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# Maximum likelihood estimation for hyperspectral remote sensing of coastal environments: a pixelwise approach

**S. JAY<sup>1</sup>, M. GUILLAUME<sup>1</sup>, A. MINGHELLI<sup>2</sup>, Y. DEVILLE<sup>3</sup>,**  
**M. CHAMI<sup>4,5</sup>, B. LAFRANCE<sup>6</sup>, V. SERFATY<sup>7</sup>**

<sup>1</sup> Aix-Marseille Université, CNRS, Centrale Marseille, Institut Fresnel UMR 7249

<sup>2</sup> Université de Toulon, CNRS, SeaTech, LSIS UMR 7296

<sup>3</sup> IRAP, Observatoire Midi-Pyrénées, Université Paul Sabatier, Université de Toulouse, CNRS

<sup>4</sup> Sorbonne Universités, UPMC Univ Paris 06, INSU-CNRS, Laboratoire d'Océanographie de Villefranche

<sup>5</sup> Institut Universitaire de France

<sup>6</sup> CS Systèmes d'Information

<sup>7</sup> DGA/DS/MRIS

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# Introduction

## □ Characterization of marine environments from optical remote sensing

### ✓ Open ocean :

- Characterization of water turbidity (phytoplankton pigments, colored dissolved organic matter and suspended matter).
- Ok with multispectral imagery using a few well-positioned spectral bands in the VIS, e.g., O'Reilly *et al.* 1998; Lee *et al.* 2002; Werdell *et al.*, 2013...

### ✓ Coastal areas :

- Characterization of water turbidity + depth + bottom cover,
- Decoupling these effects more accurate with hyperspectral imagery, i.e., using more (a few dozen) and narrower spectral bands in the VIS (Hochberg & Atkinson, 2003; Kutser *et al.*, 2003; Hedley *et al.*, 2012; Botha *et al.*, 2013),

## □ Hyperspectral remote sensing of shallow waters mostly done using :

- ✓ A semi-analytical (SA) model of subsurface remote-sensing reflectance (Lee *et al.*, 1998, 1999; Albert & Mobley, 2003):  $\tilde{r}_{rs} = \tilde{r}_{rs}(\Theta)$  where  $\Theta$  = targeted parameters,
- ✓ An inversion method that solves

$$\hat{\Theta} = \operatorname{argmin}_{\Theta} f(r_{rs}, \tilde{r}_{rs}(\Theta))$$

Cost function  
Measured reflectance

Iterative optimization, e.g., Lee *et al.* (1999, 2001); Brando *et al.* (2009); Dekker *et al.* (2011); Giardino *et al.* (2012); Garcia *et al.* (2014); McKinna *et al.* (2015); Jay & Guillaume (2016)...

Look-Up Tables (LUT), e.g., Mobley *et al.*, (2005); Hedley *et al.*, (2009, 2012)...

# Introduction

## □ About the cost function...

- ✓ Mostly the Least-Square (LS) criterion (or Euclidean distance):

$$f(\mathbf{r}_{rs}, \tilde{\mathbf{r}}_{rs}(\Theta)) = \sqrt{(\mathbf{r}_{rs} - \tilde{\mathbf{r}}_{rs}(\Theta))^t (\mathbf{r}_{rs} - \tilde{\mathbf{r}}_{rs}(\Theta))} = \sqrt{\sum_{\lambda} (r_{rs}(\lambda) - \tilde{r}_{rs}(\lambda; \Theta))^2}$$

- ✓ But, LS optimal if...

- Noise variance (e.g.,  $\text{NE}\Delta r_E^2$ ) = wavelength-independent
  - ➔ Some solutions :
  - (1) remove the noisiest bands, e.g., *Mobley et al (2005)*, or
  - (2) weight each waveband by the inverse of  $\text{NE}\Delta r_E^2$  (*Brando et al., 2009; Botha et al., 2013*).

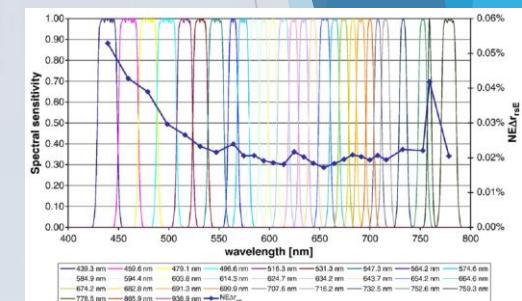
- Wavebands uncorrelated

« As homogeneous as possible »  
optically-deep water

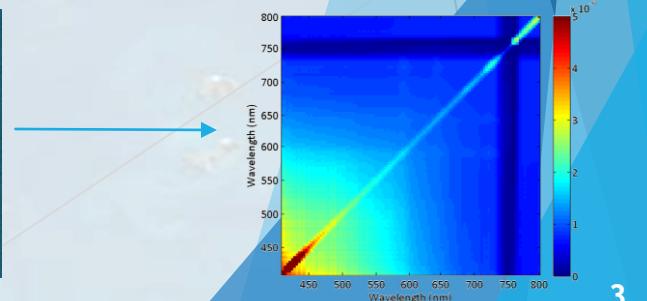
- ✓ Accounting for the full spectral covariance matrix  $\Gamma$  ?



(*Brando et al, 2009*)



Spectral covariance matrix = spectrally-correlated version of  $\text{NE}\Delta r_E^2$



# Introduction

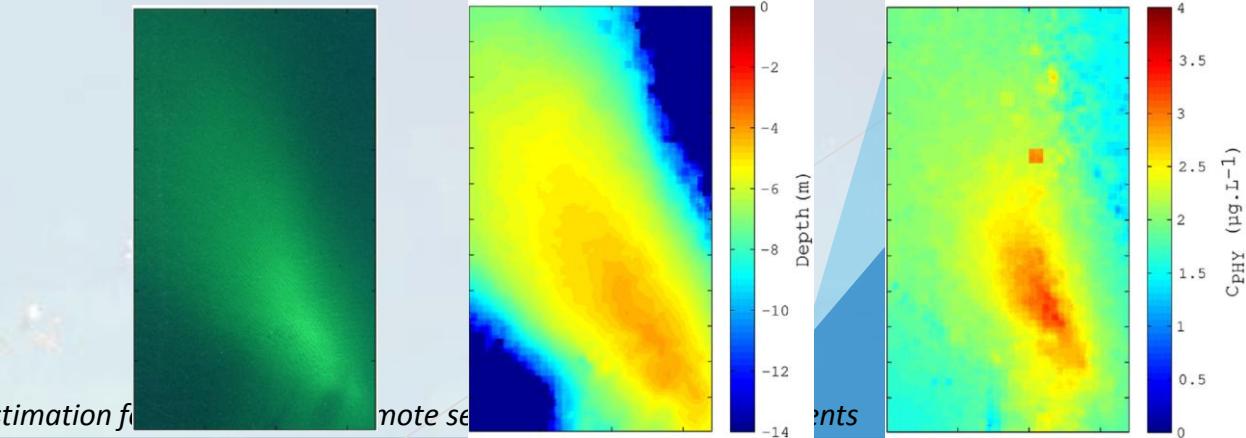
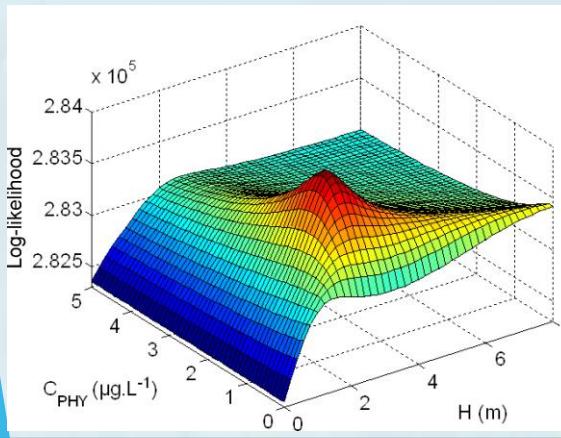
## □ Maximum likelihood (ML) estimation, some first attempts...

