A model based on stacked-constraints approach for partitioning the light absorption coefficient of seawater into phytoplankton and non-phytoplankton components

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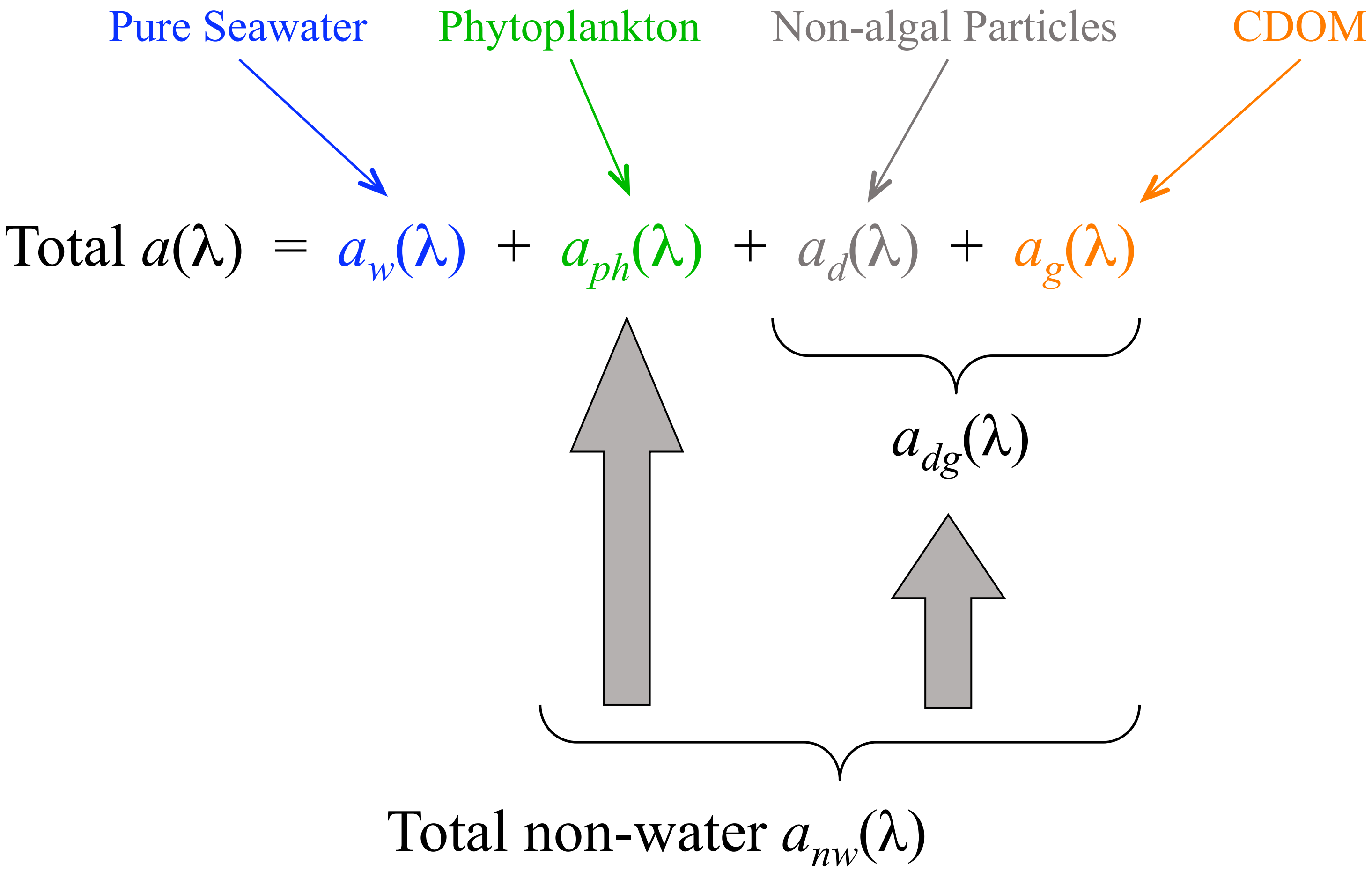
Background: Absorption Coefficient of Seawater



Pure Seawater

Phytoplankton

Non-algal Particles

CDOM

$$\text{Total } a(\lambda) = a_w(\lambda) + \underbrace{a_{ph}(\lambda) + \underbrace{a_d(\lambda) + a_g(\lambda)}_{a_{dg}(\lambda)}}_{\text{Total non-water } a_{nw}(\lambda)}$$

Existing Partitioning Models

Involve highly restrictive assumptions on spectral shape of $a_{ph}(\lambda)$ and/or spectral slope of $a_{dg}(\lambda)$, which limit the performance of these models.

