty than with uniform priors. 822

The simulation results show that the Bayesian inference provides a feasible framework to account for uncertainties in secondary reflectance model variables. In contrast to empirical VI regression methods, the proposed approach can utilize the full information content of hyperspectral data and not only (pre)selected spectral bands. Additionally, the quantified estimate uncer- 861 tainty is important in uncertainty quantification of cli-862 mate models, if remotely sensed LAI is used as an input. In the future, the proposed approach has to be tested using real measurements to validate these promising simulation results.

Acknowledgements 835

823

824

825

827

828

830

832

833

836

838

839

841

843

This work was supported in part by the University of Eastern Finland (spearhead project Multiscale geospatial analysis of forest ecosystems and the doctoral school of the University of Eastern Finland) and in part 872 by the Academy of Finland (Finnish Centre of Excel- 873 lence of Inverse Problems Research 2012-2017, project 874 number 250215, and projects 286390 and 135502). 875

[1] P. Gong, R. Pu, G. S. Biging, M. R. Larrieu, Estimation of forest leaf area index using vegetation indices de-

- rived from Hyperion hyperspectral data, IEEE Transactions on Geoscience and Remote Sensing 41 (6) (2003) 1355-1362. doi:10.1109/TGRS.2003.812910.
- [2] J. Heiskanen, M. Rautiainen, P. Stenberg, M. Mõttus, V.-H. Vesanto, Sensitivity of narrowband vegetation indices to boreal forest LAI, reflectance seasonality and species composition, IS-PRS Journal of Photogrammetry and Remote Sensing 78 (0) (2013) 1 – 14. doi:10.1016/j.isprsjprs.2013.01.001.
- [3] F. Baret, G. Guyot, Potentials and limits of vegetation indices for LAI and APAR assessment, Remote sensing of environment 35 (2-3) (1991) 161-173. doi:10.1016/0034-4257(91)90009-U.
- [4] G. Zheng, L. M. Moskal, Retrieving leaf area index (LAI) using remote sensing: Theories, methods and sensors, Sensors 9 (4) (2009) 2719-2745. doi:10.3390/s90402719.
- [5] P. D'Odorico, A. Gonsamo, A. Damm, M. E. Schaepman, Experimental evaluation of Sentinel-2 spectral response functions for NDVI time-series continuity, IEEE Transactions on Geoscience and Remote Sensing 51 (3) (2013) 1336-1348. doi:10.1109/TGRS.2012.2235447.
- [6] M. E. Schaepman, S. L. Ustin, A. J. Plaza, T. H. Painter, J. Verrelst, S. Liang, Earth system science related imaging spectroscopy - an assessment, Remote Sensing of Environment 113, Supplement 1 (0) (2009) S123 - S137. doi:10.1016/j.rse.2009.03.001.
- [7] Y. Knyazikhin, M. A. Schull, P. Stenberg, M. Mttus, M. Rautiainen, Y. Yang, A. Marshak, P. Latorre Carmona, R. K. Kaufmann, P. Lewis, M. I. Disney, V. Vanderbilt, A. B. Davis, F. Baret, S. Jacquemoud, A. Lyapustin, R. B. Myneni, Hyperspectral remote sensing of foliar nitrogen content, Proceedings of the National Academy of Sciences 110 (3) (2013) E185E192. doi:10.1073/pnas.1210196109.
- [8] F. Baret, S. Buis, Estimating canopy characteristics from remote sensing observations: Review of methods and associated prob-

