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Linking in situ LAI and Fine Resolution Remote Sensing Data to Map Reference LAI over Cropland and Grassland Using Geostatistical Regression Method

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1. Introduction

 Leaf Area Index (LAI), defined as half the total leaf area per unit ground surface areas [\(Chen and Black, 1992\)](#page-30-0), is an important parameter of vegetation structure and function [\(Abuelgasim et al., 2006\)](#page-30-1). LAI provides substantial information on the exchange of energy, mass, and momentum flux between the Earth's surface and its atmosphere [\(Morisette et al., 2006;](#page-32-0) [Myneni et al., 1997\)](#page-32-1). LAI has been widely used as an input in climate, hydrology, and biogeochemistry models [\(Berterretche et al., 2005;](#page-30-2) [Knyazikhin et](#page-31-0) [al., 1998;](#page-31-0) [Morisette et al., 2006\)](#page-32-0). To date, a number of global and regional moderate- resolution LAI products have been produced, including Moderate Resolution Imaging Spectroradiometer (MODIS), Carbon Cycle and Change in Land Observational Products from and Ensemble of Satellites (CYCLOPES), Canada Centre for Remote Sensing (CCRS), and Global Land Surface Satellite (GLASS) [\(Chen et al., 2002;](#page-30-3) [Tian et al.,](#page-32-2) [2000;](#page-32-2) [Weiss et al., 2007;](#page-33-0) [Xiao et al., 2014\)](#page-33-1). Owing to the influence of model algorithms, vegetation heterogeneity, and observation conditions, these LAI products inevitably have inherent uncertainties [\(Chen et al., 2002\)](#page-30-3), which subsequently may impact the accuracy of any resulting modeling activities. Specifying the uncertainties of these coarse spatial resolution LAI products is essential for users to determine the most appropriate dataset for their applications, and for producers to improve methodological algorithms. However, a direct comparison between in situ LAI measurements and these corresponding moderate resolution LAI products is not recommended because of scale-mismatch, geolocation errors, and land surface heterogeneity [\(Huang et al., 2006;](#page-31-1) [Yang et al., 2006\)](#page-33-2). The proposed way to validate coarse resolution remote sensing products is using fine reference maps derived from up-scaling in situ measurements [\(Fernandes et al., 2014;](#page-30-4)

 There are three categories of methods for estimating reference LAI maps using in situ LAI observations and fine spatial resolution remote sensing data, including regression, vegetation radiation transfer equation inversion, and geostatistical methods [\(Cohen et al., 2003;](#page-30-8) [Martinez et al., 2010;](#page-32-5) [Yang et al., 2006\)](#page-33-2). Of these, the radiation transfer equation inversion method is not used widely due to the difficulty in collecting certain model parameters (e.g. canopy structure) and the fact that the solution of the model is not unique [\(Yang et al., 2006\)](#page-33-2). Geostatistical methods have become popular in linking field data to image data, and been applied to estimate forest parameters (basal area, height, health conditions, etc), detect land use and land cover change, and map vegetation index (e.g., normalized difference vegetation index: NDVI and LAI) [\(Van der](#page-32-6) [Meer, 2012\)](#page-32-6). Traditional geostatistical methods, such as Kriging, predict unknown points 83 through spatially interpolating surrounding field observations [\(Berterretche et al., 2005;](#page-30-2) [Li et al., 2013a;](#page-31-4) [Li et al., 2013b\)](#page-31-5). The limited number of field observations and the spatial non-stationarity of in situ observations distribution could lead to uncertainty of predicting results. Regression methods, such as ordinary least squares regression, attempt to improve the predicting accuracy through accounting for high resolution remote sensing 88 data (e.g., reflectance or vegetation indices (VI) derived from Landsat ETM+). Cohen et

 [al. \(2003\)](#page-30-8) compared three regression methods (i.e., traditional ordinary least squares regression, inverse ordinary least square regression, and reduced major axis: RMA) over the BigFoot AGRO and NOBS sites. They reported that the performance of RMA method was superior to the other two. However, none of the regression methods consider the spatial/temporal correlation of in situ observations and high resolution reflectance or VI data, which may lead to an underestimation of the uncertainty along with the regression coefficients [\(Chatfield, 2003\)](#page-30-9).