- ✓  $r_{rs} \sim \mathcal{N}(\mu(\Theta); \Gamma(\Theta))$  where (1)  $\mu(\Theta) = \tilde{r}_{rs}(\Theta)$  = SA model  
(2)  $\Gamma(\Theta)$  estimated on a local neighborhood, within which  $\Theta$  is assumed to be constant (Jay et Guillaume., 2012) or to vary linearly (Jay & Guillaume, 2014).

$$\check{\Theta}_{ML} = \underset{\Theta}{\operatorname{argmax}} \prod_i \frac{1}{\sqrt{(2\pi)^L |\Gamma|}} e^{-0.5(r_{rs,i} - \tilde{r}_{rs}(\Theta))^T \Gamma^{-1} (r_{rs,i} - \tilde{r}_{rs}(\Theta))}$$

- ✓ ++ (1) Account for spectral and spatial correlations, (2) Accuracy  $\nearrow$  if assumptions are fully met
- ✓ -- (1) Loss in spatial resolution, (2) Accuracy  $\searrow$  if assumptions are not fully met...

## □ A pixelwise ML method ?



# Outlines

- Methods

- ✓ Proposed ML methods,
- ✓ Comparison methods,
- ✓ Implementation,

- Data

- Results

# Proposed ML methods

- Assumption:  $\mathbf{r}_{rs} \sim \mathcal{N}(\boldsymbol{\mu}(\Theta); \boldsymbol{\Gamma}(\Theta)) \Leftrightarrow \mathbf{r}_{rs} = \boldsymbol{\mu}(\Theta) + \mathbf{n}$  where  $\mathbf{n} \sim \mathcal{N}(\mathbf{0}; \boldsymbol{\Gamma}(\Theta))$
- Goal: parameterize  $\boldsymbol{\mu}(\Theta)$  and  $\boldsymbol{\Gamma}(\Theta)$  as a function of water column parameters
- Mean vector parameterized by a SA model (*Lee et al, 1998; 1999*)
  - ✓  $\boldsymbol{\mu}(\lambda; \Theta) = \tilde{\mathbf{r}}_{rs}(\lambda; \Theta) = r_{rs,\infty}(\lambda)(1 - e^{-(k_d(\lambda) + k_u^c(\lambda))H}) + (1/\pi)[B_1\rho_{b,1}(\lambda) + B_2\rho_{b,2}(\lambda)]e^{-(k_d(\lambda) + k_u^b(\lambda))H}$
  - ✓ Or in matrix notation  $\boldsymbol{\mu}(\Theta) = \tilde{\mathbf{r}}_{rs}(\Theta) = (\mathbf{I} - \mathbf{K}_c)\mathbf{r}_{rs,\infty} + (1/\pi)\mathbf{K}_b(B_1\boldsymbol{\rho}_{b,1} + B_2\boldsymbol{\rho}_{b,2})$
  - ✓  $\Theta = (H, P, G, X, B_1, B_2)$
  - ✓ Importantly, two options for bottom parameterization:
    - $\sum_i B_i = 1$  (*Klonowski et al, 2007; Goodman & Ustin, 2007; Brando et al, 2009; Hedley et al, 2009; 2012*)
      - ➔ ++ : only one parameter  $B = B_1 = 1 - B_2$  (= fractional cover of substratum 1)
      - ➔ -- : bottom within-class variability is poorly accounted for.
    - $\sum_i B_i \neq 1$  (*Fearns et al, 2011; Garcia et al, 2014*)
      - ➔ ++ : the bottom within-class variability is accounted for through a brightness factor.
      - ➔ -- : two parameters  $B_1$  and  $B_2$  (= fractional cover + within-class variability)

# Proposed ML methods

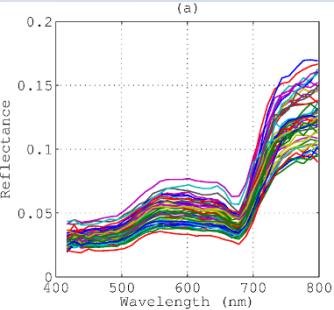
## □ Parameterization of covariance matrix

- ✓ Case 1: No bottom within-class variability (if sum-to-one) / bottom within-class variabilities perfectly described by brightness factors (if no sum-to-one)

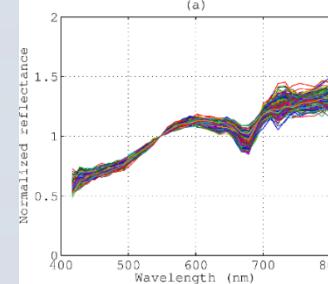
$$\triangleright \mathbf{r}_{rs} = \underbrace{(\mathbf{I} - \mathbf{K}_c)\mathbf{r}_{rs,\infty} + (1/\pi)\mathbf{K}_b(B_1\boldsymbol{\rho}_{b,1} + B_2\boldsymbol{\rho}_{b,2})}_{\text{deterministic}} + \underbrace{\mathbf{n}_s}_{\text{random}}$$

- $\mathbf{n} = \mathbf{n}_s \sim \mathcal{N}(\mathbf{0}; \boldsymbol{\Gamma}_s)$ , where  $\boldsymbol{\Gamma}_s$  is a spectrally-correlated version of the environmental noise  $N\Delta r_E^{-2}$  and is estimated over an « as homogeneous as possible » area of optically-deep water.
- $\mathbf{n}_s$  describes the sensor noise and scene-specific above-water variabilities (residuals from imperfect ATM, air-water interface and sun glint corrections, effects related to the rough water surface, etc) (Brando & Dekker, 2003; Wettle et al, 2004)

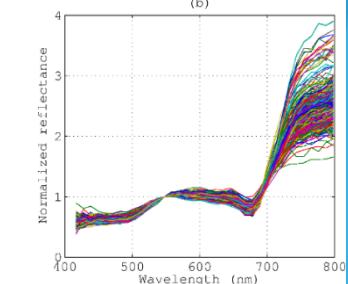
Actual seagrass spectra



Sand spectra normalized at 550 nm



Seagrass spectra normalized at 550 nm

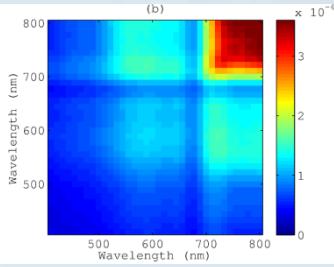


# osed ML methods



## Parameterization of covariance matrix

Seagrass covariance matrix

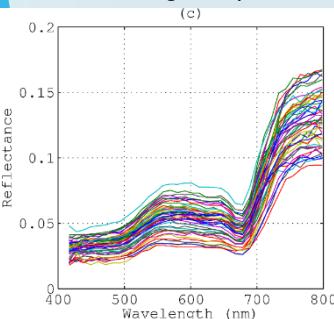


Case 2: bottom within-class variabilities not perfectly represented using brightness factors ✓