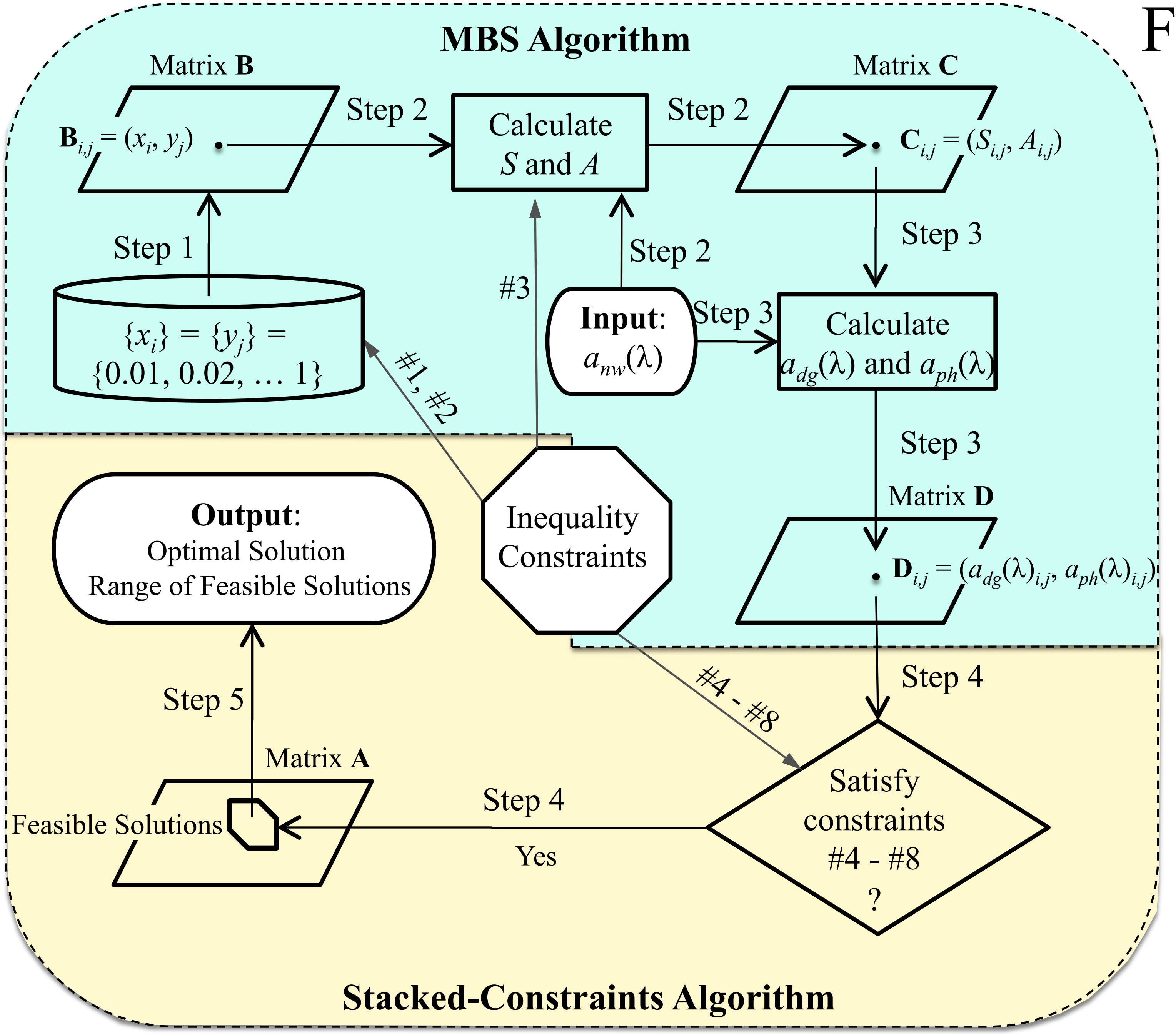
Model	Minimum Input	Key Assumptions for Phytoplankton Absorption	Key Assumptions for Non-Phytoplankton Absorption
Roesler et al., 1989	[Chl-a], [Pheo], and $a_{nw}(\lambda)$ at 436, 676 nm	1. The ratio $a_{ph}(436)$:$a_{ph}(676)$ is a specified function of the ratio [Pheo]:[Chl *a*]. 2. $a_{ph}(676) = a_{nw}(676)$	$a_{dg}(\lambda)$ is an exponential function of λ with fixed slope, $S_{dg} = 0.015$ nm^{-1}.
Lee et al., 2002, 2007	$a_{nw}(\lambda)$ at 410, 440 nm, and $r_{rs}(\lambda)$ at 440, 555 nm	The ratio $a_{ph}(410)$:$a_{ph}(440)$ is a function of the ratio $r_{rs}(440)$:$r_{rs}(555)$.	$a_{dg}(\lambda)$ is an exponential function of λ with fixed slope, $S_{dg} = 0.015$ nm^{-1}.
Maritorena et al., 2002	$a_{nw}(\lambda)$ at 412, 443, 490, 510, 555, 670 nm	The Chl-specific absorption coefficients for phytoplankton are specified.	$a_{dg}(\lambda)$ is an exponential function of λ with fixed slope, $S_{dg} = 0.015$ nm^{-1}.
Gallegos and Neale, 2002*	$a_{nw}(\lambda)$ at 412, 440, 488, 676, 715 nm	$a_{ph}(\lambda)$ are specified linear functions of $a_{ph}(676)$.	$a_d(\lambda)$ and $a_g(\lambda)$ are specified linear functions of $a_d(440)$ and $a_g(440)$, respectively.
Schofield et al., 2004*	$a_{nw}(\lambda)$ at 412, 440, 488, 510, 555, 630, 650, 676, 715 nm	$a_{ph}(\lambda)$ is a linear combination of three specified absorption spectra representing phytoplankton containing Chl *a-c*, phycobilin, and Chl *a-b*, respectively.	1. Both $a_d(\lambda)$ and $a_g(\lambda)$ are exponential functions of λ with variable slopes, S_g and S_d. 2. $S_g > S_d$ 3. $a_d(676) = a_g(676)$
Ciotti and Bricaud, 2006	[Chl] and $a_{nw}(\lambda)$ at 412, 443, 490, 510, 555 nm	1. $a_{ph}(490)/a_{ph}(412) = 0.919$ $[\mathrm{Chl}]^{.012}$ 2. $a_{ph}(510)/a_{ph}(412) = 0.581$ $[\mathrm{Chl}]^{.047}$	$a_{dg}(\lambda)$ is an exponential function of λ with variable slope, S_{dg}.
		1. $a_{ph}(\lambda)$ is a linear combination of two specified absorption spectra representing picoplankton and microplankton, respectively. 2. $a_{ph}(505) = 0.0185$ $[\mathrm{Chl}]^{0.684}$	

Objective

Develop a partitioning model that

- does not require highly restrictive assumptions on $a_{ph}(\lambda)$ and $a_{dg}(\lambda)$
- can be applied to data at past and current satellite ocean color bands, as well as data with higher spectral resolution including future satellite data

Flowchart



Derive a large number of speculative solutions.

First identifies feasible solutions, then optimal solution and range of feasible solutions.

