Ocean Optics Inversion Algorithm

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Outline

- Introduction to analytic algorithms
- Ocean optical properties
- The new algorithm
- Tests of the algorithm
- Conclusions
Rehm PhD project: Characterize constituents of ocean waters from wavelength-dependent optical measurements

Tasks:

- Perform unique set of in-water light field measurements (i.e., NAB08) for an iterative optical inversion method against a limited data set of water optical properties acquired simultaneously with different detectors
- Compare iterative optical inversion method results against those of limited data set

The problem: His iterative inversion method sometimes did not converge to a global minimum
General objectives of (semi-)analytic inversion algorithms

- To obtain an initial estimate sometimes needed for convergence to a global minimum estimate from an iterative algorithm
- To minimize or eliminate iterative forward problem calculations (e.g., steepest descent, Levenberg-Marquardt, etc.) for obtaining *approximate* optical property estimates
- To retain the physical insights from analytical methods (e.g., eigenfunction method) that provide an opportunity for analytic error estimation techniques
Brief history of 1-D analytic algorithms
(1-D is good enough for ocean optics)

(One wavelength with notation suppressed,
depth \( z \geq 0 \) and \( -1 \leq \mu \leq 1, \ 0 \leq \varphi \leq 2\pi \))

Algorithms for full angle-dependent angular fluxes \( L(z, \mu, \varphi) \):
Developed in 1974–1985 by Case, Kuščer, Siewert, McCormick, Sanchez, Larsen, and others

But \( L(z, \mu, \varphi) \) impractical to measure in an ocean environment
Low-order angular moments for ocean optics

Algorithms for hemispherical fluxes and partial currents:
Developed in 1990s by Sanchez, McCormick and students Tao and Leathers

Downward scalar flux : \( E_{0d}(z) = \int_{0}^{2\pi} \int_{0}^{1} L(z, \mu, \varphi) \, d\varphi \, d\mu \)

Upward scalar flux : \( E_{0u}(z) = \int_{0}^{2\pi} \int_{0}^{-1} L(z, \mu, \varphi) \, d\varphi \, d\mu \)

Downward partial current : \( E_{d}(z) = \int_{0}^{2\pi} \int_{0}^{1} \mu L(z, \mu, \varphi) \, d\varphi \, d\mu \)

Upward partial current : \( E_{u}(z) = \int_{0}^{2\pi} \int_{0}^{-1} |\mu| L(z, \mu, \varphi) \, d\varphi \, d\mu \)

But \( E_{0d}(z) \) and \( E_{0u}(z) \) impractical to measure in an ocean environment
Constraints on our new analytic algorithm

1. Rehm had depth-dependent data in “spatially uniform waters” only for

   Downward partial current: \( E_d(z) = \int_0^{2\pi} \int_0^1 \mu L(z, \mu, \varphi) d\varphi d\mu \)

   Vertically–upward angular flux: \( L_u(z) = L(z, -1, \varphi = 0) \)

2. To eliminate surface illumination magnitude, need ratio

   \[ r_{rs}(z) = \frac{\text{Vertically–upward angular flux}}{\text{Downward partial current}} = \frac{L_u(z)}{E_d(z)} \]

   with which only one optical property can be determined
Objective of new algorithm

Use measurements of $E_d(z)$, dominated by absorption,

and $L_u(z)$, dominated by scattering,

to see if they are sufficient to characterize an optical property in an ocean environment
Ocean optical properties

What optical properties is the light field most sensitive to?

Rehm had data for $r_{rs}(z)$ and also limited data for

- Absorption coefficient $a$
- Backscattering coefficient $b_b$, as computed from the scattering phase function $\tilde{\beta}(\mu', \mu)$

$$\tilde{\beta}(\mu', \mu) = \int_0^{2\pi} \tilde{\beta}(\mu', \phi', \mu, \phi = 0) d\phi'$$

with

$$b_b = b \int_{-1}^{0} \tilde{\beta}(\mu', \mu) d\mu$$
For average oceanic particles (Petzold 1972), most scattering is in the forward direction. (Source: C.D. Mobley, private comm.)
Implications of ocean properties

