Inversion (spectral matching) ocean color algorithms

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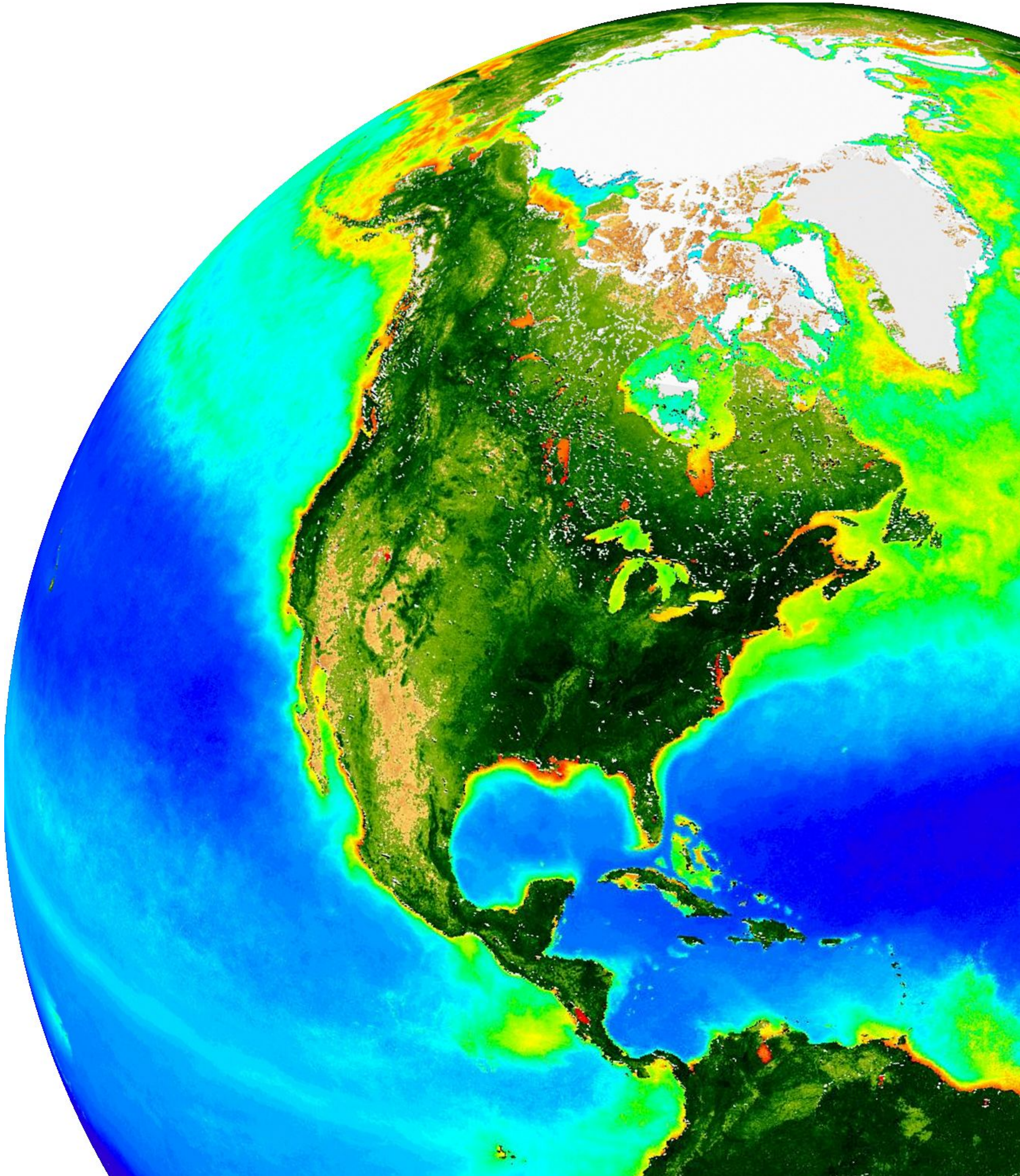
Acknowledgements: **Collin Roesler**

