Hyperspectral Visible Derivative Spectroscopy for compositional analysis of CPAs in aquatic systems

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Algal bloom on Lake Erie
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(AGU Blogosphere)
Thanks to…

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Collaborators:
- NASA Glenn, OhioView Institutions
- Donna Witter, Sapphire Geoscience Informatics
- Khalid Adem Ali, College of Charleston
- Sushma Parab, KSU Postdoc
- Nick Tufillaro and Curtis Davis
  - Hyperspectral Imager for Coastal Oceanography (HICO) Oregon State University
- Mandy Razzano, Ohio EPA
- Students: N. Bonini, R. Craine, J. Sadallah, N. Wijikoon, D. Fuecht and others
Growing Water Quality Concerns in Lake Erie

- Lake Erie is once more increasingly plagued by toxic algal blooms (CyanoHABs)
- Reduce oxygen levels and cause unwanted taste, color, and odor
- Researchers are looking for ways to monitor, assess, and predict algal blooms

August, 2014
Grand Lake St Marys (photo J. Ortiz)
The problem...

- Remote sensing of lake color gives information on plant biomass, but...

- Lake water is a complex “organic soup”
  - Various types of phytoplankton
  - Colored dissolved organic matter
  - Suspended sediment

All natural samples are mixtures!
Spectral identification of phytoplankton from space

- Different types of phytoplankton have different pigments.
- Pigments have specific absorption and reflectance patterns.
- Spectral shapes can be used to identify different algal phyla.
- Capitalizes on all information available in hyperspectral-resolution spectra.
- But, must **unmix** reflectance spectra.

Graphics: Courtesy of NASA/GSFC.
Our Approach

- **Goal:** Quantify the relationship between phytoplankton pigments and phytoplankton assemblages from Field Samples, Field Spectroradiometers, Remote Sensing data

- **Objectives –**
  - Measure water samples by Visible Near-infrared (VNIR) derivative spectroscopy
  - Match spectral pigment assemblages to known signatures for classes of phytoplankton
  - Compare pigment assemblages to measures of concentration in the lake (chl a, degradation products of chl a and other pigments).
Varimax-rotated Principal Component Analysis (VPCA)

- VPCA is a multivariate statistical technique for extracting important information regarding the dataset.

- This method lets us “unmix” the data!

- We can use VPCA to determine in-water constituents (pigments, clays, iron oxides, etc.) using the visible part of the spectrum.
Case Study 1: Akron Water supply

Collaboration with M. Razzano (OEPA) and D. Witter

Lab-based measurements
Pigment components in Lake Rockland, West Branch and La Due Reservoir
We can identify which types of phytoplankton are present in the pigment assemblages.

- For each sample we have:
  - Pigment assemblage information
  - Cell count assemblages

- We can “unmix” both of these data and compare them to see how they relate...
VPCA of algal data indicates Four Algal Cell Assemblages are present

<table>
<thead>
<tr>
<th>Cell Grouping</th>
<th>Communality</th>
<th>Algal Component 1 (Cyanophytes)</th>
<th>Algal Component 2 (CyanoHAB/Cryptophyte s)</th>
<th>Algal Component 3 (Heterokonts)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Synebra</td>
<td>0.86</td>
<td>0.90</td>
<td>0.04</td>
<td>0.00</td>
<td>-0.23</td>
</tr>
<tr>
<td>Chlorophyta</td>
<td>0.79</td>
<td>-0.83</td>
<td>0.15</td>
<td>-0.03</td>
<td>-0.26</td>
</tr>
<tr>
<td>Cryptophyta</td>
<td>0.90</td>
<td>-0.25</td>
<td>0.36</td>
<td>-0.84</td>
<td>0.05</td>
</tr>
<tr>
<td>Other Cyanophyta</td>
<td>0.97</td>
<td>0.73</td>
<td>0.64</td>
<td>0.15</td>
<td>-0.01</td>
</tr>
<tr>
<td>Dinofyta</td>
<td>0.73</td>
<td>-0.21</td>
<td>-0.55</td>
<td>0.14</td>
<td>0.60</td>
</tr>
<tr>
<td>Euglenophyta</td>
<td>0.76</td>
<td>0.26</td>
<td>0.52</td>
<td>0.59</td>
<td>0.27</td>
</tr>
<tr>
<td>Flagellates</td>
<td>0.97</td>
<td>0.08</td>
<td>0.12</td>
<td>-0.06</td>
<td>0.98</td>
</tr>
<tr>
<td>Other Heterokonts</td>
<td>0.66</td>
<td>-0.17</td>
<td>0.18</td>
<td>0.77</td>
<td>-0.04</td>
</tr>
<tr>
<td>Aphanizomenon&amp;Anabaena</td>
<td>0.79</td>
<td>0.14</td>
<td>-0.88</td>
<td>-0.02</td>
<td>-0.01</td>
</tr>
</tbody>
</table>
Compare the Pigments and Cell Assemblages

