Inherent Optical Properties (IOPs)

Lecture 2: Inversion

Empirical
(explicit or implicit)

No need: Bio-optical models

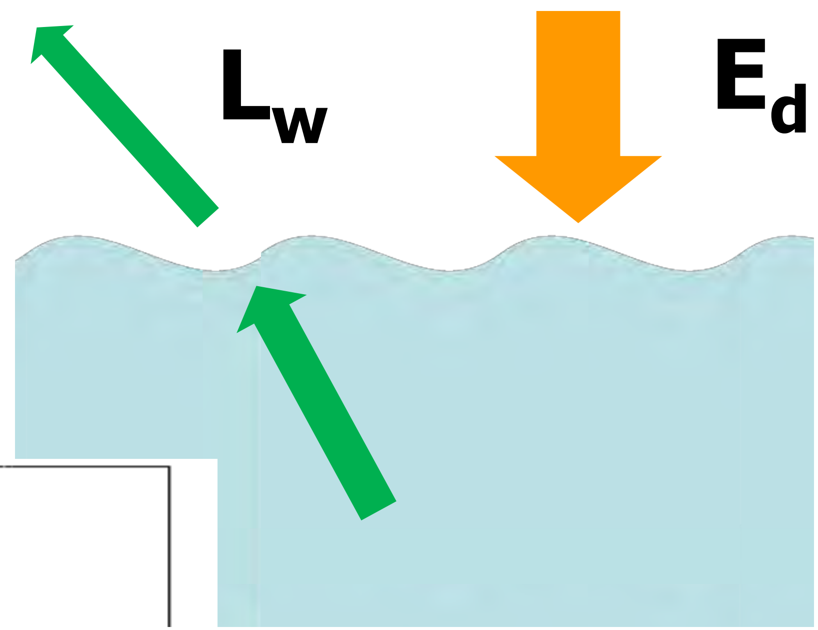
Semi-analytical
(algebraic or optimization)

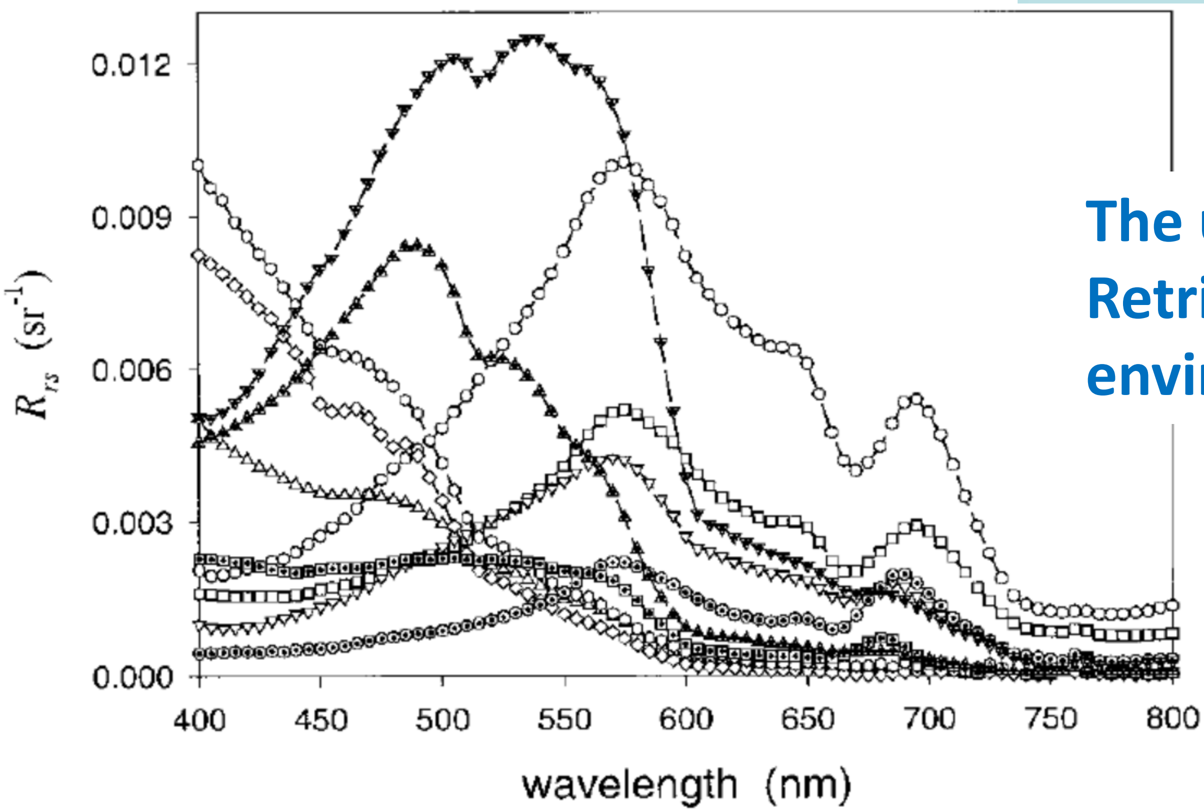
Yes: Bio-optical models

- **Bottom Up Strategy (BUS)**
- **Top Down Strategy (TDS)**

Remote-sensing reflectance (sr^{-1}):

$$R_{rs}(\lambda) = \frac{L_w(\lambda, 0^+)}{E_d(\lambda, 0^+)}$$

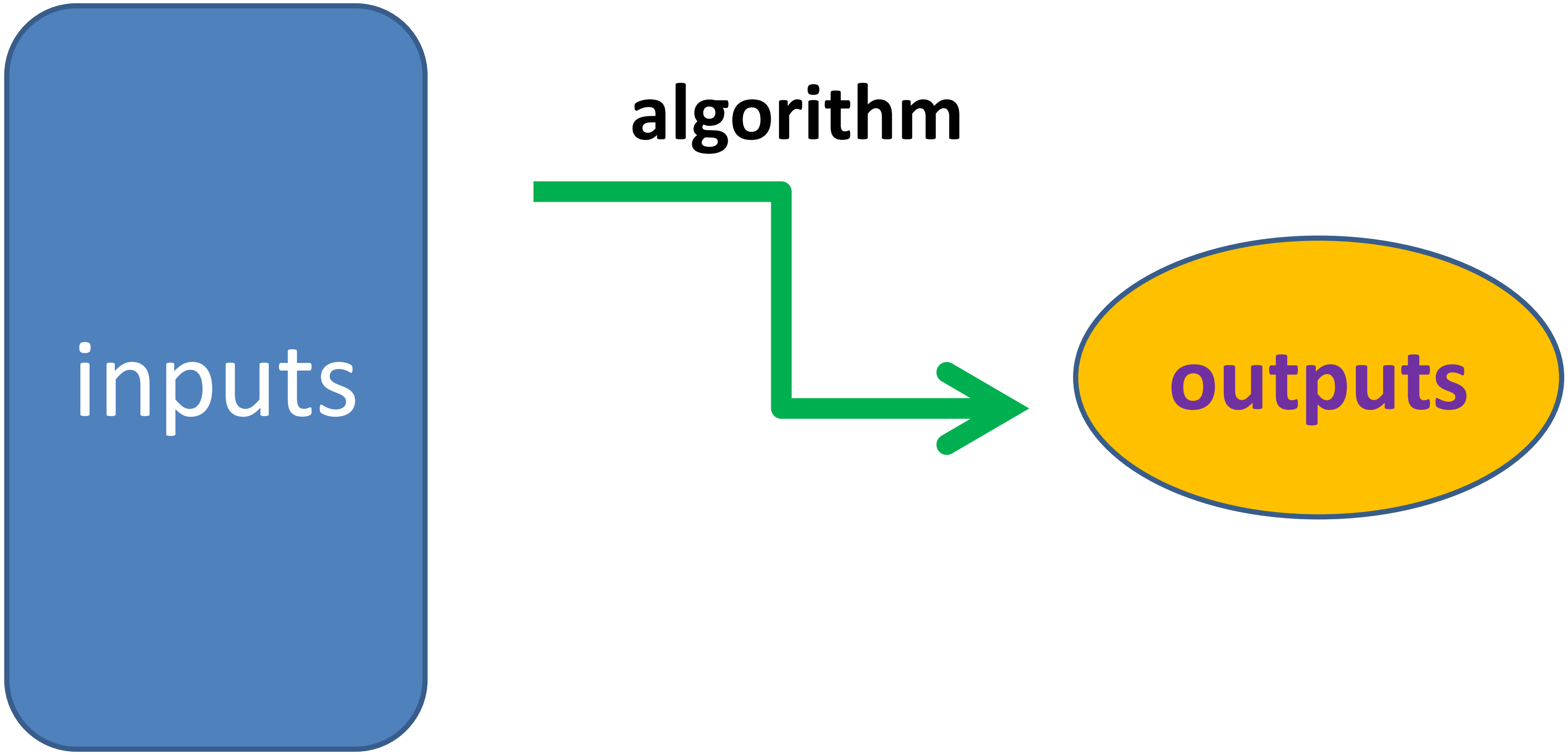




The ultimate objective: Retrieval useful/important environmental information

How?