- Two Gaussian distributions with covariances  $\Gamma_{b,1}$  and  $\Gamma_{b,2}$  are used to describe within-class variabilities,
- A single factor  $B$  is used to describe the fractional cover of substratum 1 ( $B \leq 1$ )
- $\mathbf{r}_{rs} = (\mathbf{I} - \mathbf{K}_c)\mathbf{r}_{rs,\infty} + \mathbf{K}_b(1/\pi)[B(\boldsymbol{\rho}_{b,1} + \mathbf{n}_{b,1}) + (1 - B)(\boldsymbol{\rho}_{b,2} + \mathbf{n}_{b,2})] + \mathbf{n}_s$
- $\mathbf{r}_{rs} = \underbrace{\mathbf{r}_{rs,\infty}(\mathbf{I} - \mathbf{K}_c) + (1/\pi)(B\boldsymbol{\rho}_{b,1} + (1 - B)\boldsymbol{\rho}_{b,2})\mathbf{K}_b}_{\text{deterministic}} + \underbrace{\mathbf{K}_b(B\mathbf{n}_{b,1} + (1 - B)\mathbf{n}_{b,2}) + \mathbf{n}_s}_{\text{random}}$
- In this case, it can be shown that

$$\boldsymbol{\Gamma} = \underbrace{\mathbf{K}_b[B^2\boldsymbol{\Gamma}_{b,1} + (1 - B)^2\boldsymbol{\Gamma}_{b,2}]\mathbf{K}_b}_{\text{bottom variability} = f(\Theta)} + \underbrace{\boldsymbol{\Gamma}_S}_{\text{above-water variability} \neq f(\Theta)}$$

Simulated seagrass spectra



- Decoupling of the influences of within-class variabilities and fractional covers !
  - ✓ Only one parameter to estimate for bottom parameterization (= fractional cover), AND
  - ✓ Bottom within-class variability is accounted for (but not estimated).

# Proposed ML methods / Comparison methods

- ML 1:  $\mu(\Theta) = \tilde{r}_{rs}(\Theta)$ ,  $\Gamma = \Gamma_s$  and  $\Theta = (H, P, G, X, B_1, B_2)$

✓  $\widehat{\Theta}_{ML1} = \underset{\Theta}{\operatorname{argmax}} \frac{1}{\sqrt{(2\pi)^L |\Gamma_s|}} e^{-0.5(r_{rs} - \tilde{r}_{rs}(\Theta))^t \Gamma_s^{-1} (r_{rs} - \tilde{r}_{rs}(\Theta))} = \underset{\Theta}{\operatorname{argmin}} (r_{rs} - \tilde{r}_{rs}(\Theta))^t \Gamma_s^{-1} (r_{rs} - \tilde{r}_{rs}(\Theta))$

- ML 2:  $\mu(\Theta) = \tilde{r}_{rs}(\Theta)$ ,  $\Gamma = \Gamma_s + K_b [B^2 \Gamma_{b,1} + (1-B)^2 \Gamma_{b,2}] K_b$  and  $\Theta = (H, P, G, X, B)$

✓  $\widehat{\Theta}_{ML2} = \underset{\Theta}{\operatorname{argmax}} \frac{1}{\sqrt{(2\pi)^L |\Gamma|}} e^{-0.5(r_{rs} - \tilde{r}_{rs}(\Theta))^t \Gamma^{-1} (r_{rs} - \tilde{r}_{rs}(\Theta))}$

- LS  $\approx$   $\mu(\Theta) = \tilde{r}_{rs}(\Theta)$ ,  $\Gamma = \sigma^2 I$  and  $\Theta = (H, P, G, X, B)$  or  $\Theta = (H, P, G, X, B_1, B_2)$

✓  $\widehat{\Theta}_{LS} = \underset{\Theta}{\operatorname{argmin}} (r_{rs} - \tilde{r}_{rs}(\Theta))^t (r_{rs} - \tilde{r}_{rs}(\Theta)) = \underset{\Theta}{\operatorname{argmin}} \sum_{\lambda} (r_{rs}(\lambda) - \tilde{r}_{rs}(\lambda; \Theta))^2$

# Implementation

- ❑ Model inversion using iterative optimization (trust-region reflective algorithm, Matlab®),
- ❑ Pairwise estimation of the two bottom types,
- ❑ Initialization
  - ✓ Initial guesses derived from reflectance values (*Lee et al, 1999*), OR
  - ✓ Latin Hypercube Sampling (*Garcia et al, 2014*)
    - ➔ Generation of LUTs of 100,000 spectra/parameters.
    - ➔ Initial guesses corresponding to the closest spectrum in the LUT.

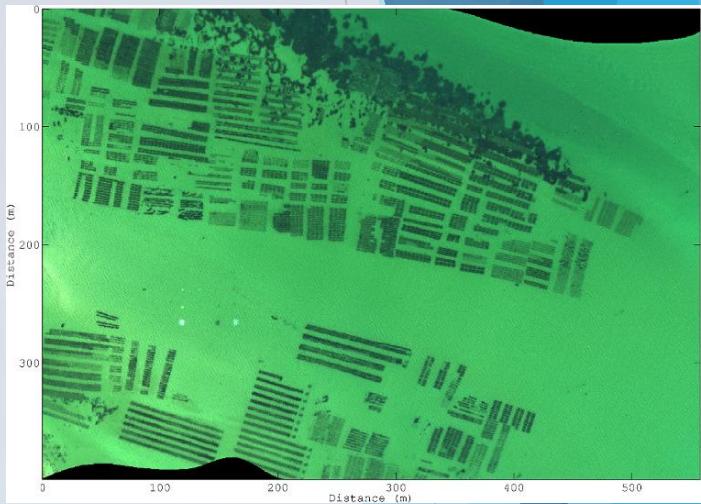
# Data

## Real data set

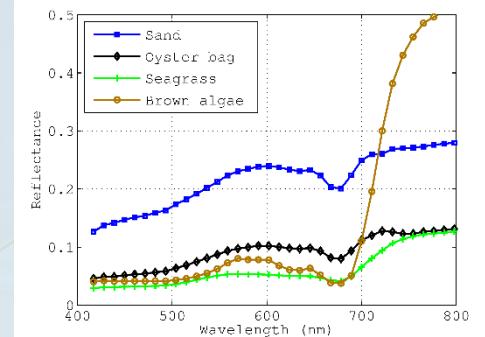
- ✓ Airborne Hypspx image collected over the Quiberon Peninsula, France (Actimar, HypLitt 2012),
- ✓ Spatial resolution = 0.50 m,
- ✓ 36 spectral bands between 400 et 800 nm (spectral sampling interval  $\approx$  11 nm),
- ✓  $1 \text{ m} < H < 5 \text{ m}$ ,
- ✓ Four bottom types: sand, oyster bags, seagrass, brown algae,
  - Estimation of bottom reflectance spectra and covariance matrices from spectral data.
- + 14 additionnal Hypspx images of other areas of the Peninsula to validate bathymetry retrieval ( $0.44 \text{ m} < H < 12 \text{ m}$ )