 Geostatistical regression (GR) method conserves merits from both traditional geostatistical methods and regression methods. It has been used in examining the relationships between terrestrial carbon dioxide flux and its primary environmental drivers [\(Mueller et al., 2010\)](#page-32-7), and estimating snow cover and gross primary productivity [\(Erickson et al., 2005;](#page-30-10) [Yadav et al., 2010\)](#page-33-4). Compared to traditional regression methods, the GR method is improved in one distinct way, which is the ability to account for the spatial/temporal correlation of the residuals from in situ observations (such as field LAI measurements) and auxiliary data (such as NDVI) [\(Erickson et al., 2005;](#page-30-10) [Mueller et al.,](#page-32-7) [2010;](#page-32-7) [Yadav et al., 2010\)](#page-33-4). Unlike traditional geostatistcal methods (e.g., Kriging), the GR method attempts to provide better estimating of unknown points by exploring the correlation between high resolution remote sensing data and field observations. To our knowledge, no attempts have been made to use the GR method to estimate LAI reference maps. This study applied the GR method to estimate high resolution LAI reference maps over cropland and grassland sites through fusing in situ LAI measurements and high resolution remote sensing images (i.e., Landsat TM/ETM+ and SPOT). To investigate the discrepancy of employing different VIs on estimating LAI reference maps, this study

- established the GR models for the following VIs: difference vegetation index (DVI),
- NDVI, and ratio vegetation index (RVI). To robustly assess the performance of the GR
- model, the results from GR and RMA models were compared.
-

2. Methodology

- *2.1. Geostatistical regression method*
- The GR method not only models the relationships between auxiliary variables (DVI, NDVI, and RVI in this study) and field measurements (in situ LAI measurements in this study), but also accounts for the spatial/temporal correlation of the regression residuals [\(Erickson et al., 2005\)](#page-30-10). As with the linear regression method, the GR method decomposes LAI into a deterministic and a stochastic component: 123 $LAI = X\beta + \varepsilon$ (1)
-

124 Where $X(n \times P)$ is the DVI, NDVI, and RVI, respectively, $\beta(P \times 1)$ is the 125 corresponding regression coefficient, and ε ($n \times 1$) is assumed to be second-order

stationary and zero-mean residuals for DVI, NDVI, and RVI [\(Leung and Cooley, 2014;](#page-31-6)

[Mueller et al., 2010;](#page-32-7) [Yadav et al., 2010\)](#page-33-4). Unlike the traditional linear regression

128 approach, which regards ε as white noise, the GR method uses spatial covariance to

129 recognize the spatial autocorrelation structure of the regression residuals ε . The

- 130 experimental covariance of residuals ε for DVI, NDVI and RVI, respectively, is:
- 131 $Q(h) = E(\varepsilon(X)\varepsilon(X+h))$ (2)

132 Where h is the spatial and/ or temporal distance, $Q(h)$ is the covariance of 133 residual at separation distance h [\(Erickson et al., 2005\)](#page-30-10). Many theoretical covariance functions (such as nugget, exponential, spherical, and Gaussian functions) can be used to model the experimental covariance [\(Schabenberger and Pierce, 2001\)](#page-32-8). In this study, a linear combination of nugget and exponential functions is used following the previous studies [\(Erickson et al., 2005;](#page-30-10) [Li et al., 2013a;](#page-31-4) [Mueller et al., 2010\)](#page-32-7). This function is defined as:

139
$$
Q(h) = \begin{cases} \sigma_N^2 + \sigma_S^2, h = 0\\ \sigma_S^2 \exp\left(-\frac{h}{l}\right), h > 0 \end{cases}
$$
 (3)

140 σ_N^2 is the measurement error or the variability at small scale that is uncorrelated in 141 space and/or time, σ_S^2 is the variance of the variability correlated in space and/or time, 142 and *l* is the correlation range parameters [\(Leung and Cooley, 2014\)](#page-31-6). The Restricted 143 Maximum Likelihood (RML), which maximizes the marginal distribution of the 144 covariance function parameters, is used to estimate the parameters (σ_N, σ_S, l) (Kitanidis 145 [and Shen, 1996\)](#page-31-7).