2023 Ocean Optics Summer Course

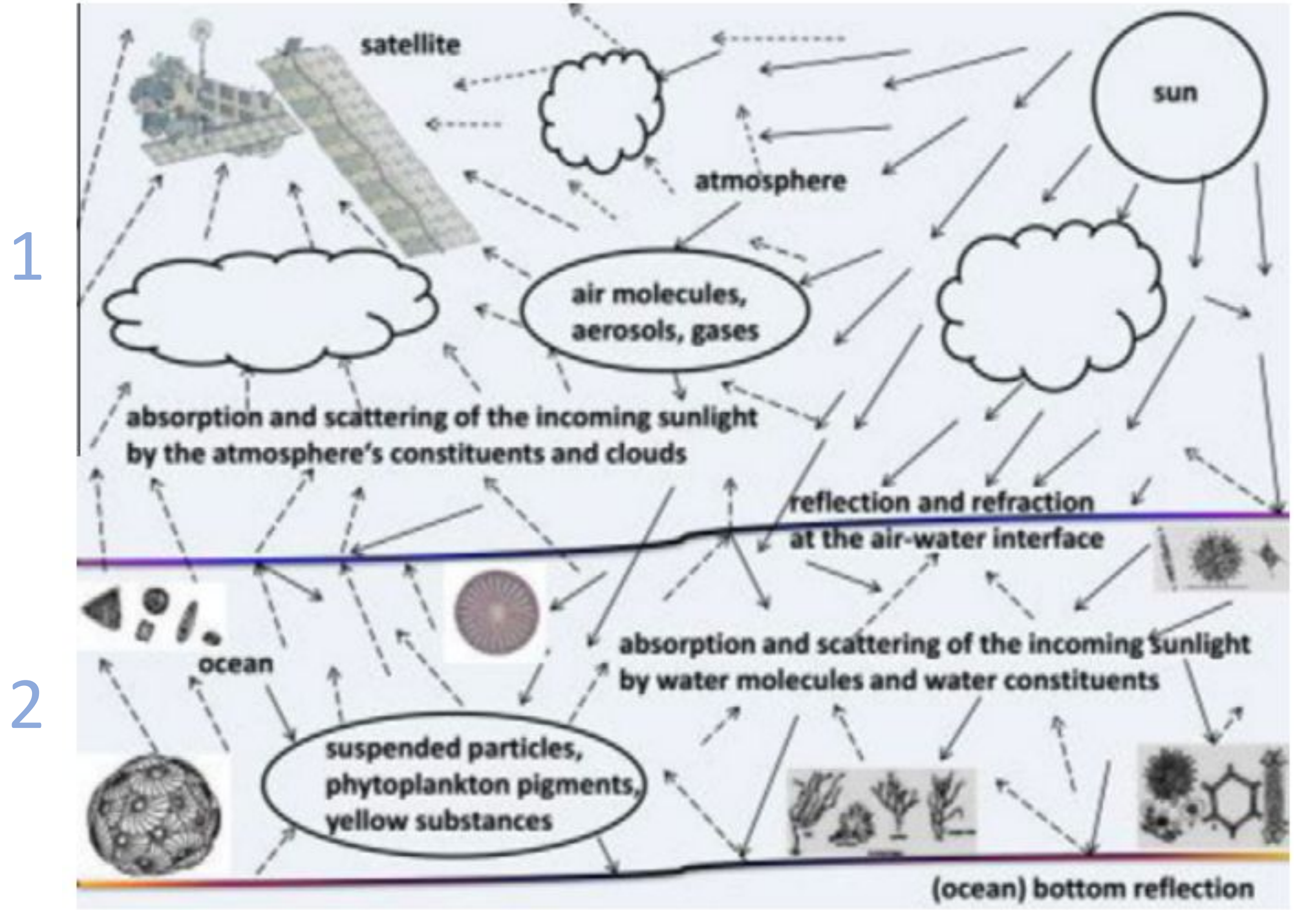


Satellite instruments measure the spectral radiant flux leaving the top of Earth's atmosphere

This includes contributions from everything directly in or directed into its instantaneous field of view

Ideally, forward models representing the combined ocean-atmosphere system (COAS) could be repeatedly run to find the combination that best reproduces the measured top-of-atmosphere radiance

Historically, this has been (and in many ways still is) too computationally expensive



Blum et al. 2012, Advances in Space Research

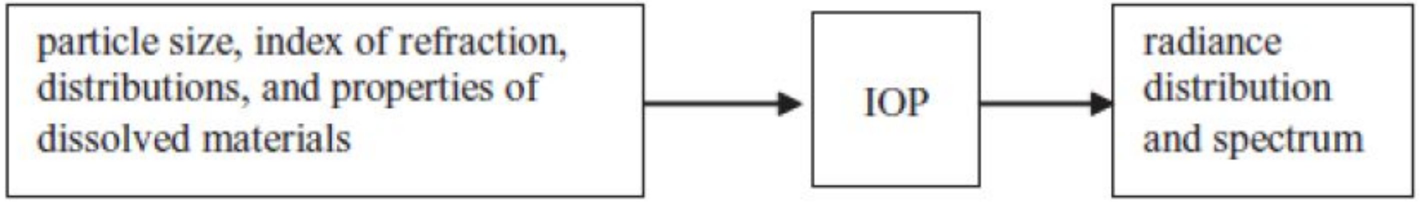
IOCCG Report Number 5, 2006

Remote Sensing of Inherent Optical Properties: Fundamentals, Tests of Algorithms, and Applications

Chapter 1

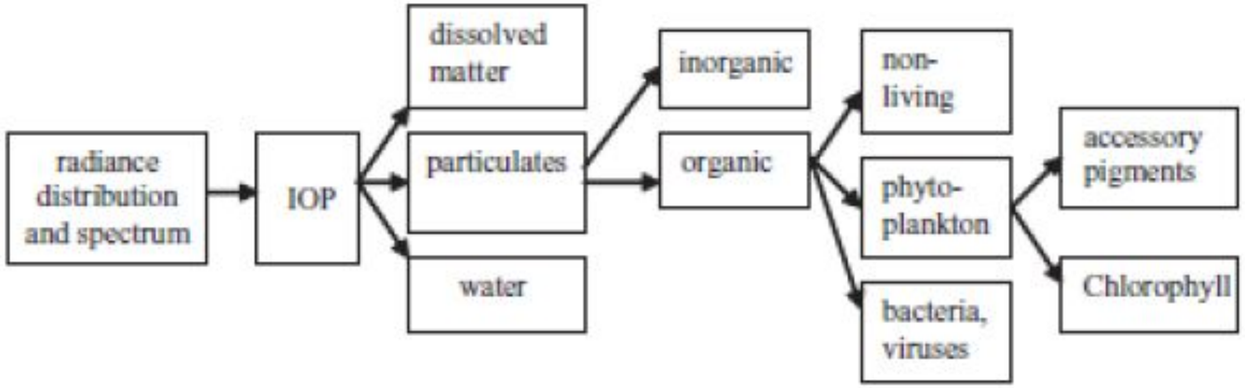
Why are Inherent Optical Properties Needed in Ocean-Colour Remote Sensing?

Ronald Zaneveld, Andrew Barnard and ZhongPing Lee



IOP(λ)[chl, whatever] → *forward model* → Rrs(λ)

Rrs(λ) → *inverse model* → IOP(λ), chl, whatever



inverse (adjective): opposite or contrary in position, **direction**, **order**, or effect

Solve RTE for Reflectance

Remember this from day 1?

$$\cos\theta \frac{dL(\theta,\phi)}{dz} = -aL(\theta,\phi) - bL(\theta,\phi) + \int_{4\pi} \beta(z,\theta,\phi;\theta',\phi')L(\theta,\phi)d\Omega'$$

- Successive order scattering, SOS
  - Separate radiance into unscattered (L_o), single scattered (L_1), doubly scattered (L_2),...(L_n) contributions
- Single scattering approximation, SSA
  - Consider only the unscattered and singly scattered radiance terms, L_o and L_1
- Quasi-single scattering approximation, QSSA
  - Note volume scattering functions are highly peaked in forward direction (diffraction)
  - For upward light field, forward scattered like unscattered
  - So, replace b with b_b

The RTE describes how the light field varies with a and b using very sophisticated math.
The QSSA has historically provided a useful simplification for use in, e.g., ocean color remote sensing.
Here's a gross oversimplification of how it works …

$$R = \frac{E_u}{E_d} \equiv \text{irradiance reflectance (unitless)}$$

Upward light field $\quad E_u \propto E_d \times b_b$

backscattered downward light

Downward light field $\quad E_d \times c$

Ed attenuated by beam-c $\quad E_d \times (a + b_b + b_f)$

However, forward scattered light looks unattenuated $\quad E_d \times (a + b_b + b_f)$

$$\downarrow$$

$$E_d \times (a + b_b)$$

$$R = \frac{E_u}{E_d} \propto \frac{E_d \times b_b}{E_d \times (a + b_b)} \propto 6\,\frac{b_b}{a + b_b}$$

The RTE describes how the light field varies with a and b using very sophisticated math.
The QSSA has historically provided a useful simplification for use in, e.g., remote sensing.
Here's a gross oversimplification of how it works …

$$R = \frac{E_u}{E_d} \propto \frac{E_d \times b_b}{E_d \times (a + b_b)} \propto G \frac{b_b}{a + b_b}$$

The proportionality coefficient G depends on how reflectance is defined and on the properties of the light field and forward model.