1. Need to develop algorithm to determine $b_b/a$

2. Assume “isotropic plus delta forward” phase function with single adjustable factor $F$:

$$
\tilde{\beta}(\mu', \mu) = \frac{1}{2} \left[ \frac{\tilde{b}_b}{F} + 2 \left( 1 - \frac{\tilde{b}_b}{F} \right) \delta(\mu' - \mu) \right]
$$

where $\tilde{b}_b = b_b/b$ is backscattering fraction

3. Apply to measurement data not near the surface so asymptotic transport approximation is applicable
The algorithm

1. Substitute phase function in one-speed, plane geometry equation. Get effective optical depth $\tau$ and albedo $\varpi$

$$\tau = a \left[ 1 + \frac{b_b}{a} \right] z \quad \text{and} \quad \varpi = \frac{b_b/a}{b_b/a + F}$$

2. Multiply transport equation for $\mu$ by $\mu L(\tau, -\mu)$ and one for $-\mu$ by $\mu L(\tau, \mu)$, integrate both over $-1 \leq \mu \leq 1$, and subtract results

$$\frac{d}{d\tau} \int_{-1}^{1} \mu^2 L(\tau, \mu) L(\tau, -\mu) d\mu =$$

$$-\varpi \int_{-1}^{1} \mu L(\tau, \mu) d\mu \int_{-1}^{1} L(\tau, \mu') d\mu'$$
The algorithm, cont’d

3. Multiply transport equation by unity and integrate over $-1 \leq \mu \leq 1$ to obtain

$$
\int_{-1}^{1} L(\tau, \mu) d\mu = -(1 - \varpi)^{-1} \frac{d}{d\tau} \int_{-1}^{1} \mu L(\tau, \mu) d\mu
$$

and substitute to get

$$
\frac{d}{d\tau} \left[ 4 \int_{0}^{1} \mu^2 L(\tau, \mu) L(\tau, -\mu) d\mu - \frac{\varpi}{1 - \varpi} \left( \int_{-1}^{1} \mu L(\tau, \mu) d\mu \right)^2 \right] = 0
$$

and convert $\tau$ to measurement depth $z_m$.
4. Divide by $[E_d(z_m)/2\pi]^2$ and substitute

$$\varpi \quad \frac{b_b}{a} = \frac{b_b/a}{F}$$

1 - \varpi

for each measurement depth $z_m$. 

$$\frac{b_b}{a} \left[ 1 - 2\pi \int_0^1 \frac{\mu L(z_m, -\mu)}{E_d(z_m)} \, d\mu \right]^2 = 16\pi^2 \int_0^1 \frac{\mu L(z_m, \mu)}{E_d(z_m)} \frac{\mu L(z_m, -\mu)}{E_d(z_m)} \, d\mu.$$
The algorithm, cont’d

5. A big problem: no data for \( L(z_m, \mu) \) and \( L(z_m, -\mu) \), \( 0 \leq \mu \leq 1 \), so define two new radiometric functions

\[
\Lambda(z_m) = 2\pi \int_0^1 \mu \frac{L(z_m, -\mu)}{L_u(z_m)} \, d\mu = \frac{E_u(z_m)}{L_u(z_m)},
\]

\[
\Omega(z_m) = 16\pi^2 \int_0^1 \mu^2 \frac{L(z_m, \mu)}{E_d(z_m)} \frac{L(z_m, -\mu)}{L_u(z_m)} \, d\mu,
\]

to get final algorithm in terms of measured \( r_{rs}(z_m) \)

\[
\frac{b_b/a}{F} = \frac{\Omega(z_m) r_{rs}(z_m)}{[1 - \Lambda(z_m) r_{rs}(z_m)]^2}
\]

\[
\approx \frac{\Omega(z_{as}) r_{rs}(z_m)}{[1 - \Lambda(z_{as}) r_{rs}(z_m)]^2}
\]
6. Compute asymptotic $\Omega(z_{as})$ and $\Lambda(z_{as})$ using isotropic-scattering classic asymptotic eigenmode

\[ L(\tau, \mu) \propto \phi(\nu_0, \mu) \exp(-\tau/\nu_0) = \frac{\omega \nu_0/2}{\nu_0 - \mu} \exp(-\tau/\nu_0) \]

for asymptotic eigenvalue $\nu_0$ to get:

