The Times They Are A-Changin':
Scaling Seasonality of Plant Physiology from Leaf to Satellite and
Implications for Terrestrial Carbon Cycle

By Xi Yang

B.A. Beijing Normal University, 2006
M.E. Beijing Normal University, 2009
M.S. Brown University, 2012

A Dissertation Submitted in Partial Fulfillment of the Requirements
for the Degree of Doctor of Philosophy
in the Department of Geological Sciences at Brown University

Providence, Rhode Island
May, 2014
© Copyright 2014 by Xi Yang
This dissertation by Xi Yang is accepted in its present form by the Department of Geological Sciences as satisfying the dissertation requirement for the degree of Doctor of Philosophy.

Date________________________  Dr. John F. Mustard, Advisor

Date________________________  Dr. Jim Tang, Advisor

Recommended to the Graduate Council

Date________________________  Dr. Meredith Hastings, Reader

Date________________________  Dr. Jung-Eun Lee, Reader

Date________________________  Dr. Joseph Berry, Reader

Approved by the Graduate Council

Date________________________  Dr. Peter M. Weber, Dean of the Graduate School
Xi Yang

The Ecosystem Center, Marine Biological Laboratory
7 MBL Street, Woods Hole, MA, 02543
Office: 508-289-7732, Cell: 517-515-2110
xyang@mbl.edu
http://xi-yang.net

I. Education

2012- PhD Candidate Ecology Brown University-Marine Biological Laboratory
2009-2012 Master of Science Ecology Brown University-Marine Biological Laboratory
2006-2009 Master of Engineering Geoscience Beijing Normal University
2002-2006 Bachelor of Science Geography Beijing Normal University

II. Awards

2. Best Student Paper Award, Phenology 2012 Conference. 2012.

III. Publications


In review & In preparation


Updated February 20th, 2014

**IV. Conferences and seminars**

*Invited Oral Presentations*

1. **Yang, X.** (2014), The times they are a-changin’: what can we learn about the seasonality of plant functioning using remote sensing?. Harvard University Herbaria.

*Oral Presentations*

4. **Yang, X.** (2013) The times they are a-changin’: monitoring and modeling of vegetation phenology under changing climate. The Ecosystem Center Seminar, Marine Biological Laboratory, Woods Hole, MA.

*Poster Presentations*

V. Teaching

- Teaching Assistant, Brown University, GE132 Introduction to Geographic Information Systems 2010
- Graduate Mentor, Harvard Forest, Harvard Forest REU Program 2012
- Mentor, Woods Hole Partnership Education Program (PEP) 2011, 2012

VI. Posthoc Reviewer


VII. Professional Organizations

- American Geophysical Union
- Sino-Eco (Sino-Ecologists Association Overseas)
- Ecological Society of America

VIII. References

- Dr. Jianwu Tang, Marine Biological Laboratory, Woods Hole, Massachusetts, USA. (jtang@mbl.edu. +1 508 289 7162)
- Dr. John F. Mustard, Brown University, Providence, Rhode Island, USA. (john_mustard@brown.edu. +1 401 863 1264)
- Dr. Christopher Neill, Marine Biological Laboratory, Woods Hole, Massachusetts, USA. (cneill@mbl.edu. +1 508 289 7481)
ACKNOWLEDGEMENTS

Gratitude is not only the greatest of virtues, but the parent of all others.

-Marcus Tullius Cicero

When I applied to Brown, Jack Mustard emailed me enthusiastically about the study of phenology, and introduced me to the Brown-MBL program. Jack kept discussing science with me almost every week, even after I moved to MBL. After I started my own project in MBL, whenever I had needs of the support for fieldwork and scientific discussions, my co-advisor Jim Tang at MBL was always available and supportive. Thanks to Jack and Jim for the guidance and support in the last five years’ wonderful journey.

Thanks to my committee members, Annie Schmitt, Meredith Hastings, Tim Herbert, Stephen Porder, Jung-Eun Lee, and Joe Berry for the time to read about my research and the inputs to generate new ideas.

“You need mentors and collaborators, not just your advisors”. I learnt this from the academic training workshop in MBL. Adrian Rocha understands my research and always gave critical and extremely useful comments on my manuscripts. Andrew Richardson and Trevor Keenan and I shared same interests in vegetation phenology, and they are always willing to share their ideas and data. Hong Xu put my interests in phenology in an ecosystem modeling perspective.

Friends and colleagues in the Department of Geological Sciences and Brown-MBL program are always helpful and supportive. They include (but certainly not limited
to): Li Gao, Yun Wang, Chenguang Sun, Lijing Yao, Marc Mayes, Stephanie Spera, Mengdi Cui, Will Daniels, Will Longo, Elizabeth Thomas, Susie Theroux, Janette Wilson, Gillian Galford, Bethany Ehlmann, Mark Salvatore, Rebecca Greenberger, Tim Goudge, Andre Burnier, David Chatlet and Chelsea Nagy.

I spent my last three years in the Ecosystem Center of MBL. I thank Chris Neill, the director of the center and the Brown-MBL program, for making it a wonderful place for students like me. I thank Ed Rastetter for teaching me a new tool – ecosystem modeling; and I thank Zoe Cardon for insightful comments on my works. When I first came to MBL, I knew little about wet chemistry work. Thanks to the help of Matthew Erickson, Rich McHorney, Jessica Drysdale, Sam Kelsey, Marshall Otter, Coralie Barth-Jensen, Jane Tucker, Kate Morkeski, Susanne Thomas, Jim Laundre, Yueyang Jiang, Jerome Girard and Will Werner, I can now claim myself to be the “Guru” of several instruments in the center. I thank students and RAs in the Tang Lab for the help with my fieldwork: Skyler Hackley, Tim Savas, Zhunqiao Liu, and Hualei Yang. I thank REU students in Harvard Forest, MBL and SEA for the help with fieldwork: Katie Laushman, Lakiah Clark, Ellen Tisdale and Shalanda Grier.

Thanks to all the administrative staffs in Brown and MBL, my PhD life got much easier. I thank Nancy Fjeldheim, Pat Davey, Ruth Craine, Pauline Fennelly, and Bonnie Horta at Brown, and Kelly Holzworth, Mary Ann Seifert, Debbie Scanlon, Alison Maksym at MBL.

I thank my friends in the Brown Dragon Soccer Team (but certainly not limited to): Cong Cao, Huaiyong Zhao, Yuzhen Guan, Mingming Jiang, Lu Lu, Dongfang Li,
Zhen Ye, Wenjun Tong, Guang Yang, Hao Tu, Qiang Hao and Sirui Tan. We fought for glory, and we played for fun. And many of them helped me with my fieldwork. I thank friends in Brown for the help to make it easier to get settled in a completely new environment: Chang Liu, Jiachen Zhou, and Xiaoai Zhao.

Many of my friends since college are always there for me, and I appreciate it very much. Qingxu Huang and Yin Yi are always available for scientific discussions and suggestions to find jobs.

I owe a huge debt to my wife, Hong Bao, who offered me love and unconditional support in the past years, and our son Ryan. They are always there to cheer me up whenever I need it. My parents are supportive of my decisions to study abroad (and far away from home); although I know they prefer their son to stay close by. I am grateful for their endless support.

Xi Yang

April 16th, 2014

Woods Hole, MA
# Table of Contents

**Curriculum Vitae** .......................................................................................................................... iv  

**Acknowledgement** ............................................................................................................................ vii  

**List of Tables** ................................................................................................................................. xii  

**List of Figures** .................................................................................................................................. xiii  

**Chapter 1** ......................................................................................................................................... 15  
  *Modeling phenological responses to climate change* ............................................................... 16  
  *Leaf color is just part of the story: leaf traits matter* .............................................................. 18  
  *Seasonality of plant photosynthesis: from canopy to satellite* ............................................. 20  
  *Concluding remarks* .................................................................................................................... 22  

**Chapter 2** ......................................................................................................................................... 29  
  *Abstract* ........................................................................................................................................ 30  
  *Introduction* .................................................................................................................................. 31  
  *Methods and materials* .................................................................................................................. 33  
    *PhenoCam and related climate data* ....................................................................................... 33  
    *Bayesian Change Point Detection* ......................................................................................... 34  
    *Ground-based manual observations in Harvard Forest* ....................................................... 38  
    *Spring Warming model* ............................................................................................................ 38  
  *Results and discussion* ................................................................................................................ 39  

**Chapter 3** ......................................................................................................................................... 57  
  *Abstract* ........................................................................................................................................ 58  
  *Introduction* .................................................................................................................................. 59  
  *Materials and methods* ................................................................................................................ 61  
    *Site description* ......................................................................................................................... 61  
    *Digital camera observations of plant phenology* .................................................................. 62  
    *Leaf spectral, biophysical, and biochemical properties* ....................................................... 63  
    *Satellite data* ............................................................................................................................. 65  
    *Statistical method* ..................................................................................................................... 66  
  *Results* ......................................................................................................................................... 66
<table>
<thead>
<tr>
<th>Chapter 4</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abstract</td>
<td>93</td>
</tr>
<tr>
<td>Introduction</td>
<td>94</td>
</tr>
<tr>
<td>Study area and methods</td>
<td>98</td>
</tr>
<tr>
<td>Study area</td>
<td>98</td>
</tr>
<tr>
<td>Measurements of leaf optical properties and traits</td>
<td>98</td>
</tr>
<tr>
<td>Methods to estimate leaf traits using leaf optical properties</td>
<td>100</td>
</tr>
<tr>
<td>Results</td>
<td>102</td>
</tr>
<tr>
<td>Temporal and spatial variability of leaf traits</td>
<td>102</td>
</tr>
<tr>
<td>Seasonal variability of leaf spectral properties</td>
<td>103</td>
</tr>
<tr>
<td>Comparisons of methods to estimate leaf traits</td>
<td>104</td>
</tr>
<tr>
<td>Implications for field sampling design</td>
<td>106</td>
</tr>
<tr>
<td>Discussion</td>
<td>107</td>
</tr>
<tr>
<td>Conclusion</td>
<td>110</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Chapter 5</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abstract</td>
<td>134</td>
</tr>
<tr>
<td>Introduction</td>
<td>135</td>
</tr>
<tr>
<td>Methods</td>
<td>136</td>
</tr>
<tr>
<td>Harvard forest environmental and CO₂ exchange measurements</td>
<td>137</td>
</tr>
<tr>
<td>Ground-based measurements of solar-induced fluorescence</td>
<td>138</td>
</tr>
<tr>
<td>Satellite measurements of solar-induced fluorescence</td>
<td>139</td>
</tr>
<tr>
<td>Results</td>
<td>140</td>
</tr>
<tr>
<td>Discussion and conclusion</td>
<td>141</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Chapter 6</th>
<th>Page</th>
</tr>
</thead>
</table>

---

Seasonal trajectories of canopy-level indices ..............................................66
Seasonal trajectories of leaf biochemical and biophysical properties ..........68
Seasonal trajectory of vegetation spectra ..................................................69
Comparisons between canopy color and leaf biochemical, biophysical and spectral properties .................................................................70
Discussion ........................................................................................................71

---

**CHAPTER 4** ............................................................................................................................93

**Abstract** ........................................................................................................................94
**Introduction** ..................................................................................................................96
**Study area and methods** ..............................................................................................98
  **Study area** ...............................................................................................................98
  **Measurements of leaf optical properties and traits** ............................................98
  **Methods to estimate leaf traits using leaf optical properties** .........................100
**Results** ......................................................................................................................102
  **Temporal and spatial variability of leaf traits** .................................................102
  **Seasonal variability of leaf spectral properties** .............................................103
  **Comparisons of methods to estimate leaf traits** .............................................104
  **Implications for field sampling design** ............................................................106
**Discussion** .............................................................................................................107
**Conclusion** ..............................................................................................................110

**CHAPTER 5** .......................................................................................................................134

**Abstract** ......................................................................................................................135
**Introduction** .............................................................................................................136
**Methods** .....................................................................................................................137
  **Harvard forest environmental and CO₂ exchange measurements** .......................137
  **Ground-based measurements of solar-induced fluorescence** ...........................138
  **Satellite measurements of solar-induced fluorescence** ....................................139
**Results** .....................................................................................................................140
**Discussion and conclusion** ......................................................................................141

**CHAPTER 6** .......................................................................................................................158
LIST OF TABLES

Chapter 2

Table 1 PhenoCam sites used in this study .............................................................50
Table 2 Extracted dates of budburst using Bayesian Change Point analysis .......51

Chapter 3

Table 1 Vegetation indices calculated in this study ..............................................84
Table 2 Partial correlation coefficients between g_{cc}/T_{cc} and individual bands at the canopy scale ...........................................................................................................85
Table 3 Partial correlation coefficients between g_{cc}/T_{cc} and individual bands at the leaf scale ................................................................................................................86

Chapter 4

Table 1 Simple vegetation indices used in this study ..........................................119
Table 2 Comparisons of goodness-of-fit among four methods using data from Martha’s Vineyard (MV) .................................................................................................120
Table 3 Comparisons of goodness-of-fit among four methods using data from Harvard Forest (HF) ........................................................................................................121
Fig.S1 Coefficient of determination (R^2) between the mean values of observed leaf traits and predicted leaf traits at both MV and HF .........................................................122
LIST OF FIGURES

Chapter 1

Fig. 1 GPP of Harvard Forest .................................................................28

Chapter 2

Fig. 1 Examples of PhenoCam images ....................................................52
Fig. 2 Examples of Bayesian Change Point method ...............................53
Fig. 3 Comparisons between ground and camera observations ..........54
Fig. 4 Spring warming model results .......................................................55
Fig. 5 Prediction of budburst dates in the future ....................................56

Chapter 3

Fig. 1 Examples of images taken by digital repeat photography ..........87
Fig. 2 Comparisons between camera and leaf traits ............................88
Fig. 3 Comparisons between camera and satellite observations ..........89
Fig. 4 Examples of leaf spectra ..............................................................90
Fig. 5 Comparisons between anthocyanin index and canopy redness ....91
Fig. S1 Comparisons between anthocyanin indices and canopy redness ..92

Chapter 4

Fig. 1 Seasonal patterns of pigments ....................................................123
Fig. 2 Seasonal patterns of pigment ratios ............................................124
Fig. 3 Seasonal patterns of N_{mass}, C_{mass} and LMA .........................125
Fig. 4 Examples of leaf reflectance and transmittance .......................126
Fig. 5 Seasonal patterns of leaf reflectance at individual bands ..........127
Fig. 6 Comparisons between observation and prediction of Martha’s Vineyard datasets .................................................................128
Fig. 7 Comparisons between observation and prediction of Harvard Forest datasets .................................................................129
Fig. 8 Weighting of Bayesian Model Averaging results ......................130
Fig. 9 Changes of RMSE and R^2 under different scenarios of Martha’s Vineyard datasets .................................................................131
Fig. S1 Comparisons of pigment concentrations between sunlit and shaded leaves ........................................................................132
Fig. S2 Changes of RMSE and $R^2$ under different scenarios of Harvard Forest datasets ................................................................. 133

Chapter 5

Fig. 1 Examples of FluoSpec ................................................................. 148
Fig. 2 Seasonal patterns of SIF ................................................................. 150
Fig. 3 Comparisons between SIF and GPP, SIF and APAR ...................... 151
Fig. 4 Diurnal patterns of SIF and GPP .................................................... 152
Fig. 5 Comparisons between ground and satellite SIF .......................... 153
Fig. S1 Seasonal patterns of SIF comparing with environmental factors ....... 154
Fig. S2 Relationships between SIF and PAR, VPD and Air T .................. 155
Fig. S3 Relationship between daily EVI and (a) NDVI, and (b) EVI .......... 156
Fig. S4 Relationship between daily APAR and PAR ............................... 157
CHAPTER 1

Introduction

Xi Yang$^{1,2}$

$^1$Department of Geological Sciences, Brown University, Providence, RI, USA, 02912

$^2$The Ecosystems Center, Marine Biological Laboratory, Woods Hole, MA, USA, 02543
Phenology is the periodic events in the life cycle of plants, for example, leaf-out and senescence (Cleland et al., 2007). This definition can be extended to the related vegetation physiological changes throughout the season, for example, photosynthesis (Richardson et al., 2013). One of the ubiquitous impacts of climate change on the terrestrial ecosystem is the shifting plant phenology, most notably in the spring (Walther et al., 2002). Extensive research based on ground-based observations and satellite data documented the changes of phenology. It has been found that most notably leaf-out dates have been generally advancing in recent decades (Fitter & Fitter, 2002, Myneni et al., 1997). This change in return could potentially exert feedbacks to the climate system through affecting the length and magnitude of photosynthesis and net CO₂ exchanges, surface energy balance, and the emission of biogenic volatile organic compounds (Churkina et al., 2005, Peñuelas et al., 2009). As an important component in the climate change study, vegetation phenology was surprisingly poorly modeled in the terrestrial biosphere models (Richardson et al., 2012). Observations of vegetation seasonality (i.e., changes of leaf colors and physiology) at the appropriate scales are thus important to help us to assess the impact of climate change.

The following four chapters are a journey for myself to gain deeper understandings of the impacts of climate change on the seasonality of ecosystem functioning. I focused on using leaf optical properties to study the seasonality of plant physiology, and how it is controlled by environmental factors.

*Modeling phenological responses to climate change*
The response of vegetation phenology to the climate change largely depends on what types of environmental cues it responds to. For temperate deciduous forests, temperature is considered to be the dominant control over spring budburst, while although still in debate, the importance of photoperiod has been recognized in recent years (Blümel & Chmielewski, 2012, Chuine et al., 2010, Körner & Basler, 2010, Laube et al., 2014). For some species, during the dormancy, the air temperature needs to be cold enough for a certain period of time to fulfill the chilling requirement, as a strategy to prevent precocious budburst susceptible to frost during the early spring (Polgar & Primack, 2011). Based on the above theories, phenology models have been developed for individual species (Chuine, 2000, Chuine et al., 1999).

One of the main issues to study the impact of climate change on vegetation phenology is the lack of phenology observations at the appropriate spatial scale. In addition, traditional way of phenological observations (i.e., observers routinely check the status of a few plants every several days) is time-consuming and only covers limited areas. The development of remote sensing technique and recent popularity of digital repeat photography provided means to monitor vegetation activities at larger scales (Xu et al., 2013, Yang et al., 2012, Zhou et al., 2001). Digital repeat photography uses digital cameras to automatically take pictures of the plant canopies, and can provide observations at higher temporal resolutions – daily or even hourly (Ahrends et al., 2008, Richardson et al., 2009, Yang et al., 2014). A network of the digital cameras (e.g., PhenoCam) thus provides a unique dataset to examine what environmental cues are driving the timing of budburst, and how it will change as the environmental cues change (or not change) in the future.
To understand the phenological responses to climate change, I started with using digital repeat photography to monitor the change of phenology; and to understand how environmental cues drive the shift of phenology (Chapter 2). I developed a statistical method – Bayesian Change Point detection – to extract the timing of key phenological stages from the time-series of canopy greenness from digital repeat photography data. Using the extracted timing of budburst from PhenoCam network data in New England area, I built a regional phenology model for budburst. And I predicted the change of vegetation phenology in New England in the future under different emission scenarios.