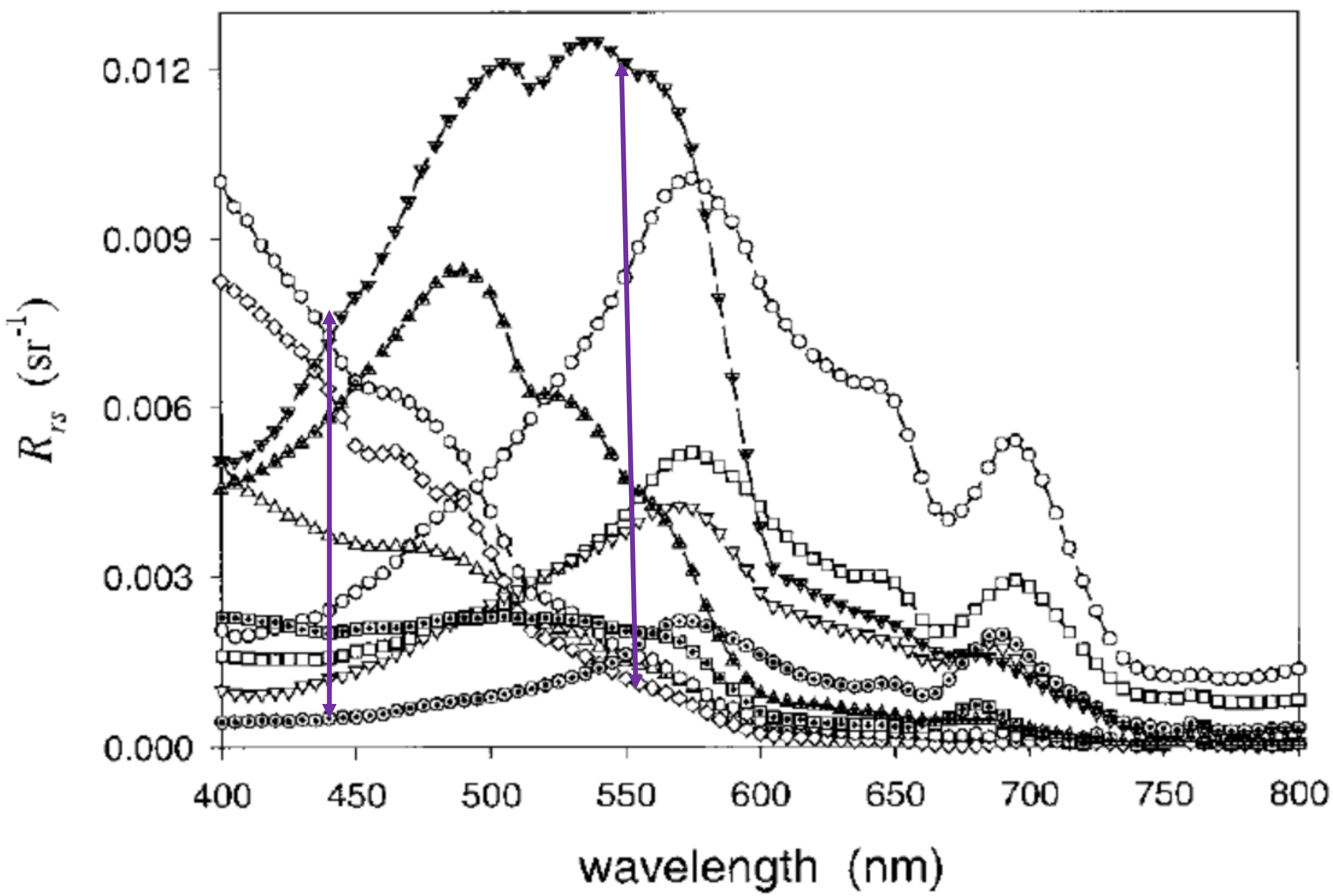
algorithm!