Usually $b_b \ll a$, so the relationship is simplified

$$R \propto \frac{b_b}{a}$$

← proportional to back scattered light (b_b)

↖ inversely proportional to absorbed light (a)

* note: this only holds for the surface

You have heard how to estimate chl from spectral reflectance ratios, but back in 1977 Morel and Prieur were already investigating the $IOPs \leftrightarrow R$ relationship

$$R = \frac{E_u}{E_d}$$

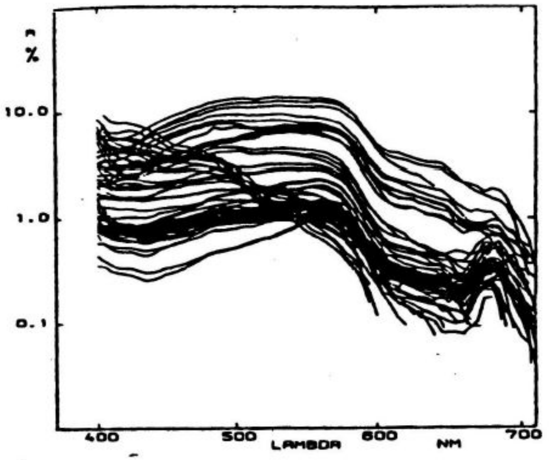


Fig. 1. Reflectance ratio $R(\lambda)$, expressed in percent, plotted with logarithmic scale vs. wavelength λ in nm, for 81 experiments in various waters. Same units and scales also used in Figs. 4, 5, 6, 7, and 11.

Goals of paper

- Explain variations in R with respect to b_b, a
- Model IOPs to predict R (→forward model)
- results became basis for semi-analytic inversions

Analysis of variations in ocean color[1]

André Morel and Louis Prieur

Laboratoire de Physique et Chimie Marines, Station Marine de Villefranche-sur-Mer, 06230 Villefranche-sur-Mer, France

Read this paper… many times

Abstract

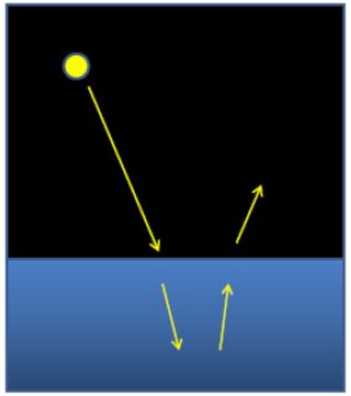
Spectral measurements of downwelling and upwelling daylight were made in waters different with respect to turbidity and pigment content and from these data the spectral values of the reflectance ratio just below the sea surface, $R(\lambda)$, were calculated. The experimental results are interpreted by comparison with the theoretical $R(\lambda)$ values computed from the absorption and back-scattering coefficients. The importance of molecular scattering in the light back-scattering process is emphasized. The $R(\lambda)$ values observed for blue waters are in full agreement with computed values in which new and realistic values of the absorption coefficient for pure water are used and presented. For the various green waters, the chlorophyll concentrations and the scattering coefficients, as measured, are used in computations which account for the observed $R(\lambda)$ values. The inverse process, i.e. to infer the content of the water from $R(\lambda)$ measurements at selected wavelengths, is discussed in view of remote sensing applications.

LIMNOLOGY AND OCEANOGRAPHY 709 JULY 1977, V. 22(4)

- $R(\lambda) = \frac{E_u(\lambda)}{E_d(\lambda)} = 0.33 \times \frac{b_b(\lambda)}{a(\lambda)}$

measurements of ↑ … led to ↑

- “Howard Gordon” Ocean
  - Homogeneous water
  - Plane parallel geometry
  - Level surface
  - Point sun in black sky
  - No internal sources (e.g., fluorescence, Raman)



- $r_{rs}(\lambda) = \frac{L_u(\lambda)}{E_d(\lambda)} (sr^{-1})$
  - $= \sum_{i=1}^{2} g_i(\lambda)[u(\lambda)]^i$
  - $u = \frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}, \; g_i(sr^{-1})$
  - $g_1 = 0.0949$
  - $g_2 = 0.0794$, generally ignored

$\rightarrow 0.0794 \times \left(\frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}\right)^2$

You have heard how to estimate chl from spectral reflectance ratios, but back in 1977 Morel and Prieur were already investigating the $IOPs \leftrightarrow R$ relationship

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LIMNOLOGY AND OCEANOGRAPHY 709 JULY 1977, V. 22(4)

- $R(\lambda) = \frac{E_u(\lambda)}{E_d(\lambda)} = 0.33 \times \frac{b_b(\lambda)}{a(\lambda)}$

$$\frac{R(\lambda)}{\pi} = \frac{0.33}{\pi} \frac{b_b(\lambda)}{a(\lambda)} = 0.105 \frac{b_b(\lambda)}{a(\lambda)}$$

1. relate Rrs to a and bb

$$r_{rs}(\lambda) = \frac{R_{rs}(\lambda)}{0.52 + 1.7R_{rs}(\lambda)}.$$

$$r_{rs}(\lambda) = \sum_{i=1}^{2} G_i(\lambda)[u(\lambda)]^i, \quad u(\lambda) = \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

2. IOPs are additive. Define a and bb.

$$b_b(\lambda) = b_{bw}(\lambda) + \sum_{i=1}^{N_{ph}} b_{bph,i}(\lambda) + \sum_{i=1}^{N_{nap}} b_{bnap,i}(\lambda).$$

$$a(\lambda) = a_w(\lambda) + \sum_{i=1}^{N_{ph}} a_{ph,i}(\lambda) + \sum_{i=1}^{N_{nap}} a_{nap,i}(\lambda) + \sum_{i=1}^{N_{cdom}} a_{cdom,i}(\lambda),$$

3. IOPs are proportional to component concentrations, so redefine as a function of concentration and spectral shapes

$$\begin{aligned} IOP_{component} &= [concentration] \times IOP_{concentration-specific} \\ &= scalar \times vector \\ &= magnitude \times spectral\ shape \\ &= eigenvalue \times eigenvector \end{aligned}$$

$$b_b(\lambda) = b_{bw}(\lambda) + \sum_{i=1}^{N_{ph}} B_{bph,i} b^*_{bph,i}(\lambda) + \sum_{i=1}^{N_{nap}} B_{bnap,i} b^*_{bnap,i}(\lambda).$$

$$a(\lambda) = a_w(\lambda) + \sum_{i=1}^{N_{ph}} A_{ph,i} a^*_{ph,i}(\lambda) + \sum_{i=1}^{N_{nap}} A_{nap,i} a^*_{nap,i}(\lambda) + \sum_{i=1}^{N_{cdom}} A_{cdom,i} a^*_{cdom,i}(\lambda),$$