*Leaf color is just part of the story: leaf traits matter*

Leaf color change is the most obvious indicator of seasonality in a deciduous forest. Beyond those lights visible to human eyes, the changes in the infrared regions are also quite significant (Asner, 1998). The driving factors of these changes are leaf traits that are central to facilitate plant functioning including photosynthesis. Chlorophyll is the major machinery to photosynthesize; carotenoids protect plants from excessive sunlight. Both pigments constitute the dominant signal in the visible (400-700 nm) as seen from optical sensors onboard airplane or satellite (Asner & Martin, 2008). Nitrogen content is the key element in both chlorophyll and photosynthetic enzyme Rubisco, while carbon is the indispensible element in building the cell walls (for example, cellulose and hemicellulose). The allocation of these elements in the leaves – as indicated by so-called leaf economic spectrum – can be important to understand terrestrial biogeochemical cycles (Wright et al., 2004).
Vegetation spectroscopy, which exploits the reflected leaf spectra from visible to infrared, provides a way to non-destructively measure those leaf traits. A plethora of studies used ground-based measurements of leaf spectra to estimate leaf pigments and nitrogen concentrations (e.g., Dillen et al., 2012, Ustin et al., 2009). Spectroradiometers onboard satellite or aircraft enable inferences of leaf traits at large scales (e.g., Asner & Martin, 2009, Ollinger & Smith, 2005). However, most of these studies focused on the mid-season instead of the full growing season. I argue that the dataset that provides a combination of leaf traits at high temporal resolution (~weekly) was rare, limiting the assessment of the ability to use vegetation spectroscopy to capture the seasonality of leaf traits.

One may argue that the photosynthesis during the spring or the fall seasons is not as important as those in the summer, as in temperate deciduous forests the maximum photosynthesis occurs in the mid season. To address this issue, I did some calculation using the estimated Gross Primary Production (GPP) from the net CO₂ exchange in Harvard Forest (EMS tower) to test this hypothesis (Fig.1). To define spring, I used the ground observations of leaf phenology in Harvard Forest (Munger and Wofsy, 1999)¹. If the spring is defined as the time between the start of leaf budburst to 95% of the leaves reaching their maximum size, GPP during this period accounted for 25.3% of annual GPP. If the spring is defined as the time between the start of leaf budburst to 100% leaf budburst (earlier than reaching the full size), GPP during this period still accounted for about 10.3% of annual GPP. In the fall, GPP between leaves started to senescence (changing color) to 100% coloring equaled 16.7% of annual GPP. The total

¹ Data were downloaded from Harvard Forest data archive: http://harvardforest.fas.harvard.edu/ (visited Apr. 15th, 2014)
photosynthesis during spring and fall is a substantial component in the annual GPP (25% - 40%). Since the leaf traits mentioned above are highly correlated with the photosynthetic capacity, the changes of leaf traits during the spring and fall need to be captured to understand the annual carbon budget in the forest.

In light of the arguments above, I assessed the ability of digital repeat photography to track the seasonality of leaf traits (Chapter 3). I found that there was a mismatch between canopy greenness measured by digital cameras and key leaf traits such as chlorophyll content. In the fall season, canopy redness was found to be a good indicator of senescence. The results from Chapter 2 left an important question that “how to better use leaf optical properties to capture the seasonality of key leaf traits such as pigment and nitrogen content?” To answer this question, I used leaf spectra collected weekly in the growing seasons of two deciduous forests in New England to test whether the full leaf reflectance spectra tell us more information about the leaf traits than the digital camera that only covers the visible region of light (Chapter 4). I found that statistical methods utilizing the full leaf spectra successfully capture the seasonality of key leaf traits.

*Seasonality of plant photosynthesis: from canopy to satellite*

Leaf traits such as nitrogen content indicate the maximum photosynthetic capacity (Wright *et al.*, 2004), which may not always be achieved under natural conditions due to environmental stress. For example, leaf chlorophyll content may remain stable while photosynthesis showed a decline during the late summer in a deciduous forest (Bauerle *et al.*, 2012). Other methods to estimate photosynthesis have their own caveats. For example,
GPP estimation from eddy covariance method is based on assumptions that may not be true (e.g., extrapolating night-time respiration to daytime) (Reichstein et al., 2005). Terrestrial biosphere models suffered from structural uncertainties (Richardson et al., 2012). Thus an independent and spatially explicit measurement of photosynthesis is necessary.

Chlorophyll fluorescence, as the by-product of photosynthesis, is emitted back to the atmosphere by the leaves (Baker, 2008). Recently, developments of remote sensing techniques made it possible to extract solar-induced fluorescence (SIF) from the satellite imagery, and a strong correlation between SIF and GPP estimation from other methods suggested the possibility to directly estimate photosynthesis from satellite (Frankenberg et al., 2011, Joiner et al., 2011). Ground-based experiments and field measurements also suggested SIF could be used to improve the estimation of GPP (e.g., Damm et al., 2010). However, most of the ground measurements have been limited to a few biome types such as cropland, grassland and shrub (e.g., Meroni et al., 2009, Middleton et al., 2009, Zarco-Tejada et al., 2013). In addition, continuous measurements of the seasonal and diurnal patterns of SIF are still rare, hampering our assessment of using SIF as a proxy for GPP under varying environmental conditions (e.g., cloudy vs. sunny days), different times of growing season, and various vegetation types.

I explored whether SIF can be used as an indicator of in-vivo photosynthesis in a temperate deciduous forest (Chapter 5). I was able to show that daily mean SIF was well correlated with both canopy photosynthesis and absorbed photosynthetically active radiation. I also vicariously validated the SIF measurements from the satellite by showing
that the temporal patterns of ground-based and satellite measurements agreed well from June to November, 2013.

Concluding remarks

This series of chapters presented in the dissertation represent a wide range of topics of different scales. However, these chapters shared the same tool – remote sensing – on addressing a common topic: the seasonality of plant physiology and its environmental drivers. This is the basic framework of my work: using remote sensing (combined with ground-based measurements) as a tool to understand basic processes in terrestrial ecosystems. Scale is a central issue in the study of ecology and climate science (Chave, 2013, Levin, 1992). Remote sensing can provide spatially explicit estimates of properties which are related to key ecological processes, while the mechanistic understandings of how environmental factors control these processes can help to understand how terrestrial ecosystem will respond to climate change.

References


throughout the growing season of a temperate deciduous forest. *Journal of Geophysical Research: Biogeosciences*, 2013JG002460.


Figure 1 Daily Gross Primary Productivity (GPP) estimated from measurements by eddy covariance tower in Harvard Forest, 2006. The green boxes indicate the spring period defined in the text. The red box indicates the fall period. Spring and fall are defined based on the ground-based phenology observations in Harvard Forest.
CHAPTER 2

Regional phenology modeling and prediction using digital repeat photography

Xi Yang\textsuperscript{1,2}, Jim Tang\textsuperscript{2,1}, John F. Mustard\textsuperscript{1}, Miao Tai\textsuperscript{3}, Xiaoxing Cheng\textsuperscript{3}, Trevor F. Keenan\textsuperscript{4}, Andrew D. Richardson\textsuperscript{5}

\textsuperscript{1}Department of Geological Sciences, Brown University, Providence, RI, USA, 02912

\textsuperscript{2}The Ecosystems Center, Marine Biological Laboratory, Woods Hole, MA, USA, 02543

\textsuperscript{3}Center for Statistical Sciences, Brown University, Providence, RI, USA, 02912

\textsuperscript{4}Department of Biological Sciences, Macquarie University, Sydney, Australia, 2109

\textsuperscript{5}Department of Organismic and Evolutionary Biology, Harvard University, 22 Divinity Avenue, Cambridge, MA, USA

To be submitted to \textit{Global Change Biology}
Abstract

Vegetation phenology is changing with the climate, and can potentially exert feedbacks to the carbon, water cycle and other ecosystem services. The impact of changing phenology extends from the scale of individual tree to landscape. Comparing with the extensive species-level phenology models, those applicable to the regional scale have been less available. Digital repeat photography from PhenoCam network provides unique records of canopy greenness throughout the year, and thus the timing of phenological events such as leaf-out can potentially be identified. In this study we used Bayesian Change Point (BCP) analysis to extract the timing of leaf-out from digital repeat photography archives of four temperate deciduous forests sites in New England. We found good agreement between the ground observation in Harvard Forest and the Phenocam data. The change points (CPs) identified from the camera-based canopy greenness time-series were able to capture the start of budburst (~50% buds broke). Using CPs from all four sites, we parameterized a regional phenology model for spring budburst. The spring warming models were able to capture both the spatial and temporal variability of vegetation phenology (with a root mean square of error of ~4.52 days). We used the parameterized models to predict the change of start of season under different future emission scenarios. This work demonstrated the use of digital repeat photography for understanding the impact of climate change on vegetation phenology.

Keywords: spring warming model, temperature, photoperiod, Bayesian methods.
Introduction

Vegetation phenology is one of the most ubiquitous indicators of climate change (Parmesan, 2006, Walther et al., 2002). The advancement of spring (and in some cases, the lengthening of growing season length) has been documented using various observation methods including ground-based observations and remote sensing (Barichivich et al., 2012, Jeong et al., 2011, Menzel et al., 2006). Growing season length is one of the key factors controlling both the temporal and spatial patterns of ecosystem carbon uptake (Baldocchi, 2008, Chapin et al., 2008, Churkina et al., 2005). In addition, changing phenology exerts feedbacks to the climate system by changing the water cycle and surface energy balance (Peñuelas et al., 2009, Richardson et al., 2013). Different phenological responses of different species may also affect the competitive interactions between them (Pau et al., 2011). It is thus necessary to both accurately observe and model vegetation phenology, and improve our understanding of climate-vegetation interactions (Medvigy et al., 2013, Randerson et al., 2009).

There are mainly three major phenological observation methods: ground observation; near-surface remote sensing using digital cameras (hereafter “PhenoCam”); and satellite remote sensing. Ground observations are based on the observations of leaf size and color change of individual trees by routine visits (usually 1~7 days’ interval) to certain species and tagged individuals (O'Keefe, 2000, Richardson et al., 2006); PhenoCam monitors color changes at the ecosystem scale, making it possible to capture the change of canopy greenness at an interval of days (Richardson et al., 2009, Yang et al., 2014); Satellite remote sensing utilizes vegetation indices such as NDVI (Normalized Difference Vegetation Index) at an interval of several days (e.g., 8 days) to quantify
vegetation phenology at the landscape scale (Shen, 2011, Yang et al., 2012, Zhang et al., 2003). Each method has its advantages and disadvantages. For example, ground observations provide the timing of phenological events of individuals, but the spatial and temporal coverage are limited, especially in North America. While remote sensing supports phenology observations at a global scale, each pixel is considered to be at least a mixture of different plant species (Keshava & Mustard, 2002). PhenoCam might be able to bridge the gap between the above two methods (Hufkens et al., 2012, Sonnentag et al., 2012).

Information on the timing of phenological stages gleaned from phenological observations above can be used to inform the development of phenology models. These models are based on the hypothesis that plant phenology responds to environmental cues (e.g., temperature, photoperiod, and precipitation) in a predictable manner. Phenology models can be used to both predict the changes of phenology in the future (Migliavacca et al., 2012) and for historical reconstruction (Vitasse et al., 2011). Phenology models are commonly optimized for specific species (Archetti et al., 2013, Chuine, 2000, Richardson et al., 2006), yet regional scale modeling is limited (but see Caldararu et al., 2012, Stöckli et al., 2011) because of the scarcity of the phenological observations at the appropriate scale. Due to the lack of observations, the representation of phenology in land surface models is notoriously poor (Keenan et al., 2012, Picard et al., 2005, Richardson et al., 2012). Bridging the gap between individual/species-level modeling and ecosystem scale modeling requires assessing the robustness of regional-scale phenology models that utilize the structure of species-level phenology model (Chuine et al., 2000).
Time-series of phenological metrics derived from both satellite and digital camera data have been used to extract key phenological stages (Elmore et al., 2012, Zhang et al., 2003). The common method is to fit data with certain mathematical function (e.g., logistic function), and then the timings of phenological stages are extracted based on certain criteria (e.g., 50% threshold between the seasonal maximum and minimum (Fisher & Mustard, 2007, Yang et al., 2012); maximum of the 2nd derivative of the time-series (Zhang et al., 2003)). Recently, Bayesian change point detection has been applied to various aspects of ecological research (Beckage et al., 2007, Thompson & Katul, 2011), including the analysis of PhenoCam data (Henneken et al., 2013). However, it is still unclear the phenological meaning of these change points, how these change points are related to ground observations, and whether the timing of these change points can be valuable input for phenology models.

Using the data from four temperate deciduous forest sites of the PhenoCam network, we attempted to answer two questions (1) how do species-level phenology model perform at a regional-scale (in New England)? (2) How will spring phenology in New England change in the long term under different emission scenarios?

Methods and materials

PhenoCam and related climate data

PhenoCam is a network of automated digital cameras monitoring the vegetation canopy (Richardson et al., 2009). In this study we used four sites including Harvard Forest (HF), Bartlett Experimental Forest (BA), Cary Institute (CA) and Arbutus Lake in Huntington Forest (AR) (Table 1). Digital cameras were fixed at a location (usually a
tower) where they can take several pictures per day. Daily air temperature data during the period of camera record were obtained from the sites listed in Table 1.

The digital camera images were processed in the following steps: first, images in which tree canopies are indiscernible were excluded. Second, one main region of interest (ROI) was selected from the images of each site (Fig. 1); Third, the Green Chromatic Coordinate (gcc) of each pixel within the ROIs was calculated and the averaged gcc of all pixels within the ROI was calculated for each ROI in each image. The gcc was calculated as (Richardson et al., 2009):

$$gcc = G / (R + G + B) \quad (1)$$

where R, G and B are the raw digital number from the three bands (red, green and blue) of the digital camera image.

The historical and projected temperature records for New England were downloaded from the Downscaled CMIP3 and CMIP5 Climate and Hydrology Projections (Maurer et al., 2007). We used the data for Coupled Model Intercomparison Project Phase 5 (CMIP5) between 1950 and 2099 – the daily maximum and minimum air temperature under three different Representative Concentration Pathways (RCPs): RCP 2.6, RCP 6.0 and RCP 8.5. These data will be used in the calibrated phenology model to assess the historical and projected phenology changes (see section “Spring Warming phenology model”)

Bayesian Change Point Detection of the camera data
We are interested in the date that the linear trend of $g_{cc}$ is changing (i.e., the change point), as it might correspond to the timing of phenological stages. We used Bayesian change point detection to detect the change points on the time-series of $g_{cc}$. The method we used is a modified version of Thomson et al. (2010), focusing only on the change of the slope of the time-series. First, as we are only interested in the spring budburst, we took the $g_{cc}$ values between the day of year (DOY) 80 to DOY 160. Second, as the original $g_{cc}$ takes the value between 0 and 1, which does not satisfy our assumption that the data is normal (which should be between –inf and inf). A common approach is to apply logit-transform to the $g_{cc}$ time-series (i.e., logit($g_{cc}$)), which only changes the value of each $g_{cc}$ data point but not the shape of the time-series. The transformed logit($g_{cc}$) takes the value between -inf and inf. We then calculated the 90th percentile of all the logit($g_{cc}$) values from images within a day. In addition, the standard deviation of the logit($g_{cc}$) was calculated using Monte Carlo method. The time-series of logit($g_{cc}$) was fitted using piecewise linear regression. A hierarchical model was constructed as follows (Thomson et al., 2010):

In the first level, the observed logit($g_{cc}$) was modeled as a logit-normal distribution:

$$logit(g_{cc}) \sim \text{logit-normal}(\mu, \sigma^2_t)$$  \hspace{1cm} (2)

Here, $\mu_t$ is the true value of logit($g_{cc}$), which also takes the value between -inf and inf. $\sigma^2_t$ is the standard deviation of logit($g_{cc}$). We estimated the standard deviation of each day when there was more than one image available. Then we used a local polynomial
regression to estimate the standard deviations of the days with only one image. Then $\sigma_i^2$ is calculated using 1000 Monte Carlo simulations, based on the sampled standard deviation.

$\mu_i$ was modeled as:

$$
\mu_i \sim \text{normal}(f(t), \tau^2)
$$

(3)

$\tau^2$ is the standard deviation of $\mu_i$. $f_i(t)$ is the piecewise linear regression that addresses the changes in the intercept and slope, i.e., $f(t) = \alpha(t) + \beta(t)$. $\alpha(t)$ is the change in intercept, which addresses the discontinuity in the logit(gcc) time-series:

$$
\alpha(t) = \alpha_1 + \sum_{j=1}^{k_\alpha} \chi_j I(t \geq \delta_j)
$$

(4)

$\alpha_1$ is the initial value of logit(gcc), $k_\alpha$ is the number of changes each year. $\delta_j$ is the DOY of the $j^{th}$ change. $\chi_j$ is the value of change. Indicator function $I(t \geq \delta_j)$ equals 1 when the logical calculation in the parenthesis is true, and 0 if otherwise. We used $\beta(t)$ to address the slope change in the logit(gcc) time-series:

$$
\beta(t) = \beta_1 t + \sum_{j=1}^{k_\beta} \beta_{j+1}(t - \theta_j)
$$

(5)

where $\beta_1$ is the initial slope. $k_\beta$ is the number of linear trend change points. $\theta_j$ is the timing of the change points. $(t - \theta_j)_+$ is calculated as $I(t \geq \delta_j)(t - \delta_j)$. Equation (5) and (6) together form the piecewise linear regression to fit the logit(gcc) time-series.
Several model parameters need prior distributions, including $k_a$, $k_b$, $\delta_j$, and $\theta_j$. Prior distributions of the above four parameters were set based on the preliminary visual examination of the logit($g_{cc}$) time-series. Visual analysis suggested that the abrupt intercept change (discontinuity in the time-series) was rare, and thus $k_a=1$. The change in slope was what we expected to capture, and the maximum number of change points was set to $k_b=2$. The reason is that we are only interested in the rapid increase of greenness in the early spring, which we assumed that it was related to the budbreak. The prior distributions of the number of two types of change points were set as binomial ($k_a \sim \text{Binomial}(1, 0.01)$ and $k_b \sim \text{Binomial}(2, 0.5)$). The prior distribution for $k_a$ reflects our expectation that the possibility of step change is very small (the probability of change is 0.01 comparing to 0.99 of the no-change). While the prior distribution for $k_b$ is non-informative (as the probability of that there is a change point is 0.5). We also set the prior distributions of the magnitude of the intercept ($\chi_j$) and slope ($\beta_j$) changes as 

$$[(\text{logit}(g_{cc})_{\text{max}} - \text{logit}(g_{cc})_{\text{min}})/(1.96\times10000)] \quad \text{and} \quad [(\text{logit}(g_{cc})_{\text{max}} - \text{logit}(g_{cc})_{\text{min}})/(1.96)],$$


where $\text{logit}(g_{cc})_{\text{max}}$ and $\text{logit}(g_{cc})_{\text{min}}$ are the seasonal maximum and minimum value. In this way, the intercept changes greater than 1/10000 of the magnitude of the logit($g_{cc}$) are unlikely. For slope change, we set that the change larger than the magnitude of the logit($g_{cc}$) is unlikely. Reversible jump Markov Chain Monte Carlo sampling (MCMC) was used to assess the posterior probabilities of all possible piecewise linear regression models (Lunn et al., 2009). This hierarchical model allows the calculation of the posterior probability of the number of change points, the posterior probability of a certain day is a change point, the locations of the change points given the most likely number of change points, and the uncertainty of the locations of the change points.
Ground-based manual observations in Harvard Forest

Phenological observation records in Harvard Forest were used to interpret the results from the change point analysis. Since 1991, spring leaf development were recorded by routine visits (3–7 days) to the tagged trees (O'Keefe, 2000). In this study, we used the records of dominant species Quercus rubra (Red oak, 5 individuals) and Acer rubrum (Red maple, 4 individuals) during 2008–2011. The phenological metric for spring are BBRK, which is the percentage of budbreak leaves on each individual tagged tree (range: 0-1).