inputs
algorithm
outputs

Chl based on band ratio

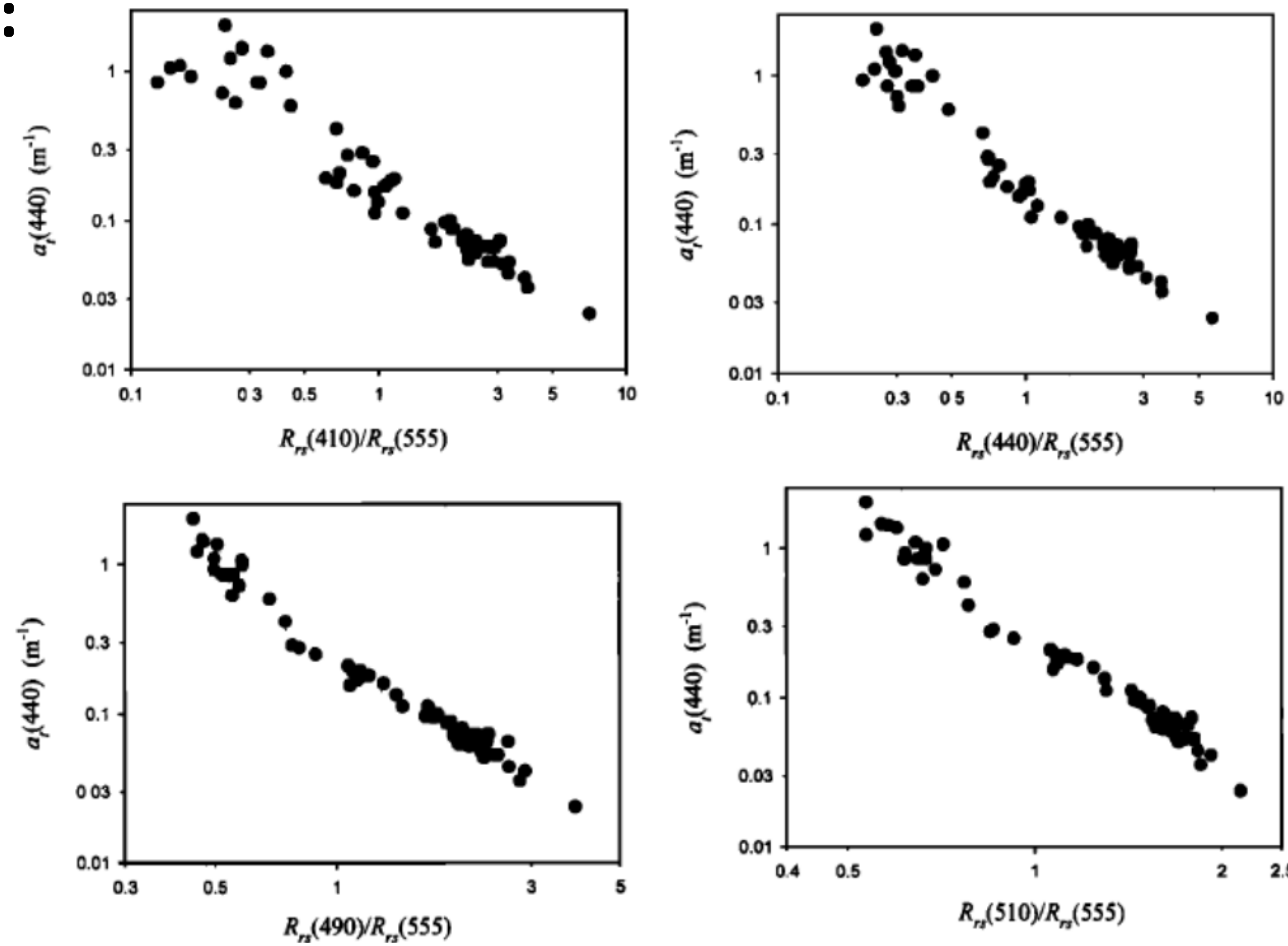
Algorithm	Type	Result Equation(s)	Band Ratio (R), Coefficients (a)
Global processing (GPs)	power	$C_{13} = 10^{(a0+a1*R1)}$ $C_{23} = 10^{(a2+a3*R2)}$ $[C + P] = C_{13}$; if C_{13} and $C_{23} > 1.5\ \mu g\ L^{-1}$ then $[C + P] = C_{23}$	$R1 = \log(Lwn443/Lwn550)$ $R2 = \log(Lwn520/Lwn550)$ $a = [0.053, 1.705, 0.522, 2.440]$
Clark three-band (C3b)	power	$[C + P] = 10^{(a0+a1*R)}$	$R = \log((Lwn443 + Lwn520)/Lwn550)$ $a = [0.745, -2.252]$
Aiken-C	hyperbolic + power	$C_{21} = \exp(a0 + a1*\ln(R))$ $C_{23} = (R + a2)/(a3 + a4*R)$ $C = C_{21}$; if $C < 2.0\ \mu g\ L^{-1}$ then $C = C_{23}$	$R = Lwn490/Lwn555$ $a = [0.464, -1.989, -5.29, 0.719, -4.23]$
Aiken-P	hyperbolic + power	$C_{22} = \exp(a0 + a1*\ln(R))$ $C_{24} = (R + a2)/(a3 + a4*R)$ $[C + P] = C_{22}$; if $[C + P] < 2.0\ \mu g\ L^{-1}$ then $[C + P] = C_{24}$	$R = Lwn490/Lwn555$ $a = [0.696, -2.085, -5.29, 0.592, -3.48]$
OCTS-C	power	$C = 10^{(a0+a1*R)}$	$R = \log((Lwn520 + Lwn565)/Lwn490)$ $a = [0.55006, 3.497]$
OCTS-P	multiple regression	$[C + P] = 10^{(a0+a1*R1+a2*R2)}$	$R1 = \log(Lwn443/Lwn520)$ $R2 = \log(Lwn490/Lwn520)$ $a = [0.19535, -2.079, -3.497]$
POLDER	cubic	$C = 10^{(a0+a1*R+a2*R^2+a3*R^3)}$	$R = \log(Rrs443/Rrs565)$ $a = [0.438, -2.114, 0.916, -0.851]$
CalCOFI two-band linear	power	$C = 10^{(a0+a1*R)}$	$R = \log(Rrs490/Rrs555)$ $a = [0.444, -2.431]$
CalCOFI two-band cubic	cubic	$C = 10^{(a0+a1*R+a2*R^2+a3*R^3)}$	$R = \log(Rrs490/Rrs555)$ $a = [0.450, -2.860, 0.996, -0.3674]$
CalCOFI three-band	multiple regression	$C = \exp(a0 + a1*R1 + a2*R2)$	$R1 = \ln(Rrs490/Rrs555)$ $R2 = \ln(Rrs510/Rrs555)$ $a = [1.025, -1.622, -1.238]$
CalCOFI four-band	multiple regression	$C = \exp(a0 + a1*R1 + a2*R2)$	$R1 = \ln(Rrs443/Rrs555)$ $R2 = \ln(Rrs412/Rrs510)$ $a = [0.753, -2.583, 1.389]$
Morel-1	power	$C = 10^{(a0+a1*R)}$	$R = \log(Rrs443/Rrs555)$ $a = [0.2492, -1.768]$
Morel-2	power	$C = \exp(a0 + a1*R)$	$R = \ln(Rrs490/Rrs555)$ $a = [1.077835, -2.542605]$
Morel-3	cubic	$C = 10^{(a0+a1*R+a2*R^2+a3*R^3)}$	$R = \log(Rrs443/Rrs555)$ $a = [0.20766, -1.82878, 0.75885, -0.73979]$
Morel-4	cubic	$C = 10^{(a0+a1*R+a2*R^2+a3*R^3)}$	$R = \log(Rrs490/Rrs555)$ $a = [1.03117, -2.40134, 0.3219897, -0.291066]$

(O'Reilly et al 1998)



0.012
0.009
0.006
0.003
0.000
R_{rs} (sr^{-1})
400
450
500
550
600
650
700
750
800
wavelength (nm)

Empirical:



$$a_t(440) = 10^{-0.674-0.531\rho_{25}-0.745\rho_{25}^2-1.469\rho_{35}+2.375\rho_{35}^2}, \qquad (14)$$

$$a_\phi(440) = 10^{-0.919+1.037\rho_{25}-0.407\rho_{25}^2-3.531\rho_{35}+1.579\rho_{35}^2}, \qquad (20)$$

(Lee et al 1998)

Basics of physics-based algorithms

'Accurate' Rrs model

$$r_{rs} = \frac{L_u(0^-)}{E_d(0^-)}$$

$$r_{rs} = \frac{f}{Q}\frac{b_b}{a+b_b}$$

$$r_{rs} = g\frac{b_b}{a+b_b} = \left(g_0 + g_1\frac{b_b}{a+b_b}\right)\frac{b_b}{a+b_b}$$

Exact solution:

$$r_{rs}(\lambda,\Omega') \equiv \frac{D_d(\lambda,\theta_S')}{c(\lambda)+k_L(\lambda,\Omega')-f_L(\lambda,\Omega')b_f(\lambda)} \frac{\int_0^{2\pi}\int_0^{\pi/2}\beta(\Omega',\Omega)\,L(\lambda,\Omega')\sin(\theta')\,d\theta'\,d\varphi'}{E_{od}(0^-,\lambda,\theta_S')}$$

Albert and Mobley (2003) :

$$r_{rs}(\lambda,\Omega') = q(\Omega',w)\sum_{i=1}^{4} p_i \left(\frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}\right)^i$$

Lee et al (2004)

$$r_{rs}(\lambda,\Omega') = g_w(\Omega')\frac{b_{bw}(\lambda)}{a(\lambda)+b_b(\lambda)} + g_p(\lambda,\Omega')\frac{b_{bp}(\lambda)}{a(\lambda)+b_b(\lambda)}$$

Park and Ruddick (2005)

$$r_{rs}(\lambda,\Omega') = \sum_{i=1}^{4} g_i(\Omega',\nu_b)\left(\frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}\right)^i$$

Van Der Woerd and Pasterkamp (2008)

$$\ln[r_{rs}(\lambda,\Omega')] = \sum_{i=1}^{4}\sum_{j=1}^{4} P_{ij}(\Omega')[\ln(a(\lambda))]^i[\ln(b(\lambda))]^j$$

Accurate Rrs model

$$R_{rs} = \frac{L_w}{E_d(0^+)}$$

$$E_d(0^-) = t_E E_d(0^+) + \gamma E_u(0^-)$$

$$L_w = \frac{t_L}{n_w^{\ 2}} L_u(0^-)$$

$$R_{rs} = \frac{t_E t_L}{n_w^{\ 2}} \frac{r_{rs}}{1 - \gamma R} = \frac{0.52\, r_{rs}}{1 - 1.7\, r_{rs}}$$

Solve Rrs for IOPs or in-water constituents?