3A. Define a reduced number of concentration spectral shapes

$$b_b(\lambda) = b_{bw}(\lambda) + \sum_{i=1}^{N_p} B_{bp,i} b^*_{bp,i}(\lambda).$$

$$a_{dg}(\lambda) = a_{nap}(\lambda) + a_{cdom}(\lambda), \quad a(\lambda) = a_w(\lambda) + \sum_{i=1}^{N_{ph}} A_{ph,i} a^*_{ph,i}(\lambda) + \sum_{i=1}^{N_{dg}} A_{dg,i} a^*_{dg,i}(\lambda).$$

N_p, N_{ph}, N_{dg} = 1

in a hyperspectral world, there's potential for multiply deconstructing each component if the IOPs differ …
… but some IOPs do not significantly differ, and we've lived in a multispectral world

3. IOPs are proportional to component concentrations, so redefine as a function of concentration and spectral shapes

$$\begin{aligned} IOP_{component} &= [concentration] \times IOP_{concentration-specific} \\ &= scalar \times vector \\ &= magnitude \times spectral\ shape \\ &= eigenvalue \times eigenvector \end{aligned}$$

$$b_b(\lambda) = b_{bw}(\lambda) + \sum_{i=1}^{N_{ph}} B_{bph,i} b^*_{bph,i}(\lambda) + \sum_{i=1}^{N_{nap}} B_{bnap,i} b^*_{bnap,i}(\lambda).$$

$$a(\lambda) = a_w(\lambda) + \sum_{i=1}^{N_{ph}} A_{ph,i} a^*_{ph,i}(\lambda) + \sum_{i=1}^{N_{nap}} A_{nap,i} a^*_{nap,i}(\lambda) + \sum_{i=1}^{N_{cdom}} A_{cdom,i} a^*_{cdom,i}(\lambda),$$

4. Put it all together

$$\sum_{i=1}^{N_{bbp}} b^*_{bp_i}(\lambda) \times B_{bp_i}$$

$$u(\lambda) = \frac{b_{bw}(\lambda) + B_{bp} \times b^*_{bp}(\lambda)}{a_w(\lambda) + A_{phyt} \times a^*_{phyt}(\lambda) + A_{nap} \times a^*_{nap}(\lambda) + A_{CDOM} \times a^*_{CDOM}(\lambda) + b_{bw}(\lambda) + B_{bp} \times b^*_{bp}(\lambda)}$$

$$\sum_{i=1}^{N_{phyt}} a^*_{phyt_i}(\lambda) \times A_{phyt_i} \qquad \sum_{i=1}^{N_{nap}} a^*_{nap_i}(\lambda) \times A_{nap_i} \qquad \sum_{i=1}^{N_{CDOM}} a^*_{CDOM_i}(\lambda) \times A_{CDOM_i}$$

water values are known and "constant"

spectral shapes (eigenvectors) are "known" and defined

magnitudes (eigenvalues) are unknown and to be retrieved

5. Input the "known" spectral shapes (eigenvectors) and perform a regression (spectral matching technique) against the reference (input) Rrs spectrum to estimate best-fit magnitudes (eigenvalues)

Additional components or nuances for consideration:

1. the cost or merit function used in least-squares regression

$$\chi^2 = \sum_{i=1}^{N_\lambda} \frac{(\hat{R}_{rs}(\lambda_i) - R_{rs}(\lambda_i))^2}{\sigma^2(\lambda_i)},$$

for future exploration:
- only considers absolute differences
- could be spectrally weighted (e.g., by SNRs)

2. quality control of the output eigenvectors and their IOP products

$$\Delta R_{rs} = \frac{100\%}{N_\lambda} \sum_{i=1}^{N_\lambda} \frac{|\hat{R}_{rs}(\lambda_i) - R_{rs}(\lambda_i)|}{R_{rs}(\lambda_i)},$$

- $-0.05 b_{bw}(\lambda) \le b_{bp}(\lambda) \le 0.05\ \mathrm{m}^{-1}$
- $-0.05 a_w(\lambda) \le a_{dg}(\lambda) \le 5\ \mathrm{m}^{-1}$
- $-0.05 a_w(\lambda) \le a_\phi(\lambda) \le 5\ \mathrm{m}^{-1}$
- $\Delta R_{rs} \le 33\%,$

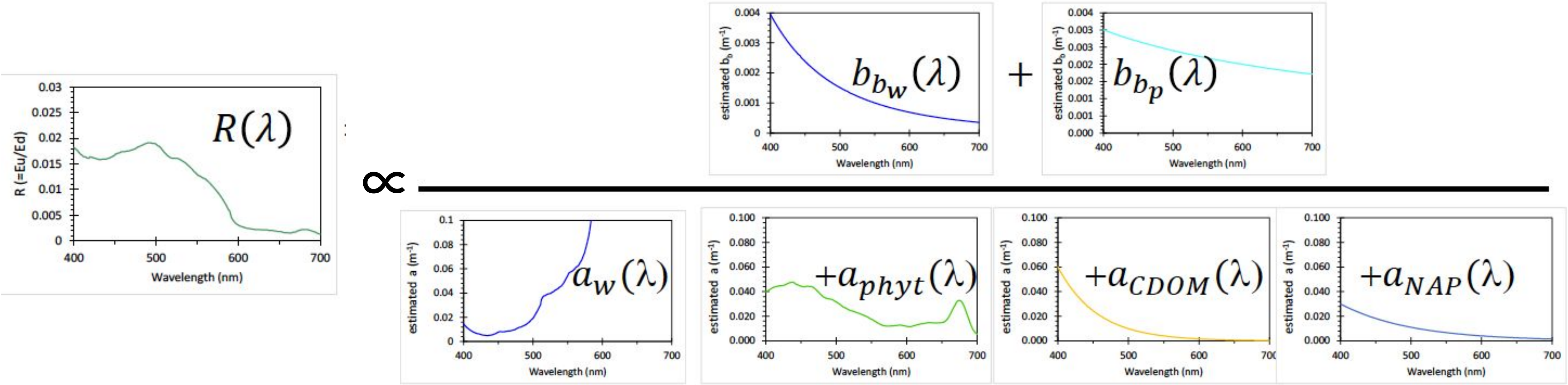
3. uncertainties calculations (more later)

4. performance assessments (more later)

one sentence summary of this inversion paradigm: How much of each absorbing and backscattering component is needed (in a least squares sense) to reconstruct the measured reflectance spectrum?