Spring Warming model

The phenology models used in this study assume that temperature and photoperiod are two main control factors. We used a modified version of the Spring Warming model (SW model) that photoperiod is implicitly included, as the starting date of heat accumulation is a parameter (Fisher et al., 2007, Yang et al., 2012). SW model is:

\[ S_f = \sum_{t_0}^{t_b} R_f(x_t) \text{ where } R_f = \max(0, x_t - T_{\text{heat}}) \text{ when } S_f \geq F^* \text{ budburst occurs} \]

where \( S_f \) is the accumulated heat forcing units (unit: °C); \( R_f \) is the rate of heat forcing (unit: °C/day); \( x_t \) is the temperature at time \( t \); \( T_{\text{heat}} \), base temperature (unit: °C) required by heat accumulation process; \( t_0 \) is the starting date (day of year, unit: day) of accumulation; \( t_b \) is the date of budburst (day of year, unit: day); \( t_h \) is the date when the heating accumulation is completed (day of year, unit: day). \( F^* \) is the critical threshold of heating process (budburst) (unit: °C). The Spring Warming model only needs three parameters: \( T_{\text{heat}}, t_0, F^* \). By including \( t_0 \) – the start date of heat accumulation – SW model
implicitly has a requirement on photoperiod that temperature can only have effect when the day is long enough.

The change points and the air temperature data were used to parameterize the spring warming model. We used simulated annealing to find the optimum value for the parameters (Xiang et al., 2013). After parameterization using the whole set of data, we used bootstrap method to assess the robustness of the models as following (Archetti et al., 2013): for a total of n site-year data, each time we took out one site-year and use the remaining n-1 site-year to parameterize the model, and then use the model to predict the absent site-year. By doing this repeatedly for all n sites, we assessed the accuracy of the model by calculating the averaged root mean square error (RMSE) between the observed and simulated data from all n runs. In addition, we calculated the Model Efficiency (ME), which compares the model with a null model (only calculating the interannual and intersite variation, or the spatial-temporal variation) (Nash & Sutcliffe, 1970). ME is between 0 and 1, and the higher the value is, the more effective the model is to capture the spatial-temporal variability of phenology.

**Results and discussion**

Bayesian Change Point detection successfully picked up the critical change points on the logit(gcc) time-series (Fig.2). There were mainly two change points in the spring: logit(gcc) showed a rapid increase around DOY 100–120 after a quite stable period in the winter; in the late spring logit(gcc) reached a peak and then started to decrease. Both change points were clearly identified as the time when the posterior probability (PP) of that day being a change point reached the peak (Fig.2 lower panel). Most days other than the identified change points had a PP of close to zero. We tuned the model parameters
(especially the maximum number of change points, $k_b$) to identify the most significant changes along the logit($g_{cc}$) time-series. However, it is possible to change the parameters if subtle changes in the logit($g_{cc}$) time-series are of interests.

We compared the change points estimated from logit($g_{cc}$) time-series with the ground-based observations of budbreak (BBRK) in Harvard Forest. BBRK showed the ‘logistic’ type increase during spring: it started flat and followed by a rapid increase (starting around DOY 115-125, Fig. 3), and then reached a plateau (Richardson et al., 2006). During the rapid increase stage, there were obvious discrepancies between each individual, as indicated by the wide range of standard deviation. The first change point in Harvard Forest from 2008 to 2011 occurred in a time window that on average 50%–80% of the bud broke. We used the first change point as the indicator of the start of the season. This comparison between the identified change point and the ground-based phenology observations suggested that major changes of canopy color occurred when half or more of the bud turns green, so that the dominating signal received by the camera came from leaves instead of soil or branches.

Spring warming model was able to capture ~70% of the variance in the observed budburst dates in the four sites in New England area (Fig. 4). The bootstrap (i.e., leave-one-out) validation with a mean RMSE of 4.52 days suggested that spring warming model can be a robust method to capture the variability of budburst, which extends from ~DOY 100 in the southern site (CA) to ~DOY 130 the northern site (AR). The base temperature was about 5°C, the date to start the heat accumulation was DOY 86 (March 26th, or 25th on a leap year), and the critical amount of heat accumulation was about ~100. These parameters were similar to those in the spring warming model parameterized in a
past study using remote sensing and climate data in New England area (Yang et al., 2012), further supporting the use of spring warming model to predict the budburst dates in this area. We acknowledged there were uncertainties in the modeling process: (1) the uncertainty in the structure of the model (Migliavacca et al., 2012). Spring warming model in this study did not include any parameters on the chilling requirement of the budburst. It has been suggested that the number of days below a certain temperature threshold needs to reach a critical amount during the winter (i.e., satisfying the chilling requirement), otherwise more heat accumulation is needed to trigger budburst. However, several past studies suggested that the chilling requirement in New England area was always fulfilled (Zhang et al., 2007), and adding parameters for chilling requirement in the phenology model did not improve the model performance (Yang et al., 2012). (2) Uncertainty in the extracted budburst date. The uncertainties in the budburst date extracted from the logit(\(g_{cc}\)) time-series may propagate into uncertainties in the modeling results. Our results suggested that the uncertainties in this category were small: most of the 95% intervals were within 1 day (Table 2). However, the next step is to examine how this uncertainty can be propagated to affect the final model results.

We used the downscaled historical and projected temperature data under different emission scenarios as inputs to the parameterized spring warming model to reconstruct the budburst date since 1950, and predict how budburst dates will change in the future (Fig. 5). Budburst dates from 1950 to 2010 advanced 6.64 days (0.1106 days/year) in New England, which is consistent with previous finding using remote sensing and phenology models (Richardson et al., 2006, Yang et al., 2012). As expected, phenology advanced most under RCP 8.5 (0.2528 days/year), and thus by 2100 the overall
advancement will be 22.75 days. Under RCP 6.0 and RCP 2.6 the budburst date advanced 0.1648 days/year (14.83 days from 2010 to 2100) and 0.0958 days/year (8.622 days from 2010 to 2100), respectively. Under RCP 2.6 the advance rate was even smaller than that from the historical assessment. One important note is that in the future, as the winter is predicted to get warmer, the chilling requirements under current climate conditions for many plants might not be fulfilled in New England area, which can lead to large uncertainties in model prediction if phenology models with chilling requirements were used. If the chilling requirement is not fulfilled, it can lead to the unrealistic model prediction that budburst will not occur (Migliavacca et al., 2012). Mechanistic understandings of the genetic controls of the budburst could help to improve the model structure (Wilczek et al., 2009).

Phenological models are important tools for the understanding how sensitive plants are to climate change and predicting how plants will respond to future climate change. In the past several decades, phenological modeling has been focusing on the species-level (e.g., Chuine, 2000, Kramer, 1994, Schwartz et al., 2006, Vitasse et al., 2011) or the genetic perspective (Chew et al., 2012, Wilczek et al., 2009). From the global change perspective, regional-scale phenological models could potentially be used to understand how plant phenology exerts feedbacks to the changing climate by modifying carbon and water cycle (Picard et al., 2005, Richardson et al., 2013, Yang et al., 2012). Our work demonstrated that regional-scale phenology models at least for the Northeastern US are robust, and can capture the spatial-temporal variability of vegetation phenology. Our work is based on species-specific phenology models designed for temperate forests. Indeed, under different climate conditions and for different vegetation
types, the environmental factors that control vegetation phenology can be different, calling for specific phenology models for certain biome. For instance, in tropical forest, the phenology of plants is mainly controlled by radiation and precipitation (Kim et al., 2012); for a Mediterranean-type biome, temperature is the major driver, but precipitation plays a role (Gordo & Sanz, 2010). Similar framework of analysis can be applied to the datasets of PhenoCam from other geographic locations, and other webcam datasets such as those from public camera (Graham et al., 2010), the ongoing projects from NEON (Keller et al., 2008), and ICOS (Integrated Carbon Observation System, http://www.icos-infrastructure.eu/proj_doc).

Acknowledgements

We would like to thank Cary Institute of Ecosystem Studies and Huntington Forest for providing climate data, and we thank the PhenoCam collaborators at these sites for their help with installation and maintenance of the cameras used in this study. Research at the Bartlett Experimental Forest tower is supported by the National Science Foundation’s LTER program (grant DEB-1114804), and the USDA Forest Service’s Northern Research Station. Research at Harvard Forest is partially supported by the National Science Foundation’s LTER program (grant DEB-0080592). We also would like to thank Dr. Jim Thomson for the help with Bayesian change point detection method. A.D.R. acknowledges support from the National Science Foundation, through the Macrosystems Biology program, award EF-1065029; the Northeastern States Research Cooperative; and the US Geological Survey Status and Trends Program, the US National Park Service Inventory and Monitoring Program, and the USA National Phenology Network through grant number G10AP00129 from the United States Geological Survey.
References


Table 1  Phenocam sites used in this study. Note that the data from Bartlett during year 2010 were excluded since the time-series is incomplete.

<table>
<thead>
<tr>
<th>Site name</th>
<th>Coordinate (Lon, Lat)</th>
<th>Elevation (m)</th>
<th>Years</th>
<th>Vegetation types*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Arbutus Lake (AR), Huntington Forest</td>
<td>-74.23, 43.98</td>
<td>535</td>
<td>2009-2013</td>
<td>Mixed deciduous and conifer</td>
</tr>
<tr>
<td>Bartlett Forest (BA)</td>
<td>-71.29, 44.06</td>
<td>268</td>
<td>2006-2012</td>
<td>Mixed deciduous and conifer</td>
</tr>
<tr>
<td>Cary institute (CA)</td>
<td>-73.73, 41.78</td>
<td>127</td>
<td>2009-2013</td>
<td>Deciduous</td>
</tr>
<tr>
<td>Harvard Forest EMS tower (HF)</td>
<td>-72.17, 42.54</td>
<td>340</td>
<td>2008-2013</td>
<td>Mixed deciduous and conifer</td>
</tr>
</tbody>
</table>

* The vegetation types are limited to those in the field of view of the camera
Table 2  Extracted budburst dates from logit($g_{sc}$) time-series and the width of 95% confidence intervals. See Table 1 for the full names of the acronyms.

<table>
<thead>
<tr>
<th>Site ID</th>
<th>Year</th>
<th>Budburst Date (StdDev)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AR</td>
<td>2009</td>
<td>135 (0.796)</td>
</tr>
<tr>
<td></td>
<td>2010</td>
<td>120 (0.605)</td>
</tr>
<tr>
<td></td>
<td>2012</td>
<td>131 (0.318)</td>
</tr>
<tr>
<td></td>
<td>2013</td>
<td>124 (1.786)</td>
</tr>
<tr>
<td></td>
<td>2006</td>
<td>124 (2.533)</td>
</tr>
<tr>
<td></td>
<td>2007</td>
<td>126 (1.391)</td>
</tr>
<tr>
<td></td>
<td>2008</td>
<td>124 (0.640)</td>
</tr>
<tr>
<td>BA</td>
<td>2009</td>
<td>116 (0.728)</td>
</tr>
<tr>
<td></td>
<td>2010</td>
<td>119 (1.904)</td>
</tr>
<tr>
<td></td>
<td>2011</td>
<td>125 (0.966)</td>
</tr>
<tr>
<td></td>
<td>2012</td>
<td>123 (1.325)</td>
</tr>
<tr>
<td></td>
<td>2009</td>
<td>113 (1.121)</td>
</tr>
<tr>
<td></td>
<td>2010</td>
<td>95 (0.961)</td>
</tr>
<tr>
<td>CA</td>
<td>2011</td>
<td>116 (0.578)</td>
</tr>
<tr>
<td></td>
<td>2012</td>
<td>105 (0.834)</td>
</tr>
<tr>
<td></td>
<td>2013</td>
<td>117 (2.276)</td>
</tr>
<tr>
<td></td>
<td>2008</td>
<td>124 (0.582)</td>
</tr>
<tr>
<td></td>
<td>2009</td>
<td>122 (0.582)</td>
</tr>
<tr>
<td>HF</td>
<td>2010</td>
<td>119 (0.578)</td>
</tr>
<tr>
<td></td>
<td>2011</td>
<td>127 (0.719)</td>
</tr>
<tr>
<td></td>
<td>2012</td>
<td>124 (0.614)</td>
</tr>
<tr>
<td></td>
<td>2013</td>
<td>124 (0.751)</td>
</tr>
</tbody>
</table>
**Figure 1** Example pictures of the PhenoCam images from four sites (HF: Oct. 2\(^{nd}\), 2010; AR: Jun. 4\(^{th}\), 2009; BA: Sep. 22\(^{nd}\), 2010; CA: May 20\(^{th}\), 2010). The red boxes indicate the selected region of interest (ROI).
Figure 2  Examples of Bayesian change point (BCP) detection at four sites. The green dots indicate the logit($g_{cc}$) value in the spring (DOY 100 – DOY 160). The solid red lines are the piecewise linear regression model fits from BCP, with standard deviations as black lines on each side of the red line. The dashed blue lines indicate the locations of the change points. In the lower panels of each plot, we plotted the posterior probability (PP) of the change point. Higher PP indicates higher chance that this day is the change point.
Figure 3  Comparisons between camera greenness index, logit(gcc), with ground-based observations of percentage of leaf budburst (BBRK) in Harvard Forest from year 2008 to 2011. The green dots indicate the logit(gcc) value in the spring (DOY 100 – DOY 160). The solid red lines are the piecewise linear regression model fits from BCP, with standard deviations as black lines on each side of the red line. The dashed blue lines indicate the locations of the change points. The black dots are mean values of the percentage of budburst from nine trees, with whiskers indicating standard deviations of BBRK.
Figure 4 Comparisons between the observed budburst from four sites and the modeled budburst using SW model. Colors indicate data from different sites. The mean values of RMSE, ME and three parameters of SW model were given, with standard deviation of the values from bootstrap validations.
Figure 5 Historical and predicted change of the budburst time (start of season) for the New England under various Representative Concentration Pathways (RCPs). The shaded areas indicate the standard deviations of the historical or predicted changes.
Beyond leaf color: comparing camera-based phenological metrics with leaf biochemical, biophysical and spectral properties throughout the growing season of a temperate deciduous forest

Xi Yang\textsuperscript{1,2}, Jianwu Tang\textsuperscript{2,1}, John Mustard\textsuperscript{1}

\textsuperscript{1}Department of Geological Sciences, Brown University, Providence, RI, USA, 02912

\textsuperscript{2}The Ecosystems Center, Marine Biological Laboratory, Woods Hole, MA, USA, 02543

Published in

Journal of Geophysical Research – Biogeosciences

2014
Abstract

Plant phenology, a sensitive indicator of climate change, influences vegetation-atmosphere interactions by changing the carbon and water cycles from local to global scales. Camera-based phenological observations of the color changes of the vegetation canopy with throughout the growing season have become popular in recent years. However, the linkages between camera phenological metrics and leaf biochemical, biophysical and spectral properties are elusive. We measured key leaf properties including chlorophyll and carotenoids concentrations and leaf reflectance on a weekly basis from June to November, 2011 in a white oak forest on the island of Martha’s Vineyard, Massachusetts, USA. Concurrently, we used a digital camera to automatically acquire daily pictures of the tree canopies. We found that there was a mismatch between the camera-based phenological metric for the canopy greenness (green chromatic coordinate, gcc) and the total chlorophyll and carotenoids concentration and leaf mass per area during late spring/early summer. The seasonal peak of gcc is approximately 20 days earlier than the peak of the total chlorophyll concentration. During the summer we observed a gradual decline of gcc and leaf-level vegetation index in a period of insignificant change in total chlorophyll concentration. During the fall, both canopy and leaf redness (red chromatic coordinate, rcc) were significantly correlated with the vegetation index for anthocyanin concentration, opening a new window to quantify vegetation senescence remotely. Satellite and camera-based vegetation indices agreed well, suggesting that camera-based observations can be used as the ground validation for satellites. Using the high temporal resolution dataset of leaf biochemical, biophysical and spectral properties, our results show the strengths and potential uncertainties to use
canopy color as the proxy of ecosystem functioning. Our results suggest an urgent need for additional research that bridges the gap between leaf physiological properties and camera-based phenological metrics.

**Keywords:** green-up, senescence, phenology, leaf physiology, vegetation spectroscopy, carbon cycle, chlorophyll, carotenoids

1. **Introduction**

Plant phenology, the timing of periodic events in the life cycle of plants such as leaf-out, flowering and senescence, is a widely-used indicator of climate change [Rosenzweig et al., 2007; Walther et al., 2002]. It is reported that leaf-out and flowering in the northern hemisphere are advancing as a result of climate change [Fitter and Fitter, 2002; Schwartz et al., 2006; Yang et al., 2012]. These changes can exert feedbacks to the climate system through photosynthesis, canopy albedo, surface energy balance, canopy conductance, and emissions of volatile organic compounds [Peñuelas et al., 2009; Richardson et al., 2013]. Consequently, accurate characterization of vegetation phenology, especially the seasonal trajectories of key biophysical and biochemical properties (e.g., leaf area index and chlorophyll concentration), could improve the performance of terrestrial biosphere models [Richardson et al., 2012].
Plant phenology has been documented at different scales, including manual observations at the species level (<1 m²) (e.g., [Richardson and O'Keefe, 2009]), remote sensing at regional and global scale (1-10 km² per pixel) [Elmore et al., 2012; Fisher et al., 2006; Yang et al., 2012; Zhang et al., 2003], and near-surface remote sensing of leaf phenology using digital cameras at the ecosystem scale (10-1000 m²) [Hufkens et al., 2012; Richardson et al., 2009]. Digital cameras record the color changes of the vegetation canopy as an indicator of vegetation phenology. However, leaf reflectance in the visible and near-infrared bands may not be an accurate proxy for the plant physiology and biochemistry, as the physiological changes (e.g., photosynthetic capacity) could occur even when the leaf color is constant [Bauerle et al., 2012]. Leaf biochemical and biophysical properties, such as leaf nitrogen content, leaf chlorophyll and carotenoids concentrations, and leaf mass per area, are directly related to the plant physiology. For example, nitrogen and chlorophyll are both key components in plant photosynthesis [Chapin et al., 2011; Wright et al., 2004]; carotenoids protect leaves from environmental stress [Demmig-Adams and Adams III, 2002]; and leaf mass per area measures the investment of plant dry-mass per leaf area and is usually related to the rate of photosynthesis [Poorter et al., 2009]. Thus, field measurements of key leaf properties are necessary to understand whether and how leaf color change are related to plant physiological change during the growing season.

Leaf biophysical and biochemical properties change throughout the season, so does the leaf spectral properties [Zhang et al., 2007]. Traditional phenological observations focus on several phenological stages such as leaf-out and flowering, while ignoring the change during the growing season. However, climate-induced phenological
shift could potentially affect not just the start and end of the growing season, but also the mid-season when ecosystem productivity has been considered to be relatively constant [Richardson et al., 2010]. In addition, some of the changes in leaf properties happen within weeks (e.g., Jurik [1986]). Thus a high temporal resolution (~1 week) dataset of these properties is critical for understanding the plant physiological processes and the camera-based phenological metrics.