*True color composite image (deglinted, subsurface)*



*Bottom reflectance spectra*



# Data

## □ Simulations

### ✓ Statistical modeling #1

$$\triangleright \quad \mathbf{r}_{rs} = \underbrace{(\mathbf{I} - \mathbf{K}_c)\mathbf{r}_{rs,\infty} + (1/\pi)\mathbf{K}_b(B_1\boldsymbol{\rho}_{b,1} + B_2\boldsymbol{\rho}_{b,2})}_{\text{deterministic}} + \underbrace{\mathbf{n}_s}_{\text{random}}$$

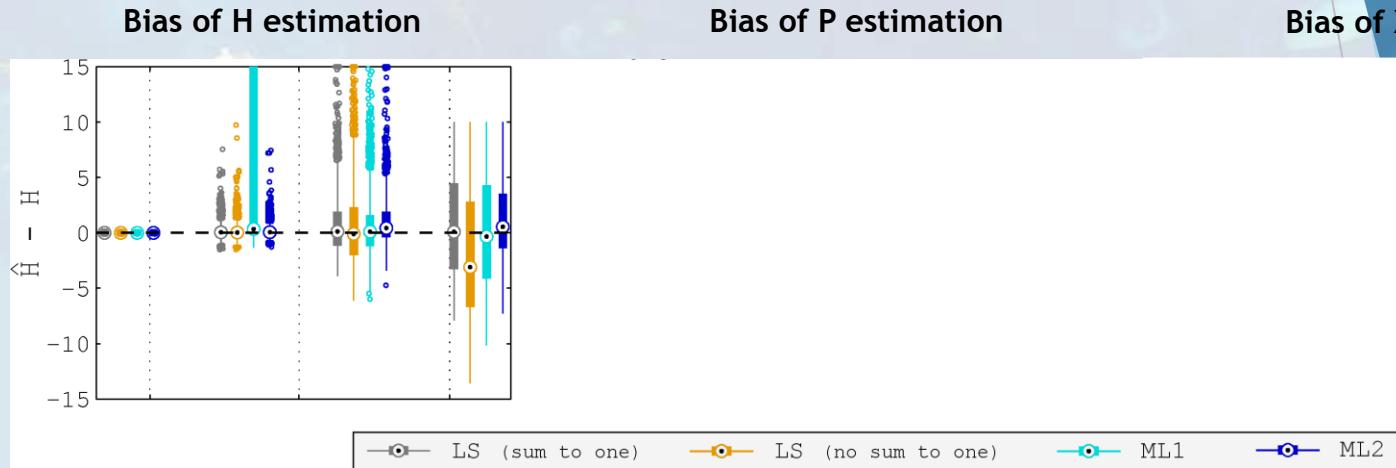
### ✓ Statistical modeling #2

$$\triangleright \quad \mathbf{r}_{rs} = \underbrace{\mathbf{r}_{rs,\infty}(\mathbf{I} - \mathbf{K}_c) + (1/\pi)(B\boldsymbol{\rho}_{b,1} + (1-B)\boldsymbol{\rho}_{b,2})\mathbf{K}_b}_{\text{deterministic}} + \underbrace{\mathbf{K}_b(B\mathbf{n}_{b,1} + (1-B)\mathbf{n}_{b,2}) + \mathbf{n}_s}_{\text{random}}$$

- ✓  $H = 1; 5; 10; 15 \text{ m}$
- ✓ Intermediate water turbidity (*Garcia et al, 2015*) :  $P = 0.05 \text{ m}^{-1}$ ;  $G = 0.1 \text{ m}^{-1}$ ;  $X = 0.01 \text{ m}^{-1}$
- ✓ 4 pure bottom spectra + 6 mixtures of two bottom spectra (50%-50%)  
→ 10 bottom spectra in total
- ✓ For each statistical modeling, 2,000 simulations for each depth.