Two basic strategies:

1. Bottom-up strategy (BUS):

Assume we know the spectral shapes of the optically active components

2. Top-down strategy (TDS):

Only need the spectral shape information when it is necessary

What are we facing in RS algorithms?

$$R_{rs}(\lambda) = F(a(\lambda), b_b(\lambda))$$

$$R_{rs}(\lambda) = F(a_w(\lambda), a_{ph}(\lambda), a_{dg}(\lambda), b_{bw}(\lambda), b_{bp}(\lambda))$$

$$\begin{cases} R_{rs}(\lambda_1) = F(a_w(\lambda_1), a_{ph}(\lambda_1), a_{dg}(\lambda_1), b_{bw}(\lambda_1), b_{bp}(\lambda_1)) \\ R_{rs}(\lambda_2) = F(a_w(\lambda_2), a_{ph}(\lambda_2), a_{dg}(\lambda_2), b_{bw}(\lambda_2), b_{bp}(\lambda_2)) \\ \vdots \\ R_{rs}(\lambda_n) = F(a_w(\lambda_n), a_{ph}(\lambda_n), a_{dg}(\lambda_n), b_{bw}(\lambda_n), b_{bp}(\lambda_n)) \end{cases}$$

# of unknowns > # of equations!

An ill formulated math problem!

Have to increase # of equations or decrease # of unknowns!

1. Bottom-up strategy (BUS):

Build-up an Rrs spectrum block-by-block:

$$a(\lambda) = a_w(\lambda) + \sum a_{xi}(\lambda) \qquad b_b(\lambda) = b_{bw}(\lambda) + \sum b_{bxi}(\lambda)$$

$$a(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + a_{dg}(\lambda)$$

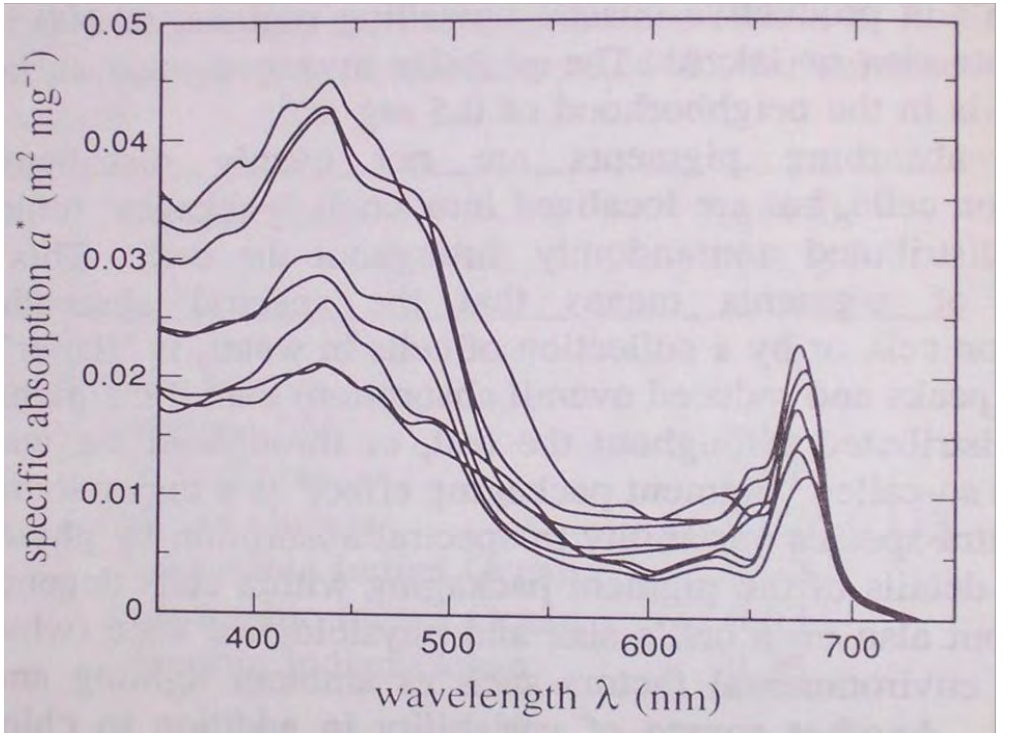
$$a(\lambda) = a_w(\lambda) + M_1 \left\langle a_{ph}(\lambda) \right\rangle + M_2 \left\langle a_{dg}(\lambda) \right\rangle$$

$$b_b(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda)$$

$$b_b(\lambda) = b_{bw}(\lambda) + M_3 \left\langle b_{bm}(\lambda) \right\rangle + M_4 \left\langle b_{bo}(\lambda) \right\rangle$$

$$R_{rs}(\lambda) = G \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

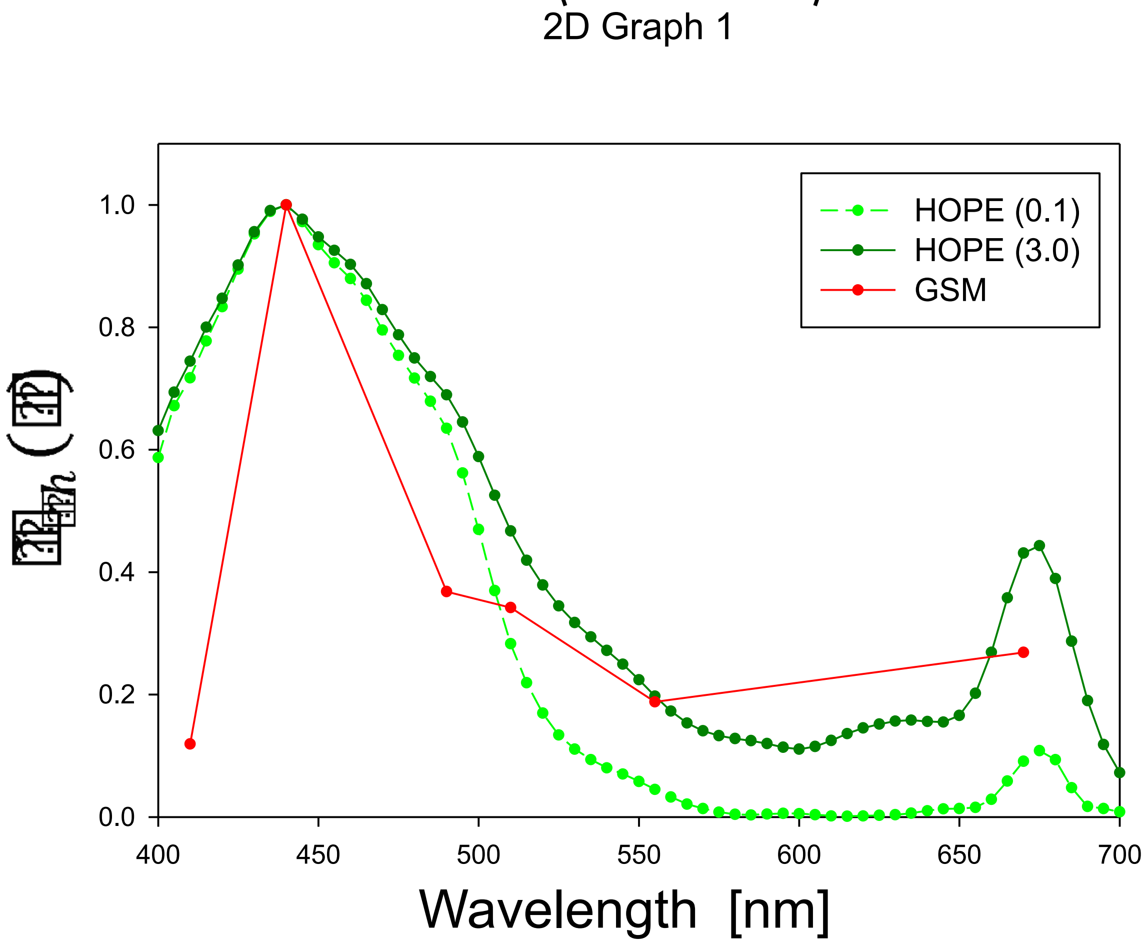
Bio-optical models (forward model)