Input and Output

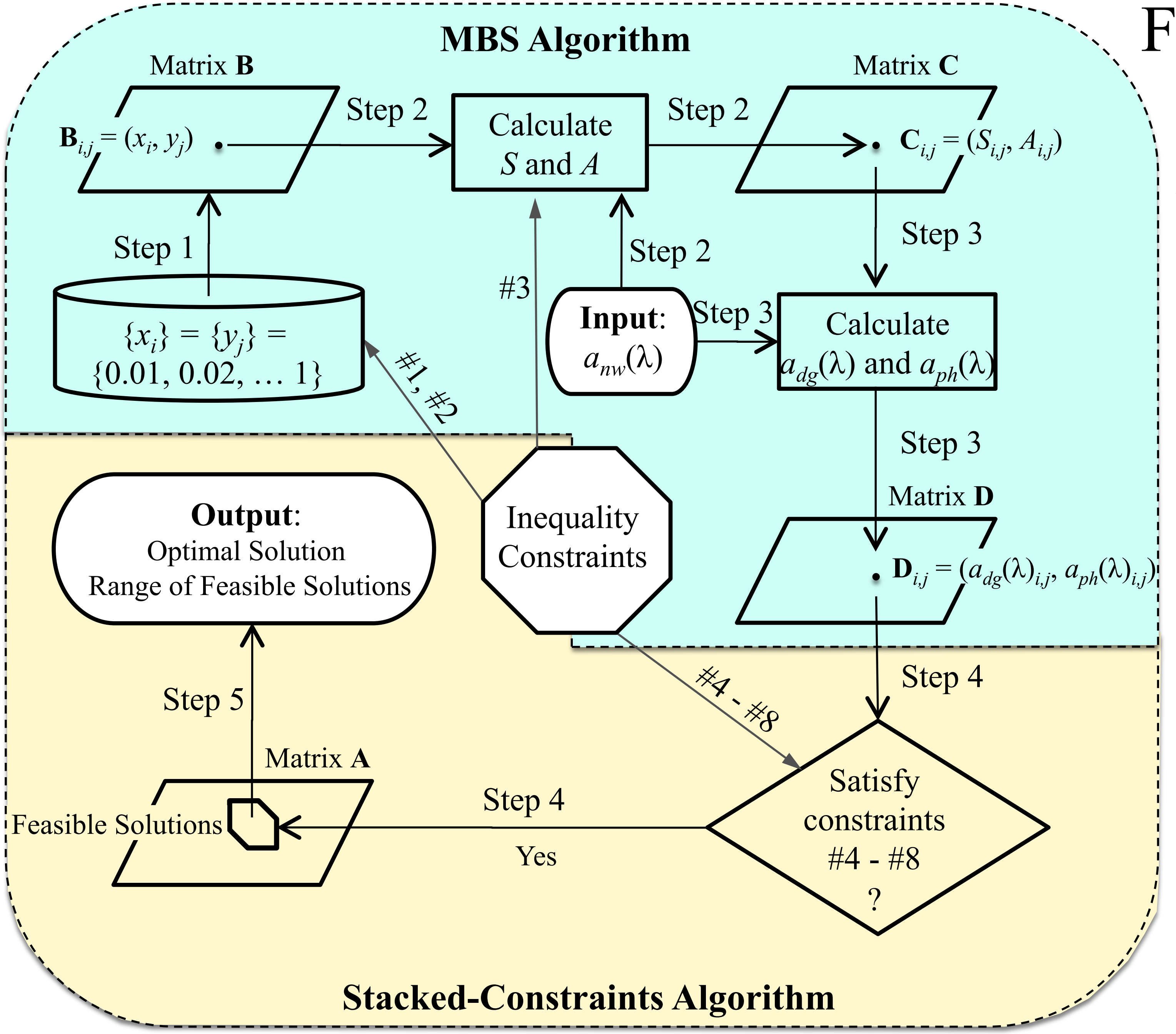
- Input
  - $a_{nw}(\lambda)$ at a minimum of six wavelengths

    412 nm, 443 nm, 490 nm, 510 nm, 555 nm, and 670 nm
  - or $a_{nw}(\lambda)$ with higher spectral resolution

- Output
  - $a_{dg}(\lambda)$ with arbitrarily high spectral resolution because

    $$a_{dg}(\lambda) = A \exp(- S \lambda)$$
  - $a_{ph}(\lambda)$ with same spectral resolution as input $a_{nw}(\lambda)$

Flowchart



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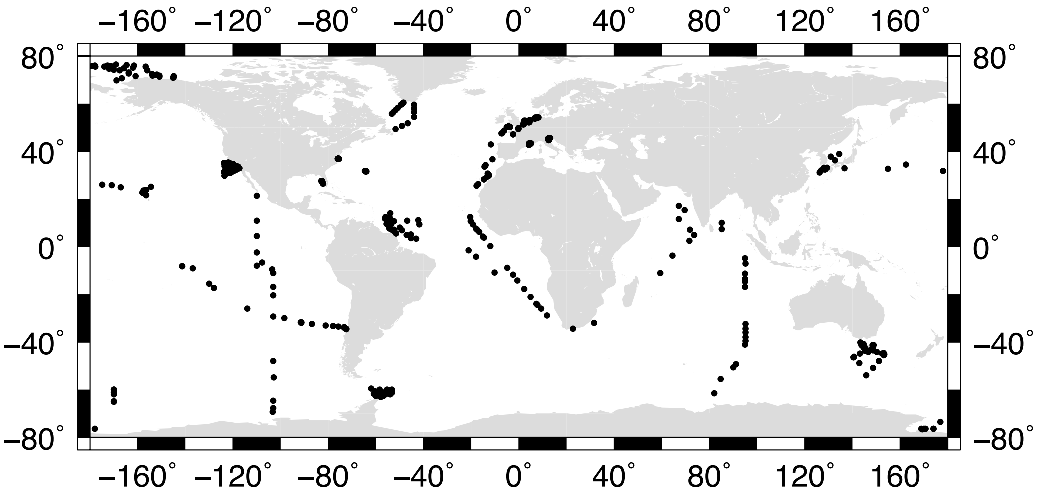
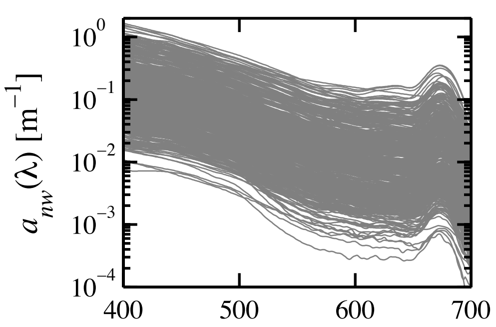
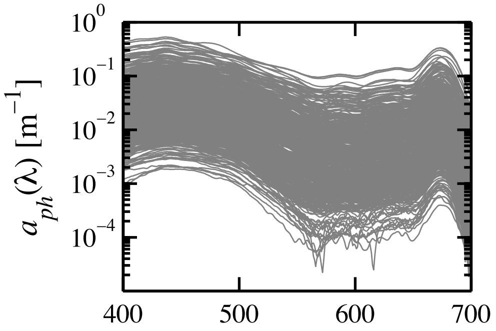
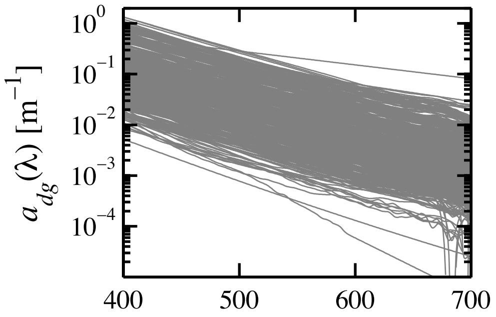
Field Data and Inequality Constraints



