Ocean Optics 2015: Semi-Analytic Reflectance Inversion

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Goals of Laboratory

To experiment with reflectance model inversion by examining the output sensitivity to basis vectors, initialization, reflectance models.

Exercise 1.

You are supplied with an Excel file that provides you with the opportunity to perform a non-linear optimization for reflectance inversion by hand.

The eigenvector worksheet provides you with the constituent absorption and backscattering spectra used as eigenvector inputs for the model.

There are three worksheets each with a measured irradiance reflectance spectra from Roesler and Perry 1995 which span a large optical range. These are the spectra you will model using the provided eigenvectors. Your job is to find the best set of eigenvalues that best reconstruct the measured reflectance spectrum. To help get you going, the OC4 algorithm for chlorophyll estimation is provided for each spectrum.

When you think you have achieved the best fit, (note that rms errors are computed for you), write you eigenvalues on the board with you initials. As each student finds an improved rms, replace the values on the board. These will be compared with those determined by non-linear regression using the Matlab code provided.

Exercise 2.

Now use the Matlab code provided to perform the inversions on a range of reflectance spectra. Use the Rrs_inversion_RP95.m (runs Roesler Perry 1995 with variable wavelengths, data sets) program to run the inversion on the data sets provided. Note that the data set you inverted by hand in Exercise 1 is the West Coast data set (spectra 1, 6 and 11). The following exercises should be performed on these three spectra at minimum. You may also use the other data sets if you are interested and have time.

1. Run the inversion model using 2 nm resolution. How do the retrieved eigenvalues compare with those you determine in the excel file? How well are the reflectance spectra modeled
2. Run the inversion with reduced wavelength resolution:
    a. SeaWiFS wavelengths
    b. MODIS wavelengths

   How different are the retrieved eigenvalues between your hyperspectral inversion and those retrieved at satellite wavelengths? Do the modeled reflectance spectra match the measured spectra to a greater or lesser degree than the hyperspectral results? How do SeaWiFS and MODIS compare to the hyperspectral, which is closer, why do you think this is so?
3. Select the same three spectra as above. Investigate how the retrieved eigenvalues and modeled reflectance spectra vary depending upon how many eigenvectors you use (number of retrieved parameters). Do you find a better fit between modeled and

measured reflectance spectra if you increase the number of fitted parameters? Is there a difference if you use hyperspectral versus MODIS wavelengths?