… can reconstruct this?

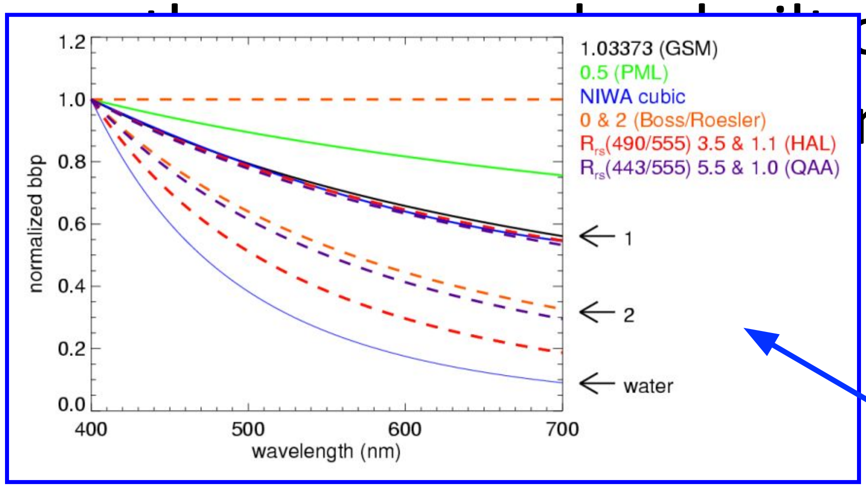
what combination of these …



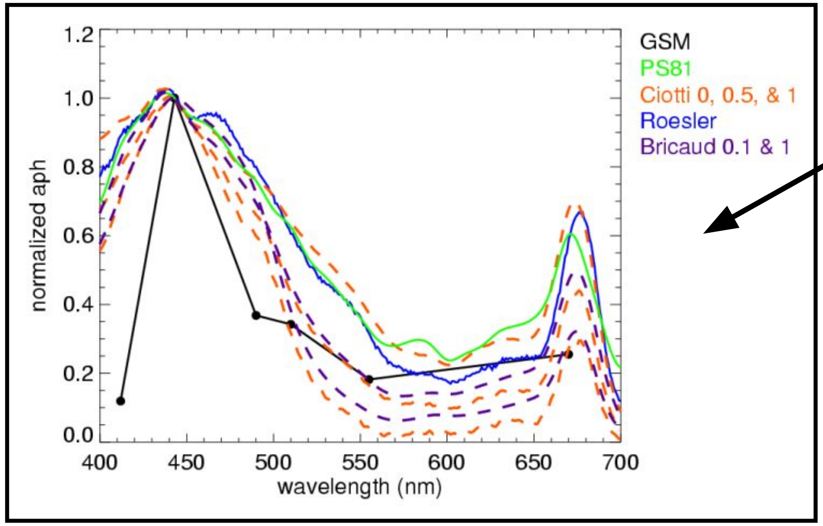
Explosion of papers in the mid-1990's to mid-2000's on ocean color inversion modeling:

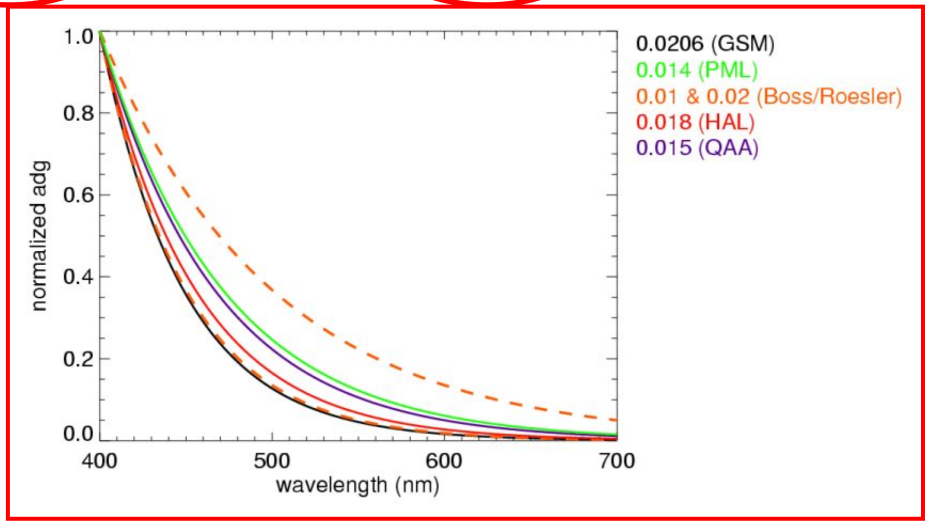
- Roesler and Perry 1995 – two component backscattering; thoughtful re: fluorescence
- Lee et al. 1996 → Lee et al. 2002 = QAA
- Hoge and Lyon 1996
- Garver and Siegel 1997 → Maritorena et al. 2002 = GSM
- Roesler and Boss 2003 – shift focus from bb to beam-c and its spectral slope
- Roelser et al. 2004 – use component aph to infer phytoplankton community structure

In the broadest se… on each other or experienced convergent evolut… n common and key places …



$$r_{rs}(\lambda) = G(\lambda)\,\frac{b_{bw}(\lambda) + B_{bp}\,b^{*}_{bp}(\lambda)}{a_{w}(\lambda) + A_{ph}\,a^{*}_{ph}(\lambda) + +A_{dg}\,a^{*}_{dg}(\lambda)}$$





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$$r_{rs}(\lambda) = G(\lambda) \frac{b_{bw}(\lambda) + B_{bp} b^*_{bp}(\lambda)}{a_w(\lambda) + A_{ph} a^*_{ph}(\lambda) + +A_{dg} a^*_{dg}(\lambda)}$$

Table 1
Example methods for deriving normalized $a_{ph}(\lambda)$.

Reference	Uses measured data (Y/N)	Input data required	Description
Prieur and Sathyendranath (1981)	Y	C_a	Single $a^*_{ph}(\lambda)$ vector
Roesler et al. (1989)	Y	C_a	Single $a^*_{ph}(\lambda)$ shape
Lee et al. (1996a, b)	N	C_a	Blends two Gaussian basis vectors
Bricaud et al. (1995)	Y	C_a	Blends two basis vectors
Bricaud et al. (1998)	Y	C_a	Blends two basis vectors
Hoge and Lyon (1996)	N	C_a	Single Gaussian basis vector (Hoepffner and Sathyendranath, 1993)
Sathyendranath et al. (2001)	Y	C_a	Blends $a^*_{ph}(\lambda)$ basis vectors for two phytoplankton populations
Ciotti et al. (2002)	Y	Size parameter, S_f	Blends $a^*_{ph}(\lambda)$ basis vectors for micro- and picophytoplankton

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$$r_{rs}(\lambda) = G(\lambda) \frac{b_{bw}(\lambda) + B_{bp} b^*_{bp}(\lambda)}{a_w(\lambda) + A_{ph} a^*_{ph}(\lambda) + +A_{dg} a^*_{dg}(\lambda)}$$

Table 3
Example methods for deriving normalized S_{bp}.