\[
\begin{align*}
\Lambda(z_{as}) &= 2\pi(\nu_0 + 1) \int_0^1 \mu (\nu_0 + \mu)^{-1} d\mu \\
\Omega(z_{as}) &= \frac{16\pi^2(\nu_0 + 1) \int_0^1 \mu^2(\nu_0^2 - \mu^2)^{-1} d\mu}{\int_0^1 \mu (\nu_0 - \mu)^{-1} d\mu}
\end{align*}
\]
7. Determine factor $F$ from $\Omega(z_{as})$ and $\Lambda(z_{as})$ and $r_{rs}(z_m)$ obtained by Ecolight© calculations by minimizing cost function $g_F = G_F^T G_F$

$$G_F = \begin{bmatrix} \frac{b_b}{a} - \frac{\Omega(z_{as}) r_{rs}(z_m)}{F} \\ [1 - \Lambda(z_{as}) r_{rs}(z_m)]^2 \\ 1 - \frac{\omega \nu_0}{2} \ln \left( \frac{\nu_0 + 1}{\nu_0 - 1} \right) \\ (b_b/a) - (b_b/a)_{measured} \end{bmatrix}$$

and parameterize $F$ as a function of $b_b/a$ with

$$F = p_1(b_b/a) + p_2$$
Tests of the algorithm

- With computer generated data sets: 63 different simulations (7 different chlorophyll concentrations, 3 depths, 3 incident illumination directions with no simulated noise or natural variability) and selected phase functions
  - $\beta_{FF}$ (training set)
  - $\beta_{Petzold}$ (validation set)
- With Rehm’s 2008 North Atlantic Bloom (NAB08) data for
  - $L_u(z), E_d(z)$
  - $a(z)$
  - $b_b(z)$ estimated from measurements at two wavelengths
Test of algorithm: synthetic data

$F$ tuned with training set: $L_u$, $E_d$ using ($\beta_{FF}$)

Absolute retrieval error for $b_b/a$ with:

- Training set ($\beta_{FF}$)
- Validation set ($\beta_{Petzold}$)

**Conclusion:** It appears delta-isotropic phase function is not bad
NAB08 vertical IOPs and radiometric data

\[ b_a(488) (m^{-1}) \]

\[ L_u (\mu w \text{ cm}^{-2} \text{ sr}^{-1}), \ E_d (\mu w \text{ cm}^{-2}) \]

(A) \[ a(488), \ b(488), \ b/a(488) \]

(B) \[ L_u, E_d \]
Determination of $F$ from NAB08 field data

(A) $F(b/b/a, 488)$ vs $b/b/a$

(B) $F(b/b/a, \lambda)$ vs $b/b/a$

<table>
<thead>
<tr>
<th>$\lambda$ (nm)</th>
<th>$p_1$</th>
<th>$p_2$</th>
<th>$R^2$</th>
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<tr>
<td>412</td>
<td>0.582</td>
<td>0.0313</td>
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<tr>
<td>510</td>
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<td>0.0190</td>
<td>0.84</td>
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<tr>
<td>532</td>
<td>1.12</td>
<td>0.0145</td>
<td>0.82</td>
</tr>
</tbody>
</table>
$b_b / a$ validation from NAB08 field data

(A) Scatter plot showing $b_b / a_{\text{meas}} (488)$ versus $b_b / a_{\text{est}} (488)$. The dashed line represents the ideal 1:1 relationship.

(B) Relative Absolute Error (%) for different datasets.

(C) Relative Error (%) for different datasets.

(D) Depth (m) vs. Relative Absolute Error (%). Each line represents a different dataset (1 to 7).
Use in global optimization algorithms

- Local minima (error > 5%): start (open circles), end (solid dots).
- Global minimum (error < 5%): start (unmarked gray dots)
- Using analytical algorithm: start points inside gray box
Conclusions

- One-parameter delta-isotropic phase function acceptable
- $F$ factor is spectrally dependent
- Algorithm works OK approaching asymptotic regime with best results in deeper waters
- Algorithm gives useful estimate for starting and constraining iterative algorithms
- Algorithm doesn’t work well for wavelengths where inelastic (Raman) scattering important
Future work?

- Extend algorithm to multigroup theory so can treat inelastic scattering for wavelengths > 550 nm or so
- $b_a/a$ is the optical property typically obtained from satellite data so develop algorithm for near-surface measurements by computing approximate $\Lambda(0^+)$ and $\Omega(0^+)$ factors with singular eigenfunction half-space albedo problem angular flux
Want more details?

- If accepted, see Rehm and McCormick, *Optics Express* (2011 or 2012)

- Ask a question
Raman scattering wavelength redistribution function

(Source: Mobley, Light and Water, 1994)