Absorption coefficients data collected from 505 open ocean and coastal surface stations from low to high latitudes.







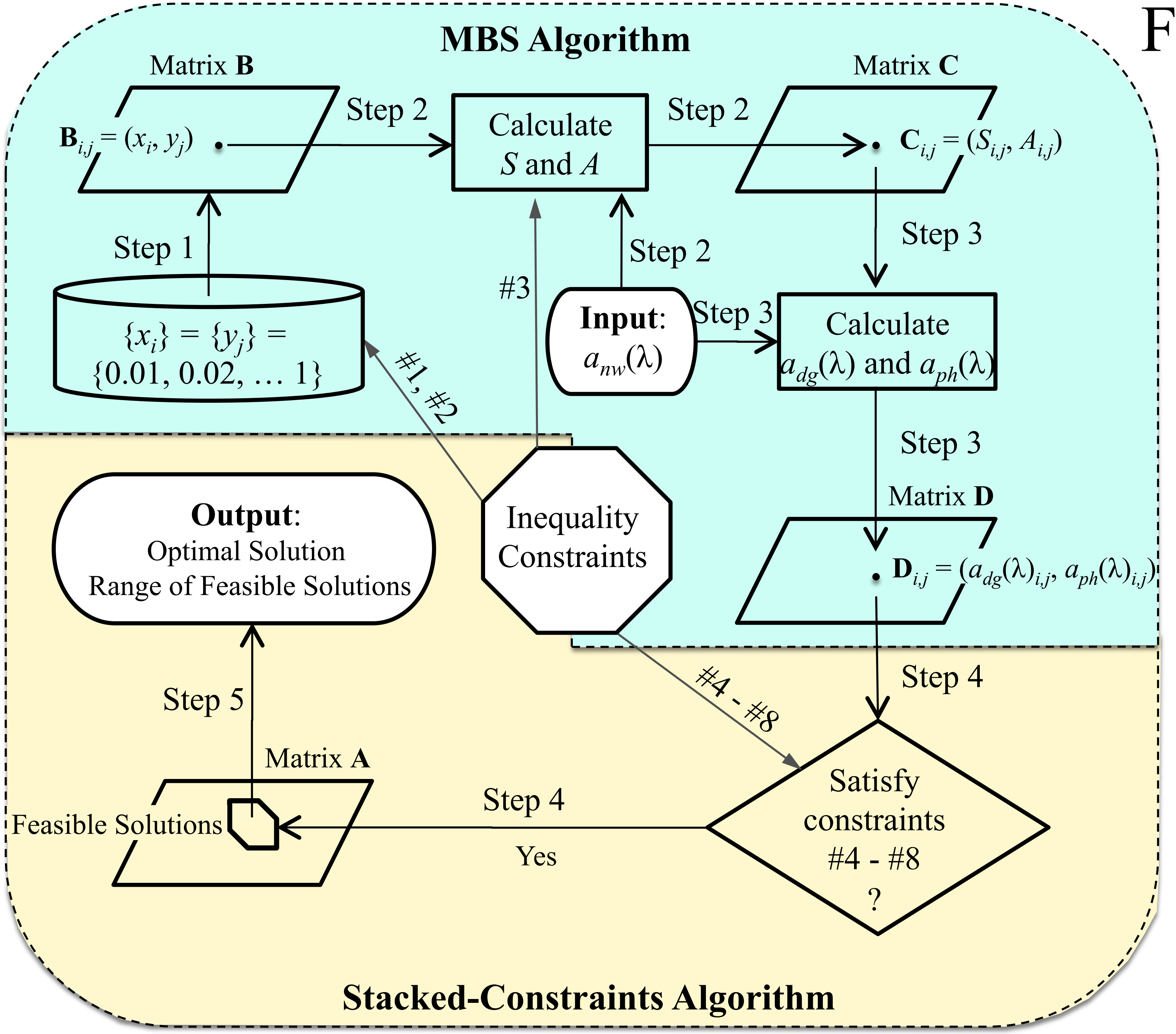
Hyperspectral measurements spanning a wide range of variability in spectral shape and magnitude.