876

867

- lems, in: S. Liang (Ed.), Advances in Land Remote Sensing, 911
- 879 Springer, 2008, pp. 173–201.
- 880 [9] K. M. Vanhatalo, M. Rautiainen, P. Stenberg, Monitor- 913
- ing the broadleaf fraction and canopy cover of boreal 914
- 882 forests using spectral invariants, Journal of Quantitative 915
- Spectroscopy and Radiative Transfer 133 (2014) 482–488. 916
- doi:10.1016/j.jqsrt.2013.09.011.
- 885 [10] J. P. Kaipio, E. Somersalo, Statistical and Computational Inverse 918
- Problems, Springer, New York, 2005.
- 887 [11] Q. Zhang, X. Xiao, B. Braswell, E. Linder, F. Baret, B. Moore, 920
- 888 Estimating light absorption by chlorophyll, leaf and canopy in 921
- a deciduous broadleaf forest using MODIS data and a radiative 922
- transfer model, Remote Sensing of Environment 99 (3) (2005) 923
- 891 357–371. doi:10.1016/j.rse.2005.09.009.
- [12] M. Rautiainen, P. Stenberg, Application of photon recol- 925
- 893 lision probability in coniferous canopy reflectance simula- 926
- tions, Remote Sensing of Environment 96 (2005) 98-107.
- doi:10.1016/j.rse.2005.02.009.
- 896 [13] T. Manninen, P. Stenberg, Simulation of the effect of
- snow covered forest floor on the total forest albedo,
- Agricultural and Forest Meteorology 149 (2009) 303–319.
- doi:10.1016/j.agrformet.2008.08.016.
- 900 [14] P. Stenberg, Simple analytical formula for calculating av-
- erage photon recollision probability in vegetation canopies,
- Remote Sensing of Environment 109 (2007) 221–224.
- 903 doi:10.1016/j.rse.2006.12.014.
- 904 [15] M. Mõttus, P. Stenberg, A simple parameterization of
- canopy reflectance using photon recollision probability, Re-
- 906 mote Sensing of Environment 112 (2008) 1545–1551.
- 907 doi:10.1016/j.rse.2007.08.002.
- 908 [16] P. Lukeš, P. Stenberg, M. Rautiainen, M. Mõttus, K. M. Van-
- hatalo, Optical properties of leaves and needles for boreal tree
- species in Europe, Remote Sensing Letters 4 (7) (2013) 667–

- 676. doi:10.1080/2150704X.2013.782112.
- [17] J. I. Peltoniemi, J. Suomalainen, E. Puttonen, J. Näränen, M. Rautiainen, Reflectance properties of selected arctic-boreal land cover types: field measurements and their application in remote sensing, Biogeosciences Discuss. 5 (2008) 1069–1095. doi:10.5194/bgd-5-1069-2008.
- [18] M. Thérézien, S. Palmroth, R. Brady, R. Oren, Estimation of light interception properties of conifer shoots by an improved photographic method and a 3D model of shoot structure, Tree physiology 27 (10) (2007) 1375–1387. doi:10.1093/treephys/27.10.1375.
- [19] W. Gilks, S. Richardson, D. Spiegelhalter (Eds.), Markov Chain Monte Carlo in Practice, Chapman & Hall, 1996.
- [20] H. Haario, M. Laine, A. Mira, E. Saksman, DRAM: efficient adaptive MCMC, Statistics and Computing 16 (4) (2006) 339– 354. doi:doi:10.1007/s11222-006-9438-0.

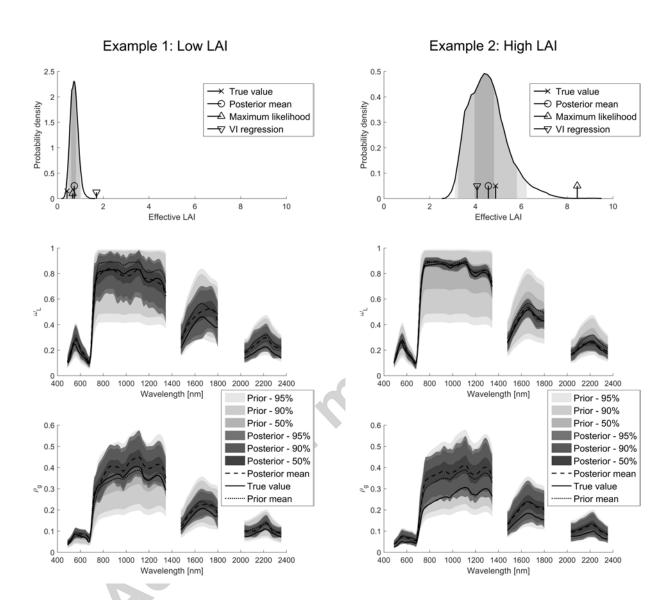


Figure 5: Posterior marginal densities of effective LAI (top), leaf albedo (center), and understory reflectance (bottom) for Example 1. The shaded areas in the top picture correspond to the 50%, 90% and 95% posterior CIs from dark to light grey, respectively.

Figure 6: Posterior marginal densities of effective LAI (top), leaf albedo (center), and understory reflectance (bottom) for Example 2. The shaded areas in the top picture correspond to the 50%, 90% and 95% posterior CIs from dark to light grey, respectively.