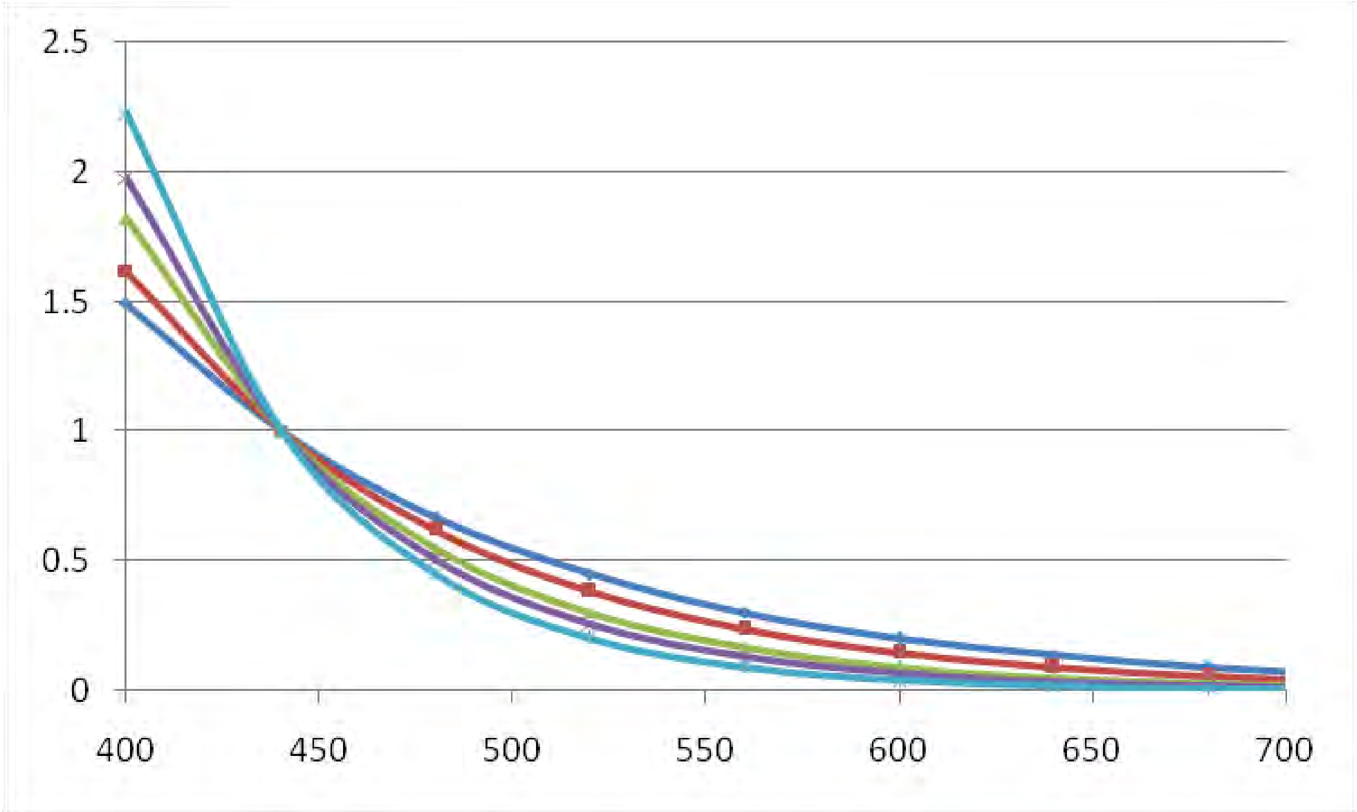
One variable: $$a_{ph}(\lambda) = P\left\langle a_{ph}(\lambda)\right\rangle$$

Two variables: $$a_{ph}(\lambda) = P_1\left\langle a_{ph1}(\lambda)\right\rangle + P_2\left\langle a_{ph2}(\lambda)\right\rangle$$

Examples of $\left\langle a_{ph}(\lambda) \right\rangle$ spectra



Absorption components: a_g spectrum shapes



$$\langle a_g(\lambda) \rangle = e^{-S(\lambda - 440)}$$

S: 0.01 – 0.02 nm^{-1}

(*Bricaud et al* 1981)

$$\left\langle b_{bp}(\lambda) \right\rangle = \left(\frac{440}{\lambda} \right)^{\eta}$$

$$\begin{cases} R_{rs}(\lambda_1) = F(a_w(\lambda_1), b_{bw}(\lambda_1), P, G, X) \\ R_{rs}(\lambda_2) = F(a_w(\lambda_2), b_{bw}(\lambda_2), P, G, X) \\ \vdots \\ R_{rs}(\lambda_n) = F(a_w(\lambda_n), b_{bw}(\lambda_n), P, G, X) \end{cases}$$

3-variables model to describe an Rrs spectrum

$$R_{rs}(\lambda) = G \frac{b_{bw}(\lambda) + M_3 \langle b_{bm}(\lambda) \rangle + M_4 \langle b_{bo}(\lambda) \rangle}{a_w(\lambda) + M_1 \langle a_{ph}(\lambda) \rangle + M_2 \langle a_{dg}(\lambda) \rangle + b_{bw}(\lambda) + M_3 \langle b_{bm}(\lambda) \rangle + M_4 \langle b_{bo}(\lambda) \rangle}$$

$M_{1\text{-}4}$ (or $M_{1\text{-}3}$) are wavelength independent variables!

Then they could be derived by comparing the modeled Rrs spectrum with the measured Rrs spectrum.

Spectral ranges used for solutions (e.g. examples of BUS):

The **blue-green** domain: e.g., Hoge and Lyon (1996), Carder et al (1999)

The **red-infrared** domain: e.g., Binding et al (2012)

The **entire spectrum** (**spectral optimization**): e.g., Bukata et al (1995), Lee et al (1994,1996,1999), Maritorena et al (2002), Boss and Roesler (2006), Brando et al (2012)

Look-Up-Tables (LUT): e.g., Carder et al (1991); Mobley et al (2005)

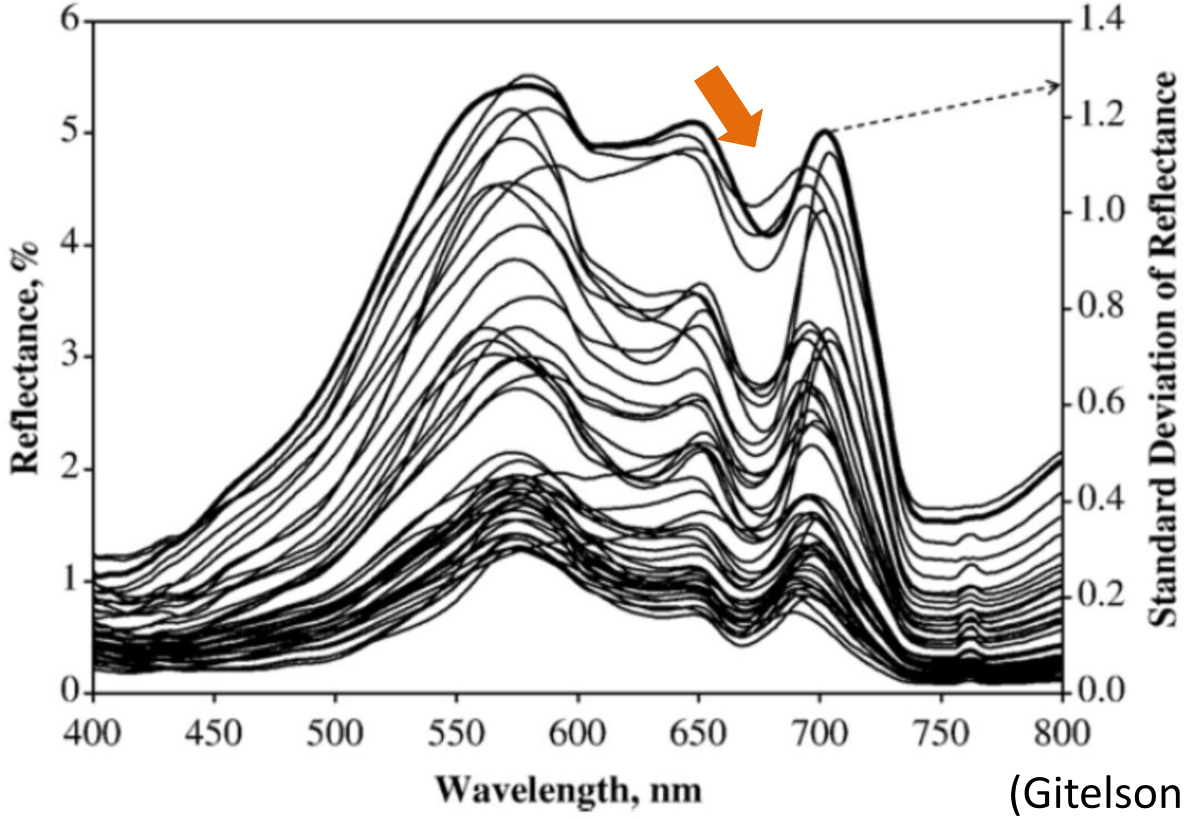
Spectral Optimization

Matching between measured and modeled R_{rs}

Quantitative measure of the closure (**error function**):

$$\delta_{R_{rs}} = \frac{\sqrt{\Lambda_{\lambda 1}^{\lambda 2}\left|\widetilde{R}_{rs}(\lambda) - R_{rs}(\lambda)\right|^2}}{\Lambda_{\lambda 1}^{\lambda 2} R_{rs}(\lambda)} = \sqrt{n}\,\frac{\sqrt{\sum_{\lambda 1}^{\lambda 2}\left|\widetilde{R}_{rs}(\lambda) - R_{rs}(\lambda)\right|^2}}{\sum_{\lambda 1}^{\lambda 2} R_{rs}(\lambda)}$$