Inequality Constraints

# 1	$0 < a_{ph}(412)/a_{ph}(443) < 1$
# 2	$0 < a_{ph}(510)/a_{ph}(490) < 1$
# 3	$0.006\ \text{nm}^{-1} < S < 0.03\ \text{nm}^{-1}$
# 4	$0.74 < a_{ph}(467)/a_{ph}(412) < 1.54$
# 5	$1.3 < a_{ph}(510)/a_{ph}(555) < 10$
# 6	$1.4 < a_{ph}(443)/a_{ph}(670) < 9.1$
# 7	$0.33\ a_{nw}(412)/a_{nw}(443) < a_{dg}(412)/a_{nw}(412) < 0.78\ a_{nw}(412)/a_{nw}(443)$
# 8	$0.003 < (na_{ph}(510) - na_{ph}(555))/(555 - 510) < 0.0087$

Account for the wide range of variability.

Flowchart



Derive a large number of speculative solutions.

First identifies feasible solutions, then optimal solution and range of feasible solutions.

Modified Bricaud & Stramski (MBS) Algorithm

Original *Bricaud and Stramski* [1990] Algorithm

$$a_d(\lambda) = A \exp(-S\lambda)$$

$$a_p(\lambda) \rightarrow \boxed{\begin{array}{l} a_{ph}(505)/a_{ph}(380) = 0.99 \\ a_{ph}(580)/a_{ph}(693) = 0.92 \end{array}} \rightarrow S, A \rightarrow a_d(\lambda) \rightarrow a_{ph}(\lambda)$$

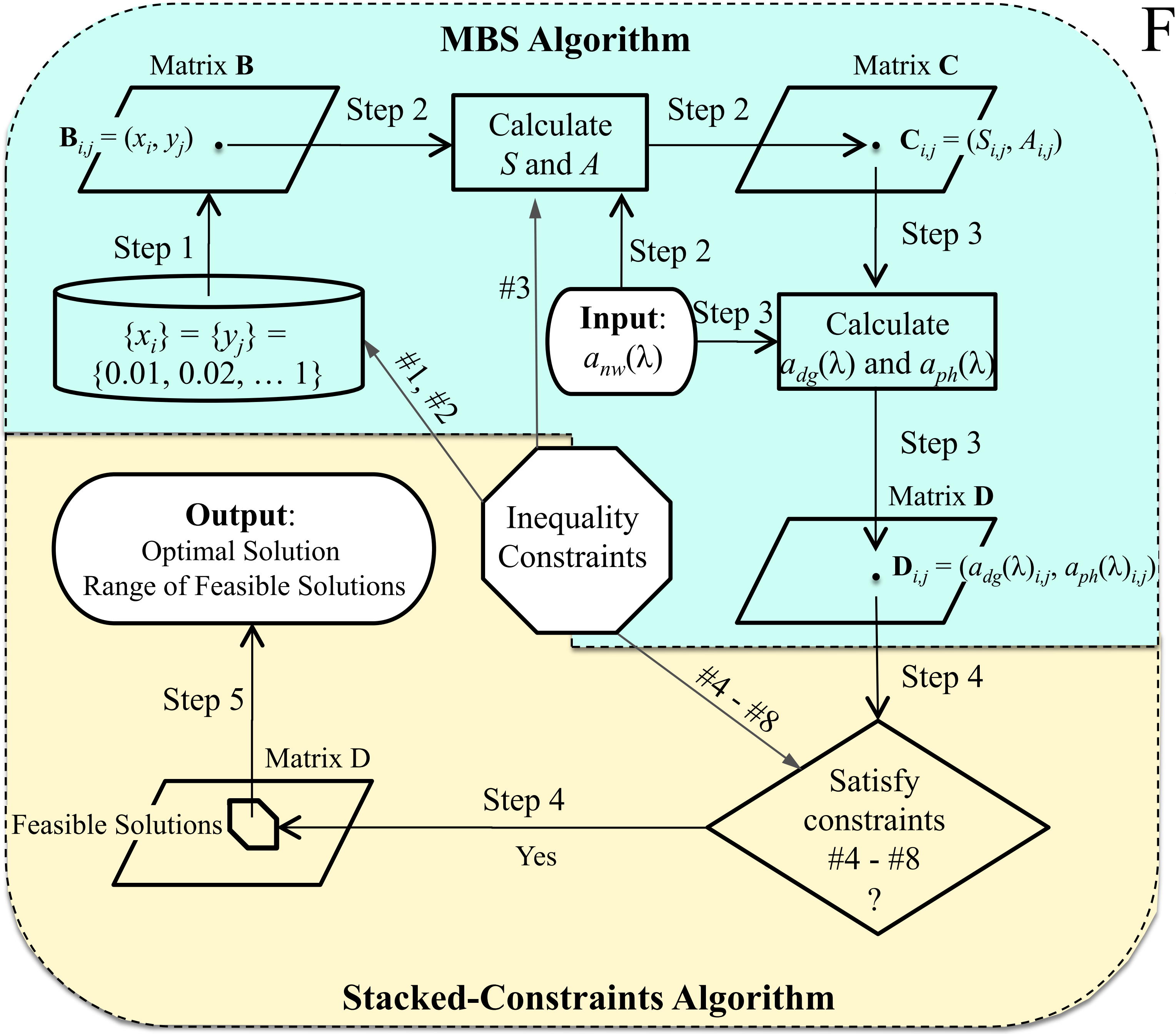
Modified Bricaud & Stramski Algorithm, MBS

$$a_{dg}(\lambda) = A \exp(-S\lambda)$$

$$a_{nw}(\lambda) \rightarrow \boxed{\begin{array}{l} a_{ph}(412)/a_{ph}(443) = x \\ a_{ph}(510)/a_{ph}(490) = y \end{array}} \rightarrow S, A \rightarrow a_{dg}(\lambda) \rightarrow a_{ph}(\lambda)$$

Inequality Constraints	
# 1	$0 < x = a_{ph}(412)/a_{ph}(443) < 1$
# 2	$0 < y = a_{ph}(510)/a_{ph}(490) < 1$
# 3	$0.006\ \mathrm{nm}^{-1} < S < 0.03\ \mathrm{nm}^{-1}$