Recently, given the relative simplicity of installing and maintaining digital cameras for automatically monitoring vegetation phenology, camera-based phenological observation is emerging as a mainstream approach (e.g., in NEON [Keller et al., 2008], PhenoCam [Richardson et al., 2009], and ICOS (Integrated Carbon Observation System, http://www.icos-infrastructure.eu)). Therefore, it is important to examine the physiological meanings of the phenological metrics derived from camera images. In this study, we aim to integrate the phenological observations at leaf, canopy and satellite levels. Specifically, our objectives are to (1) understand the relationship between canopy-level camera phenological metrics and relevant leaf physiological properties; and (2) examine the relationship between camera phenological metrics and remote sensing data.

2. Materials and methods

2.1. Site description

The study site (41°21'42.6"N, 70°34'41.7"W) was a deciduous white oak (Quercus alba) dominated forest located in the Manuel F. Correllus State Forest on the island of Martha’s Vineyard, Massachusetts, USA. The forest age was 80-115 years after natural recovery from abandoned cropland and pasture [Foster et al., 2002]. Mean
temperatures were 20°C in the summer and 0°C in the winter, and annual precipitation was about 1,200 mm from 1981 to 2010\(^2\).

2.2. Digital camera observations of plant phenology

Ground based observations of plant phenology were documented with a north-facing digital camera (Netcam MP, Stardot Inc., Buena Park, CA, USA) that was mounted with 15° downward view from the horizontal plane on top of a 50-foot tower (~25 feet above the canopy). The camera took pictures hourly from 10AM to 3PM every day from April to November 2011, and images were stored in a USB network storage system (TS-U100, Trendnet, Torrance, CA, USA). The system was powered by an 85W solar panel (Suntech STP085B-12/BEA, Suntech, San Francisco, CA, USA) and two deep cycle batteries that were attached to an electrical timer (GE 15079, General Electric, Fairfield, CT, USA) that powered down the system during inactive periods for energy conservation.

Images from the camera system described above were processed in three steps. First, images where tree canopies are indiscernible because of rain drops on the protection case, heavy fog and overexposed sky were identified manually and excluded from further analysis. Second, green and red chromatic coordinates (\(g_{cc}\) and \(r_{cc}\), Gillespie et al., [1987]; Sonnentag et al., [2012]) for each image were calculated as the averaged \(g_{cc}\) and \(r_{cc}\) of all the pixels within the Region of Interest (ROI), which contains most of the tree canopies in the picture (Fig.1). \(g_{cc}\) and \(r_{cc}\) were calculated from every image as follows (Eq. 1),

\[ \text{Eq. 1} \]

\[ \text{Retrieved from National Climate Data Center: http://www.ncdc.noaa.gov.} \]
\[ g_{cc} = \frac{G}{R + G + B} \]
\[ r_{cc} = \frac{R}{R + G + B} \]

where R, G, and B are red, green and blue layer of the JPEG image. Leaf biochemical properties such as chlorophyll concentration and biophysical properties such as leaf mass per area (LMA) can affect the reflectance in the visible wavelength, including R, G, and B, and thus could potentially be linked to \( g_{cc} \) and \( r_{cc} \) [Asner et al., 2009]. Third, we calculated the 90th percentile of all the values within a 3-day moving window based on the method of Sonnentag et al. [2012]. By doing so, we acquired the smoothed time-series of \( g_{cc} \) and \( r_{cc} \) (Fig. 2a).

2.3. Leaf spectral, biophysical, and biochemical properties

A high temporal resolution dataset of leaf spectral, biophysical and biochemical properties was collected. The weekly (biweekly in August) sampling of leaves throughout the growing season (June, 2011 - November, 2011) was conducted on three white oak trees located within 5 meters of the camera tower. For each sampling period, two fully-sunlit branches (each having ~6 leaves) were randomly cut from each tree using a tree pruner, and then immediately placed in a plastic bag containing a moist paper towel. All the samples were stored in a cooler filled with ice to keep the leaves from desiccation [Foley et al., 2006].

Each branch was divided into two subsets. One subset (3 leaves) was immediately used for leaf reflectance measurements in the field with a spectroradiometer (FS-3, ASD Inc. Boulder, CO, USA; spectral range: 300-2500 nm, spectral resolution: 3 nm@700 nm, 10 nm@1400/2100 nm) and an integrating sphere (ASD Inc.). Each leaf spectrum was the average of 50 measurements. At least six leaf discs (~0.2827 cm² each) from the same
subset of leaves were taken from each leaf using a hole puncher and then kept in the dry ice for the pigment analyses. Back in the lab, three leaf discs were ground in a mortar with 100% acetone solution and MgO [Asner et al., 2009]. After an 8-minute centrifugation, the absorbance of the supernatant was measured using a spectrophotometer (Shimadzu UV-1201, Kyoto, Japan). Chlorophyll a, b and carotenoids concentrations were calculated using the readings from 470, 520, 645, 662 and 710 nm [Lichtenthaler and Buschmann, 2001]. The other subset (3 leaves) was scanned using a digital scanner (EPSON V300, EPSON, Long Beach, CA, USA), and oven-dried (65° C) for at least 48 hours for quantification of leaf dry mass. LMA was calculated based on the following equations:

\[
LMA = \frac{W_{\text{dry}}}{A_{\text{leaf}}} \tag{2}
\]

where \(W_{\text{dry}}\) is leaf dry mass weight, \(A_{\text{leaf}}\) is the leaf area calculated from the scanned leaf using ImageJ [Schneider et al., 2012]. Dried leaves were then ground and analyzed for nitrogen percentage of dry mass (%N) with a CHNS/O analyzer (FLASH 2000, Thermo Scientific, Waltham, MA, USA).

The narrow-band (<10 nm) leaf spectra were convoluted to produce broadband (the bandwidth is usually 30-100 nm for MODIS) reflectance using the spectral response functions \(f_s(\lambda)\) from the digital camera and MODIS (Table 1). The convolution from narrow-band \(R_N\) to broad-band \(R_B\) reflectance can be described as [Liang, 2003]:

\[
R_B = \frac{\sum_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} R_N(\lambda)f_s(\lambda)}{\sum_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} f_s(\lambda)} \tag{3}
\]
where $\lambda$ is the wavelength (nm). Broadband red, green and blue reflectances from the leaves were calculated to simulate the signal from leaves as received by the camera. Similarly, red, green, blue, and near-infrared (NIR hereafter) were calculated using the MODIS spectral response function, and were then used to calculate Normalized Difference Vegetation Index (NDVI) and Enhanced Vegetation Index (EVI) [Huete et al., 2002; Sims and Gamon, 2002]. We used three vegetation index (Anthocyanin Reflectance Index, ARI; modified Anthocyanin Reflectance Index, mARI; and Red:Green Ratio, RGR) as indicators of the anthocyanin concentration in the leaves [Gitelson et al., 2006; Sims and Gamon, 2002; Ustin et al., 2009]. Using the scanned images of the leaves, we calculated the scanned leaf $g_{cc}$ and $r_{cc}$.

We randomly collected six branches and measured the reflectance of their surfaces. In addition, we measured the reflectance of two surface soil samples. The stem and soil spectra were used to calculate the corresponding $g_{cc}$ (Fig. 3a).

2.4. Satellite data

Satellite data of the study area were used for comparison with the camera-derived indices. MODIS 8-day 500 m surface reflectance data (MOD09A1) of year 2011 were downloaded (http://modis-land.gsfc.nasa.gov/, tile no.: h12v04). The pixel where the camera tower was located was obtained, and the pixel covered a homogenous area in terms of plant phenology [Fisher and Mustard, 2007]. Quality control was conducted by using the quality assessment (QA) layers: only days that were indicated as ideal quality (00 in first two bits of QA of MOD09A1, and 0 in first bit of QA of MOD15A2) were
included in the analysis. Savitzky-Golay filter was used to smooth the time-series [Chen et al., 2004].

2.5. Statistical method

Pearson’s Partial Correlation Coefficient (PCC) was used to estimate the relative contribution of each individual band (R, G and B) on the seasonal patterns of $g_{cc}$ and $r_{cc}$, at both canopy level and leaf level [Shipley, 2002]. In this study, PCC is an estimate of partial correlation coefficient between individual band (e.g., R) and $g_{cc}$ (or $r_{cc}$), controlling the effect of other individual bands. PCC takes the value between -1 and 1. The higher the absolute value is, the more important the individual band is to the patterns of $g_{cc}$ or $r_{cc}$. PCC was calculated as follows:

$$
\rho_{XZ,Y} = \frac{\rho_{XZ} - \rho_{XY}\rho_{ZY}}{\sqrt{1 - \rho_{XY}^2}(1 - \rho_{ZY}^2)}
$$

(4)

$\rho_{XZ,Y}$ is PCC between X and Z, with other variables (i.e., Y) fixed. In this study, X (or Y) is each individual band while Z could be $g_{cc}$ or $r_{cc}$. $\rho_{XY}$, $\rho_{XZ}$, $\rho_{ZY}$ are the correlations between XY, XZ and ZY, respectively. PCC was calculated using a commercial software package (Matlab R2012b, The MathWorks Inc., Natick, MA, 2000).

3. Results

3.1. Seasonal trajectories of canopy-level indices

The digital camera recorded the seasonal trajectories of canopy greenness and redness. $g_{cc}$ and $r_{cc}$ in our site showed the typical seasonal patterns reported for deciduous forests (e.g., Henneken et al., [2013]; Richardson et al., [2009]). We divided the entire
growing season into four stages based on the trajectories of \(g_{cc}\) and leaf chlorophyll concentration (Fig. 2). The \(g_{cc}\) trajectory consists of a rapid increase in the spring due to leaf-out (Stage 0, Fig. 2a & 3); a seasonal peak in the early summer followed by a rapid decline (Stage I); a gradual decline in the mid-to-late summer (Stage II) and a rapid decline of \(g_{cc}\) in the autumn (Stage III). The general seasonal pattern of \(r_{cc}\) was the opposite to \(g_{cc}\). \(r_{cc}\) reached a local peak in the early spring. \(r_{cc}\) was highest when 100% of the leaves on the tree changed to red color in the fall and lowest when the canopy was fully covered by green leaves. Although the seasonal cycles of \(g_{cc}\) and \(r_{cc}\) were inversely correlated over the course of the year, there were several important differences between \(r_{cc}\) and \(g_{cc}\) trajectories within the season. For example, after DOY 160 (June 9\textsuperscript{th}, 2011), \(g_{cc}\) started to decline gradually until DOY 237 (Aug. 25\textsuperscript{th}, 2011), while \(r_{cc}\) remained stable during this period. During DOY 240-310, \(g_{cc}\) exhibited another decline, while \(r_{cc}\) increased to its seasonal peak. The period after the spring \(g_{cc}\) peak can be divided into three stages (Fig. 2a). Stage I was the period during which the \(g_{cc}\) started a rapid decline after the seasonal peak. During this period, \(r_{cc}\) remained stable. Stage II was a gradual decline of \(g_{cc}\) and stable \(r_{cc}\). Stage III was marked as another gradual decline of \(g_{cc}\) and a rapid increase of \(r_{cc}\) to its seasonal peak. As both leaf and canopy level measurements overlap in these three stages, we focus the comparison (Section 3.4) in Stage I-III.

The contribution of individual bands to canopy color varied at different stages (Table 2). The green and red were consistently important factors driving the seasonal changes of \(g_{cc}\) and \(r_{cc}\), respectively. However, the blue band played a more important role for both \(g_{cc}\) and \(r_{cc}\) during certain stages. For example, the decline of blue in Stage 0 drove the increase in \(g_{cc}\). Note that for camera data, the value for each individual band is
the raw digital number, not necessarily reflecting the actual reflectance of each individual band.

The color as seen from the satellite showed a good agreement with that from the camera (Fig. 3b). Overall the agreement in $g_{cc}$ between the satellite and camera was higher than that of the $r_{cc}$ (MODIS vs. Camera, $r^2 = 0.878$ for $g_{cc}$, $r^2 = 0.531$ for $r_{cc}$). The three distinct stages similar to those in camera $g_{cc}$ were observed in the MODIS $g_{cc}$ time-series. For $g_{cc}$, a spring peak and the following summer greendown was also obvious in the MODIS data. The spring local peak was not obvious in MODIS $r_{cc}$ time-series. However, a fall $r_{cc}$ peak (and a $g_{cc}$ minimum) was obvious in the MODIS $r_{cc}$ time-series.

We compared MODIS NDVI and EVI with the camera $g_{cc}$ (Fig. 3c). In stage I, NDVI reached its seasonal peak and started to decline, which is similar to that of the camera $g_{cc}$. However, EVI was stable or even increasing during this period. In stage II, like camera $g_{cc}$, NDVI and EVI both decreased. In stage III, there was another gradual decline of MODIS NDVI and EVI.

3.2. **Seasonal trajectories of leaf biochemical and biophysical properties**

The seasonal trajectories of leaf biochemical and biophysical properties were similar to those in the previous research on deciduous trees [Damesin, 2003; Jurik, 1986; Poorter et al., 2009]. Area-based leaf total chlorophyll concentration ($\mu$g/cm$^2$) increased steadily in Stage I, reaching a plateau in Stage II, and gradually declined in Stage III (Fig. 2b). The seasonal trajectory of area-based carotenoids concentration ($\mu$g/cm$^2$) was similar to that of the total chlorophyll. The only difference was in Stage II, when carotenoids started to decrease. The ratio between chlorophyll a and b (Chl a:b) generally varied
between 2.5 to 3.0. During Stage I and early Stage II, Chl a:b increased to its seasonal peak at 3.0, and then was followed by a decrease to ~2.7 in Stage III (Fig. 2c). The Carotenoids-to-Chlorophyll ratio (Car/Chl) was conservative through Stage I and II. In Stage III, a gradual increase of Car/Chl was followed by a rapid increase to the seasonal peak with a mean value of ~0.5.

The mean value of %N decreased from 4 to 2 in stage I (Fig. 2d). After a stable Stage II, %N started to decrease during the end of Stage III, which presumably could be the result of nitrogen resorption during senescence [Killingbeck, 1996]. The seasonal trajectory of LMA is conservative compared to the other biochemical and biophysical properties (Fig. 2d). LMA increased in Stage I to a plateau in Stage II and III, and only showed a slight decrease by the end of the growing season.

3.3. Seasonal trajectory of vegetation spectra

Leaf spectra at different times of the growing season exhibited distinct features (Fig. 4). Each leaf biophysical and biochemical property contributes to different wavelengths of leaf spectra [Jacquemoud and Baret, 1990]. During the period between leaf budburst and maturity (May-August), the most significant change in the visible wavelength (VIS thereafter, 400~700nm) was the decrease of green reflectance (Fig. 2f; Fig. 4). During the fall senescence, there was a sharp increase in the red reflectance, presumably caused by the decrease of total chlorophyll (Fig. 2b). Similarly, there was a moderate increase of green reflectance.

The contributions of each individual band (R, G, and B) from leaf spectra changed at different stages (Table 3). For $g_{cc}$, the green reflectance was the major
contributor throughout the three stages. The green reflectance – gc relationship was significantly positive. The contribution of R to gc increased significantly throughout the season from non-significant (Stage I) to the dominant (Stage III). For rc, R was the major contributor. Blue also significantly affected the seasonal pattern of rc (Fig. 2e, 2f). The green band contributed to the first two stages for rc, but not the last stage.

NIR reflectance increased during DOY 159~187, which was followed by a gradual decrease till DOY 269 (September 26th). After that, NIR reflectance increased until the end of the growing season (Fig. 2f, Fig. 4). The spectra between 1,300 nm to 2,000 nm were conservative during most times of the season; only by the end of the season did reflectance in this region start to increase (Fig. 4).

3.4. Comparisons between canopy color and leaf biochemical, biophysical and spectral properties

Although both the canopy gc and the pigment concentrations showed a similar “bump” shape throughout the growing season, there were obvious discrepancies between the two types of time-series. In stage I, while the gc started to decline from its annual peak, the total chlorophyll concentration in the leaves was still increasing (Fig. 2b). At the same time, both carotenoids concentration and LMA increased, and the %N decreased. For leaf reflectance, an increase in the NIR (on average by 0.050) was accompanied by a decrease of R and G (on average by 0.029 and 0.040, respectively, Fig. 2f, Fig. 4). Spectral indices such as NDVI and EVI showed an increase during this period.

Stage II is the “summer greendown”. Between DOY 189 and 236, similar decreases of gc were observed at both canopy (Fig. 3a) and leaf level (Fig. 2e). At the
canopy level, $g_{cc}$ gradually declines from 0.44 to 0.40 (~36% decrease compared to the seasonal amplitude). When taking the autocorrelation in data points into consideration [Bence, 1995], there is still a significant decline of carotenoids during stage II ($p < 0.0001$), but no significant change of chlorophyll ($p = 0.159$). Similarly, there is a significant decline of EVI during this period. Both LMA and N content showed no significant change during this period.

Stage III is the “senescence” stage (DOY 237~311). Leaf-level $r_{cc}$ was significantly correlated with the mARI ($r^2 = 0.635$, $p < 0.0001$), while for the entire growing season (including Stage I and II) the correlation was lower but still significant ($r^2 = 0.565$, $p <0.0001$) (Fig. 5). Although leaf-level $g_{cc}$ and $r_{cc}$ started to diverge from the canopy metrics (Fig.3a), there is still a significant correlation between the canopy $r_{cc}$ and the median of leaf-level mARI ($r^2 = 0.533$, $p = 0.016$). Similarly, we found a good correlation between $r_{cc}$ and the other two anthocyanin indices (Fig. S1).

Both chlorophyll and carotenoids showed significant decrease at the senescence stage. The carotenoids/chlorophyll ratio shows a consistent increase during this period (on average from 0.201 to 0.497). LMA did not show significant decrease until ~DOY 300. %N content started to decrease at ~DOY 285. During this period, NDVI and EVI all showed a consistent decline, while all three anthocyanin indices increased. Canopy $g_{cc}$ decreased while $r_{cc}$ increased to its seasonal peak.

4. Discussion

Aiming to examine the physiological meaning of camera-based phenological metrics in this study, we found a mismatch between camera-based canopy greenness and
leaf biochemical and biophysical properties: in the spring, the seasonal peak of camera $g_{cc}$ was approximately 20 days earlier than the peak of total chlorophyll and carotenoids concentration and LMA. During the fall, we found a significant correlation between the anthocyanin indices (mARI, ARI and RGR) and $r_{cc}$ at both canopy and leaf level.

Leaf biochemical and biophysical properties are major contributors to the amount of (1) the reflected solar radiation [Asner and Martin, 2008; Jacquemoud et al., 2009], the visible part of which is seen by digital camera; and (2) the absorbed solar radiation by leaves, which is used for photosynthesis [Demmig-Adams and Adams, 2000; Peng et al., 2011]. Thus, we might expect that canopy colors (greenness or redness) show the same pattern as leaf pigmentation. However, the observed mismatch between canopy greenness and leaf biochemical properties suggests that the relationship between canopy color and leaf pigmentation is nonlinear. At the leaf level, pigments like chlorophyll and carotenoids are major contributors in the visible wavelength [Asner, 1998; Jacquemoud and Baret, 1990]. At the canopy level, LAI (along with factors such as leaf inclination angle distribution) is considered to be the major contributor [Asner and Martin, 2008; Jacquemoud et al., 2009], especially with the oblique view of the digital camera, more layers of leaf can be seen, changing both the rate and magnitude of $g_{cc}$ and $r_{cc}$. In Stage I and II, leaf level $g_{cc}$ matched well with canopy level $g_{cc}$, indicating that leaf-level color change largely controlled the signal received by digital camera, though it is still possible that LAI could have an impact on the signal during these stages [Samanta et al., 2012].