Algorithms using information in the red-infrared bands



(Gitelson et al 2007)

Two bands

$$Chl = f\left(\frac{Rrs(75x)}{Rrs(67x)}\right)$$

Three bands

$$Chl = f\left(\frac{Rrs(75x)}{Rrs(67x)} - \frac{Rrs(75x)}{Rrs(70x)}\right)$$

Two-, three-, four-band ratios in the red-infrared domain:

$$R_{rs}(\lambda) = G \frac{b_{bw}(\lambda) + M_3 \langle b_{bm}(\lambda) \rangle + M_4 \langle b_{bo}(\lambda) \rangle}{a_w(\lambda) + M_1 \langle a_{ph}(\lambda) \rangle + M_2 \langle a_{dg}(\lambda) \rangle + b_{bw}(\lambda) + M_3 \langle b_{bm}(\lambda) \rangle + M_4 \langle b_{bo}(\lambda) \rangle}$$

$$R_{rs}(\lambda) \approx G \frac{M_3 \langle b_{bp}(\lambda) \rangle}{a_w(\lambda) + M_1 \langle a_{ph}(\lambda) \rangle}$$

$$\frac{R_{rs}(\lambda_{red1})}{R_{rs}(\lambda_{red2})} = \frac{\langle b_{bp}(\lambda_{red1}) \rangle}{\langle b_{bp}(\lambda_{red2}) \rangle} \frac{a_w(\lambda_{red2}) + M_1 \langle a_{ph}(\lambda_{red2}) \rangle}{a_w(\lambda_{red1}) + M_1 \langle a_{ph}(\lambda_{red1}) \rangle}$$

Proper contrast of Rrs at λ_1 and λ_2 then leads to M_1.

2. Top-down strategy (TDS):

$$R_{rs} = G \frac{b_b}{a + b_b}$$

$$R_{rs} \rightarrow b_b \& a \rightarrow a_x$$

$$\Downarrow$$

Clarity (Secchi depth, light depth, TSM/SPM, etc)

Remote sensing measures the *total* effect:

Water clarity (or turbidity) is also a measure of total effect.

Examples of TDS:

Loisel & Stramski (2000), QAA (Lee et al, 2002); Smyth et al (2006); Doran et al (2007).

The Quasi-Analytical Algorithm (QAA)

Forward modeling:

$(a, b_b, \text{etc}) \rightarrow Rrs$

$$R_{rs} \approx 0.05 \frac{b_b}{a + b_b}$$

QAA:

$(a, b_b) \leftarrow Rrs$

The data flow of QAA:

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

$$\eta$$

$$a(\lambda_0) = a_w(\lambda_0) + \delta a(\lambda_0)$$

$$b_{bp}(\lambda_0) = F_2\left(r_{rs}(\lambda_0), a(\lambda_0), b_{bw}(\lambda_0)\right)$$

$$b_{bp}(\lambda) = b_{bp}(\lambda_0)\left(\frac{\lambda_0}{\lambda}\right)^{\eta}$$

$$a(\lambda) = F_3\left(r_{rs}(\lambda), b_{bp}(\lambda), b_{bw}(\lambda)\right)$$

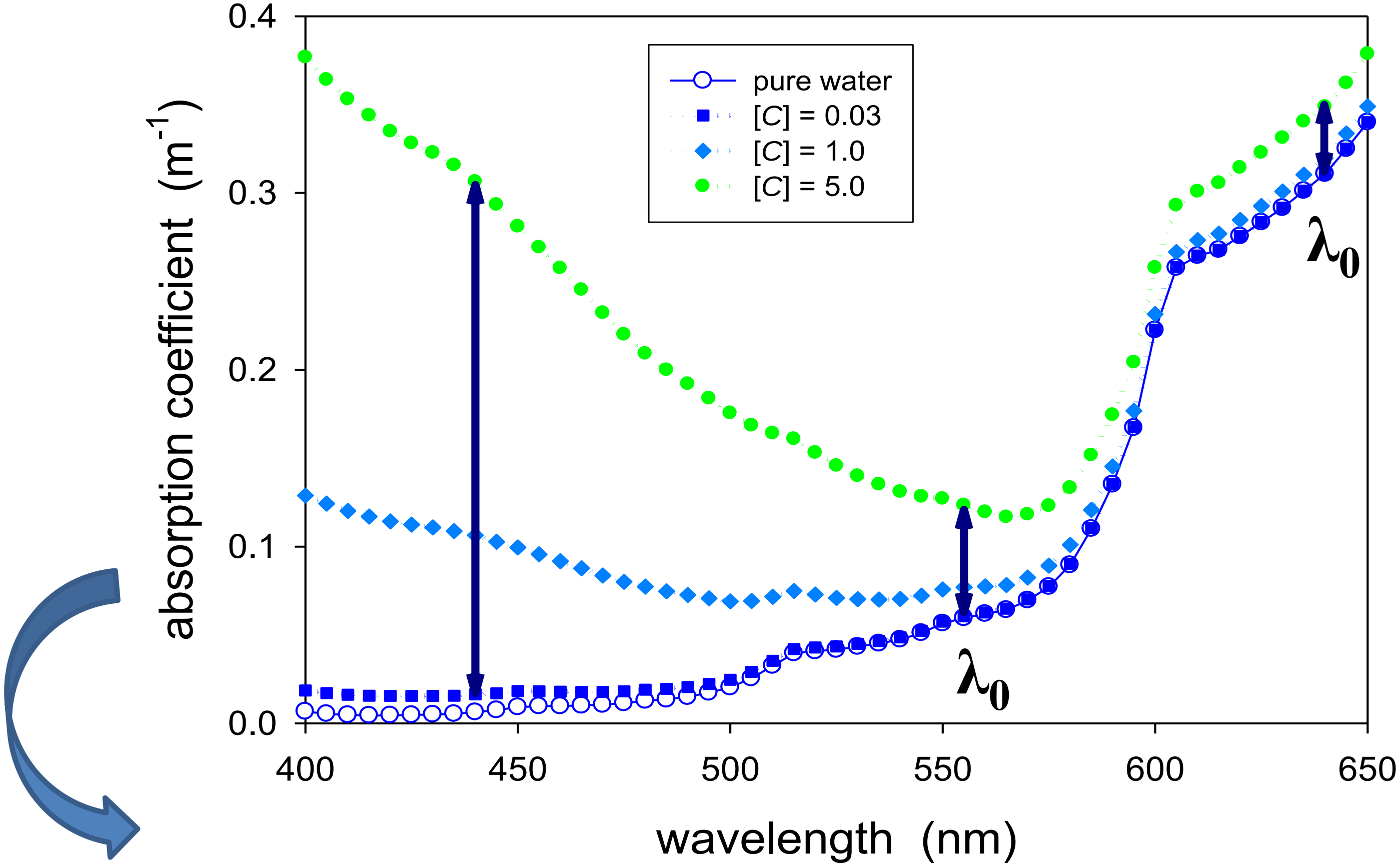
$$\begin{cases} a(411) = a_w(411) + \zeta a_{ph}(443) + \xi a_{dg}(443) \\ a(443) = a_w(443) + a_{ph}(443) + a_{dg}(443) \end{cases}$$

$$\zeta = \frac{a_{ph}(411)}{a_{ph}(443)}$$

$$\xi = \frac{a_{dg}(411)}{a_{dg}(443)}$$

(Lee et al 2002)

Logic behind QAA:



For a reference wavelength, λ_0, variation of $a(\lambda_0)$ is limited.