- 146 The best linear unbiased estimator of β on the basis of [Aitken \(1935\)](#page-30-11) is the
- 147 generalized-least-squares estimator, that is, the value of β that minimizes (LAI –
- $(148 \t X\beta)^T Q^{-1} (LAI X\beta)$. Thus,

$$
\hat{\beta} = (X^T Q^{-1} X)^{-1} X^T Q^{-1} L A I \tag{4}
$$

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- 150
151 2.2. Reduced major axis method

 To robustly assess the performance of the GR model, we compare the results from GR and RMA models. We choose RMA method because it is regarded as the 'standard' method for estimating LAI reference map in BigFoot project [\(Berterretche et al., 2005;](#page-30-2) [Cohen et al., 2003\)](#page-30-8), which is a well known project linking in situ measurements, remote sensing and models to validate MODIS products including LAI product. The form of RMA is identical to a simple linear regression method:

158 $LAI = \beta_0 + \beta_1 X + \varepsilon$ (5)

159 Where *X* is DIV, NDVI, and RVI, respectively. ε is white noise residual. RMA method is superior to traditional ordinary least squares regression when 161 both dependent (LAI in this study) and independent variables (DVI, NDVI, and RVI in 162 this study) are measured with errors [\(Cohen et al., 2003;](#page-30-8) [Smith, 2009\)](#page-32-9). The estimating of 163 β_0 and β_1 is different with the traditional ordinary least square regression. The traditional ordinary least square regression estimates the regression coefficients by minimizing the sum of squares of the residuals, while RMA minimizes the areas of triangles formed by the deviation of a point from the regression line in both horizontal and vertical directions 167 [\(Smith, 2009\)](#page-32-9). The equations for calculating β_0 and β_1 are $\beta_0 = \overline{LAI} - \frac{\sigma_Y}{\sigma_X} \overline{X}$ and $\beta_1 = \frac{\sigma_Y}{\sigma_X}$.

3. Data

3.1. Study Sites

 Two cropland sites (AGRO and Plan-de-dieu sites) and two grassland sites (Hulun Buir and Zhangbei sites) were used in this study. The AGRO site is from the BigFoot project [\(http://www.fsl.orst.edu/larse/bigfoot/index.html\)](http://www.fsl.orst.edu/larse/bigfoot/index.html), which is funded by NASA'S Terrestrial Ecology Program [\(Morisette et al., 2006;](#page-32-0) [Pisek and Chen, 2007\)](#page-32-4). 175 Nine validation sites are in the BigFoot project with each of them covering a 5 km \times 5 km extent [\(Morisette et al., 2006\)](#page-32-0). The field LAI values in the AGRO site were measured by the allometric destructive method. The Hulun Buir site is one of the validation sites for the GLASS LAI product, which is a newly released LAI product generated by Beijing Normal University, China [\(Liang et al., 2014\)](#page-31-8). The coverage of the Hulun Buir site is 180 about 32 km \times 28 km. The in situ LAI values in the Hulun Buir were measured by LAI-

2000. The Plan-de-dieu and Zhangbei sites are from the VALERI project

[\(http://w3.avignon.inra.fr/valeri/\)](http://w3.avignon.inra.fr/valeri/), which has served to provide high spatial resolution

maps of biophysical variables (e.g., LAI, fAPAR, fCover) to validate products derived

from satellite observations (e.g., VEGETATION, MERIS, POLDER, AVHRR, and

- MODIS) [\(Baret et al., 2005\)](#page-30-5). The VALERI project has 33 sites, each of them covering
- 186 around 3 km \times 3 km. The in situ LAI values in the VALERI project were measured by
- LAI-2000 or hemispherical images.