During the fall, as leaves start to drop in Stage III, the signal received by the camera is from a mixture of leaves, branches and background soil (Fig. 3a). Thus the leaf $g_{cc}$ started to deviate from the camera $g_{cc}$, which is the averaged value from leaves with higher $g_{cc}$.
and branches/soil background with lower $g_{cc}$. The contribution of leaves to the canopy $g_{cc}$ decreased during Stage III (Fig. 3d). To disentangle the contributions of leaf chemistry and LAI, concurrent measurements of LAI from instruments like LAI-2000 can be helpful [Gond et al., 1999]. In addition, with the input of LAI and leaf biochemical, biophysical and spectral properties, canopy radiative transfer models might be able to provide the mechanistic understanding for this mismatch [Jacquemoud et al., 2009].

At the leaf-level, leaf biochemical and biophysical properties control the leaf color changes throughout the season. The decline of $g_{cc}$ at Stage I was the result of greater decline of G, compared to the relatively stable R and B (Fig. 2f, Table 3). Presumably, it can be explained by the change of leaf biochemical and biophysical properties: the increase of chlorophyll concentration is an indicator of leaf maturity, which is supported by the increase of LMA [Ellsworth and Reich, 1992; Jurik, 1986] and carotenoids concentration [Lewandowska and Jarvis, 1977], and the decline of the nitrogen concentration measured as the percentage of dry weight [Field and Mooney, 1983; Schultz et al., 1982]. Could this mismatch simply be a result of the saturation of the $g_{cc}$ as the pigments accumulate, like the saturation of NDVI as chlorophyll accumulates [Gamon et al., 1995]? Our results did not support this hypothesis. First, if $g_{cc}$ saturates as the pigments accumulate in Stage I, $g_{cc}$ should neither increase nor decrease as adding more pigments would have no effect. However, we observed a decline of $g_{cc}$ at both leaf and canopy level. Second, there were significant increases in both NDVI and EVI during stage I, when chlorophyll increased. Both NDVI and EVI did not show saturation during this stage (data not shown).
Since total chlorophyll concentration is considered to be related to Gross Primary Production (GPP), we might expect a similar mismatch between the canopy greenness and GPP in the spring [Toomey et al., 2012; Xiao et al., 2004], even though $g_{cc}$ and GPP might have similar seasonal patterns [Richardson et al., 2009]. In addition, during Stage II, the leaf $g_{cc}$ matched well with the canopy $g_{cc}$, showing the same decline in G (Fig. 3a). This decline of $g_{cc}$ was mainly controlled by the decrease of G (R and B were relatively constant (Table 2)) which could be attributed to leaf aging, or potentially changes in leaf internal structure [Slaton et al., 2001] (as hinted by that NIR reflectance significantly declined during this period (Fig. 2f)). Similarly, leaf-level NDVI and EVI all declined, but this “summer greendown” is rarely documented in remote sensing literatures [Elmore et al., 2012]. Leaf aging, paralleled with the decline of leaf photosynthetic capacity [Wilson et al., 2001], could affect GPP even though we see little change in chlorophyll concentration [Bauerle et al., 2012]. LMA did not correlate well with the change of canopy greenness. In the spring, the mismatch between canopy $g_{cc}$ and LMA was similar to that between $g_{cc}$ and chlorophyll concentration, presumably in Stage I leaves were still building up cell materials [Poorter et al., 2009].

The good correlation between camera and satellite-based $g_{cc}$ time-series suggests the potential to use digital cameras as the ground validation for satellites, for example, Hufkens et al. [2012] found a good match between satellite vegetation indices and canopy greenness (as indicated by another metric, ExG). However, our results suggest that the $g_{cc}$ time-series from both methods could mismatch with leaf pigmentations in the spring. In contrast, the $r_{cc}$ and anthocyanin relationship could potentially be used to monitor fall senescence remotely just using reflectance at visible wavelength, at least in
certain species with anthocyanin in the leaves [Zhang and Goldberg, 2011]. To further
test the robustness of this observation, in-situ measurements of leaf anthocyanin
concentration can be helpful. To capture the seasonality of leaf physiology, ground-based
measurements of leaf biochemical, biophysical and spectral properties should
complement near-surface and remote sensing data with high temporal and spatial
resolutions.

Acknowledgements

We thank Dr. Dennis Baldocchi, the associate editor and three anonymous reviewers for
their constructive comments. We would like to thank Johanna Schmitt for the discussion
and Adrian Rocha for commenting on an earlier version of this manuscript. We thank
Katie Laushman, Lakiah Clark, Skyler Hackley, and Tim Savas for assisting with
fieldwork. We thank Matthew Erickson, Marshall Otter, Rich McHorney, Jane Tucker
and Sam Kelsey for the help with lab work. We also thank the Manuel F. Correllus State
Forest, the Nature Conservancy Hoft Farm Preserve, and Mr. Colbert for the permission
to use the forests in the island of Martha’s Vineyard in Massachusetts for our research.
This research was supported by the Brown University–Marine Biological Laboratory
graduate program in Biological and Environmental Sciences, Brown–ECI phenology
working group, Brown Office of International Affairs Seed Grant on phenology, and
Marine Biological Laboratory start-up funding for JT.

References

Asner, G., and R. Martin (2008), Spectral and chemical analysis of tropical forests:
Scaling from leaf to canopy levels, Remote Sensing of Environment, 112(10), 3958-3970.


Peñuelas, and R. Valentini (1995), Relationships between NDVI, canopy structure, and
Gillespie, A. R., A. B. Kahle, and R. E. Walker (1987), Color enhancement of highly
correlated images. II. Channel ratio and “chromaticity” transformation techniques,
noninvasive estimation of chlorophyll, carotenoids, and anthocyanin contents in higher
Gond, V., D. G. G. de Pury, F. Veroustraete, and R. Ceulemans (1999), Seasonal
variations in leaf area index, leaf chlorophyll, and water content; scaling-up to estimate
fAPAR and carbon balance in a multilayer, multispecies temperate forest, *Tree
physiology*, 19(10), 673-679.
Henneken, R., V. Dose, C. Schleip, and A. Menzel (2013), Detecting plant seasonality
from webcams using Bayesian multiple change point analysis, *Agricultural and Forest
Meteorology*, 168(0), 177-185.
Overview of the radiometric and biophysical performance of the MODIS vegetation
Hufkens, K., M. Friedl, O. Sonnentag, B. H. Braswell, T. Milliman, and A. D.
Richardson (2012), Linking near-surface and satellite remote sensing measurements of


Richardson, A. D., et al. (2010), Influence of spring and autumn phenological transitions on forest ecosystem productivity, *Philosophical Transactions of the Royal Society B: Biological Sciences, 365*(1555), 3227-3246.


Schwartz, M. D., R. Ahas, and A. Aasa (2006), Onset of spring starting earlier across the Northern Hemisphere, *Global Change Biology, 12*(2), 343-351.


### Table 1

Broadband and narrowband reflectance used for the calculation of vegetation indices

<table>
<thead>
<tr>
<th>Sensors</th>
<th>Reflectance (and bandwidth(^1))</th>
<th>Indices(^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Digital camera</strong></td>
<td>R (577-698nm), G (494-585nm), and B (411-505nm)</td>
<td>(g_{cc} = G/(R+G+B); r_{cc} = R/(R+G+B))</td>
</tr>
<tr>
<td><strong>MODIS</strong></td>
<td>R (620-670nm), G (459-479nm), B (545-565nm), NIR (841-876nm)</td>
<td>NDVI = (NIR-R)/(NIR+R); EVI = 2.5×(NIR-R)/(NIR+6×R-7.5×B+1)</td>
</tr>
</tbody>
</table>
| **ASD**   | \(\rho_{530-570} (530-570nm), \rho_{690-710} (690-710nm), \rho_{760-800} (760-800nm)\) | mARI = \((1/\rho_{530-570} - 1/\rho_{690-710}) \times \rho_{760-800}\)  
ARI = 1/\(\rho_{550}\) - 1/\(\rho_{700}\)  
RGR = \(\rho_{600-699}/\rho_{500-599}\) |

1 Spectral response function for the camera was retrieved from: [http://s1.archive.theimagingsource.com/publications/sensors-ccd/icx205ak/0eedde64522190fb3cd9076af716619/icx205ak.en_US.pdf](http://s1.archive.theimagingsource.com/publications/sensors-ccd/icx205ak/0eedde64522190fb3cd9076af716619/icx205ak.en_US.pdf) (Accessed on Nov. 28th, 2012); and spectral response function for MODIS was retrieved from: [http://mcst.gsfc.nasa.gov/calibration/parameters](http://mcst.gsfc.nasa.gov/calibration/parameters) (Accessed on Nov. 28th, 2012). The bandwidth of digital camera was estimated using a simple calculation of FWHM (Full Width at Half Maximum), which is based on the spectral response function of the band (Liang, 2003).

2 \(g_{cc}\): green chromatic coordinate; \(r_{cc}\): red chromatic coordinate; NDVI: Normalized Difference Vegetation Index; EVI: Enhanced Vegetation Index; mARI: modified Anthocyanin Reflectance Index; ARI: Anthocyanin Reflectance Index; RGR: Red-to-Green Ratio.
Table 2

Partial Correlation Coefficient (Pearson’s Partial Correlation) between camera-based $g_{cc}/r_{cc}$ and each individual band (R, G, B). Statistics in bold indicate that $p < 0.05$.

<table>
<thead>
<tr>
<th></th>
<th>Stage 0</th>
<th>Stage I</th>
<th>Stage II</th>
<th>Stage III</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g_{cc}$ R</td>
<td>-0.6843</td>
<td>0.0509</td>
<td>0.1187</td>
<td><strong>-0.7710</strong></td>
</tr>
<tr>
<td>G</td>
<td>0.7265</td>
<td>0.5388</td>
<td><strong>0.4817</strong></td>
<td>0.6448</td>
</tr>
<tr>
<td>B</td>
<td>-0.9266</td>
<td>-0.6748</td>
<td><strong>-0.6894</strong></td>
<td>0.0691</td>
</tr>
<tr>
<td>$r_{cc}$ R</td>
<td>0.9434</td>
<td>0.7595</td>
<td><strong>0.8939</strong></td>
<td>0.9664</td>
</tr>
<tr>
<td>G</td>
<td>-0.7118</td>
<td>-0.5559</td>
<td><strong>-0.6675</strong></td>
<td>-0.5394</td>
</tr>
<tr>
<td>B</td>
<td>-0.9149</td>
<td>-0.5142</td>
<td><strong>-0.7005</strong></td>
<td>-0.7962</td>
</tr>
</tbody>
</table>
Table 3

Partial Correlation Coefficient (Pearson’s Partial Correlation) between leaf-level $g_{cc}/r_{cc}$ and each individual band (R, G, B). Leaf-level reflectance in R, G and B were calculated based on MODIS spectral response function using spectra collected by ASD spectrometer. Statistics in bold indicate that $p < 0.05$. Note that leaf spectra were collected since the beginning of Stage I.

<table>
<thead>
<tr>
<th></th>
<th>Stage I</th>
<th>Stage II</th>
<th>Stage III</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g_{cc}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R</td>
<td>-0.5426</td>
<td>-0.7517</td>
<td>-0.9113</td>
</tr>
<tr>
<td>G</td>
<td>0.8159</td>
<td>0.9788</td>
<td>0.8977</td>
</tr>
<tr>
<td>B</td>
<td>-0.4300</td>
<td>-0.6730</td>
<td>-0.6822</td>
</tr>
<tr>
<td>$r_{cc}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R</td>
<td>0.9285</td>
<td>0.9402</td>
<td>0.9445</td>
</tr>
<tr>
<td>G</td>
<td>-0.7448</td>
<td>-0.7941</td>
<td>-0.0168</td>
</tr>
<tr>
<td>B</td>
<td>-0.9087</td>
<td>-0.9217</td>
<td>-0.6441</td>
</tr>
</tbody>
</table>
Fig. 1 An example of the images acquired by the digital camera. The red rectangle indicates the Region of Interest (ROI) used to calculate camera phenological metrics such as Green chromatic coordinate ($g_o$). Pictures in the lower panel are images from different times of the year (time format: mm-dd).
Fig. 2 Comparisons between leaf biochemical, biophysical, spectral properties and camera-based metrics. (a) Green chromatic coordinate ($g_{cc}$) and red chromatic coordinate ($r_{cc}$) calculated from camera time-series. (b) Leaf total chlorophyll and carotenoids concentration ($\mu$g/cm$^2$). Solid dots are average from the 18 leaves sampled each time. The whiskers are the standard deviations; (c) Car/chl ratio and chl a/b ratio. (d) Mass-based total nitrogen content (%N), leaf mass per area (LMA). (e) Normalized Vegetation Index (NDVI), Enhanced Vegetation Index (EVI), $g_{cc}$ (green chromatic coordinate) and $r_{cc}$ (red chromatic coordinate) calculated from leaf spectra; (f) Green, red, near-infrared and blue reflectance from the leaf spectra, see Section 2.3 for details.
Fig. 3 Comparisons of vegetation indices at the canopy-level. (a) Green/red dots are $g_{cc}/r_{cc}$ from digital camera. Pink triangles are $g_{cc}$ calculated from scanned leaves. The whiskers are the standard deviation of 18 leaves each date. The horizontal dashed lines are $g_{cc}$ of stem and soil calculated from spectra. (b) MODIS $g_{cc}$ and $r_{cc}$ calculated from the MOD09A1 reflectance product. (c) MODIS NDVI and EVI calculated from MOD09A1 product. (d) Raw digital number (DN) from red, green, and blue bands of digital camera images.
Fig. 4 Examples of the leaf spectra (400–2,000 nm) collected using ASD spectroradiometer throughout the season. Only a subsample of the spectra was plotted for the best visual effect. Curves in different colors represent leaf directional-hemispherical reflectance at different dates.
Fig. 5 Comparisons of leaf- and canopy-level $r_{cc}$ with modified Anthocyanin Reflectance Index (mARI) throughout the growing season. The dots are mean values and the whiskers are standard deviations. The inset shows the scatter plot of entire growing season leaf $r_{cc}$~mARI (black dots + pink dots) and the linear regression (black line); Stage III only leaf $r_{cc}$~mARI (pink dots) and the linear regression (pink line); and canopy $r_{cc}$~mARI (dark yellow triangle) and the linear regression (dark yellow line).
**Fig.S1** Comparisons of leaf- and canopy-level $r_{cc}$ with Anthocyanin Reflectance Index (ARI) (Upper Panel) and Red-to-Green Ratio (RGR) (Lower Panel) throughout the growing season. The dots are mean values and the whiskers are standard deviations. The inset shows the scatter plot of entire growing season leaf $r_{cc}$~ ARI (Upper Panel, or RGR, lower panel, black dots + pink dots) and the linear regression (black line); Stage III only leaf $r_{cc}$~ ARI (Upper Panel, or RGR, lower panel, pink dots) and the linear regression (pink line); and canopy $r_{cc}$~ ARI (Upper Panel, or RGR, lower panel, dark yellow triangle) and the linear regression (dark yellow line).
CHAPTER 4

Temporal variability of leaf traits captured by leaf optical properties

Xi Yang$^{1,2}$, Jianwu Tang$^{1,2}$, John Mustard$^1$, Kaiguang Zhao$^3$

$^1$Department of Geological Sciences, Brown University, Providence, RI, USA, 02912

$^2$The Ecosystems Center, Marine Biological Laboratory, Woods Hole, MA, USA, 02543

$^3$School of Environment and Natural Resources, Ohio Agricultural and Research Development Center, The Ohio State University, Wooster, OH, USA, 44691

To be submitted to

*Remote Sensing of Environment*
Abstract

Leaf biochemical and biophysical traits are tightly linked with plant functioning under various environmental conditions. Hyperspectral remote sensing provides a non-destructive way to infer leaf traits from leaf optical properties. Although there is a large body of studies that link leaf traits with optical properties, the ability of using leaf optical properties to capture the seasonal variability of leaf traits was less well tested. Moreover, a few literatures that partially addressed this question only focused on a few leaf traits, especially leaf chlorophyll concentration. We collected a dataset of leaf traits (chlorophyll, carotenoids, total nitrogen by mass ($N_{mass}$), total carbon by mass ($C_{mass}$), and leaf mass per area (LMA)) and leaf optical properties (directional-hemispherical reflectance and transmittance) at a high temporal frequency (~weekly) during the growing season of two deciduous forests (Martha’s Vineyard in 2011, and Harvard Forest in 2012). We compared three categories of methods to use leaf optical properties to estimate leaf traits: simple indices that were calibrated with multiple datasets, statistical methods that exploit the full reflectance spectra (Partial Least Square, PLS; Bayesian Model Averaging, BMA), and a leaf optical model (PROSPECT). We found that all the leaf traits varied significantly throughout the growing season. Chlorophyll and carotenoids showed similar seasonal patterns. $C_{mass}$ and LMA showed similar seasonal patterns. The seasonal pattern of $N_{mass}$ was characterized with a peak in the early spring, followed by a relatively stable summer and a further decline in the fall. Leaf spectra also changed considerably throughout the season, especially for the visible and near-infrared wavelengths. Among all the methods, BMA consistently outperformed other methods in estimation all the leaf traits at both sites. In addition, BMA was able to capture the shape
of the seasonal patterns of leaf traits, which were defined by the mean values of leaf traits at each sampling date. Using the dataset, we further offered suggestions on the field sampling design: for most leaf traits, biweekly sampling of leaf samples allowed accurate characterization of the leaf seasonal patterns. These results highlight the importance of the use of full spectra to estimate leaf traits, which are highly variable throughout the growing season. This work has implications to remote sensing applications that use leaf optical properties to estimate leaf traits.

**Keywords:** phenology, leaf physiology, vegetation spectroscopy, carbon cycle, chlorophyll, carotenoids, nitrogen, leaf mass per area
Introduction

Leaf traits are important indicators of plant physiology (Wright et al., 2004). Leaf chlorophyll concentration and nitrogen concentration are essentially related to photosynthetic activities. Carotenoids are used to protect leaves from excessive sunlight. Leaf mass per area (LMA) is considered as the investment to the leaves in terms of carbon and nutrients to intercept sunlight. These leaf traits vary at different phenological stages of the leaves and under different light conditions (e.g., Lewandowska & Jarvis, 1977; Poorter et al., 2009; Yang et al., 2014). Capturing the temporal variations of these leaf traits is important to understand the ecosystem functioning (Baurele et al. 2012).