Method	Uses measured data (Y/N)	Input data required	Description
Morel and Maritorena (2001)	Y	C_a	• S_{bp} defined in terms of $\tilde{b}$
Gordon et al. (1988)	N	C_a	• Defines $b_p(\lambda)$ from C_a • Assumes $\tilde{b} = F(Ca)$
Ciotti et al. (1999)	Y	C_a	• Logarithmic function from −2 where $C_a = 0.05\,mg\,m^{-3}$ to 0 where $C_a = 20\,mg\,m^{-3}$
Lee et al. (2002)	Y	$r_{rs}(\lambda)$	• Empirical relationship
Roesler and Boss (2003)	N	$\tilde{b}(\lambda)$, $c_p(\lambda)$, $a_p(\lambda)$	• Solves for for $b_{bp}(\lambda)$ and S_c
Antoine et al. (2011)	Y	C_a or $b_b(555)$	• Empirical relationship
Brewin et al. (2012)	Y	C_a	• Empirical relationship for $b_{bp}(\lambda)$

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$$r_{rs}(\lambda) = G(\lambda)\frac{b_{bw}(\lambda) + B_{bp}b^*_{bp}(\lambda)}{a_w(\lambda) + A_{ph}a^*_{ph}(\lambda) + +A_{dg}a^*_{dg}(\lambda)}$$

Table 2
Example approaches for partitioning $a(\lambda)$ into $a_{ph}(\lambda)$ and $a_{dg}(\lambda)$.

Reference	Method and assumptions for parameterizing $a_{ph}(\lambda)$ and $a_{dg}(\lambda)$	Additional input data	Applied to ocean color data? (Y/N)
Roesler et al. (1989)	• $a_{dg}(\lambda)$ has fixed exponential slope, S_{dg} • $a_{ph}(\lambda)$ blue-to-red absorption peak defined using pigment data • Solves for $a_{dg}(\lambda)$ and $a_{ph}(\lambda)$	• C_a • Phaeophytin-a concentration	N
Lee et al. (2002)	• $a_{dg}(\lambda)$ has fixed exponential slope, S_{dg} • Empirical relationship uses $r_{rs}(\lambda)$ to parameterize band ratio of $a_{ph}(\lambda)$ • Solves for $a_{dg}(\lambda)$ and $a_{ph}(\lambda)$	• None	Y
Ciotti and Bricaud (2006) Method 1	• $a_{dg}(\lambda)$ assumed to be exponential • Empirical relationships uses C_a to parameterize band ratios of $a_{ph}(\lambda)$ • Solves for M_{dg}, S_{dg}, $a_{dg}(\lambda)$, and $a_{ph}(\lambda)$ algebraically (Bricaud and Stramski 1990)	• C_a	Y
Ciotti and Bricaud (2006) Method 2	• $a_{dg}(\lambda)$ assumed to be exponential • $a_{ph}(\lambda)$ parameterized through mixing of pico- and microphytoplankton contributions (Ciotti et al. 2002) • Solves for M_{dg}, S_{dg}, M_{ph}, and the size parameter of phytoplankton (S_f) via nonlinear optimization	• C_a	Y
Zheng and Stramski (2013b)	• $a_{dg}(\lambda)$ assumed to be exponential • $a_{ph}(\lambda)$ shape expressed through band ratios of 412:443 and 510:490 • Searches multiple speculative (feasible) solutions of M_{dg}, S_{dg}, $a_{dg}(\lambda)$, and $a_{ph}(\lambda)$ (Bricaud and Stramski, 1990) • Computes candidate and selects optimal solution for $a_{dg}(\lambda)$ and $a_{ph}(\lambda)$ using stacked inequality contstraints	• Pre-determined bounds of inequality constraints	Y
Zhang et al. (2015)	• $a_{dg}(\lambda)$ assumed to be exponential • $a_{ph}(\lambda)$ parameterized as the sum of mixing of pico-, nano-, and microphytoplankton contributions • Solves for M_{dg}, S_{dg}, $a_{dg}(\lambda)$, and $a_{ph}(\lambda)$ including contributions of pico-, nano-, and microphytoplankton using constrained least-squares optimization	• C_a-specific $a^*_{ph}(\lambda)$ for pico-, nano-, and micro-phytoplankton	N

Remember thisfrom the empirical algorithms lecture?

"Dirty secret:
- *embedded into nearly 100% of all ocean color"*

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$$r_{rs}(\lambda) = G(\lambda)$$

$a_w($

Generalized ocean color inversion model for retrieving marine inherent optical properties

Table 1. Summary of Eigenvectors Available for Use in GIOP (as of March 2011)[a]

Eigenvector	Description	Reference
$a^*_\phi(\lambda)$	User-provided $a^*_\phi(\lambda)$	
	Maritorena *et al.* (2002) tabulated $a^*_\phi(\lambda)$	[8]
	Bricaud *et al.* (1998)-derived $a^*_\phi(\lambda)$ using OC-derived C_a	[14]
	Ciotti and Bricaud (2006)-derived $a^*_\phi(\lambda)$ using user-provided size fraction	[17]
$a^*_{dg}(\lambda)$	**Eq. (5) with user-provided S_{dg}**	
	Eq. (5) with Lee *et al.* (2002)-derived S_{dg}	[7]
	Eq. (5) with Franz and Werdell (2010)-derived S_{dg}	[13]
	User-provided $a^*_{dg}(\lambda)$	
$b^*_{bp}(\lambda)$	Eq. (8) with user-provided S_{bp}	
	Eq. (8) with Hoge and Lyon (1996)-derived S_{bp}	[4]
	Eq. (8) with Lee *et al.* (2002)-derived S_{bp}	[7]
	Eq. (8) with Ciotti *et al.* (1999)-derived S_{bp}	[15]
	Eq. (8) with Morel and Maritorena (2001)-derived S_{bp}	[22]
	Eq. (8) with Loisel and Stramski (2000)-derived S_{bp}	[6]
	User-provided $b^*_{bp}(\lambda)$	
	Loisel and Stramski (2000)-derived $b^*_{bp}(\lambda)$	[6]
	Lee *et al.* (2002)-derived $b^*_{bp}(\lambda)$	[7]

[a]Boldface indicates the eigenvector used in GIOP-DC.