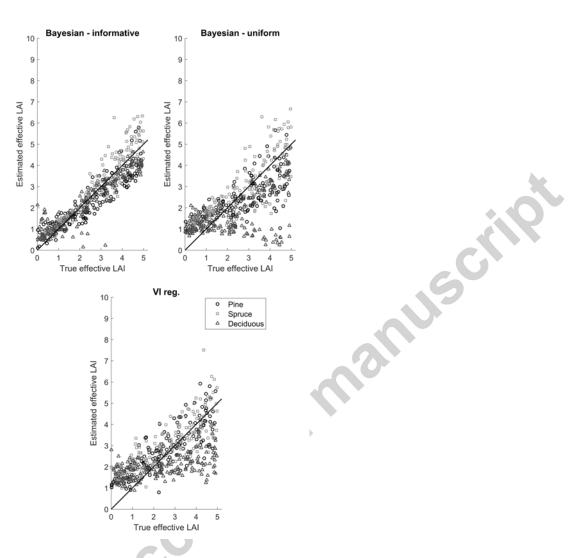


Figure 7: Estimated LAI $_{\rm eff}$ vs. true LAI $_{\rm eff}$ for the Bayesian posterior mean estimates (top left), empirical VI regression estimates (top right) and Bayesian posterior mean estimates using uniform prior (bottom), Pine dominated stands are marked with circles, spruce dominated with squares and deciduous with triangles.

Table 3: Relative RMSE and relative bias of Bayesian posterior mean estimates, and coverage percentage of 95% credible intervals, by the majority species. The spectral variables ω_L and ρ_g are divided to visible light (c. 480 – 700 nm), NIR (c. 750 – 1350 nm) and SWIR (c. 1500 – 2350 nm) components.

		Uniform prior		Informative prior			
		RMSE%	bias%	CI%	RMSE%	bias%	CI%
LAI_{eff}	pine	37.44	-5.44	63.29	23.44	-7.34	78.48
	spruce	36.02	12.24	69.51	23.51	12.44	86.59
	decid.	60.69	-27.43	46.07	26.83	-5.32	82.02
	all	45.88	-6.96	59.20	24.62	-0.0089	82.40
ω_L , vis.	pine	24.14	-2.09	99.64	12.06	2.88	99.19
	spruce	27.20	1.06	99.07	12.73	7.45	98.40
	decid.	30.95	7.03	99.01	11.25	-3.89	89.48
	all	28.29	2.23	99.23	12.17	1.65	95.48
ω_L , NIR	pine	14.31	-7.83	86.23	9.57	-4.17	90.60
	spruce	11.80	-5.25	94.84	4.42	-1.26	99.32
	decid.	17.92	-11.25	85.59	5.26	-1.61	97.16
	all	15.35	-8.34	88.83	6.70	-2.29	95.80
ω_L , SWIR	pine	21.36	-4.80	98.88	10.17	-0.15	99.82
	spruce	21.87	0.83	98.94	12.54	4.42	99.49
	decid.	23.41	-16.7	95.73	12.32	-8.35	88.16
	all	23.37	-9.11	97.78	12.39	-2.99	95.56
ρ_g , vis.	pine	48.94	30.57	99.37	30.98	-10.71	88.16
	spruce	66.06	54.57	99.91	13.93	2.59	72.00
	decid.	112.76	88.64	99.92	28.87	24.62	97.65
	all	72.45	53.93	99.74	26.59	2.97	93.77
ρ_g , NIR	pine	52.49	42.56	85.64	25.32	21.34	88.65
_	spruce	34.58	22.13	93.69	10.03	3.28	98.88
	decid.	40.47	24.90	71.00	16.31	-6.31	92.76
	all	42.13	28.66	83.06	17.51	4.02	93.47
$ ho_g$, SWIR	pine	42.60	25.51	96.77	20.06	5.49	94.05
	spruce	46.03	32.02	98.68	17.01	13.74	99.52
	decid.	60.65	51.77	86.22	20.43	16.56	91.18
•	all	51.08	36.94	93.64	19.41	11.85	94.82
β	pine	15.62	-0.16	89.24	13.06	-3.59	98.73
	spruce	20.68	7.34	87.80	22.43	12.96	91.46
	decid.	18.86	-12.36	84.27	6.35	1.74	97.19
	all	18.87	-3.63	87.00	13.24	3.20	95.80