Collecting the leaf traits data are usually time-consuming. Traditional ways to measure leaf traits usually involve the destruction of the samples, making continuous measurements of the same leaf impossible. The limits on labor, time and costs further constrain the ability of traditional methods to capture the temporal and spatial variability of leaf traits. Remote sensing provides a non-destructive way to estimate these leaf traits, on the ground, airborne or spaceborne (Shen et al., 2009; Asner et al., 2011; Dillen et al., 2012). Many efforts have been put on using leaf optical properties to estimate leaf traits in the temperate deciduous forest, but most of them are focusing on a short time window during the summer. There have been a few attempts on using spectra to estimate chlorophyll seasonality (e.g., Belanger et al., 1995). However, there are still few datasets that provide a combination of leaf traits at high temporal resolution (~ weekly), which allows the assessment of methods using leaf optical properties to estimate the temporal variability of leaf traits.
There are mainly three categories of methods to estimate leaf traits from leaf optical properties: vegetation indices, statistical methods exploiting the full wavelength (400 – 2500 nm), and the inversion of leaf optical models. Vegetation indices are calculated using the reflectance from two or three wavelengths (Huete et al., 2002; Richardson et al., 2002; Sims & Gamon, 2002). After calibration with extensive datasets from various plant functional types, vegetation indices were associated with leaf chlorophyll, carotenoids and leaf mass per area using polynomial equations (Féret et al., 2011). Statistical methods such as Partial Least Square (PLS) regression became popular in recent years as more and more full spectra of leaves were collected (Wold et al., 2001; Asner & Martin, 2008; Couture et al., 2013). PLS avoids the collinearity between predictors (i.e., the reflectance at different wavelengths) by reducing them into a few uncorrelated variables to build the best prediction model (low root mean square error, RMSE). Similarly, another statistical method called Bayesian Model Averaging (BMA) was recently developed to use the full spectra to estimate leaf traits (Zhao et al., 2013). BMA has been found to outperform PLS for a few datasets. The last method is based on the state-of-art leaf optical model (e.g., PROSPECT). The inversion mode of PROSPECT allows for the calculating of leaf traits (i.e., in this study chlorophyll, carotenoids and LMA) using directional-hemispherical leaf reflectance and transmittance (Feret et al., 2008). Although being widely used, these methods were not thoroughly assessed and compared, especially using a dataset that covers the temporal variability of leaf traits in deciduous forests.

Here we hypothesized that using leaf optical properties we were able to track temporal variability of leaf traits at different heights of the sampled trees. We first
presented the temporal variations of leaf traits. We then compared three categories of methods that use leaf optical properties to estimate leaf traits. Finally, we discussed the implications of these dataset for field sampling strategy.

**Study area and methods**

**Study area**

Sample collection was conducted in two temperate deciduous forests in the northeastern part of United States. In 2011, the fieldwork was in a white oak (*Quercus alba*) dominated forest on the island of Martha’s Vineyard (MV, 41.362N, 70.578W). The forest age was 80-115 years after natural recovery from abandoned cropland and pasture (Foster *et al.*, 2002). Mean annual temperature was 10°C, and annual precipitation was about 1200 mm from 1981 to 2010 (Yang *et al.*, 2014). In 2012, the field work was conducted in Harvard Forest (HF, 42.538N, 72.171W) between May and late October. The dominating deciduous tree species were red oak (*Quercus rubra*) and red maple (*Acer rubrum*), with a few scattered yellow birch (*Betula alleghaniensis*). The forest age was 70-100 years. The annual mean temperature was about 7.5°C (Wofsy *et al.*, 1993), and the annual precipitation was 1200 mm. Satellite date suggested that the start of season in MV is about 10-20 days later than that of HF (Fisher & Mustard, 2007; Yang *et al.*, 2012).

**Measurements of leaf optical properties and traits**

We collected a high temporal resolution dataset of leaf traits in both years. In 2011, on Martha’s Vineyard weekly (biweekly in August) sampling of leaves throughout the growing season (June, 2011 - November, 2011) was conducted on three white oak
trees. For each sampling period, we cut two fully-sunlit branches (each having ~6 leaves) and one shaded branch using a tree pruner. The optical properties of the leaves were immediately measured (see below). Then the leaves were placed in a plastic bag containing a moist paper towel, and all the samples were kept in a cooler filled with ice until being transferred back to the lab for further measurements. In 2012, in Harvard Forest the same weekly (biweekly in the summer) measurements were made on five individuals (two red oak, two red maple and one yellow birch). For each tree, two sunlit and one shaded branch were collected each time. We measured the leaf optical properties immediately after the sampling. Directional-hemispherical leaf reflectance and transmittance were measured using a spectroradiometer (ASD FS-3, ASD Inc. Boulder, CO, USA; spectral range: 300-2500 nm, spectral resolution: 3 nm@700 nm, 10 nm@1400/2100 nm) and an integrating sphere (ASD Inc.). Each leaf spectrum was the average of 50 measurements. Using the full spectrum, we calculated the reflectance and transmittance at red, green, blue and near-infrared (R, G, B, and NIR) (Yang et al., 2014).

The measured leaf traits include total chlorophyll concentration (including chlorophyll a and chlorophyll b, μg/cm²), carotenoids (μg/cm²), leaf mass per area (LMA, g/m²), nitrogen concentration (%N, g/g), and carbon concentration (%C, g/g). Each branch was divided into two subsets. One subset was used to measure pigment concentrations. To measure the chlorophyll and carotenoids concentration, three leaf discs (~0.28 cm² each) were taken from each leaf using a hole puncher, and then ground in a mortar with 100% acetone solution and MgO (Asner et al., 2009). After an 8-minute centrifugation, the absorbance of the supernatant was measured using a spectrophotometer (Shimadzu UV-1201, Kyoto, Japan). Chlorophyll a, b and carotenoids
concentrations were calculated using the readings from 470, 520, 645, 662 and 710 nm (Lichtenthaler & Buschmann, 2001). The other subset (3 leaves) was scanned using a digital scanner (EPSON V300, EPSON, Long Beach, CA, USA), and oven-dried (65° C) for at least 48 hours for quantification of leaf dry mass. LMA was calculated based on the following equations:

\[
LMA = \frac{W_{\text{dry}}}{A_{\text{leaf}}}
\]

where \( W_{\text{dry}} \) is leaf dry mass weight, \( A_{\text{leaf}} \) is the leaf area calculated from the scanned leaf using ImageJ (Schneider et al., 2012). Dried leaves were then ground and analyzed for %N and %C with a CHNS/O analyzer (FLASH 2000, Thermo Scientific, Waltham, MA, USA).

Methods to estimate leaf traits using leaf optical properties

We used three categories of method to estimate leaf traits based on leaf optical properties: vegetation indices that utilize the reflectance from two wavelengths; statistical methods that exploit the information from the full leaf reflectance spectrum; and a leaf optical model. The details of the three methods are explained below:

Based on extensive datasets from various types of biomes and plants, Feret et al. (2011) established polynomial relationships between vegetation indices and total chlorophyll concentration, carotenoids and LMA (Table 1).

The second category of methods essentially is to build a multivariate linear regression model(s) between leaf reflectance and leaf traits (Zhao et al., 2013):

\[
y = X_{M'} \beta_{M'} + e, i = 1, 2, 3, ..., 2^n
\]
where $y$ is an $n$-by-$1$ matrix of leaf traits ($n$ equals to the number of leaf samples). $X$ is an $n$-by-$m$ matrix ($m$ equals the number of bands from each spectrum). $\epsilon$ is the $n$-by-$1$ estimation error that are to be minimized. $M_i$ is the $i^{th}$ model configuration from $2^p$ possible configurations ($p$ is the number of covariates, for example, the number of bands in the leaf reflectance). Each model has its unique set of covariates (the selection of reflectance at certain wavelengths). PLS and BMA differ in the ways that these models were chosen and the number of models used, as described in details below.

Partial Least Square (PLS) regression chooses the best model for the given dataset. The numbers of independent factors used in the regression were determined by minimizing the Prediction Residual Error Sum of Squares (PRESS). Unlike PLS, which seeks to find the single optimal regression model between spectra and leaf traits, BMA takes into account of model uncertainty by averaging several competing models. The detailed mathematic formulations of BMA can be found in Zhao et al. (2013), in which BMA was found to be superior to PLS.

For PLS and BMA, we randomly choose $2/3$ of the entire dataset in each site as the calibration dataset to optimize the regression model parameters ($\beta$), and then use the remaining $1/3$ of the dataset to validate the predictions by calculating the $R^2$, Root Mean Square Error (RMSE) and normalized RMSE (NRMSE), which is RMSE divided by the range of the estimated leaf traits. The calibration-validation process was conducted iteratively for 50 times. Then we summarized the result by averaging the $R^2$ and RMSE of the 50 runs.
Lastly, we used a leaf optical model (PROSPECT) which is based on the interactions between light and the chemical and internal structure of the leaf (Jacquemoud & Baret, 1990; Feret et al., 2008). We used the measured directional-hemispherical reflectance and transmittance as input to the PROSPECT to calculate the total chlorophyll, carotenoids, and leaf mass per area. We then compared the calculated leaf traits with the measured leaf traits.

**Results**

*Temporal and spatial variability of leaf traits*

Fig.1 showed the seasonal patterns of leaf pigments at two study sites. Overall, all the pigments from both sites showed the similar bell-shaped trajectories throughout the seasons, despite the samples are from different species and locations within the canopy. Chlorophyll and carotenoids concentration rapidly increased at the beginning of the season, and then were stable during the summer followed by a decline in the fall. The Harvard Forest samples were from three different species, and showed much larger variability in each sampling period than those from Martha’s Vineyard, especially for the shaded leaves (Fig.1 e-h). The total chlorophyll concentration was ~10 \( \mu \text{g/cm}^2 \) at the early season and the end of season for both sites; in the peak season, the total chlorophyll concentration was ~50 \( \mu \text{g/cm}^2 \) and ~40 \( \mu \text{g/cm}^2 \) in MV and HF, respectively. The carotenoids concentration was ~3 \( \mu \text{g/cm}^2 \) at the beginning/end of the season and ~10 \( \mu \text{g/cm}^2 \) at the peak season. The total chlorophyll concentration relative to the carotenoids concentration (Chl/Car) increased during the early seasons. In the fall, though both
chlorophyll and carotenoids decreased, Chl/Car decreased steadily, as a result of faster
decline of chlorophyll relative to the carotenoids.

The remaining three leaf traits (LMA, N_{mass}, and C_{mass}) had different seasonal
patterns to the leaf pigments. LMA rapidly increased in the spring, but only slightly
decrease by the end of the season. N_{mass} was high (~4-5%) at the early seasons, but stable
during the summer, followed by ~1% decrease in the fall, presumably caused by nitrogen
resorption (Eckstein et al., 1999). Similar to LMA, C_{mass} accumulated in the spring and
was stable for the rest of the seasons. The rapid increase of LMA in the spring was
accompanied with a similar increase of C_{mass} and decrease of N_{mass}, which all end at the
same time (DOY ~194 in Martha’s Vineyard, and DOY ~170 in Harvard Forest).

Sunlit leaves had more total chlorophyll and carotenoids (Fig. S1). The
carotenoids concentration relative to the total chlorophyll concentration was significantly
higher for sun-lit leaves comparing with shaded leaves (MV, p < 0.0001; HF, p = 0.0182).
Chlorophyll a/b was also significantly higher for sunlit leaves in both sites (MV, p <
0.0001; HF, p < 0.0001). Similarly, LMA and C_{mass} were significantly higher in the sun-
lit leaves. The only exception was N_{mass}, for which both sun-lit and shaded leaves were
indistinguishable throughout the two seasons (Fig. 3b).

*Seasonal variability of leaf spectral properties*

The full leaf reflectance and transmittance spectrum showed significant variability
in both amplitude and shape (Fig.4). The visible (VIS, 400 – 700 nm) and near infrared
(NIR, 700-1000 nm) changed dramatically throughout the season. While shortwave
infrared (SWIR, 1000-2500 nm) was relatively stable. Data from Martha’s Vineyard
showed stronger variability in NIR comparing to those from Harvard Forest. Leaf spectra collected in this study was in agreement with past studies (e.g., (Zhang et al., 2007; Asner & Martin, 2008)). The spectral variations in VIS were mainly related to chlorophyll, carotenoids and anthocyanins (Sims & Gamon, 2002; Gitelson et al., 2006; Feret et al., 2008). NIR was related to LMA and leaf internal structure (Slaton et al., 2001), with additional contributions from leaf water content (Cheng et al., 2011). Leaf N affects the SWIR reflectance, especially around ~2000 nm (Kokaly et al., 2009).

Fig. 5 shows the seasonal variations of individual bands. The R, G, and B reflectance at both sites showed a hump-shape pattern (Fig. 5a, 5c): all of them decreased in the beginning of the season; and increased in the end of the season after a stable summer. The NIR from MV showed a consistent decline in the mid-summer and then increased in the fall, while the NIR from HF is relatively stable throughout the season. Leaf transmittance at each band had the similar patterns to the reflectance (Fig. 5b, 5d).

Comparisons of methods to estimate leaf traits

We compared the four methods to estimate leaf traits from leaf spectra. Overall, BMA consistently outperformed the other methods in estimating leaf traits, in both MV and HF (Table 2 and Table 3). The performance of BMA and PLS were close but for a majority of leaf traits BMA was statistically significantly better than PLS. For different leaf traits, the performance of these methods varies, as described in details below.

For both sites, leaf chlorophyll were well estimated by BMA ($R^2 > 0.7$ and NRMSE < 12%) and PLS ($R^2 > 0.67$ and NRMSE < 13%). Simple index for chlorophyll showed larger estimation error, but its performance was close to BMA and PLS,
especially for the MV dataset (Table 2). PROSPECT performed poor comparing to the other methods. The two components of chlorophyll (a and b) were also well captured by leaf reflectance. Similarly, carotenoids were estimated relatively well by BMA and PLS ($R^2 > 0.65$) but the other two methods were relatively poor.

$N_{mass}$ was well presented by leaf spectra especially for the HF dataset ($R^2 > 0.7$ and NRMSE < 10%). BMA was significantly better than PLS. LMA was presented in the leaf spectra too: BMA outperformed the other three methods ($R^2 = 0.68~0.70$ and NRMSE < 13%). Comparing to the other leaf traits, $C_{mass}$ was least presented in the leaf spectra, and the performance of the two methods (BMA and PLS) were similar.

BMA was good at not just estimating the values, but also the seasonal patterns of leaf traits (Fig. 6, Fig. 7). The seasonal patterns of the mean values of measured leaf traits were well captured for all the leaf traits (Table S1): for most of the leaf traits at both sites, the mean values of each sampling date were very well captured by predictions from leaf spectra ($R^2 > 0.9$ except for $C_{mass}$ in HF that $R^2 = 0.76$).

BMA weighting gave the relative importance of each wavelength in predicting a specific leaf trait (Fig. 8). Higher absolute value of the weighting indicates more important contribution of a specific wavelength. Chlorophyll mainly absorb the light in the blue and red wavelengths (400nm and 600-700 nm), where the weighting were the highest. The two components of chlorophyll (a and b) were also mainly contributing to the red/NIR region (600-750 nm), and the main contributing bands for chl b shifted towards red comparing to those for chl a (Fig. 8c, 8d). Carotenoids were mainly represented in the wavelengths around 400-450 nm, which agreed with previous results.
(Ustin et al., 2009). LMA as a structural parameter was largely contributing to the reflectance at NIR and SWIR. $N_{\text{mass}}$ contributed to both visible ($\sim$470-500nm) and SWIR ($\sim$2050 nm). We caution the interpretation of $C_{\text{mass}}$ as this leaf trait was not well captured by the leaf spectra.

**Implications for field sampling design**

Extensive field sampling always cost a lot in terms of labor, time and money. There is always the question of “how much is good enough?” Since the measurements of leaf optical properties are easier (and non-destructive) comparing with the measurements of most leaf traits, this question became that how many destructive measurements of leaf traits to calibrate the models using full leaf spectra was good enough to capture the seasonal variability of leaf traits? We designed the following scenarios to answer this question. In all the scenarios, leaf spectra were still collected weekly, but the leaf traits that were used to calibrate the model were collected at different time of the season. As BMA is the best method for our dataset, we only used BMA to derive the regression models between leaf traits and spectra (Eq. 1).

Scenario 1 was that the leaf traits were only measured one time during the summer (DOY 190-270 in MV, DOY 160-240 in HF). Leaf samples and spectra collected that day were used to calibrate the model. Scenario 2 was that the leaf traits were sampled throughout the summer. Scenario 3 was that the leaf traits were sampled monthly from the start to the end of the season. Scenario 4 was that the leaf traits were sampled biweekly from the start to the end of the season. Scenario 5 was the same as the
sampling division when validating BMA method: 2/3 of the samples were randomly selected to calibrate the model while the remaining 1/3 was used to validate the model.

Generally as the scenarios progress from 1 to 5, RMSE decreased and $R^2$ increased for all leaf traits (Figure 9, Figure S2). The first two scenarios failed to estimate the variability of leaf traits. Scenario 4 (biweekly sampling) was close to Scenario 5, suggesting that increasing the size of calibration dataset did little to increase the predictability. Interestingly, for LMA in Martha’s Vineyard and Chlorophyll in Harvard Forest, monthly sampling (scenario 3) achieved similar predictive power to that of scenario 4 and 5, indicating that monthly sampling was enough at least for these two traits at these sites.

**Discussion**

Leaf traits are key parameters for understanding the ecosystem functioning (Wright *et al.*, 2004; Kattge *et al.*, 2011). The seasonality of leaf traits gained more and more attention recently as an effort to improve our understanding of terrestrial carbon cycle (Grassi *et al.*, 2005; Bauerle *et al.*, 2012; Medvigy *et al.*, 2013). Hyperspectral remote sensing is a useful tool to estimate leaf traits both on the ground or using airborne/spaceborne sensors (Kokaly *et al.*, 2009; Asner *et al.*, 2011; Ollinger, 2011). There has been a few studies that use leaf optical properties to estimate leaf chlorophyll concentration (e.g., Belanger *et al.*, 1995; Zhang *et al.*, 2007). However, there were few efforts to use leaf spectral properties to estimate a combination of leaf traits (pigments, LMA, and N) with high temporal sampling frequency. In addition, there have been few attempts to compare the commonly used methods.
Our two years’ weekly sampled leaf traits are valuable datasets to understand their variations with time and tree heights. The temporal patterns of total chlorophyll and its two major components (chl a and b) agreed with past findings (Zhang et al., 2007). Less commonly measured carotenoids concentration showed similar temporal patterns to that of total chlorophyll ($R^2 = 0.7661$, $p=0.0000$). At the senescence stage, the increasing car/chl ratio suggests that carotenoids were decreasing at a slower pace than chlorophyll (Fig. 2a and c). The time-series of $N_{\text{mass}}$ capture two important features: (1) the seasonal peak at the beginning of the spring, suggesting that nitrogen was allocated to the leaves early in the season. As leaves grown mature, other types of elements such as carbon accumulated at a faster ratio, result in an increase of $C_{\text{mass}}$ and decrease of $N_{\text{mass}}$. (2) A decline of $N_{\text{mass}}$ by the end of the season, which is presumably caused by the nitrogen resorption (Killingbeck, 1996). $N_{\text{mass}}$ and LMA was relatively stable in both sites during the summer (Fig. 3a and 3b), thus leaf age does not appear to be affecting the nitrogen content during the peak season (Field & Mooney, 1983). Our datasets also confirm the allocation theory that trees allocate most of the resources to the top of the canopy: sunlit leaves have higher chlorophyll concentration and LMA throughout the entire growing season (Fig. 1a, 1e and Fig. 3a and 3d) (Chapin et al., 2011). Sunlit leaves also need more carotenoids to protect themselves from high radiation (Demmig-Adams & Adams, 2000). As the seasonal changes of nitrogen and chlorophyll are the major contributors to the temporal variability of photosynthetic capacity (Feng & Dietze, 2013), high temporal frequency measurements of leaf traits could be useful for understanding the temporal and spatial variability of photosynthesis (Wilson et al., 2000).
Our results suggested that leaf optical properties can be used to capture the seasonal variability of most leaf traits (Table 2, Table 3), especially the seasonal patterns of the mean values of leaf traits (Table S1). Trivial changes on the seasonal patterns of leaf traits were clearly tracked by leaf optical properties. This is an important result as collecting leaf spectra cost less both in terms of time and money, and it allows repeat sampling of the same leaves throughout the season. The result also has implications for the current and future use of field spectrometers that measure leaf reflectance at high temporal frequency (e.g., Hilker et al., 2009). Our well calibrated model using BMA can be used on leaf reflectance to track the seasonality of multiple leaf traits. Simple indices can be an alternative for the estimation of total chlorophyll concentration when there are limits on the instruments and budget (ASD costs about $50k while two-band LED sensors can be as cheap as ~$700, e.g., Garrity et al., 2010; Ryu et al., 2010).