Werdell et al. 2013, Applied Optics

Table 4
Example of semi-analytical solution classes used in ocean-color algorithms.

Class	Methodology	Example usage
Non-linear spectral optimization	Levenberg Marquardt	Roesler and Perry (1995) Garver and Siegel (1997) Maritorena et al. (2002)
	Nelder-Mead	Evers-King et al. (2014)
	Particle swarm	Slade et al. (2004)
	Genetic algorithm	Lee et al. (1999) Haigang et al. (2003)
	Simulated annealing	Salinas et al. (2007)
Direct linear inversion	Linear matrix inversion	Hoge and Lyon (1996) Wang et al. (2005)
Spectral deconvolution	Step-wise algebraic	Lee et al. (2002) Smyth et al. (2006) Pinkerton et al. (2006)
Bulk inversion	Step-wise algebraic solving for each wavelength independently	Loisel and Stramski (2000)
Ensemble inversion	Adaptive linear matrix inversion	Brando et al. (2012)

Werdell et al. 2018, Prog. Oceanography

a tool like GIOP (its goals anyway):

- supports and consolidates critical understanding of how inversion algorithms operate
- democratizes inversion algorithm development & refinement
- simplifies sensitivity analyses
- simplifies (NASA's) code maintenance (and anyone's ability to update it)
- simplifies uncertainties calculations

Table 5. Delta Statistics for the Sensitivity Analyses[a]

		MPD				Median				
Run	N	b_{bp}	a	a_{dg}	a_ϕ	ΔR_{rs}	Δb_{bp}	Δa	Δa_{dg}	Δa_ϕ
GIOP-DC	437	NA	NA	NA	NA	1.04	8.52	8.56	27.25	35.83
$S_{bp}-33\%$	440	5.19	5.17	7.58	2.98	0.99	11.23	11.70	32.14	34.69
$S_{bp}+33\%$	436	5.65	5.70	8.82	2.90	1.14	11.40	10.70	23.51	39.12
$S_{dg}-33\%$	448	18.96	33.44	101.73	46.59	1.61	16.27	19.08	32.94	31.95
$S_{dg}+33\%$	399	3.77	8.41	40.10	32.92	1.23	9.44	8.95	79.90	59.32
S_{dg} from [7]	439	3.20	5.33	20.40	14.58	1.10	8.65	9.80	22.25	34.42
$C_a-33\%$ in [14]	419	2.02	2.92	1.48	7.25	1.19	8.79	8.83	28.62	31.10
$C_a+33\%$ in [14]	437	1.56	2.28	1.14	5.90	1.10	8.12	9.17	26.79	40.09
Fixed C_a in [14]	369	4.57	7.89	2.60	21.68	1.46	11.30	11.53	30.97	26.70
a_ϕ^* from [17]	357	8.33	12.72	7.04	22.23	1.20	14.26	16.75	38.30	23.13
G from [22]	422	9.99	6.15	7.49	14.12	1.16	11.50	13.64	37.49	36.24
Matrix inversion	475	4.60	3.68	2.24	7.41	1.73	9.15	9.43	24.79	36.82
$400 \le \lambda \le 600$ nm	424	0.23	0.21	0.08	0.38	0.92	8.76	8.78	31.94	36.55

[a] N is the sample size. MPD is the average spectral median percent difference between GIOP-DC and each alternate run, as calculated in Tables 2 and 3. Medians of the ΔIOP frequency distributions are also presented, as presented in Table 4.

some recent advances and enhancements:

- **expanded solution space** (e.g., ag and ad) – Brando et al. 2012, Zheng et al. 2013, 2015, others
- **temperature and salinity dependence of bbw** – Werdell et al. 2013
- **Raman adjustment of Rrs** – McKinna et al. 2016 (from Lee et al. 2013, Westberry et al. 2013)
- **Bayesian / Optimal Estimation retrievals** – Erickson et al. 2020, Erickson et al. 2023
- **seeding the inversion with an externally collected IOP** – Bission et al. in review
- **application to optically shallow waters** – Lee et al. 1999, McKinna et al. 2015, Barnes et al. in prep, others
- **application to PCC** – Werdell et al. 2014, Chase et al. 2019, Kramer et al. 2022, others

- still little work exploiting the fluorescence signal
- expansion of parameterization across optical water types (Moore et al. 2014)

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Merged satellite ocean color data products using a bio-optical model: Characteristics, benefits and issues

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frontiers in Earth Science

METHODS
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Approach for Propagating Radiometric Data Uncertainties Through NASA Ocean Color Algorithms

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Uncertainties of optical parameters and their propagations in an analytical ocean color inversion algorithm

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still missing components in the uncertainty budgets (e.g., in situ uncertainties used in empirical models, and fit parameters, correlations, etc.)

the Rrs wavelength suite input into the inversion will influence the values of the output IOP retrievals (Werdell and McKinna 2019)

- SeaWiFS: 412, 443, 490, 510, 555, 670
- MODIS: 412, 443, 488, 531, 547, 667
- MERIS: 412, 443, 490, 510, 560, 620, 665
- VIIRS: 410, 443, 486, 551, 671
- OLCI: 400, 412, 443, 490, 510, 560, 620, 665
- PACE: 400, 412, 425, 443, 460, 475, 490, 510, 532, 555, 583, 617, 640, 655, 665
- 410–670 nm: 5 nm intervals from 410 to 670 nm
- 410–600 nm: 5 nm intervals from 410 to 600 nm