Known $a(\lambda_0)$, enables calculation of $b_b(\lambda_0)$ from $R_{rs}(\lambda_0)$; propagate $b_b(\lambda_0)$ to $b_b(\lambda)$, then enables calculation of $a(\lambda)$ from $R_{rs}(\lambda)$.

No need of spectral model of $a_x(\lambda)$ in this process!

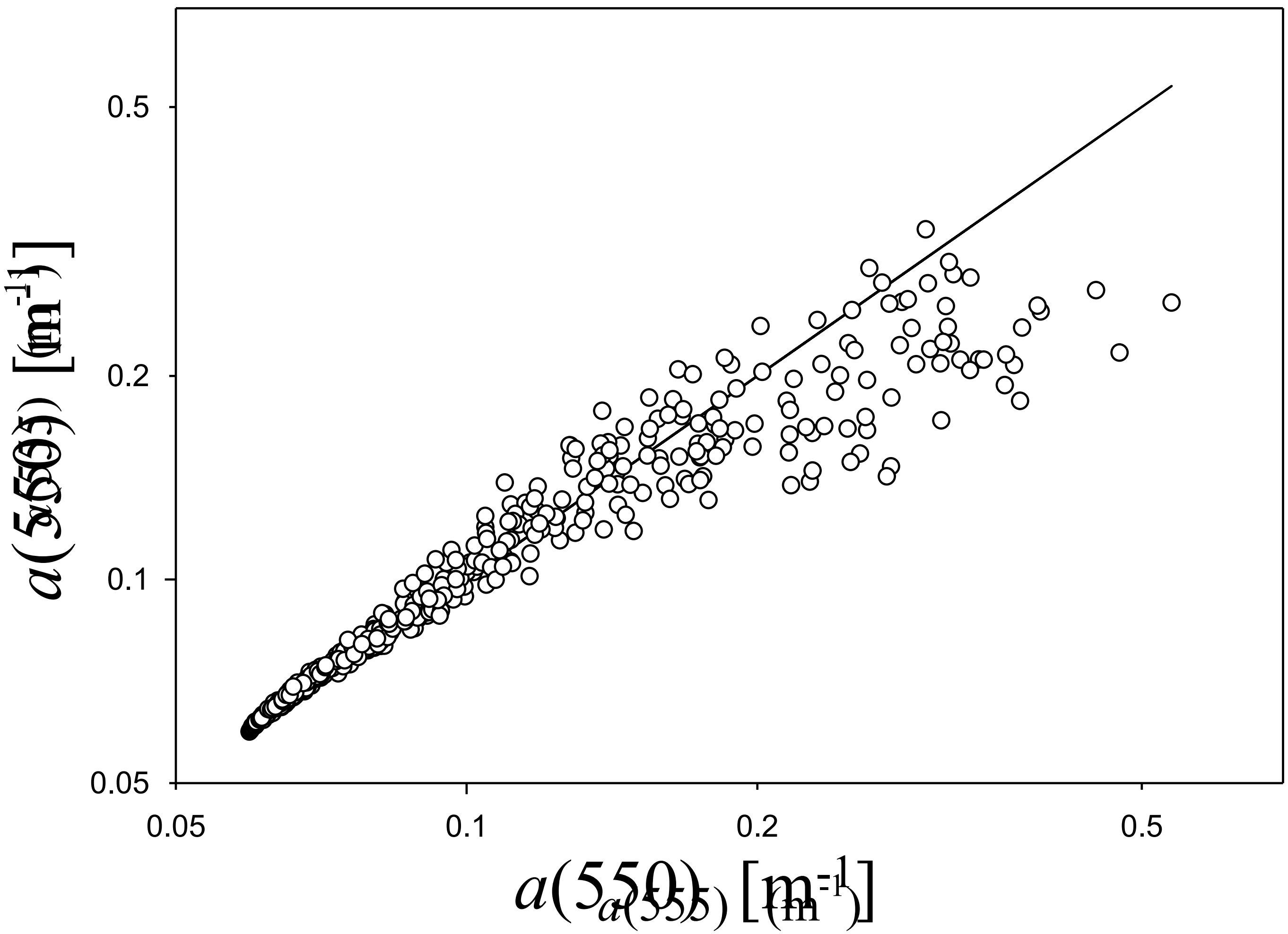
When 550 nm as the reference wavelength (λ_0)

$$a(550) = a_w(550) + 10^{-1.146-1.366\chi-0.469\chi^2}$$

$$\chi = \log\left(\frac{r_{rs}(443) + r_{rs}(490)}{r_{rs}(\lambda_0) + 5\frac{r_{rs}(667)}{r_{rs}(490)}r_{rs}(667)}\right)$$

$a_w(550) = 0.0565$

Empirical!


0.05
0.1
0.2
0.5
0.05
0.1
0.2
0.5
a(550) [m-1]
a(555) (m-1)
a(550) [m-1]
a(555) (m-1)

Invert Rrs:

R_{rs} → r_{rs} → $\{a \& b_b\}$

$r_{rs}(\lambda) = R_{rs}(\lambda)/(0.52 + 1.7\, R_{rs}(\lambda))$

$$r_{rs} = g_0\left(\frac{b_b}{a+b_b}\right) + g_1\left(\frac{b_b}{a+b_b}\right)^2$$

$g_0=0.089, g_1=0.125$

$$u(\lambda) = \frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)} = \frac{-g_0 + \sqrt{(g_0)^2 + 4g_1 * r_{rs}(\lambda)}}{2g_1}$$

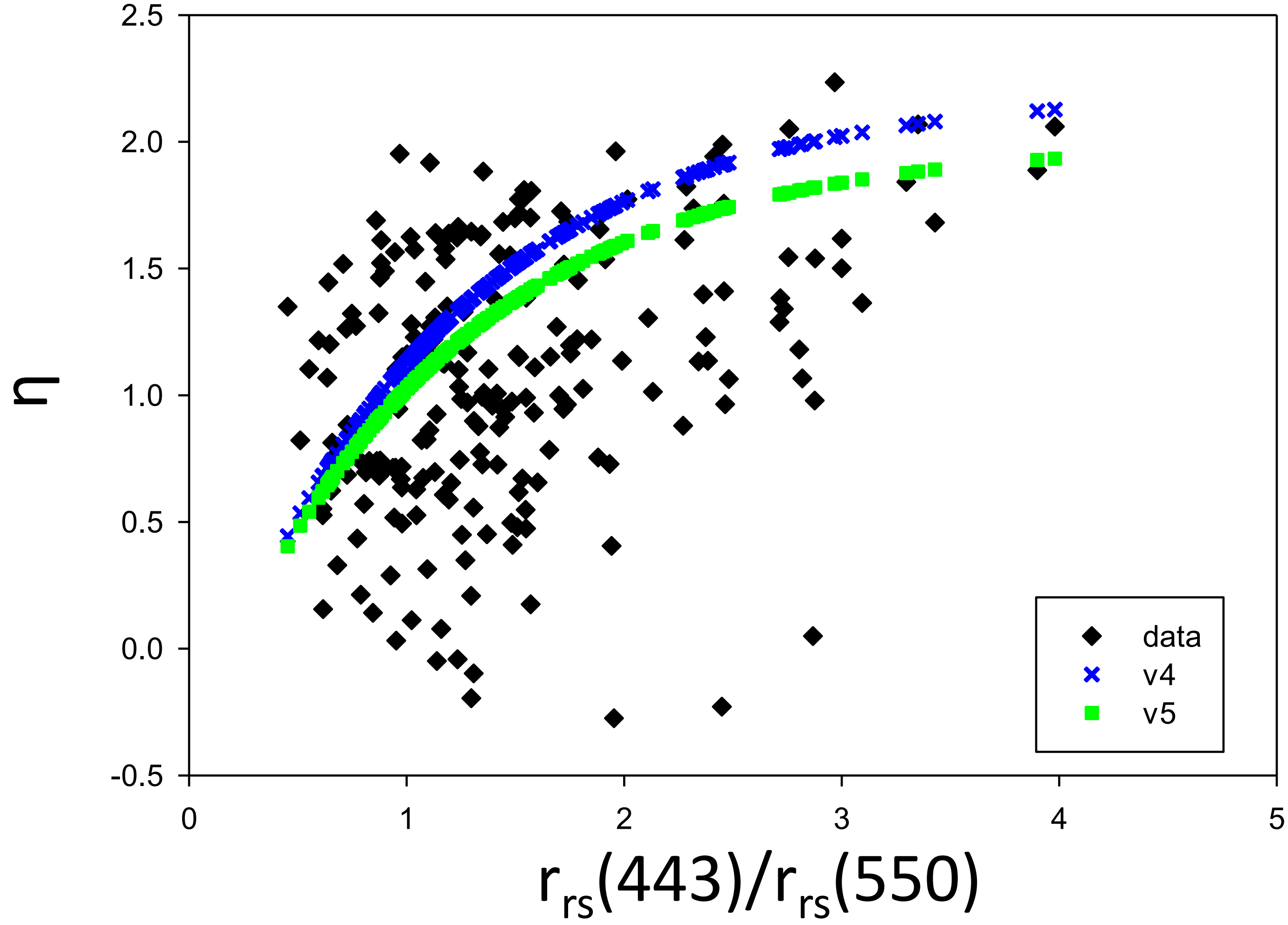
$$a(550) = a_w(550) + 10^{-1.146-1.366\,\chi-0.469\,\chi^2}$$