# Results - Simulations - Statistical modeling #1

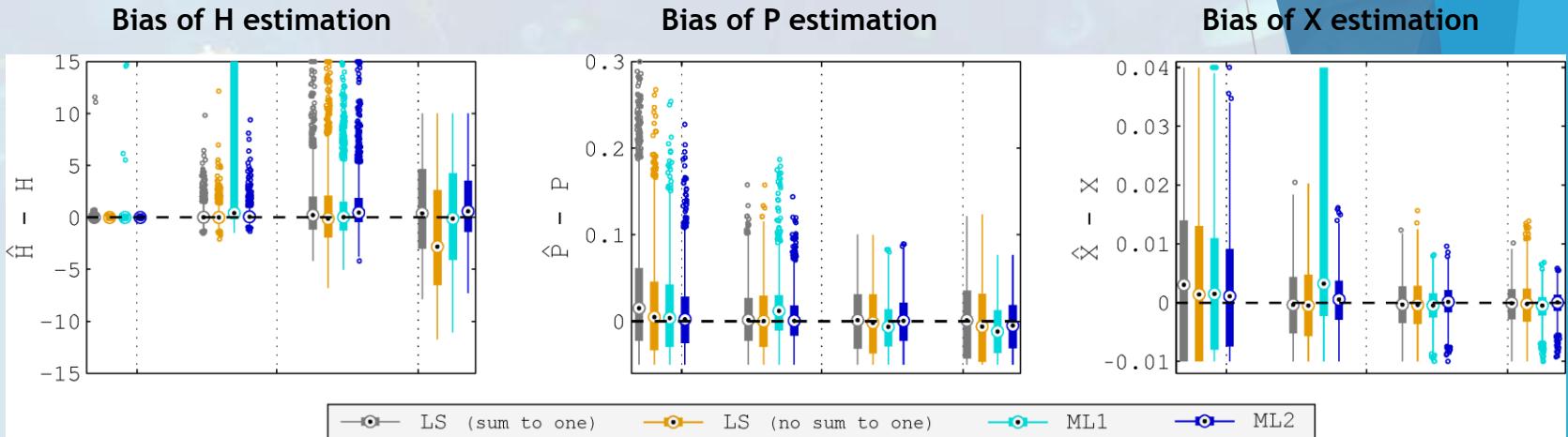
Reflectance-derived initialization



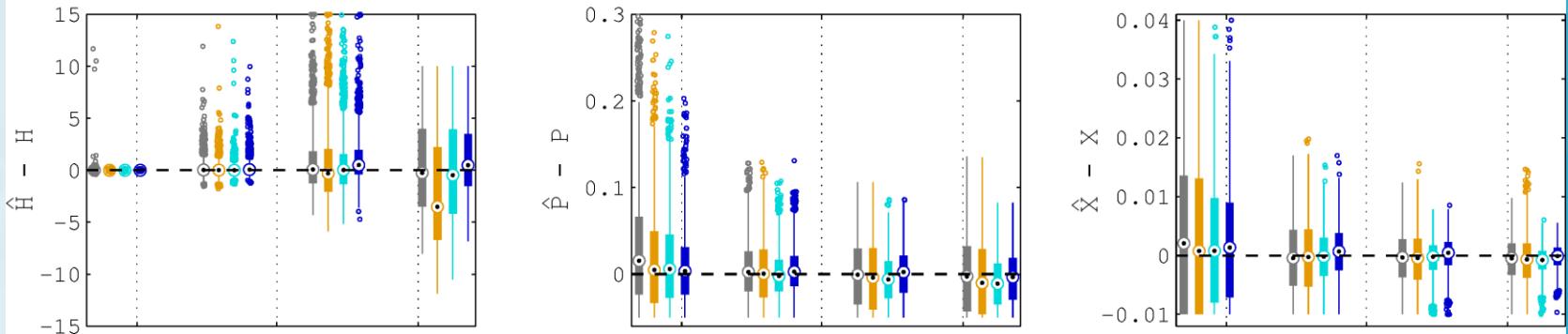
LHS sampling based initialization

# Results - Simulations - Statistical modeling #2

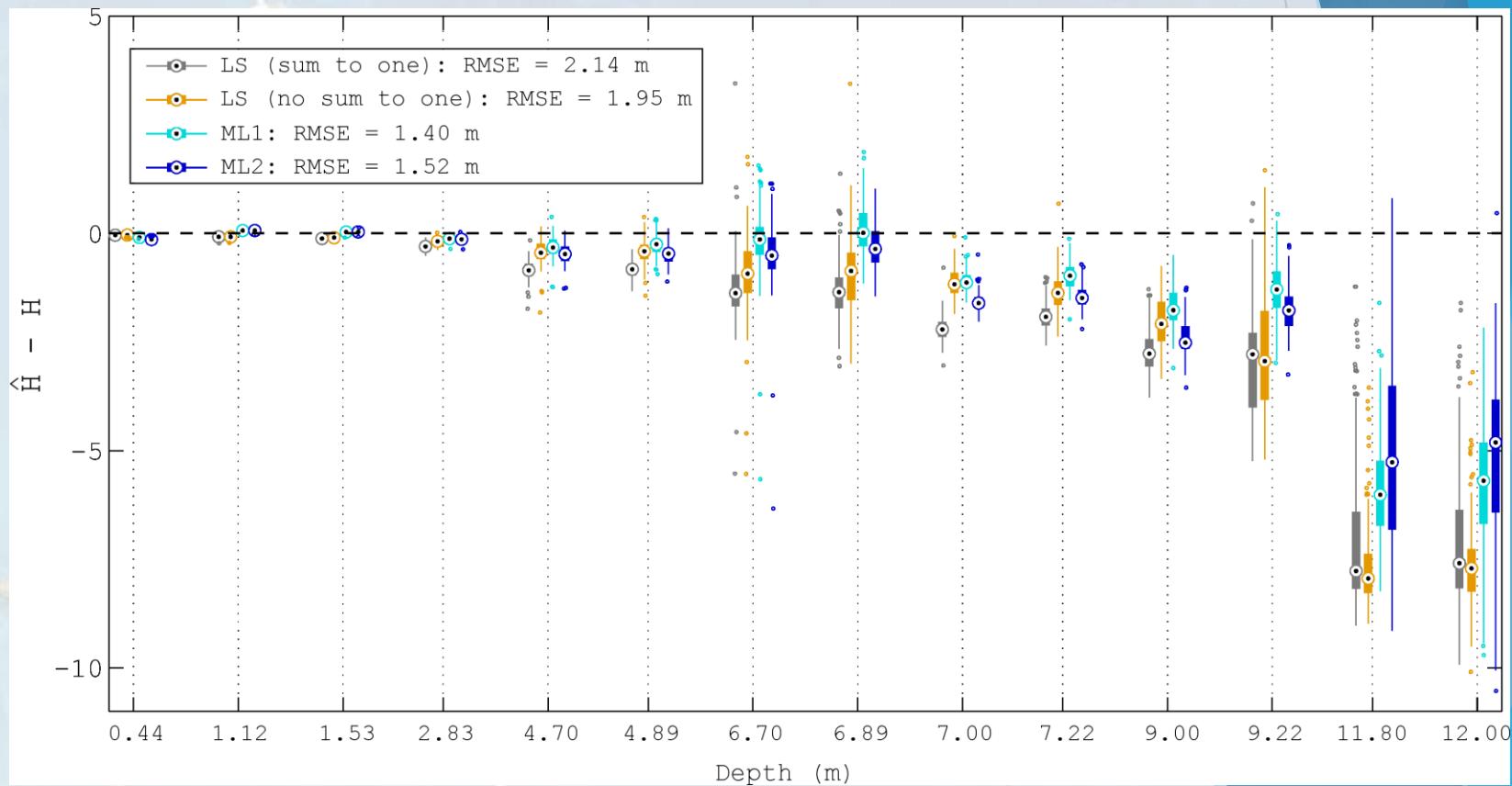
Reflectance-derived initialization



LHS sampling based initialization



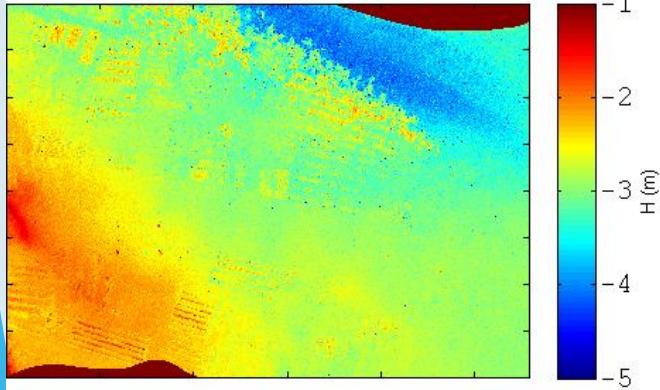
# Results - Real data - Bathymetry estimation



# Results - Real data - Bathymetry estimation

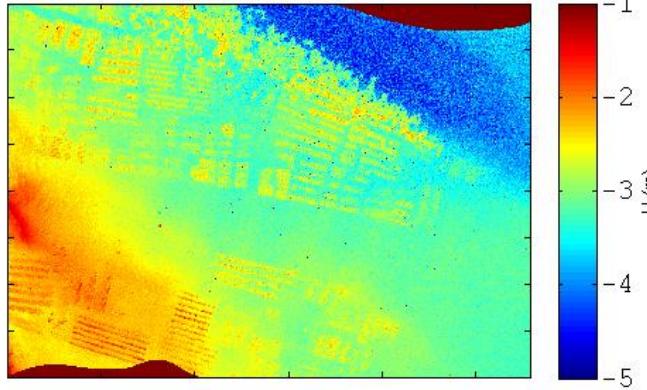
*Sum-to-one*

LS (sum to one)