The AGRO site is located in Bondville, Illinois, USA. The main crop types of the

AGRO site are corn and soybean [\(Pisek and Chen, 2007\)](#page-32-4). The Plan-de-dieu site, with its

main crop being vineyards, is located at Cotes du Rhone Village, France [\(Rossello,](#page-32-10)

[2007\)](#page-32-10). The Hulun Buir and Zhangbei grassland sites are located in Inner Mongolia and

Hebei, China, respectively. The Landsat TM/ETM+ for AGRO and Hulun Buir sites were

employed in this study as high resolution remote sensing images, because they are

commonly used in up-scaling field measurements [\(Berterretche et al., 2005;](#page-30-2) [Cohen et al.,](#page-30-8)

[2003\)](#page-30-8) and could be easily obtained. We chose SPOT-HRV for Plan-de-dieu and

Zhangbei sites because the Landsat TM/ETM+ corresponded to the date of in situ LAI in

these two sites has gaps and does not have good quality, while SPOT-HRV images have

been collected for many sites in VALERI project including Plan-de-dieu and Zhangbei

sites [\(Baret et al., 2005\)](#page-30-5) . The in situ LAI, TM/ETM+, and HRV data on the exact same

date were not available. Therefore the data on the closest dates were chosen. The detailed

information of the four sites is described in Table 1. The locations of the four study sites

and the corresponding distribution of the in situ LAI locations in each site are shown in

Figure 1.

 Figure 1. Study sites of the AGRO, Plan-de-dieu, Hulun Buir, and Zhangbei (the 207 background is the standard false color composited image, and the green points are the in 208 situ LAI locations). situ LAI locations).

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3.2. Data pre-processing

- Landsat TM/ETM+ data with 30 m spatial resolution used in this study were
- downloaded from the USGS website [\(http://glovis.usgs.gov/\)](http://glovis.usgs.gov/). The TM/ETM+ data are
- Level 1T data that have been systematically, radiometrically, and geometrically
- corrected. A large proportion of images are contaminated due to the influence of aerosols,
- clouds, and cloud shadows [\(Liang et al., 2001\)](#page-31-9). The TM/ETM+ data were
- atmospherically corrected by the Landsat Ecosystem Disturbance Adaptive Processing
- System (LEDAPS) [\(Masek et al., 2006\)](#page-32-11). The two study areas, the AGRO and Hulun Buir

241 (Table 1). As the Hulun Buir covered around 896 km^2 , which may include other types of vegetation (e.g., forest), the land cover data used in this study to mask the non-grassland regions was provided by Tsinghua University (Table 1), China [\(Gong et al., 2013;](#page-31-11) [Yu et](#page-33-5) [al., 2013\)](#page-33-5).

Figure 2. The scatter plots of DVI, NDVI, and RVI with the in situ LAI at the AGRO, 247 Plan-de-dieu, Hulun Buir, and Zhangbei sites. Plan-de-dieu, Hulun Buir, and Zhangbei sites.

- 248
249 The total in situ LAI measurements for the AGRO, Plan-de-dieu, Hulun Buir, and Zhangbei sites are 98, 26, 51, and 42, respectively. This study randomly selected around 65% of the LAI points to establish and specify the GR and RMA models. The 35% of the LAI points were used to validate the results. This was repeated another five times for the 253 GR models, in order to cross validate the robustness of performance of the models.
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4. Results and Discussion

4.1. Spatial covariance models

 As stated in 2.1, the residuals for Equation (1) were assumed to be second-order stationary with zero-mean, we calculated the experimental isotropic covariance of the residuals using least square method [\(Li et al., 2013b\)](#page-31-5). The experimental covariances were modeled with exponential functions. The parameters of exponential functions were obtained through RML method. Table 2 shows the parameters of exponential functions for different VIs at four sites, respectively. The experimental and modeled covariances are shown in Figure 3. The parameters of covariance function in the same site have very similar values, which indicate similar spatial structure happens in the same site no matter what the VI is. At different sites the parameters are quit different (Table 2), depending on 268 the locations of in situ LAI measurements and associations between LAI and VIs in that site. In addition to nugget variance for DVI at AGRO (Corn) site, all of the nugget values are larger than zero, which may be due to the heterogeneous of LAI of sub-samples within each sample, since the in situ LAI value for each sample is calculated from sub- samples in that sample [\(Baret et al., 2005;](#page-30-5) [BigFoot, 1999\)](#page-30-13). For example, each in situ LAI sample plot in Zhangbei site covers around 20 m x 20 m. In each sample plot, 12 sub- samples are used to calculate the corresponding LAI value for that sample plot [\(Baret et](#page-30-5) [al., 2005\)](#page-30-5).