Flowchart



MBS Algorithm

Matrix **B**

$\mathbf{B}_{i,j} = (x_i, y_j)$

Step 2

Calculate
S and A

Step 2

Matrix **C**

$\mathbf{C}_{i,j} = (S_{i,j}, A_{i,j})$

Step 1

$\{x_i\} = \{y_j\} = \{0.01, 0.02, \ldots 1\}$

#3

Step 2

Input:
$a_{nw}(\lambda)$

Step 3

Step 3

Calculate
$a_{dg}(\lambda)$ and $a_{ph}(\lambda)$

#1, #2

Step 3

Matrix **D**

$\mathbf{D}_{i,j} = (a_{dg}(\lambda)_{i,j}, a_{ph}(\lambda)_{i,j})$

Inequality
Constraints

Output:
Optimal Solution
Range of Feasible Solutions

#4 - #8

Step 4

Step 5

Matrix D

Feasible Solutions

Step 4

Yes

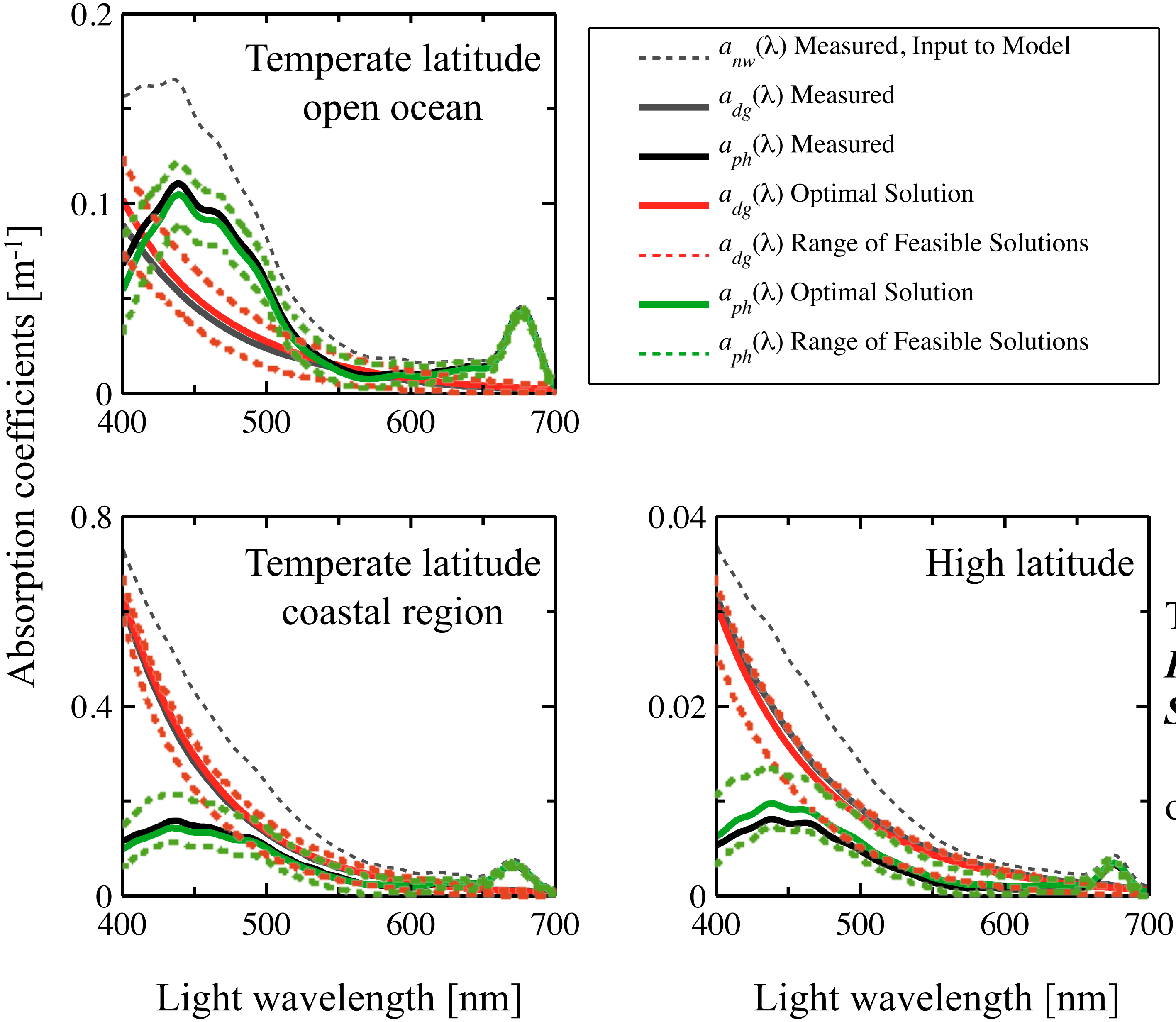
Satisfy
constraints
#4 - #8
?

Stacked-Constraints Algorithm

Derive a large number of speculative solutions.

First identifies feasible solutions, then optimal solution and range of feasible solutions.