<table>
<thead>
<tr>
<th>Pigment Component</th>
<th>Cell Component</th>
<th>Multiple Linear Correlation</th>
<th>Significance level (P-value, df=1,10)</th>
</tr>
</thead>
<tbody>
<tr>
<td>VPCA 1</td>
<td>Algal Component 2 (CyanoHAB)</td>
<td>0.83</td>
<td>0.001</td>
</tr>
<tr>
<td>VPCA 2</td>
<td>Algal Component 1 (Cyanophytes)</td>
<td>0.71</td>
<td>0.010</td>
</tr>
<tr>
<td>VPCA 3</td>
<td>Algal Component 4 (Dinos/Flagellates)</td>
<td>0.70</td>
<td>0.011</td>
</tr>
<tr>
<td>VPCA 4</td>
<td>Detritus</td>
<td>N/A</td>
<td>No significant correlation @ 0.050</td>
</tr>
</tbody>
</table>

VPCA 1-3: Algal Component 2 (CyanoHAB), Algal Component 3 (Heterokonts/Cryptophytes), Algal Component 4 (Dinos/Flagellates). Correlation 0.96, Significance level (P-value, df=1,10) 0.022.
Independent corroboration

Leading component matches derivative spectrum for cultures of HAB forming Aphanizomenon sp. and Anabena sp and a published cyanophyta spectrum

Parab et al, unpublished data
Case Study 2: 2007 and 2011 Western Basin of Lake Erie

- Samples are **mixtures** of different color producing agents (e.g. pigments, CDOM, sediment).
- Peaks and troughs in the Reflectance data relate to different Color Producing Agents.
- Derivative-transformed data accounts for scattering and particle size effects.
- Still need to “unmix” or partition the data.
- Compare Components from Field samples with HICO components.

Ortiz et al. (2013)
Lab Measurements from 2007 Field Samples

Ortiz et al. 2013
Lake Erie hyperspectral pigment assemblage comparison

Leading Component

Wavelength (nm)

VPCA Component Leading

HICO VPCA Component Loading

ASD Component 1 B-G Algae (filtered Lake water)

HICO VPCA 400-700
5nm B-G Algae Loading 1

2007 field results (green) vs.
HAB-forming Blue-Green Algae
Component extracted from HICO image 9-3-11
Lake Erie hyperspectral pigment assemblage comparison
3rd ASD component vs. HICO components

2007 field results (green)
vs. Non-HAB Blue-Green Algae
Component extracted from HICO image 9-3-11
Case study 3: Western Basin CyanoHAB during the 2014 Toledo Water Shutdown (1 Aug 2014)

Source: NOAA Experimental Lake HAB Bulletin
Field sampling from many lakes and different vessels

Photos: J. Ortiz

RV Bowfin: USGS-LEBS
Commercial Fishing boat
RV Muskie: USGS-LEBS
ODNR watercraft
Pontoon boat
Measuring with the ASD FieldSpec HH Spectroradiometer

Photo: L. Liou
Collecting water samples at Grand Lake St. Marys

- Field and Remote Sensing radiometric data is compared with water samples
- Determine how much algae, sediment and dissolved material is in the water
- Measure chemical properties

Photos: J. Ortiz
NASA Glenn S3 Viking Research Aircraft

- Converted US Navy Submarine chaser aircraft
- Equipped with a high resolution, imaging radiometer (NASA Glenn HSI) similar to satellite-based instruments
- Quantifies the color of the surfaces that the sensor images

Source: NASA Glenn
Photos: J. Ortiz
Example data: 8-12-14 USGS CSMI sampling

- Samples collected from 24’ Boston Whaler
- Winds 10-15 NW, overcast with scattered rain showers
- Samples collected at three paired stations in Maumee Bay
Reflectance vs. First Derivative spectra

- Reflectance spectra are sensitive to directional quality of the light affected by
  - Solar viewing angle
  - Sun glint
- Problem is accentuated for non-Lambertian surfaces
- Derivative spectra are less sensitive to these problems.
Influence of wave action on reflectance and first derivative spectra

At each site averaged 2-3 sets of 10 replicates with 30 spectra per replicate. Integration time at 10’s of milliseconds.
Spectral derivative signatures of different lakes

A: GLSM
B: Sandusky Bay
C: Western Basin
Summary

- VNIR derivative spectroscopy quantifies plant pigment assemblages in Case 2 aquatic systems (Akron Reservoirs, Lake Erie, OWC).
- VNIR derivative spectroscopy helps address non-Lambertian scattering effects.
- Ties optical assemblages to phytoplankton phyla.
- Developing a new means of tracking phytoplankton impacts on eutrophication, with implications for anoxia and harmful algal blooms.
- Method can be applied to lab samples, field-based spectroradiometers, Remote Sensing data.
- Well suited for application to HyspIRI: Makes use of all information present in hyperspectral spectra.
Recent Publications

- See Water quality webpage at: http://www.personal.kent.edu/~jortiz/home/wqr.html