As expected, the two methods exploiting the full wavelength to estimate leaf traits – BMA and PLS – performed the best, and BMA was significantly better than PLS (Table 2, Table 3). Although the absolute value of improvement was not large, the important finding is that BMA consistently outperform other methods, suggesting that BMA at least is a useful alternative to the other methods. The simple indices and PROSPECT were close to BMA and PLS in estimating total chlorophyll concentration, but not for the carotenoids and LMA. This suggests that the leaf traits variability in our datasets were not fully captured by the simple indices and PROSPECT, albeit being calibrated by extensive datasets (Féret et al., 2011). Incorporating more datasets to the calibration of simple indices and PROSPECT could potentially improve the performance of these methods. Another advantage of BMA is that it clearly showed the wavelengths
that were important for the estimation of certain leaf traits (Fig. 8). It has implications for the design of multi-band sensors and imagers as it can select the wavelengths that are most useful for the leaf traits of interest (Ryu et al., 2010; Nijland et al., 2014).

Our leaf traits time-series showed the critical time windows to capture their seasonality. For example, LMA showed dramatic changes in the early season, thus the sampling and calibration process needs to include the data at this stage. Similarly, Nmass was relatively stable in the mid season, and most of the variations occurred in the early and end of season, which makes the sampling at these time frames important. It is also why in the comparisons between scenarios, the first two scenarios that only consider the variability of leaf traits in the summer failed. Monthly and even biweekly sampling should be considered, at least for the four temperate deciduous species examined in this study.

**Conclusion**

The seasonality of leaf traits is an important factor to understand the plant functioning and terrestrial carbon cycle (Wilson et al., 2000; Bauerle et al., 2012). Hyperspectral remote sensing has long been used to estimate leaf traits, but fewer applications were to track the seasonal variations of leaf traits. Here we collected two years’ weekly leaf traits and spectra in two temperate deciduous forests. The leaf traits and spectra showed significant variations throughout the season. By comparing three categories of method, we found that the recently developed method – Bayesian Model Averaging – performed consistently better than the other methods. In addition, BMA successfully provided the band selection scheme for all the leaf traits that are consistent
with our current knowledge. Consequently, our results support the use of full spectra to estimate leaf traits. Current study was focusing on the leaf level relationship between leaf traits and optical properties. An important next step is to upscale the analysis from leaf level to canopy level, which will have implications for near-surface, airborne and satellite remote sensing (Verhoef & Bach, 2007).

Reference


Couture JJ, Serbin SP, Townsend PA. 2013. Spectroscopic sensitivity of real-time, rapidly induced phytochemical change in response to damage. *New Phytologist*: n/a-n/a.


Dillen SY, de Beeck MO, Hufkens K, Buonanduci M, Phillips NG. 2012. Seasonal patterns of foliar reflectance in relation to photosynthetic capacity and color index in two co-occurring tree species, Quercus rubra and Betula papyrifera. *Agricultural and Forest Meteorology* 160(0): 60-68.


Table 1 Simple indices used in this study. These indices were calibrated using extensive datasets (Feret et al. 2011). Leaf traits were calculated based on a polynomial relationship: leaf trait = a × index² + b × index + c.

<table>
<thead>
<tr>
<th>Leaf traits (µg/cm²)</th>
<th>Index</th>
<th>Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chl</td>
<td>((R_{780}-R_{712})/(R_{780}+R_{712}))</td>
<td>40.65 121.88 -0.77</td>
</tr>
<tr>
<td>Car</td>
<td>((R_{800}-R_{530})/(R_{800}+R_{530}))</td>
<td>8.09 11.18 -0.38</td>
</tr>
<tr>
<td>LMA</td>
<td>((R_{1368}-R_{1722})/(R_{1368}+R_{1722}))</td>
<td>-0.1004 0.1286 -0.0044</td>
</tr>
</tbody>
</table>


Table 2 Comparisons among three methods in terms of the goodness-of-fit (RMSE and $R^2$) for the dataset from Martha’s Vineyard of year 2011. The numbers in the parenthesis are normalized RMSE. * mark means the results are statistically different to the other methods at the significance level of $p<0.05$. Note that as simple indices were derived from independent datasets (Feret et al. 2011), the validation dataset for simple indices was the entire dataset we collected. Similarly, the validation dataset from PROSPECT inversion was the entire dataset.

| Leaf traits | RMSE (NRMSE) | | | R$^2$ | | | | |
|-------------|--------------|------------|-----------|-----------|------------|-----------|------------|-----------------|-----------------|
|             | Simple indices | BMA | PLS | PROSPECT | Simple indices | BMA | PLS | PROSPECT | Simple indices | BMA | PLS | PROSPECT |
| Total Chl   | 7.3383 (0.1257) | **7.0574*** (0.1206) | 7.4663 (0.1276) | 17.7046 (0.3025) | 0.6751 | **0.7026*** | 0.6780 | 0.4940 |
| Chl a       | **5.2045*** (0.1197) | 5.6488 (0.1290) | 0.7062* | 0.6720 |
| Chl b       | **1.9633*** (0.1176) | 2.0602 (0.1234) | 0.6764* | 0.6574 |
| Car         | 2.0040 (0.1460) | **1.4711*** (0.1072) | 1.5465 (0.1127) | 0.3647 | **0.6586*** | 0.6308 |
| Nmass       | **0.3223*** (0.0750) | 0.3582 (0.0834) | 0.5814* | 0.5165 |
| Cmass       | **0.7446*** (0.1541) | 0.7813 (0.1617) | **0.4878** | 0.4781 |
| LMA         | 32.0499 (0.2016) | **22.6712*** (0.1383) | 23.3170 (0.1464) | 72.8701 | 0.4099 | **0.7046*** | 0.6872 | 0.1512 |
Table 3 Comparisons among three methods in terms of the goodness-of-fit (RMSE and $R^2$) for the dataset from Harvard Forest of year 2012. The numbers in the parenthesis are normalized RMSE. * mark means the results are statistically different to the other methods at the significance level of $p<0.05$. Note that as simple indices were derived from independent datasets (Feret et al. 2011), the validation dataset for simple indices was the entire dataset we collected. Similarly, the validation dataset from PROSPECT inversion was the entire dataset.

| Leaf traits | RMSE (NRMSE) | | | | | R$^2$ | | | |
|-------------|--------------|--------------|--------------|--------------|--------------|
|             | Simple indices | BMA | PLS | PROSPECT | Simple indices | BMA | PLS | PROSPECT |
| Total Chl   | 6.1014 (0.1197) | 5.4861 (0.1076) | 5.5591 (0.1091) | 13.1005 | 0.7051 | 0.7641 | 0.7582 | 0.6638 |
| Chl a       | 3.9914 (0.1043) | 4.0697 (0.1063) | | | 0.7650 | 0.7568 |
| Chl b       | 2.0373 (0.0890) | 2.0734 (0.0906) | | | 0.6610 | 0.6537 |
| Car         | 1.6787 (0.2052) | 1.1890* (0.1454) | 1.2514 (0.1530) | 4.8806 | 0.2627 | 0.5305* | 0.4892 | 0.1071 |
| $N_{\text{mass}}$ | 0.3856* (0.0975) | 0.5306 (0.0890) | | | 0.7291* | 0.5627 |
| $C_{\text{mass}}$ | 1.4752* (0.1230) | 1.7210 (0.1434) | | | 0.2387 | 0.2182 |
| LMA         | 12.7339 (0.1625) | 9.6210* (0.1228) | 10.9467 (0.1397) | 37.1222 | 0.4355 | 0.6852* | 0.6120 | 0.0558 |
Table S1  Coefficient of determination ($R^2$) between the mean values of observed leaf traits and predicted leaf traits at both Martha’s Vineyard (MV) and Harvard Forest (HF).

<table>
<thead>
<tr>
<th>Leaf traits</th>
<th>MV</th>
<th>HF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Chl</td>
<td>0.9568</td>
<td>0.9540</td>
</tr>
<tr>
<td>Car</td>
<td>0.9468</td>
<td>0.8504</td>
</tr>
<tr>
<td>N_mass</td>
<td>0.9017</td>
<td>0.9439</td>
</tr>
<tr>
<td>C_mass</td>
<td>0.9185</td>
<td>0.7620</td>
</tr>
<tr>
<td>LMA</td>
<td>0.9188</td>
<td>0.9223</td>
</tr>
</tbody>
</table>
Figure 1 Seasonal patterns of pigments of sunlit/shaded leaves from two deciduous forest sites. Martha’s Vineyard, year 2011: (a) Total chlorophyll; (b) chlorophyll a; (c) chlorophyll b; (d) carotenoids. Harvard Forest year 2012: (e) Total chlorophyll; (f) chlorophyll a; (g) chlorophyll b; (h) carotenoids. Each dot is the mean value of all the samples collected that day. Error bars are standard deviations.
Figure 2 Seasonal patterns of the ratio between leaf chlorophyll and carotenoids (Chl/Car) (a) on Martha’s Vineyard and (c) in Harvard Forest, and the ratio between leaf chlorophyll a and b (Chl a/b) (b) on Martha’s Vineyard and (d) in Harvard Forest. Each dot is the mean value of all the samples collected that day. Error bars are standard deviations.
Figure 3 Seasonal patterns of biochemical and biophysical properties of sunlit/shaded leaves from two deciduous forest sites. Martha’s Vineyard, year 2011: (a) Leaf mass per area (LMA); (b) mass-based nitrogen concentration; (c) mass-based carbon concentration. Harvard Forest, year 2012: (d) Leaf mass per area (LMA); (e) mass-based nitrogen concentration; (f) mass-based carbon concentration. Each dot is the mean value of all the samples collected that day. Error bars are standard deviations.
Figure 4 Examples of leaf directional-hemispherical reflectance and transmittance measured on (a, b) Martha’s Vineyard and in (c,d) Harvard Forest.
Figure 5 Seasonal patterns of the reflectance and transmittances at individual bands. Each dot was the mean value of each day and whiskers as the standard deviation. Data from Martha’s Vineyard are (a) reflectance and (b) transmittance; data from Harvard Forest are (c) reflectance and (d) transmittance.
Figure 6 Observed leaf traits and predicted leaf traits by Bayesian Model Averaging for the data from Martha’s Vineyard, 2011. The solid dots are mean values from observations (including both sunlit and shaded leaves) with error bars indicating standard deviations; the empty circles are mean values from predictions with error bars for standard deviations.
Figure 7  Observed leaf traits and predicted leaf traits by Bayesian Model Averaging for the data from Harvard Forest, 2012. The solid dots are mean values from observations (including both sunlit and shaded leaves) with error bars indicating standard deviations; the empty circles are mean values from predictions with error bars for standard deviations.
Figure 8 The weightings of the Bayesian Model Averaging models for the data from Martha’s Vineyard. Prior to calculating the model parameters (Beta), the data were standardized so that the absolute values of Beta represent the relative importance of the specific wavelength. The first panel (a) shows an example of leaf spectra as a reference of the locations of the weightings in the lower panels.
Figure 9 The change of RMSE and $R^2$ under five scenarios using BMA for the data from Martha’s Vineyard (see section “Implications for field sampling design”) for (a) total chlorophyll; (b) carotenoids; (c) $N_{\text{mass}}$; (d) LMA. Black dots denote RMSE and black upper triangles denote $R^2$. The red dots and triangles are the mean value under scenario 5, in which 2/3 of the samples were randomly selected to calibrate the model, while the remaining 1/3 of the samples were used to validate the model.
Figure S1 Comparison between pigment concentrations of sun-lit and shaded leaves from two sites.
Figure S2 The change of RMSE and $R^2$ under five scenarios using BMA for the data from Harvard Forest (see section “Implications for field sampling design”) for (a) total chlorophyll; (b) carotenoids; (c) $N_{\text{mass}}$; (d) LMA. Black dots denote RMSE and black upper triangles denote $R^2$. The red dots and triangles are the mean value under scenario 5, in which 2/3 of the samples were randomly selected to calibrate the model, while the remaining 1/3 of the samples were used to validate the model.
Chapter 5

Seasonal pattern of solar-induced fluorescence as a proxy for canopy photosynthesis in a temperate deciduous forest

Xi Yang\textsuperscript{1,2}, Jianwu Tang\textsuperscript{2,1}, John F. Mustard\textsuperscript{1}, Jung-Eun Lee\textsuperscript{1}, Micol Rossini\textsuperscript{3}, Joanna Joiner\textsuperscript{4}, J. William Munger\textsuperscript{5}, Andrew D. Richardson\textsuperscript{6}

\textsuperscript{1}Department of Geological Sciences, Brown University, Providence, RI, USA

\textsuperscript{2}The Ecosystems Center, Marine Biological Laboratory, Woods Hole, MA, USA

\textsuperscript{3}Remote Sensing of Environmental Dynamics Laboratory, DISAT, Universit\'a degli Studi Milano-Bicocca, Milan, Italy

\textsuperscript{4}NASA Goddard Space Flight Center, Greenbelt, MD, USA

\textsuperscript{5}School of Engineering and Applied Sciences and Department of Earth and Planetary Sciences, Harvard University, Cambridge, MA, USA

\textsuperscript{6}Department of Organismic and Evolutionary Biology, Harvard University, HUH, 22 Divinity Avenue, Cambridge, MA, USA

To be submitted to

Geophysical Research Letters
Abstract

Photosynthesis in the terrestrial ecosystems contributes to the largest carbon flux in the global carbon cycle. The use of solar-induced fluorescence (SIF) as a proxy of photosynthesis at the ecosystem scale (Gross Primary Production, GPP) is a critical emerging technology. Satellite measurements of SIF were found to be significantly correlated with GPP, and several ground campaigns suggested that SIF could improve the GPP estimation. However, the robustness of using SIF as a proxy for GPP under different climate conditions, growth stages and vegetation types has not been explored. Here we presented the first-ever high temporal frequency (5 minutes) measurement of SIF in a temperate deciduous forest. Concurrently, we estimated GPP with the eddy covariance method. We found a strong linear relationship between daily mean SIF and GPP ($r^2=0.725$), and between SIF and absorbed photosynthetically active radiation ($r^2=0.705$). The seasonal patterns of ground and satellite-derived SIF matched well. These results suggest strong evidence that SIF is a good proxy for direct measurements of canopy photosynthesis.

Key words:

Plant physiology, remote sensing, spectroscopy, fluorescence

Key points:

- A novel system for continuous measurement of solar-induced fluorescence was developed
- Fluorescence is an indicator of canopy photosynthesis and absorbed photon
- The seasonal patterns of ground and satellite fluorescence matched well
1. Introduction

Photosynthesis controls the largest flux in the global carbon cycle and is the key to support most of the life on Earth [Demmig-Adams and Adams, 2000]. However, direct measurement of photosynthesis on the ecosystem scale, or gross primary production (GPP), is challenging because photosynthetic carbon fluxes is accompanied by respiratory carbon fluxes. Spatially explicit estimation of vegetation photosynthesis at the ecosystem scale can provide important information on terrestrial carbon budget about when, where and how much carbon dioxide was absorbed. Currently three methods are used for the estimation of GPP globally: (1) diagnostic models calibrated by measurements at eddy covariance tower [Beer et al., 2010]; (2) satellite measurements of vegetation activity with vegetation indices and climate variables integrated through a modeling approach [Zhao et al., 2005]; (3) process-based models integrated in the earth system models [Lawrence et al., 2011]. Uncertainties with models and vegetation indices can propagate to the process of estimating global GPP [Beer et al., 2010], calling for other independent measurements of GPP.

Fluorescence is always re-emitted as a result of leaking of photons during the photosynthesis. This phenomenon provides a way to estimate photosynthesis using fluorescence [Baker, 2008]. Recently, the development of retrieving solar-induced fluorescence (SIF) from space (e.g. the Japanese Greenhouse Gases Observing Satellite, GOSAT) provides an alternative for estimating global photosynthesis from space [Frankenberg et al., 2011; Joiner et al., 2011]. Comparisons with other estimation methods of GPP globally suggested a significant and strong correlation between SIF and GPP. However, small-scale, field-based studies to explore this SIF-GPP relationship are strongly needed to validate the satellite-based results and test the robustness of SIF-GPP.
Past works on using fluorescence to probe the photosynthesis have been intensely studied in the lab using excitation light sources [Baker, 2008]. Recently there have been some field studies on using SIF to estimate GPP [Meroni et al., 2009]. However, a year-round, high temporal frequency dataset of SIF that parallels the CO₂ flux measurements using eddy covariance towers has been left unexplored. Thus the robustness of SIF-GPP relationship has not been thoroughly assessed throughout the growing season. Furthermore, most studies have been conducted over cropland or shrub, while deciduous forests were less covered [Rascher et al., 2009; Zarco-Tejada et al., 2012]. On the other hand, there are few continuous measurements of SIF by ground-based spectrometer that has the similar spectral resolution as that of GOSAT.

In this study, we developed a novel spectrometric system and obtained the first-ever dataset of canopy solar-induced fluorescence over temperate deciduous forests at high temporal frequency every day between June and October 2013. We used data from a nearby eddy covariance tower to estimate GPP. Using these measurements we aim to address the following questions: (1) how does SIF change seasonally in a temperate deciduous forest? (2) How is SIF related to GPP and controlled by environmental factors? (3) How does the ground-based observation of SIF compare with satellite observation of SIF and GPP? Answering those questions can provide important information regarding the use of SIF as the proxy for canopy photosynthesis.

2. Methods

2.1. Harvard forest environmental and CO₂ exchange measurements

Our study site is in Harvard Forest (42.538N, 72.171W), a mixed deciduous forest. The dominating deciduous tree species were red oak (*Quercus rubra*) and red maple
(Acer rubrum), with a few scattered yellow birch (Betula alleghaniensis). The forest age was about 70-100 years. The long-term annual mean temperature was about 7.5°C, and the annual precipitation was 1200 mm.