Table 2. Parameters of the covariance function

Figure 3. The experimental and modeled covariance (blue circle is experimental covariance, and red line is modeled covariance) covariance, and red line is modeled covariance)

4.2. GR models for the four study sites

 Table 3 shows the GR models for the AGRO, Plan-de-dieu, Hulun Buir, and Zhangbei sites. The values in parentheses are standard deviations for slope and intercept.

The significance of slope and intercept are tested by Student's t test. Besides slopes for

- NDVI and RVI in the AGRO (corn) sites, all slopes are significant at 1% level, indicating
- the reliability of the models. The majority of intercepts are not significant at 1% level,
- excepting the intercepts in Zhangbei site. The insignificance may be due to small
- samples, such as the AGRO (corn) and Plan-de-dieu sites. The negative values of

 intercept may be attributed to the uncertainty of retrieving DIV, NDVI, and RVI from TM/ETM+ and HRV images, as there is no accurate atmosphere information for each sites, thereby the band reflectance from these images has errors. In addition, the in situ LAI values also have measurement errors. Therefore, the negative values of intercept are shown when conducting statistical analysis.

297 The coefficient of determination (R^2) varies among different models in different 298 sites. At the AGRO site, the R^2 value for corn ranges from 0.28 to 0.44, and for soybean 299 0.38 to 0.40. The R^2 value of DVI model is the highest for the AGRO site compared to 300 the R^2 values for NDVI and RVI models. As with the AGRO site, the R^2 value of DVI 301 model in the Plan-de-dieu site is the highest. The R^2 value for the Hulun Buir and 302 Zhangbei grassland sites ranges from 0.53 to 0.61, 0.63 to 0.69, respectively. In contrast 303 to the cropland sites (i.e., the AGRO and Plan-de-dieu sites), the R^2 values of DVI models 304 over the two grassland sites are the lowest. Excepting for Zhangbei site, the R^2 values are 305 not high, which maybe because of the poor relationships between DVI, NDVI, and RVI 306 and original in situ LAI values (Figure 2). However, the GR models with DVI perform 307 best over the two cropland sites, while for the two grassland sites, the GR models with 308 DVI have the poorest performance.

309 **Table 3.** GR models at the four study sites.

310 * significant at 5% level, ** significant at 1% level.

311 *4.3. Estimating and validating the reference LAI maps based on GR models*

312 Figure 4 presents the reference LAI maps estimated by the GR models based on 313 Table 3. The validation results are shown in Figure 5 and Table 4. Most of the \mathbb{R}^2 values 314 in Table 4 are nearly equal to the R^2 values in Table 3, which indicates that the GR 315 models are robust. However, some GR models may not be robust (e.g., GR model with 316 DVI for corn at the AGRO site). We discuss the problem in detail at the end of this

Table 4. Statistics of estimated LAI of the GR and RMA models compared to the in situ

337	LAI.							
	Site	VIs	\mathbf{R}^2		RMSE		bias	
			GR	RMA	GR	RMA	GR	RMA
		DVI.	0.23	0.23	0.88	0.89	0.05	0.10
	AGRO	NDVI	0.18	0.18	0.94	1.10	-0.17	0.01

 (1)

GRM DVI

 (4)

 (m^2/m^2)

 \mathbf{M}

 Figure 4. Reference LAI maps estimated by the GR models at the AGRO, Plan-de-dieu, Hulun Buir, and Zhangbei sites.

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 Figure 5. Validation results of the GR models at the AGRO, Plan-de-dieu, Hulun Buir, and Zhangbei sites.