$$b_{bp}(550) = \frac{u(550)\,a(550)}{1-u(550)} - b_{bw}(550)$$

$$b_{bp}(\lambda) = b_{bp}(550)\left(\frac{550}{\lambda}\right)^{\eta}$$

Empirical:

$$\eta = 2.0\left(1 - 1.2\ \exp\left(-0.9\frac{r_{rs}(443)}{r_{rs}(\lambda_0)}\right)\right)$$



$$b_b(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda)$$

$$a(\lambda) = \frac{(1 - u(\lambda))\, b_b(\lambda)}{u(\lambda)}$$

$$a(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + a_{dg}(\lambda)$$

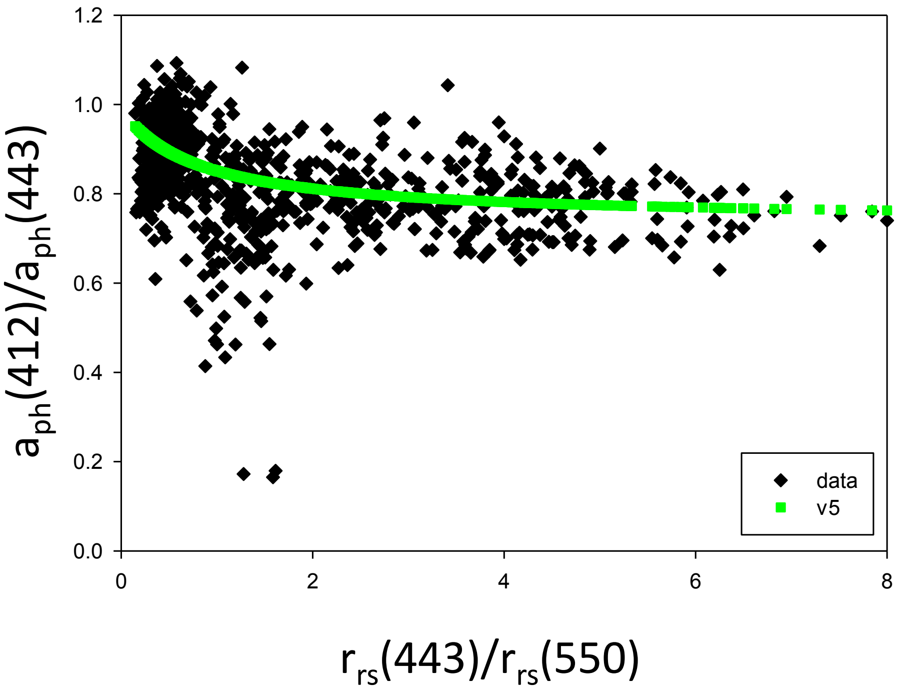
$$\begin{cases} a(410) = a_w(410) + a_{ph}(410) + a_{dg}(410), \\ a(440) = a_w(440) + a_{ph}(440) + a_{dg}(440). \end{cases}$$

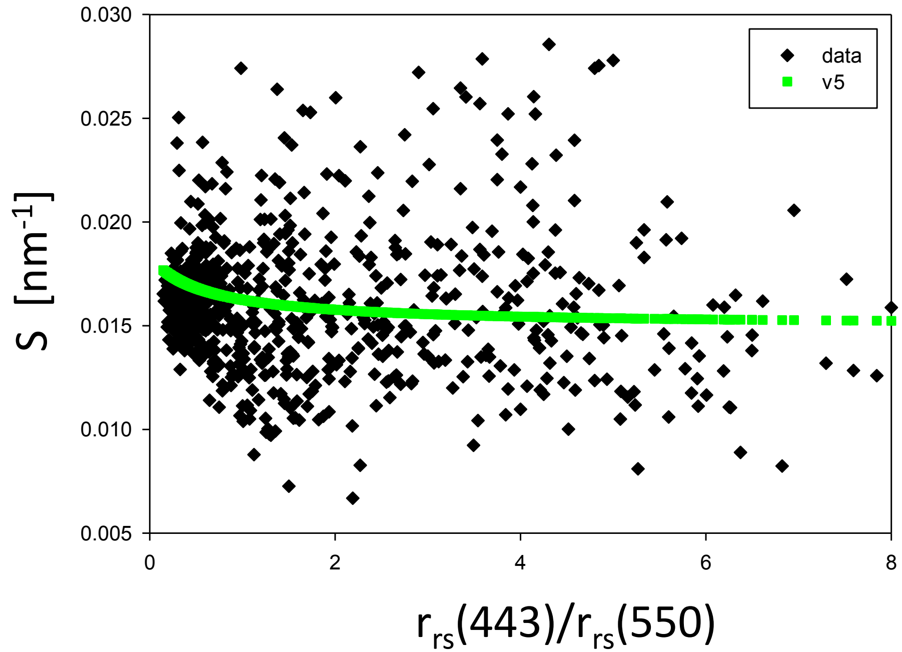
$$\zeta = \frac{a_{ph}(410)}{a_{ph}(440)} \qquad \xi = \frac{a_{dg}(410)}{a_{dg}(440)}$$

$$\begin{cases} a(410) = a_w(410) + \zeta\, a_{ph}(440) + \xi\, a_{dg}(440), \\ a(440) = a_w(440) + a_{ph}(440) + a_{dg}(440). \end{cases}$$

$$\begin{cases} a(410) = a_w(410) + \zeta\, a_{ph}(440) + \xi\, a_{dg}(440), \\ a(440) = a_w(440) + a_{ph}(440) + a_{dg}(440). \end{cases}$$

$$\begin{cases} a_g(440) = \dfrac{\left(a(410) - \zeta\, a(440)\right) - \left(a_w(410) - \zeta\, a_w(440)\right)}{\xi - \zeta}, \\ a_{ph}(440) = a(440) - a_w(440) - a_{dg}(440). \end{cases}$$





$$\xi = e^{S(443-411)},$$

$$\zeta = 0.74 + \frac{0.2}{0.8 + r_{rs}(443)/r_{rs}(550)}$$

$$S = 0.015 + \frac{0.002}{0.6 + r_{rs}(443)/r_{rs}(550)}$$

Empirical!

Key Points:

1. Various inversion algorithms for IOPs have been developed; but more/better ones are also expected.

2. BUS derives every component first, then (simultaneously) derives the total optical property.

Assume the spectral shapes of the optically active components are well characterized!
BUS relies more on forward bio-optical model

3. TDS derives total first, then decompose to separate components.

TDS relies more on Rrs measurement