Half-hourly environmental data were collected in 2013. These data include air temperature, relative humidity, air pressure, above canopy photosynthetically active radiation (PAR\text{above}), reflected PAR (PAR\text{reflect}), and the average of understory PAR (PAR\text{under}) from three PAR sensors, diffuse radiation (RAD\text{diff}) and total radiation (RAD\text{tot}). We took the days when the daily mean RAD\text{diff}/RAD\text{tot}>50% as cloudy. The absorbed PAR (APAR) was calculated as:

\[
APAR = PAR_{\text{above}} - PAR_{\text{reflect}} - PAR_{\text{under}}
\]  

In addition, CO₂ and water exchange between the forest and atmosphere every 30 minutes was measured by eddy covariance method (on Harvard Forest EMS tower). We used the method in Reichstein et al. [2005] to partition daytime NEE into GPP and ecosystem respiration. The Light Use Efficiency (LUE) was calculated as GPP/APAR. LED sensors mounted on the top of the tower measured the reflectance at 860 nm, 655 nm and 470 nm, which were used to calculate Normalized Difference Vegetation Index (NDVI), and Enhanced Vegetation Index (EVI) [Huete et al., 2002].

### 2.2. Ground-based measurements of solar-induced fluorescence

We designed a novel system (FluoSpec) to measure SIF every 5 minutes during the day from June 21th to October 26th, 2013 about 5 meters above the canopy (Fig. 1). The key component of FluoSpec is a spectrometer capable of measuring spectra at a spectral resolution of ~0.13 nm between 680 nm and 760 nm (HR2000+, OceanOptics, Inc., Dunedin, FL.). The spectrometer was connected to an inline fiber optic shutter
(FOS-2x2-TTL, OceanOptics, Inc.), which has two ports that were connected to two fiber optics, one of which was pointing towards the tree canopy (viewing zenith angle: 30°), while the other one was attached with a cosine corrector (CC-3, OceanOptics, Inc.) towards the sky. The shutter opens one port while closes the other port to collect the signal from either the canopy or sky at one time. The spectrometer first collected the solar irradiance (integrating time: 5 seconds), then immediately the shutter switched to the canopy radiance (integrating time: 5 seconds). Every 5 minute the system completed a measuring cycle with one irradiance and 59 canopy radiance, which was averaged to a single measurement. Each measurement of irradiance or radiance was accompanied by a measurement of dark current, which was subtracted from the irradiance/radiance. We performed radiometric and wavelength calibration prior to and one time during the field campaign using radiometric calibration light source (LS-1-CAL, OceanOptics, Inc.) and wavelength calibration light source (HG-1, OceanOptics, Inc.). The raw data collected by the spectrometer was then converted to irradiance (mW/m²/nm) and radiance (mW/m²/sr/nm) [Perez-Priego et al., 2005]. We used the Spectral Fitting Methods (SFM) to extract the SIF at 760nm, which is the oxygen absorption (O₂-A) band [Meroni et al., 2009]. We conducted quality control on the extracted data that when the fitting algorithm R² <0.99, we discarded the data. We calculated daily mean SIF (SIF<sub>mean</sub>) to represent the emission of SIF of each day. SIF<sub>yield</sub> was calculated as

\[ SIF_{yield} = \frac{SIF_{mean}}{APAR_{mean}} \]  

(2)

where APAR<sub>mean</sub> is the daily mean APAR (umol/m²/sec).

2.3. Satellite measurements of solar-induced fluorescence
We compared the ground-based SIF and satellite-based SIF measurements. GOME-2 (The Global Ozone Monitoring Experiment-2), is a UV/visible spectrometer that measures the top-of-atmosphere radiance between 240 and 790 nm. Level 1B data that covers 590-790 nm (resolution: 0.5 nm) were used to estimate SIF [Joiner et al., 2013]. The spatial resolution of GOME-2 product is 40×80 km. We extracted the estimated SIF for the pixel containing Harvard Forest between June and November in year 2007-2012.

3. Results

The seasonal pattern (June to November, 2013) of daily mean SIF (SIF\text{mean}) matched well with GPP estimated from the measurements by a nearby eddy covariance tower (Fig. 2a). SIF\text{mean} gradually decline from 0.8~1.0 mW/m²/sr/nm during the summer to ~0.2 mW/m²/sr/nm by the end of the growing season. Similarly, daily GPP decreased from ~12 g C/m²/day to 1 g C/m²/day. Both SIF and GPP showed large day-to-day variations, which was correlated with the variations in PAR and APAR (the R² between PAR and APAR is 0.996. Fig. S1b and Fig. S2a and S2d, and Fig.S4). VPD and air temperature only explained a small amount of the variations in SIF and GPP (for SIF, R² = 0.352 and 0.346; for GPP, R² = 0.115 and 0.306. Fig. S2).

We found a strong correlation between SIF\text{mean} and GPP (R²= 0.725, Fig. 3a), and SIF\text{mean} and APAR (R²=0.705, Fig. 3d), while the vegetation indices (NDVI, EVI) clearly saturated at high GPP and APAR (Fig. 3b-c, e-f). Specifically, when GPP > 8 g C/m²/day, NDVI and EVI showed little change, which was the case for most of the days between June and September. In contrast, SIF\text{mean} was able to track both low and high value of GPP and APAR. SIF\text{yield} and LUE were generally higher throughout the season during the
cloudy days than those during the sunny days. This resulted in a relatively stable LUE/SIF yield ratio (Fig. 2e). We found that the relationship between GPP and SIF was indistinguishable between sunny and cloudy days (Fig. 3a). On the contrary, the SIF yield given the same APAR was generally higher during cloudy days (Fig. 3d).

Diurnal SIF measurements showed a typical hump shape with a steady increase in the morning and decline in the afternoon. Fig. 4 showed two examples of the diurnal pattern of SIF from June and September, respectively. The diurnal patterns are similar to the diurnal patterns of GPP. However, the diurnal patterns of SIF do not exactly follow those of the GPP: SIF reached a peak later in the day than GPP, and declined earlier than GPP, resulting in a sharper peak. We will analyze the diurnal pattern in details in a separate analysis. The SIF yield in both days were quite stable during most of the day time.

The ground-based SIF was shared similar seasonal patterns with the satellite-based SIF from GOME-2 (Fig. 5). Overall, the mean value of GOME-2 SIF showed a decreasing trend from the mid-summer, consistent with our ground-based estimation of SIF. The mean value of GOME-2 SIF was higher than our ground measurements at 9:30AM, which the local time of GOME-2 passing, partly because that GOME-2 SIF was measured at 740nm. For example, the monthly SIF from GOME-2 around DOY 200 was about ~3 mW/m²/sr/nm, while ground-observation of SIF at 9:30 was ~0.6 mW/m²/sr/nm, and the daily mean is about 0.8 mW/m²/sr/nm.

4. Discussion and conclusion

Recent studies have provided satellite or field-based evidence suggesting that SIF could potentially improve the estimation of GPP (e.g., [Damm et al., 2010; Middleton et al., 2009; Zarco-Tejada et al., 2013]). However, to the best of our knowledge, this is the
first study to continuously measure SIF over diurnal and seasonal time scales in a temperate deciduous forest. These measurements provide us a unique dataset to examine how well the seasonal patterns of SIF and GPP match, and what are the major environmental drivers of SIF. Lastly we were able to use this measurement to vicariously validate satellite observations of SIF.

Our results demonstrated that SIF can be used as a proxy to capture the seasonal variability of canopy photosynthesis. As LUE and SIF\(_{\text{yield}}\) generally changed at same direction and similar relative magnitude, LUE/SIF\(_{\text{yield}}\) was relatively stable throughout the season (Fig. 2e). As GPP \(\approx (\text{LUE}/\text{SIF}_{\text{yield}}) \times \text{SIF}\) [Guanter et al., 2014], there is a significant linear relationship between GPP and SIF (R\(^2\) = 0.725). Our results did not rule out the possibility of other mathematical forms of the relationship between GPP and SIF, for example, a hyperbola function. Additional measurements including the spring season would provide data to establish a more robust relationship. Nonetheless, this result provided support to the future use of satellite SIF product to assess the photosynthetic activity [Guanter et al., 2014], especially over forests. Vegetation indices such as NDVI and EVI that are commonly used as indicators of canopy greenness showed clear saturation effect when comparing with GPP, APAR and fAPAR (Fig. 3, Fig. S3). This result suggested that SIF was a measurement of ecosystem functioning and not simply the change of canopy greenness.

Our measurements suggest that SIF generally decreases from mid-summer to late fall, while superimposed on this pattern was a day-to-day variation highly correlated with PAR (and thus APAR, as in our study we found a nearly 1:1 relationship between the two variables, R\(^2\) = 0.996, Fig. S4). Although the SIF-APAR relationship was different under
sunny and overcast days, a strong linear relationship between SIF and APAR regardless of sky conditions still exists. Note that the SIF we calculated were from the near infrared region (760 nm), which is completely different wavelength compared with the PAR measurement (400-700 nm). Thus, the significant linear correlation between SIF and APAR suggested that SIF could be an independent indicator of APAR, complementing the existing satellite products or ground observation methods based on the above and below canopy measurements of PAR [Frankenberg et al., 2012; Jenkins et al., 2007; Knyazikhin et al., 1998]. The observed relationships between SIF and GPP/APAR in this study were mainly focused on the seasonal patterns. To understand how the diurnal patterns of SIF are related to those of GPP/APAR, a photosynthesis model that incorporated fluorescence can be useful (Yang et al. in prep).

Since the ground-based and satellite-based measurements of SIF were essentially from different spatial scales, a comparison focusing on the seasonal patterns instead of the absolute value of SIF is more realistic. In addition, based on the theoretical spectrum of SIF, SIF around 740 nm is generally higher than that from 760 nm [van der Tol et al., 2009]. In the future, more rigorous comparisons between ground-observation, airborne and satellite measurements (e.g., OCO-2, [Frankenberg et al., 2014]), such as the FLEX mission, could be useful to further validate the use of SIF as the proxy of GPP, especially over biomes that were under-represented, for example, arctic tundra and wetlands [Rocha and Shaver, 2010; Rocha and Goulden, 2010].

Acknowledgements

We thank Dr. Pablo Zarco-Tejada for the help with the design of FluoSpec. We thank Mark Vanscoy from Harvard Forest, and Jerome Girard from MBL with the
installation of FluoSpec. We thank Marc Mayes, Shalanda Grier, Will Werner, and Zhunqiao Liu for the help with fieldwork.

References


cycle from GOSAT: Patterns of plant fluorescence with gross primary productivity, 
*Geophysical Research Letters*, 38(17), L17706.


Figure 1 FluoSpec system and an example of the collected data. (a) a sketch map shows the settings of the instruments. The two red rectangles indicate two fiber optics that were connected to the spectrometer on the ground. The tower is about 40 meters and the fiber
optics were about 30 meters above the ground. (b) The flow diagram shows the settings of the system (for details, please see the descriptions in the text); (c) an example of the irradiance (orange line) and top-of-canopy (TOC) radiance (blue line) measured by FluoSpec. Reflectance (black line) was calculated as TOC radiance/(irradiance/π). A spectrum of chlorophyll fluorescence simulated by the SCOPE model (van der Tol et al. 2009) was presented here for reference (red line). Note in this study we only extracted the fluorescence signal around 760 nm.
Figure 2 Seasonal patterns of (a) daily mean solar-induced fluorescence (SIF) compared with Gross Primary Productivity (GPP) estimated from eddy covariance tower measurements; (b) Absorbed Photosynthetic Active Radiation (APAR); (c) SIF yield (SIF/APAR), green dots are from sunny days (diffuse/total radiation < 50%), and black dots are from cloudy days (diffuse/total radiation > 50%); (d) Midday Light Use Efficiency (LUE); (e) the ratio between LUE and SIF yield; and (f) NDVI and EVI.
Figure 3 Scatter plots between daily integrated GPP and (a) Daily mean SIF; (b) NDVI; and (c) EVI. The scatter plots between daily mean APAR and (d) daily mean SIF; (e) NDVI; and (f) EVI. In (a), red dots are from sunny days, red line is the linear regression between sunny day GPP and SIF: GPP = 13.21*SIF + 0.19 (r² = 0.764, p=0.0000); blue dots are from cloudy days, and blue line is the linear regression between cloudy day GPP and SIF: GPP = 10.76*SIF + 1.97 (r² = 0.685, p=0.0000). For all the days (black line), GPP = 11.82*SIF + 1.19 (r² = 0.725, p=0.0000).

In (d), red dots are from sunny days, red line is the linear regression between sunny day APAR and SIF: APAR = 1004.73*SIF + 303.64 (r² = 0.818, p=0.0000); blue dots are from cloudy days, and blue line is the linear regression between cloudy day APAR and SIF: APAR = 741.59*SIF + 231.43 (r² = 0.786, p=0.0000). For all the days (black line), APAR = 970.36*SIF + 250.29 (r² = 0.705, p=0.0000).
Figure 4 Examples of the diurnal patterns of solar-induced fluorescence (SIF), gross primary productivity (GPP), Absorbed Photosynthetic Active Radiation (APAR), and SIF yield in (a) the summer, day of year 175; and (b) the fall, day of yield 250.
Figure 5 Comparisons between ground-measured SIF and GOME-2 derived SIF. (a) ground-measured SIF at 09:30 AM and GOME-2 SIF. (b) ground-measured daily mean SIF and GOME-2 SIF. The solid green dots are ground-measured SIF during sunny days (less than 50% diffuse radiation). The open dots are ground-measured SIF during cloudy days (more than 50% diffuse radiation). The grey solid dots are the averaged monthly GOME-2 SIF between year 2007 and 2012, with standard deviation indicated by the whiskers.
Fig. S1 The seasonal patterns of (a) daily integrated SIF; (b) Photosynthetically active radiation (PAR); (c) Vapor pressure deficit (VPD); and (d) air temperature (Air T).
Fig. S2 Relationship between daily mean solar-induced fluorescence (SIF) and (a) daily integrated photosynthetic active radiation (PAR), (b) daily average vapor pressure deficit (VPD), and (c) daily average air temperature. Relationship between daily integrated GPP and (d) PAR, (e) VPD, and (f) air temperature. Solid lines are linear regression and dashed lines indicate 95% confidence intervals.
Fig. S3 Relationship between daily EVI and (a) NDVI, and (b) EVI.
Fig. S4 Relationship between daily mean APAR and PAR. Red solid line is the linear fit.
CHAPTER 6

Epilogue

Xi Yang\textsuperscript{1, 2}

\textsuperscript{1}Department of Geological Sciences, Brown University, Providence, RI, USA, 02912

\textsuperscript{2}The Ecosystems Center, Marine Biological Laboratory, Woods Hole, MA, USA, 02543
How the terrestrial ecosystems respond to climate change, and exert feedbacks to the climate system is one of the key questions in ecology and climate science [Solomon et al., 2007]. The seasonal cycle of plant functioning, such as photosynthesis, is largely influenced by environmental factors including temperature. This work investigates the environmental drivers of the seasonality of plant functioning, using various types of remote sensing techniques at different scales. I started with using digital camera to capture the timing of the beginning of biological spring – budburst (i.e., leaf-out). The phenology model that considers temperature and photoperiod as the major controls was up-scaled to the regional level, and was used for historical reconstruction and prediction of budburst dates (Chapter 2). We were able to use leaf spectra to capture the seasonal variability of multiple key leaf traits (Chapter 3 and 4). We found that solar-induced fluorescence was a good indicator of Gross Primary Productivity (GPP) and Absorbed Photosynthetically Active Radiation (APAR) (Chapter 5).

In the following sections, I offered some thoughts on what improvements can be made based on the current status of this area.

**Phenology modeling and feedbacks to the climate system**

Current understanding of drivers of budburst in the temperate forests is good but not complete; it is still in debate that what are the controls of budburst of different species, specifically, the relative importance of photoperiod in the spring and chilling temperature in the winter [Laube et al., 2014b]. Relative humidity has also been proposed as the driver for budburst [Laube et al., 2014a]. Controlled experiments are useful to understand the relative contributions from co-varying factors, but caution needs to be made when
using saplings’ responses to environmental factors to represent the responses of mature
trees [Vitasse, 2013]. Ultimately, the study of genetic control of vegetation phenology
can provide mechanistic understandings, although current research is mainly focusing on
Arabidopsis [Wilczek et al., 2010; Wilczek et al., 2009]. In addition, understanding the
drivers of phenology of less-represented ecosystems and incorporate those factors in a
modeling framework is crucial. First and foremost thing is to establish routine phenology
observations in biomes like tropical forests and tundra, using both traditional human-
based observations and automated sensors such as digital repeat photography. Satellite
observations will become more useful as the technical and financial difficulties to build
high spatial/temporal/spectral resolution sensors are overcome.

Evidence suggested that budburst can affect the microclimate: the abrupt increase
of the diurnal temperature range ceased after budburst, i.e., the initiation of plant
photosynthesis and transpiration [Schwartz, 1996]. Quantitative analysis of the feedbacks
of shifting growing season to the surface energy balance is rare, but important for the
understanding of vegetation-atmosphere interactions [Richardson et al., 2013]. An
important next step is to examine the consequences of lengthening growing seasons on
the latent/sensible heat, surface albedo, and surface temperature using both observations
and models.

Vegetation spectroscopy and seasonality of leaf traits

Vegetation spectroscopy has been proved to be a powerful tool to estimate leaf
traits non-destructively, either on the ground or remotely (airborne or space-borne).
These efforts can be extended to capture the seasonal variability of leaf traits. On the
ground, automated spectrometers have been developed to measure canopy reflectance at various viewing angles [Hilker et al., 2010]. The planned HyspIRI provides high spectral resolution images, but still is not able to provide high temporal frequency data that can capture the temporal variability of leaf traits. The proposed CubeSat is relatively cheap and easy to build. Thus a network of geostationary CubeSats with hyperspectral capability can revolutionize the remote sensing and ecology community by providing seasonal and even diurnal patterns of leaf traits and other plant physiological properties.

**Solar-induced fluorescence (SIF): monitoring, experiments and modeling**

Comparing with the use of fluorescence in the lab, terrestrial remote sensing of vegetation fluorescence is still in its infancy. Recent developments of the use of solar-induced fluorescence are fast and promising [Frankenberg et al., 2011; Guanter et al., 2014; Joiner et al., 2013; Lee et al., 2013]. There are several important research gaps to fill: 1) sharpening the tool. Spectrometers that have high spectral resolution (~0.1nm) and signal-to-noise ratio (>1000:1) need to be deployed in the future. In addition, spectrometers need to be designed to cover a wide spectral range (ideally the full range of fluorescence, which is from 640 nm to 850nm), and the algorithm to extract fluorescence signals from multiple Fraunhofer lines (the absorption features along the solar spectrum caused by elements in the sun) needs to be developed. It can provide more information on the shape of the fluorescence signal, instead of just the information from one signal wavelength like most field-based measurements are used for (see Chapter 5). 2) Continuous measurements of vegetation fluorescence need to be made over different biomes. Concurrent measurements of plant water stress, leaf photosynthesis, vegetation-atmosphere CO₂ and water exchange can be helpful for the interpretation of fluorescence
data. 3) Measurements of fluorescence under different environmental and nutrient conditions are needed, e.g., water stress gradient, nutrient addition level, and surface warming level. It can be made using the existing controlled experiments [Melillo et al., 2002]. 4) Upscale leaf and canopy scale photosynthesis models that are capable of producing fluorescence to larger scales, and incorporate them into terrestrial biosphere models (such as ED2, Medvigy et al., 2009) and climate models (such as Community Land Model, CLM, Lawrence et al., 2011). This will allow for the use of spatially-explicit satellite measurements of SIF to constrain the models.

References