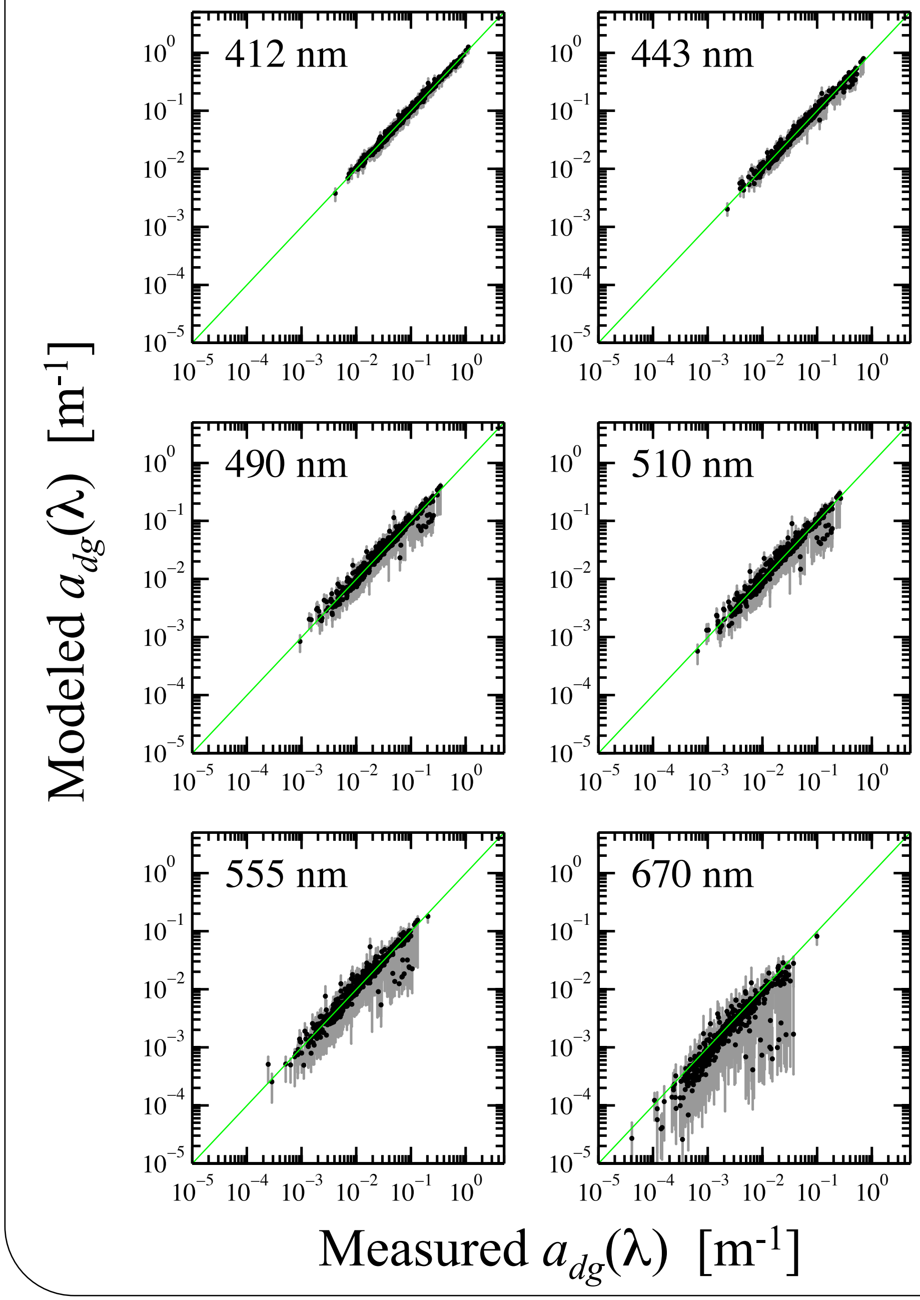
Example Partitioning Results

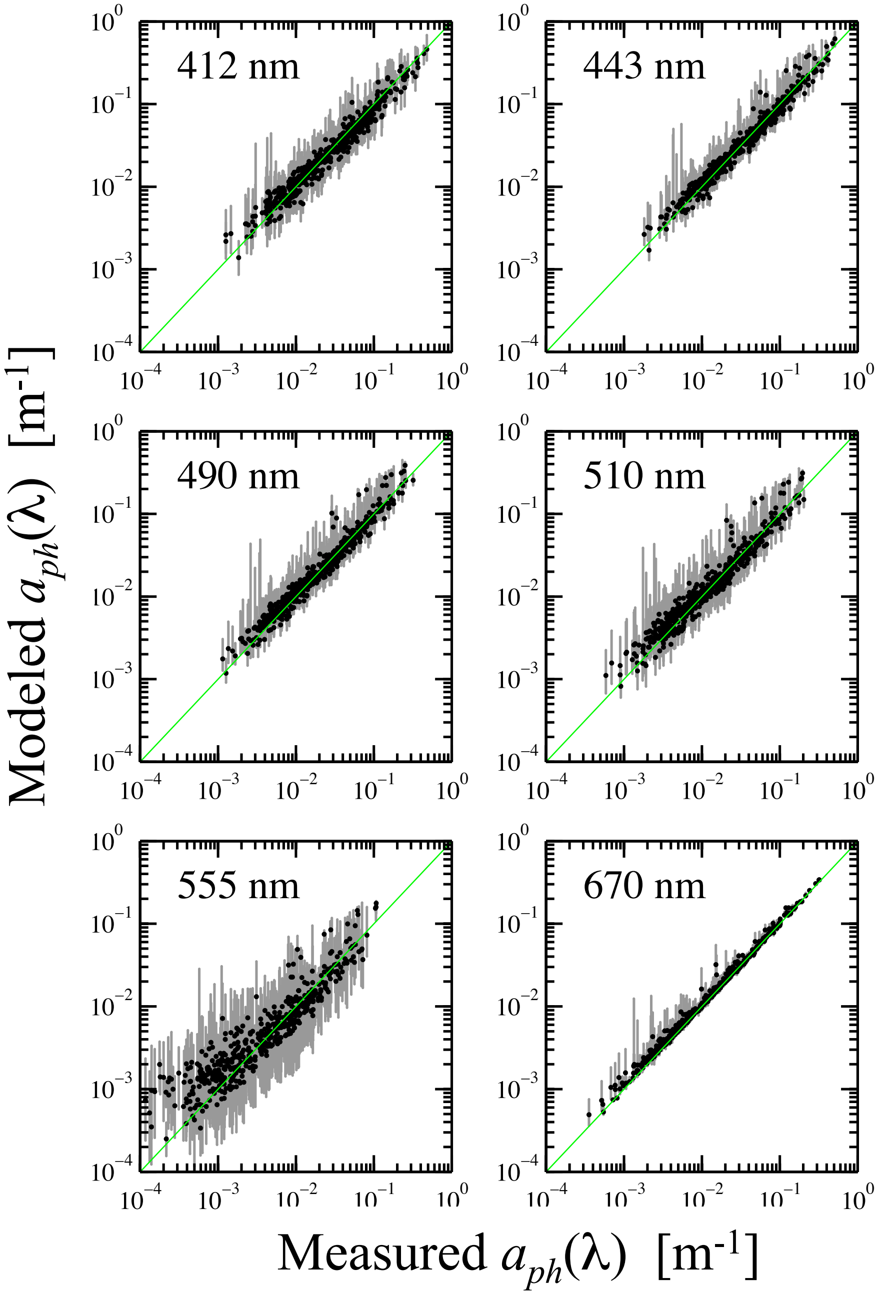


The ***Optimal Solutions*** are very close to the actual measured spectra.