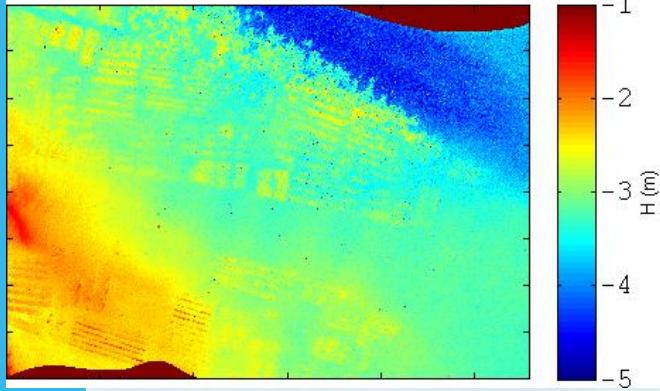


*No sum-to-one*

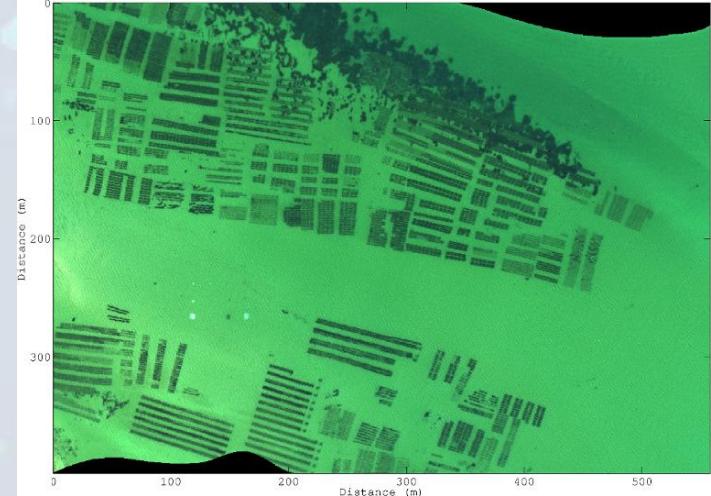
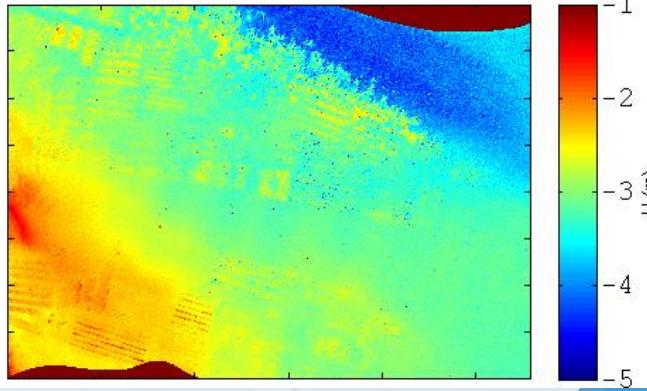
LS (no sum to one)