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350 In order to check the robustness of the predictive ability of the GR models, this study used cross validation. Considering the intensive computation of the GR models that involve spatial covariance modeling and geostatistical estimation, this study was repeated five times by randomly selecting 65% of the LAI points for establishing the GR models, with the remainder of the LAI points used for model validation. The mean RMSE values

(μ _{RMSE}) of the five repetitions were calculated following previous studies Lee et al.

356 [\(2008a,](#page-31-12) [b\)](#page-31-13). Figure 6 shows the results of cross validation. The blue bar is the μ_{RMSE} of the

357 five repetitions for each GR model, the black error bar is $\mu_{RMSE} \pm \sigma_{RMSE}$ (σ_{RMSE} is the standard deviation) of the five repetitions for each GR model, and the brown square is the 359 RMSE value from Table 4. In comparison to the μ_{RMSE} in Figure 6, most of the RMSE 360 values in Table 4 are nearly within $[\mu_{RMSE} - \sigma_{RMSE}, \mu_{RMSE} + \sigma_{RMSE}]$, which indicates that the GR models are robust. The RMSE value of the GR model for DVI at the AGRO 362 (corn) site slightly exceeds the upper limits of the error bar (μ _{RMSE} + σ _{RMSE}), which confirms that the GR model with DVI for corn at the AGRO site is not robust. This is presumably due to the poor association of DVI and the in situ LAI values (Figure 2). The RMSE values of the GR model for DVI and RVI at the Zhangbei site also exceed upper limits of the error bar, which may be due to the limited repetitions. More repetitions are needed for robust validation.

Figure 6. Cross validation for the GR models

4.4. Comparing the results of GR and RMA models

 Figure 7. Reference LAI maps estimated by the RMA models at the AGRO, Plan-dedieu, Hulun Buir, and Zhangbei sites.

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394
395 **Figure 8.** Validation results of the RMA models at the AGRO, Plan-de-dieu, Hulun Buir, and Zhangbei sites.

5. Conclusions

 Spatial scale issue commonly exits in remote sensing studies. [Van der Meer et al.](#page-32-13) [\(2001\)](#page-32-13) explored spatial scale effects on vegetation indices estimation through calculating vegetation indices, including NDVI, perpendicular vegetation index, weighted difference vegetation index, etc., from the Medium Resolution Imaging Spectrometer (MERIS) at the spatial resolutions ranging from 6 to 300 m. The proposed way to validate coarse resolution remote sensing products is using fine reference maps derived from up-scaling in situ measurements. This study up-scaled the field LAI measurements to high resolution LAI reference map through linking the in situ LAI measurements and Landsat TM/ETM+ and SPOT-HRV data using the geostatistical regression method. To analyze the discrepancy of employing different vegetation indices on estimating LAI reference maps, this study established the GR models for DVI, NDVI and RVI. To further assess the 410 performance of the GR model, this study compared the results from GR and RMA models. The results show that the performances of GR models over the cropland and grassland sites are different. The GR models based on DVI provide the best estimation at the cropland sites (AGRO and Plan-de-dieu sites), while the GR models perform poorly based on DVI at the grassland sites (Hulun Buir and Zhangbei sites). By considering the

 spatial/temporal correlations of in situ LAI observations and high resolution DVI, NDVI, and RVI data, this study reveals that the performance of the GR models is better than the RMA models in terms of RMSE and bias.

 In summary, the GR method inherits the merits from both traditional geostatistical methods and regression methods. Compared to regression methods (e.g., RMA), the GR method is improved in accounting for the spatial/temporal correlation of residuals from the regressions of LAI observations and high resolution remote sensing data (e.g., DVI, NDVI and RVI data in this study). In contrast to traditional geostatistcal methods (e.g., Kriging), the GR method attempts to provide better estimating of unknown points by exploring the association between high resolution remote sensing data and field observations. Our study confirmed the performance of the GR models is better than the RMA models in terms of RMSE and bias, which indicates the potential of GR method to 427 up-scale other in situ biophysical and geophysical measurements (e.g., fAPAR and soil moisture) to high resolution reference data to validate other coarse resolution products.

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