The ***Range of Feasible Solutions*** is a unique feature of our model.

Evaluation of the Model for 505 Samples



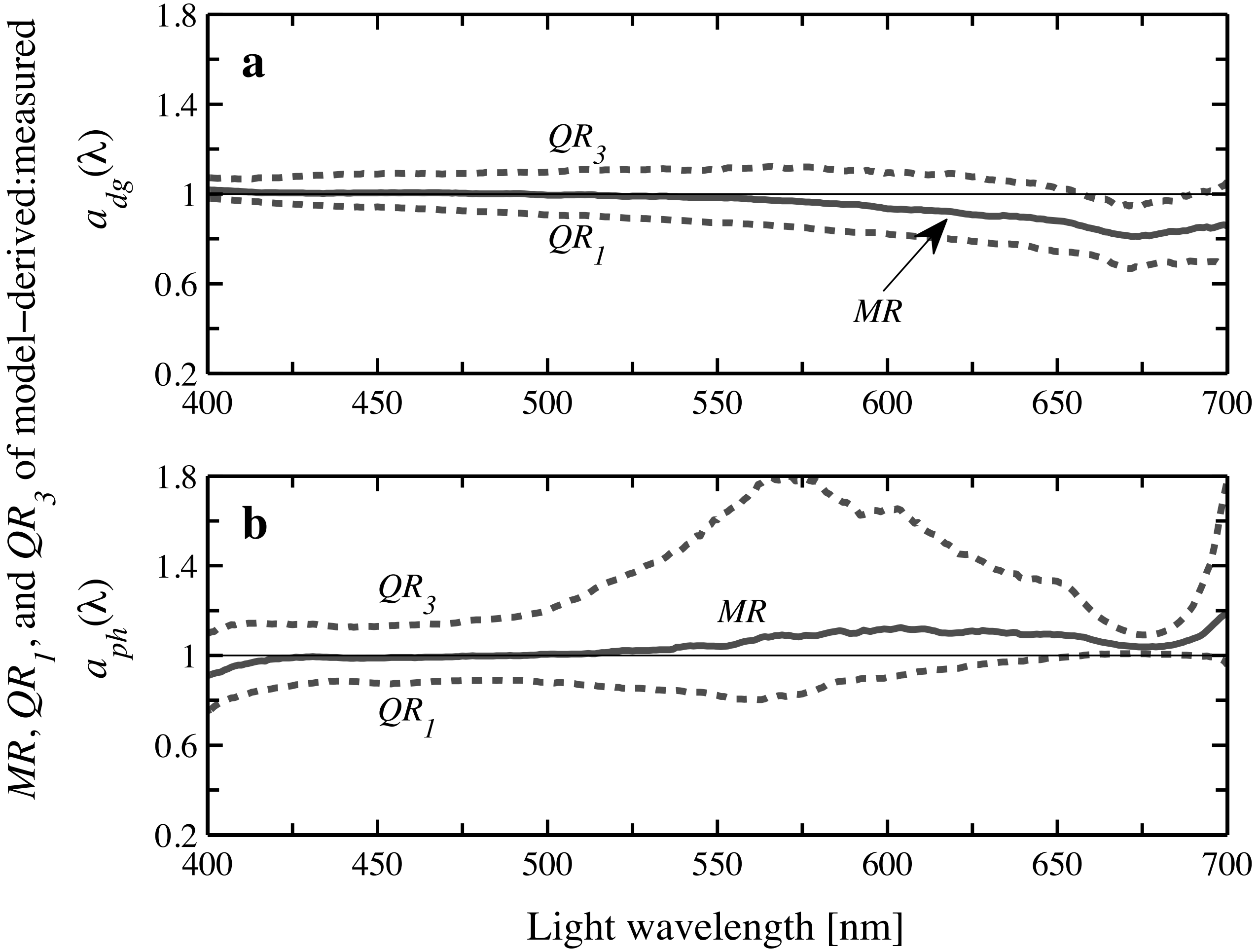


Example Error Statistics for Optimal Solutions at Two Wavelengths

Output Variables	**R**	**Median Ratio** Modeled : Measured	**Median Absolute Percent Difference (%)**
$a_{dg}(443)$	0.985	1.004	6.50
$a_{ph}(443)$	0.963	0.988	12.04
$a_{dg}(670)$	0.899	0.815	21.43
$a_{ph}(670)$	0.997	1.043	4.82

Both systematic and random errors are generally small.

Spectral Dependence for the Median and Quartile Ratios of Modeled:Measured $a_{dg}(\lambda)$ and $a_{ph}(\lambda)$ — Optimal Solutions



MR, median ratio

QR_1, 1st quartile ratio

QR_3, 3rd quartile ratio

MR, QR_1, and QR_3 are calculated based on 505 samples

Summary and Conclusions

- We have formulated a model that successfully relaxes the widely used highly restrictive assumptions on both the spectral slope S of $a_{dg}(\lambda)$ and the spectral shape of $a_{ph}(\lambda)$.
    - Our assumptions include exponential shape of $a_{dg}(\lambda)$ and eight inequality constraints that account for a wide range of variability in absorption coefficients.
    - The model requires input of $a_{nw}(\lambda)$ at a minimum of six wavelengths, but can also work with data with higher spectral resolution.
- Evaluation of the model performance with field data from diverse environments shows good error statistics.
- These results support the prospect of good performance of our model on data provided by various remote-sensing and in situ platforms.

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