4. Werdell et al. (2013) found that variations seawater absorption and backscattering due to variations in the temperature and salinity impacted retrieved eigenvalues. Note that the lines of code (53 and 54 shown below) are used to determine the absorption and backscattering by seawater for a given temperature and salinity (15 C and 33ppt by default). What is the variability in retrieved eigenvalues due to large variations in T and S? Try this for a clear water case and a high chlorophyll case.

```
%water basis vectors require temperature T and salinity S, output
water IOPs at wave resolution
 [a_w,bb_w]=water_iops_PF_TScorr(wave,15,33);
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Exercise 3

Curt generated a simulated hyperspectral radiance reflectance data set using Hydrolight (R_L_HL_simulation.dat) Open the excel file for details of each run. Compare the inversion results for this data set between the GSM, QAA and RP95 inversion models at the MODIS wavelengths by running the program Rrs_inversion_comparison_MODIS.m for this data set. Which models works best with which simulated data set? Why do you think this is?

Exercise 4

In lecture we discussed the variations in the early inversion models. One of the largest differences lies in the characterizations of the eigenvectors, particularly that of phytoplankton absorption and backscattering spectra. One of the outputs of the Rrs_inversion_comparison_MODIS.m run is figure(500) which shows the model-specific eigenvectors. Which eigenvector is the most variable in spectral shape between the models? Which the least? Given you experience thus far and in this course, comment on the shapes of these eigenvectors. What changes might you make if you were going to define new eigenvectors (recall these are about 15-20 years old!).

Exercise 5

Based upon the IOCCG workshop in 2006, Werdell et al. (2013) conceived of a generalized ocean color inversion model (gIOP) to retrieve IOPs from ocean color. Recognizing that most of the published inversions to date were more similar than they were different, they provide a code that allows users to select all of various inputs (eigenvectors), models (inversions), and input data (reflectances). Think of this model as a slick front end to the sets of code that you have been provided as part of this lab. Now that you can run the individual codes, you are equipped to be able to run gIOP which is a bit more “black box” on the front end. To run gIOP go to the gIOP_code folder. In Matlab open up the run_giop_cr.m program (note I made some changes to the original code run_giop.m to make graphs of the results). It is really well documented. By commenting and uncommenting various lines you can customize the inversion runs.

1. Run the program as provided. What are the x coefficients printed to the screen?
2. I added code to print out measured and modeled Rrs, retrieved a_{phyt}, a_{CDM}, b_{bp} spectra. How well do the default values used in gIOP do in modeling reflectance?
3. Now change inputs, one at a time, to see what changes in eigenvectors, then models provide improved inversion results. Note your results on the black board. Did other students retrieve better agreement between measured and modeled reflectance spectra using different eigenvectors or models?

Extra things you can do on your own time (not required for class, just for your interest)
You now have the explicit codes for each model and for comparisons. In addition you have all the data from Roesler and Perry 1995 as well as Curt's simulations for a broad range of reflectance spectra. More importantly, you will have your own measure reflectance spectra from the radiometry lab, from the upcoming cruise, and from you Hydrolight simulations. These are paired with IOP measurements for testing the model output. You can also begin to make modifications to the models by redefining the eigenvectors based upon your ideas (if you want to do hyperspectral, build upon the RP95 code as this was optimized for hyperspectral measurements and can be spectrally degraded more easily than taking GSM or QAA and building up to hyperspectral).

Code Supplied

1. Main programs (these call the invert and cost functions)
Rrs_inversion_comparison_MODIS.m (compares RP95, GSM, QAA at MODIS wavelengths)
Rrs_inversion_comparison_SeaWiFS.m (compares RP95 and QAA at SeaWiFS wavelengths)
Rrs_inversion_RP95.m (runs Roesler Perry 1995 with variable wavelengths, data sets)
Rrs_inversion_RB03.m (runs Roesler Boss 2003 with variable wavelengths, data sets)
Rrs_inversion_RPFG.m (runs Roesler Perry 1995 with variable wavelengths, data sets, 4 phytoplankton absorption spectra –functional groups)
GIOP (in folder GIOP, you will find the General IOP model inversion from Jeremy Werdell. See details below in #6 in assignments for more details AFTER you have run the programs above).
Linear Matrix Inversion with uncertainty (Boss and Roesler 2006)

2. Inversion Model programs called by main programs
GSM01_invert and GSM01_cost [*Garver et al. 2002*]
QAA4_MODIS and QAA4_SeaWIFS [*Lee et al. 2002*]
RP95_invert and RP95_cost [*Roesler and Perry 1995*]
RB03_invert and RB03_cost [*Roesler and Boss 2003*]
RPFG_invert and RPFG_cost [*Roesler et al. 2004*]

3. eigenvector functions provided
water_iops_PF_TScorr (called by all inversions, does varying T/S matter?)
phyto_avg_abs (implemented in RP95)
phyto_species_abs (implemented in *Roesler et al. 2004* and *Roesler and Boss 2003*))
phyto_Lee (try using it)
Also, try Bricaud et al 1995 (see next page);
a_{CDOM} and a_{nap} separate with slopes of 0.018+/- 0.002 or 0.01+/- 0.002, respectively or combined a_{cdm} with combined slope of 0.0145+/-0.002
b_{bp} with variable spectral slope (+0.5 to -1.5)

4. Regression function
Fminsearch (not Levenberg-Marquardt, does have some differences)

5. Data files supplied for experimentation and then your data sets to be loaded by you
1. Subsurface irradiance reflectance from Roesler and Perry 1995 (JGR)
    Rrs_E_PugetSound.dat (11 spectra, Puget Sound)

Rrs_E_GulfMaine (8 spectra, Gulf of Maine)
Rrs_E_DabobBay (8 spectra, Dabob Bay north of Puget Sound)
Rrs_E_WestCoast (8 spectra, transect off Oregon gyre waters to coast)

2. R_L_HL_simulation.dat Simulated hyperspectral reflectances that Curt provided from Hydrolight runs, see excel file for details of runs
3. *Your measured reflectance spectra from cruise (load in format of column 1 is wavelength, columns 2 to n are reflectance spectra 1 to (n-1)*
4. *Your reflectance spectra from Hydrolight simulation*

Exploratory activities that you can try at home

1. Using the provided data sets (from Roesler and Perry 1995 and Curt's simulations), experiment by
   a. comparing the various models on the same data sets
   b. comparing retrieved IOPs as a function of wavelength resolution
   c. comparing retrieved IOPs with inputs from Hydrolight
   d. looking at sensitivity of retrievals to input parameters (a_{phyt}, S_{cdom}, S_{nap}, n_{bb}, Temperature and/or Salinity of water…)
2. Once you are comfortable running the models, load your data sets into the models:
   a. Various ways of determining reflectance
   b. Hydrolight simulations using IOPs from cruise
3. Run supplied inversion models to retrieve IOPs (a_{phytp}, a_{cdom}, b_{bp})
4. How do the retrieved IOPs depend upon:
   a. the phytoplankton absorption eigenvector
   b. the slope of a_{cdm} (or the separation of the two)
   c. the slope of b_{bp}
   d. the number of wavelengths (try hyperspectral, then degrade to SeaWiFS, then MODIS wavelengths; what can be done with 3 wavelengths
   e. the model chosen
5. Test the QSSA. Using your IOPs from the cruise,
   a. compute $b_b/(b_b+a)$
   b. compute R = Lu(0-)/Ed(0+) from Hydrolight
   c. how do the spectral shapes of the two compare?
   d. Given R_{QSSA} (f/Q) $b_b/(b_b+a)$ and R_{HL} = Lu/Ed, what is f/Q? Does it vary spectrally?
   e. People often approximate to R_{QSSA} (f/Q) b_b/a, what do your results suggest?
6. Set up some Hydrolight runs to test the sensitivity of the inversions model retrievals to such impacts as:
   a. Sun angle. How do the retrievals vary as sun angle varies? Do Eu/Ed and Lu/Ed respond similarly?
   b. Raman. How do the retrievals respond to the presence of Raman? Is it worse or better when using MODIS versus hyperspectral retrievals? Is the effect chlorophyll-dependent?
   c. Volume scattering function. How do retrievals of each eigenvalue vary as the shape of the VSF varies?
   d. I am sure you can think of lots of fun tests.
7. In the folder 'chapter_08_syn' you will invert ZP Lee's synthetic data set using the code of Boss and Roesler (2006; all can be downloaded from: http://ioccg.org/groups/lee.html). The advantage

of this code is in that it provides for error bars in inverted parameters, based on varying the eigen-functions in the range observed and finding all the solution within the uncertainty in Rrs.

a. run 'IOCGG_ZPL_data_inversion'

b. run the same code but on a field dataset at 'chapter_08_insitu'. There it is called 'IOCGG_in_situ_data_inversion.m'.

c. try to modify these codes to invert a reflectance spectra of your choice

References

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