ML 1

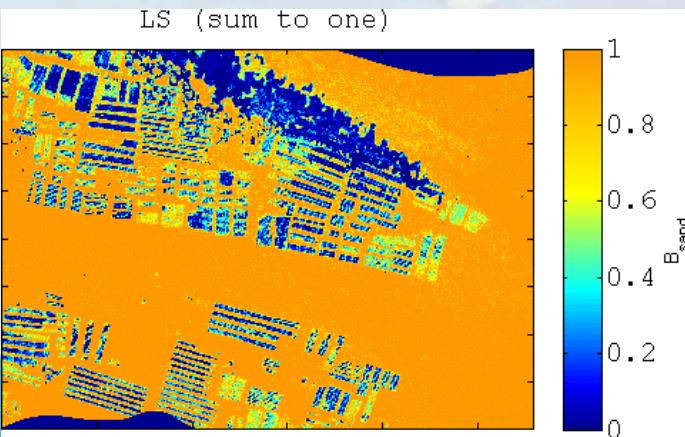


ML 2

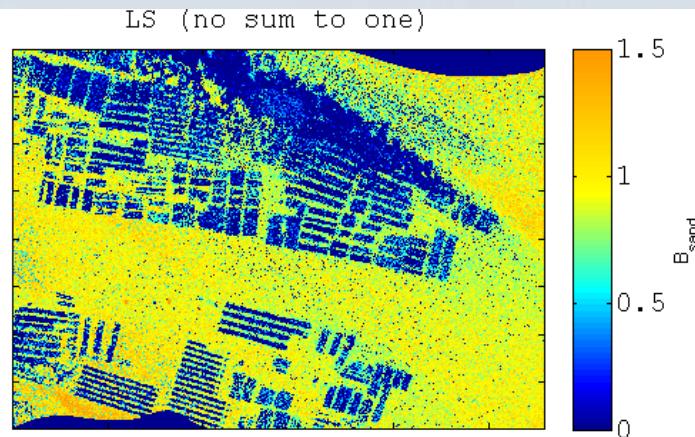


# Results - Real data - Bottom cover estimation

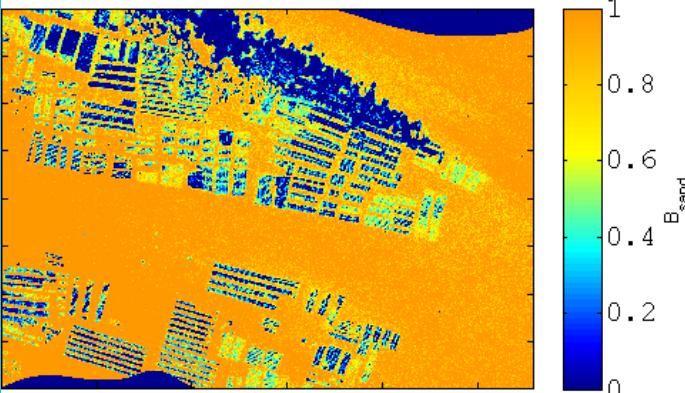
*Sum-to-one*



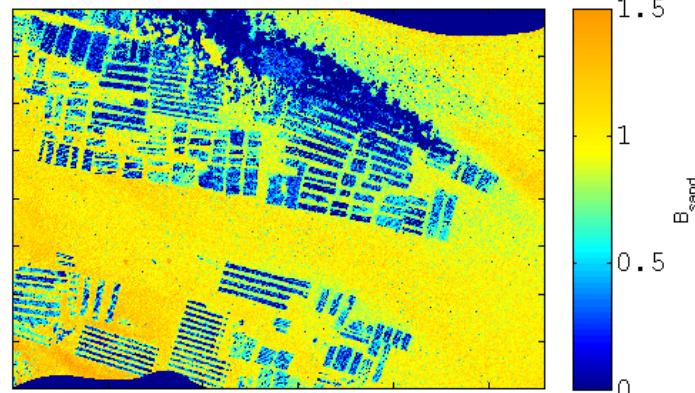
*No sum-to-one*



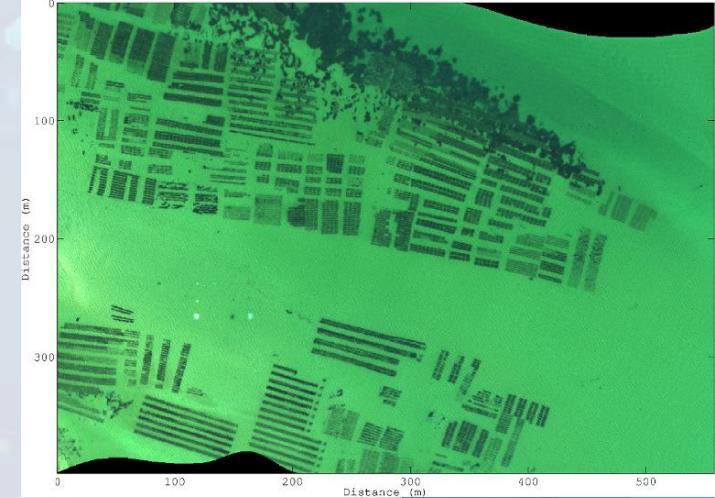
ML 2



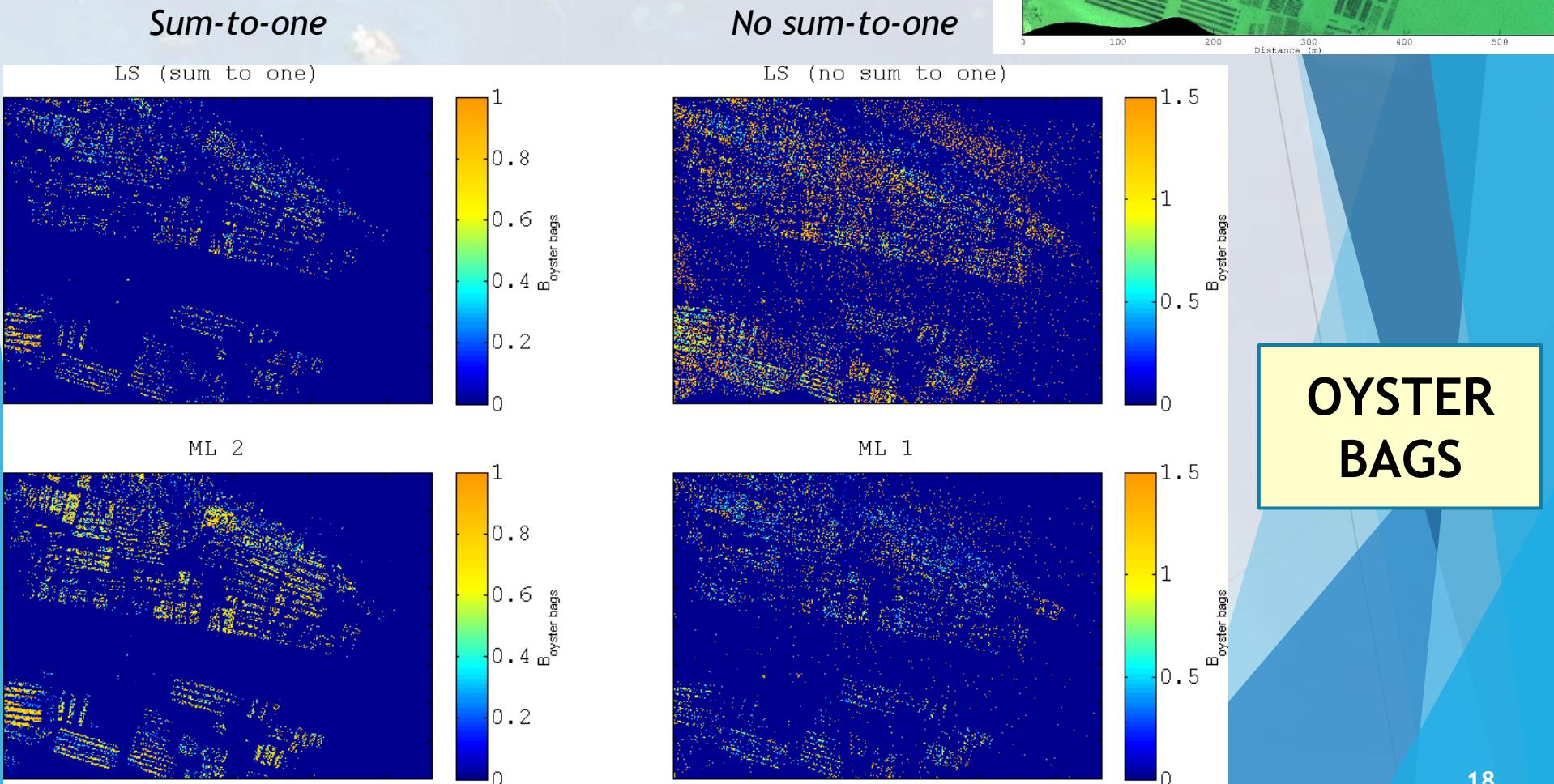
ML 1



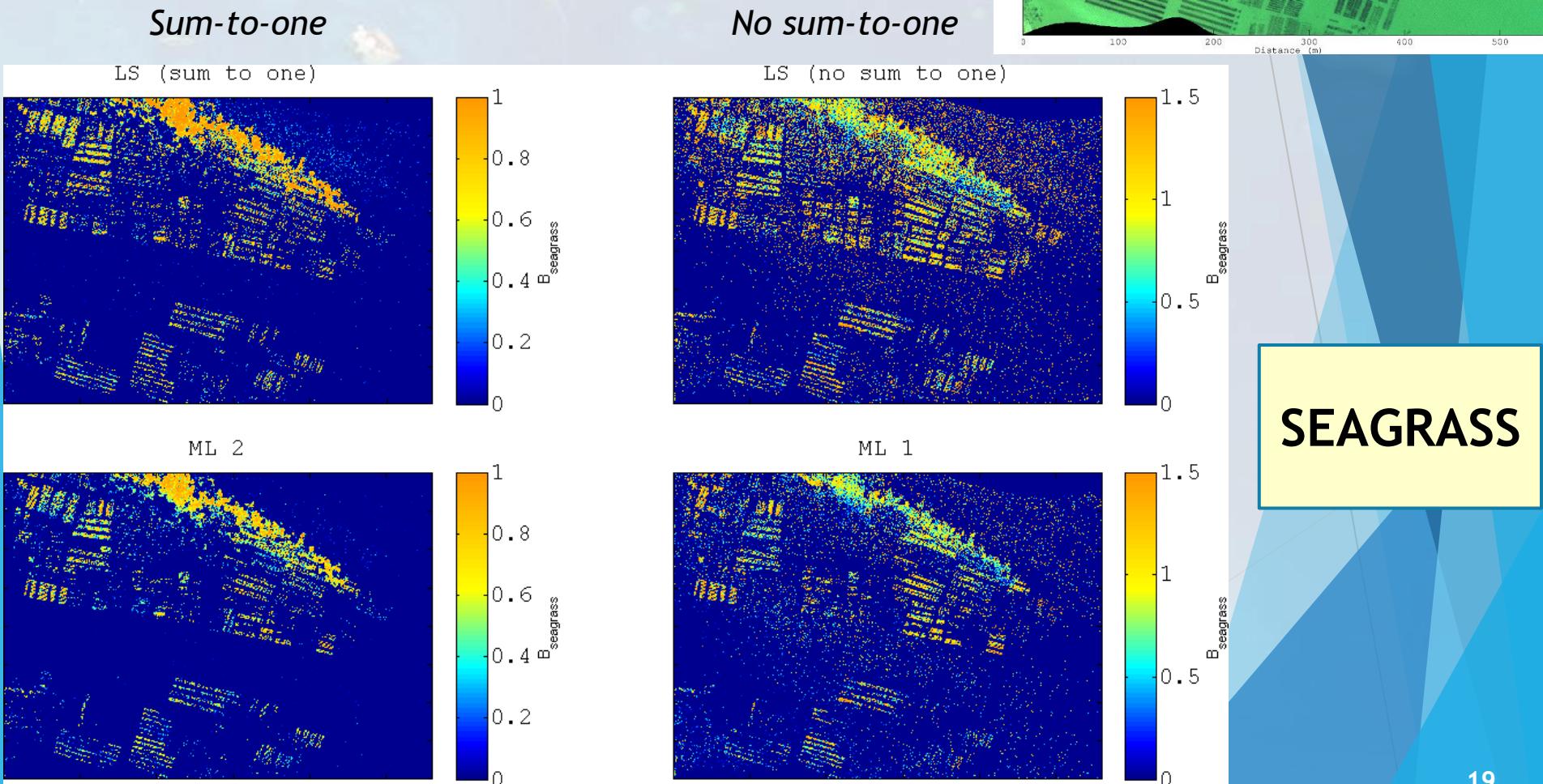
SAND



# Results - Real data - Bottom cover estimation

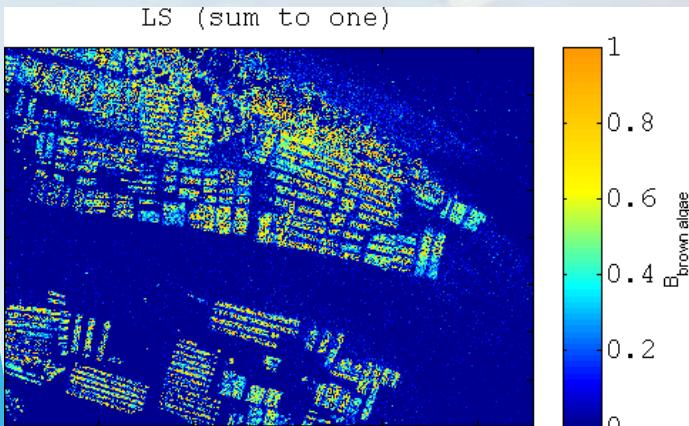


# Results - Real data - Bottom cover estimation

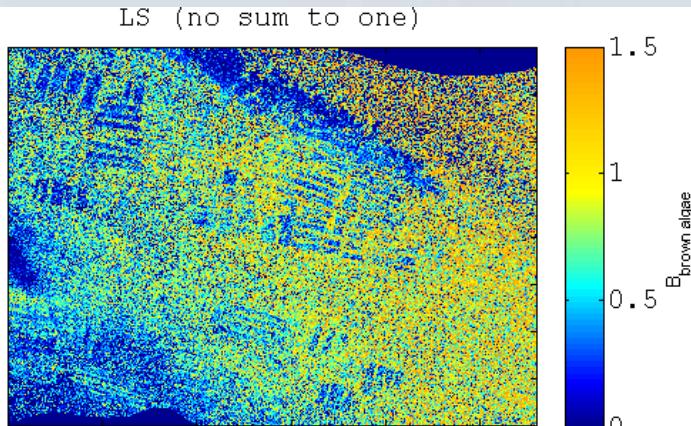


# Results - Real data - Bottom cover estimation

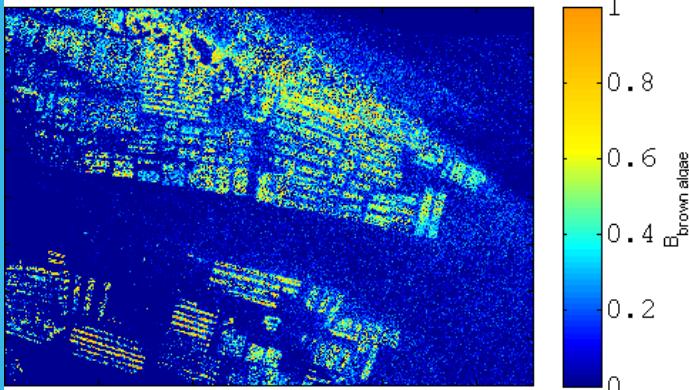
Sum-to-one



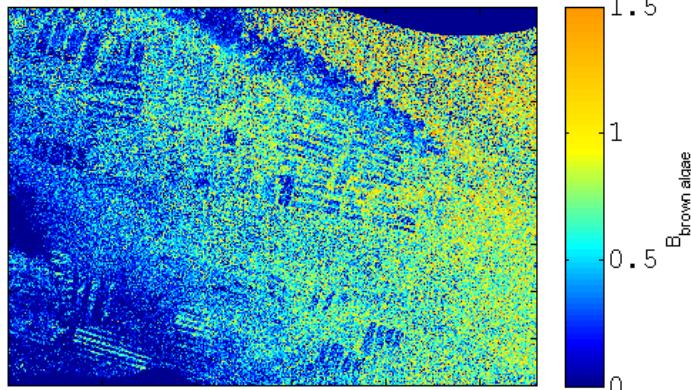
No sum-to-one



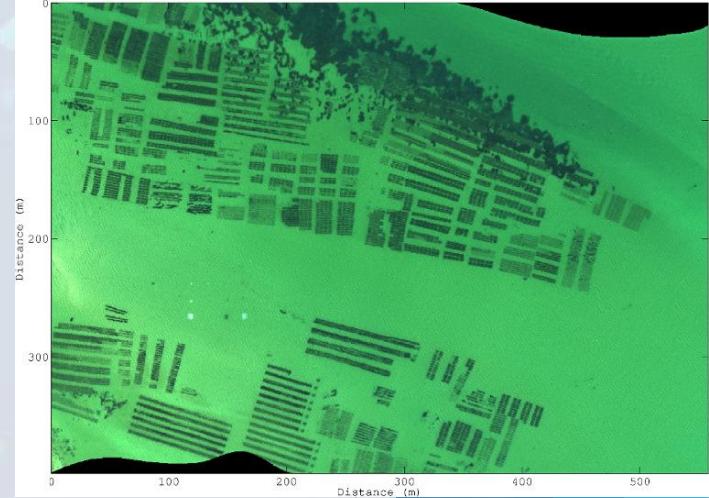
ML 2



ML 1



**BROWN  
ALGAE**



# Conclusions & Future works...

- Most inversion methods do not account for spectral covariance,
- We propose two alternative methods (ML1 and ML2) based on Maximum Likelihood estimation to invert a SA model,
- Importance of initialization, especially for ML1,
- ML2 allows accounting for (potentially complex) bottom within-class variability while limiting the ill-posedness of the inversion problem,
- Estimation accuracy generally increases compared with LS methods,
- ML2 requires estimating bottom covariance matrices beforehand (ground-based measurements ?),
- Future works include
  - ✓ Investigating how accurate the estimation of bottom covariance matrices should be ?  
Is it possible to use standard matrices ?
  - ✓ Testing LUT-based inversion to avoid local minima ?
  - ✓ ...

*Thanks for your attention !!*



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