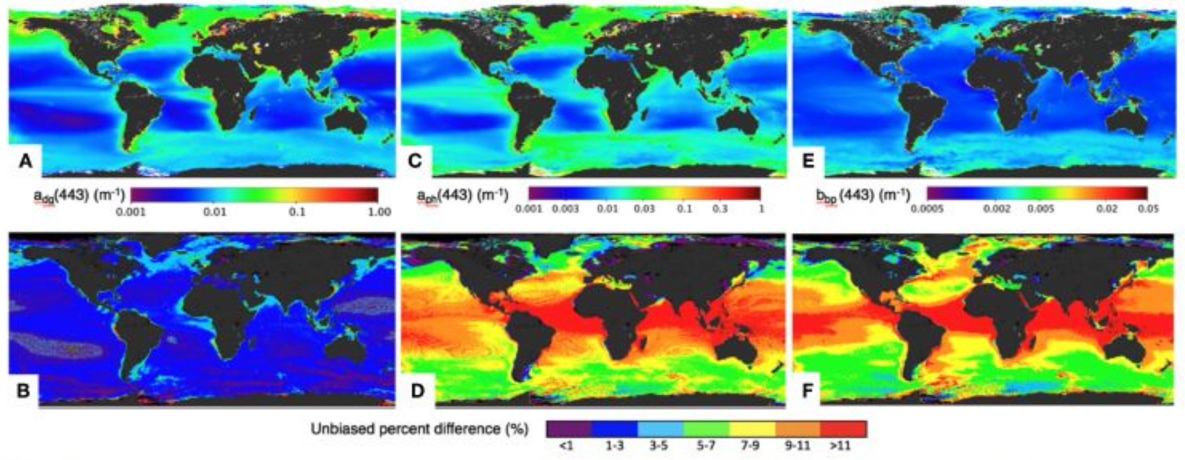


FIGURE 8 | Global IOPs calculated using SeaWiFS mission-long $R_{rs}(\lambda)$ and the UPD between IOP values calculated using SeaWiFS and VIIRS wavelength suites (SeaWiFS = satellite$_1$ and VIIRS = satellite$_2$ in Equation 7). Geophysical values and UPD for $a_{dg}(443)$ shown in **(A,B)**, for $a_{ph}(443)$ in **(C,D)**, and for $b_{bp}(443)$ in **(E,F)**.

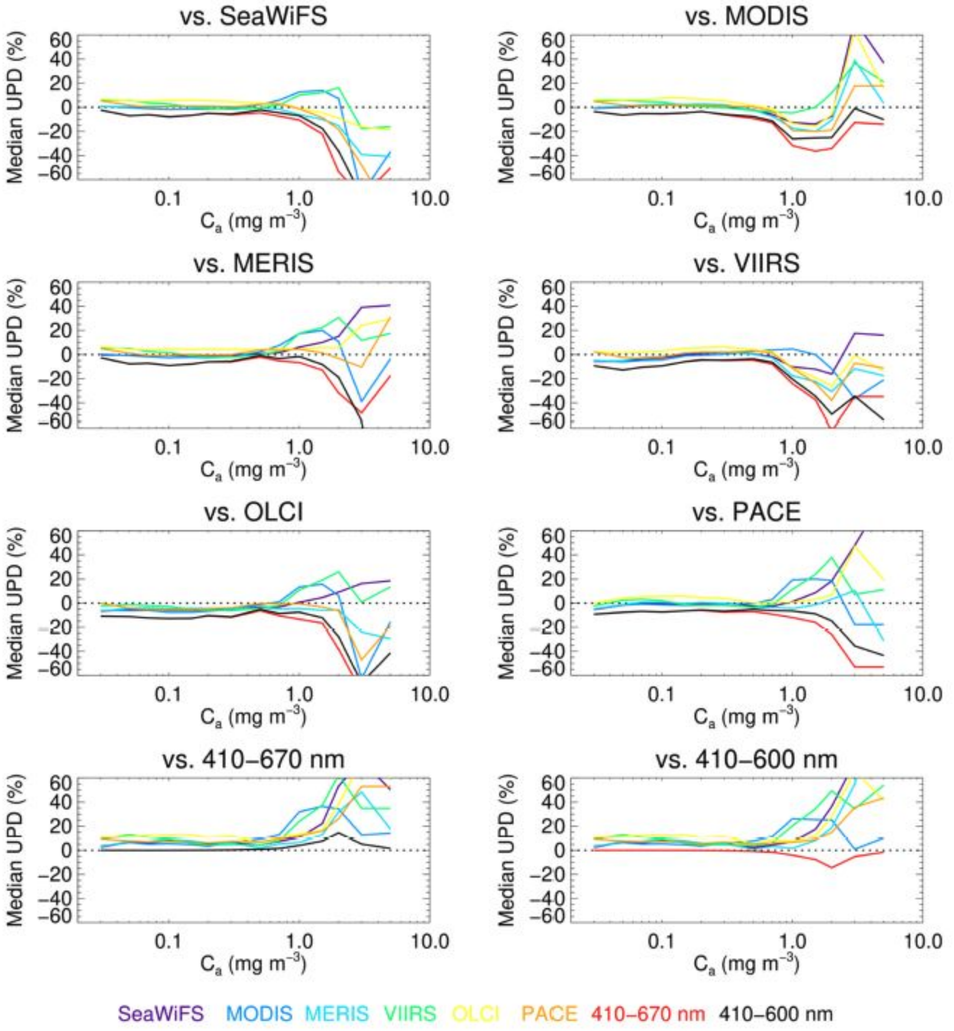
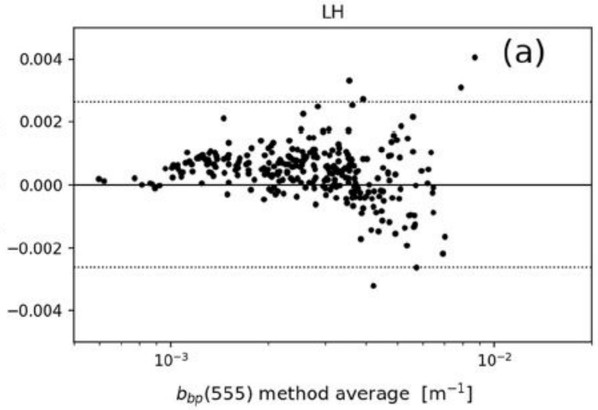
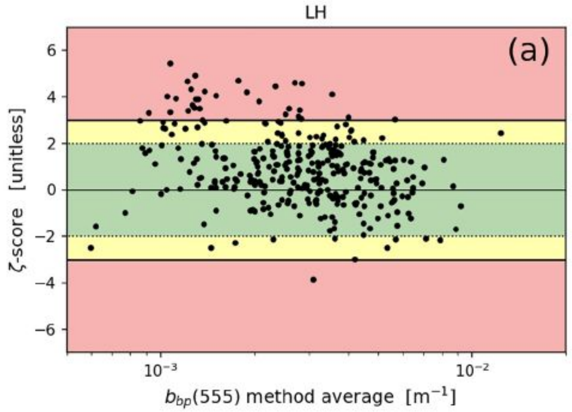


FIGURE 5 | As for **Figure 3**, but for $a_{ph}(443)$.

performance assessment of ocean color inversion models requires care:

- independent datasets
- variation in performance across spectral regions (good in blue vs. poor in red?)
- performance of one product (e.g., aph) relative to the another (e.g., bbp)
- uncertainties should consider both model and “truth” (McKinna et al. 2019)
- large of wavelengths to consider
- meaningful plots and results reporting





quick wrap-up:

- ocean color inversion algorithms are powerful tools
- the devil is in the details
    - eigenvector definitions
    - solution methods
    - over- vs. under-constrained solutions
    - choice of wavelength
    - correlations
- no-one escapes empiricism
- used properly, these methods can be made portable and predictive