PACE $R_{rs}$ Uncertainty

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Sources of uncertainties in ocean color

- Radiometric uncertainty
  - Random noise $\rightarrow$ SNR.
  - Systematic uncertainty (calibration errors).
- Non-radiometric
  - Geolocation accuracy
  - Band-to-band registration
- Modeling uncertainty
  - Radiative transfer errors.
  - Simplification of physics.

Pre-launch and on-orbit calibration

IOCCG, report 18
20+ years of diagnostic uncertainty estimates in ocean color

- Pixel-level uncertainty has been absent from the ocean color community for decades.
- The community relies on the validation data to provide diagnostic estimates of uncertainty.
- Validation data is not representative of the global oceans.
- Uncertainty varies spatially and temporal (season).

### PACE SDT Goal for $R_{rs}$(VIS)

$\Delta R_{rs}$(VIS) = 3e-4 sr$^{-1}$ or 5%

**Current Approach**

$\Delta R_{rs}$(VIS) $\sim$ 1e-3 sr$^{-1}$ or 12% (22% 412)

goal is factor of 3 reduction ... seems achievable!
Toward pixel-level uncertainty in operational products

There are various methods to estimate the pixel-level uncertainty:

- Monte Carlo sampling
- Analytical error propagation
- Bayesian Framework (Optimal Estimation)
- Machine learning (ensemble approach)
- Cramér-Rao Bounds
- ...

\[ y = f(x_1, x_1, \ldots, x_n) \]

\[
u^2(y) = \sum_{i=1}^{n} \left( \frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) + 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} u(x_i, x_j)\]
Pixel-level uncertainty in SeaDAS

\[ L_t(\lambda) = (L_r(\lambda) + L_a(\lambda) + L_{ra}(\lambda) + t(\lambda)L_f(\lambda) + T(\lambda)L_g(\lambda) + t(\lambda)L_w(\lambda)) \times T_g(\lambda) \]
Pixel-level uncertainty of OCI

One goal is to retrieve $R_{rs\_unc\_440} < 0.00076 \text{ sr}^{-1}$

$R_{rs\_440}$ includes random noise + systematic unc. + forward model unc.

$R_{rs\_unc\_440}$ includes random noise + systematic unc. + forward model unc.
Pre-launch instrument uncertainty model tells us how well we will do for PACE

<table>
<thead>
<tr>
<th>Data Product</th>
<th>Baseline Uncertainty</th>
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</thead>
<tbody>
<tr>
<td>Water-leaving reflectances centered on (±2.5 nm) 350, 360, and 385 nm (15 nm bandwidth)</td>
<td>0.0057 or 20%</td>
</tr>
<tr>
<td>Water-leaving reflectances centered on (±2.5 nm) 412, 425, 443, 460, 475, 490, 510, 532, 555, and 583 (15 nm bandwidth)</td>
<td>0.0020 or 5%</td>
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<tr>
<td>Water-leaving reflectances centered on (±2.5 nm) 617, 640, 655, 665 678, and 710 (15 nm bandwidth, except for 10 nm bandwidth for 665 and 678 nm)</td>
<td>0.0007 or 10%</td>
</tr>
</tbody>
</table>

- Remember there are requirements that we need to meet for the water reflectance.
- Remember that we can use our global PyTOAST simulations to test these requirements

Uncertainty in ocean reflectance after the Atmospheric Correction
Are we going to produce operational uncertainty products? yes

- We will be able to produce Rrs and IOPs uncertainty for L2 products from PACE and other heritage sensors.

8-day L2 binned data. This is not L3 uncertainty product.

Zhang et al (2022) in press
Validating the pixel-level uncertainty

\[ \Delta_N = \frac{R_{rs}^m - R_{rs}^f}{\Delta_D} \]

Zhang et al (2022) in press
• Developed a Bayesian version of the full-spectrum AC (combined with the GIOP forward ocean model).

  • Define the state vector:
    \[ \mathbf{x} = [RH, O_3, Pr, WS, WV, fmf, \tau_a, a_{ph}, a_{dg}, b_{bp}] \]

  • Define the objective function:
    \[ \chi^2 = [\mathbf{\rho}_{obs} - \mathbf{F}(\mathbf{x})]^T \mathbf{S}_e^{-1} [\mathbf{\rho}_{obs} - \mathbf{F}(\mathbf{x})] + [\mathbf{x} - \mathbf{x}_a]^T \mathbf{S}_a^{-1} [\mathbf{x} - \mathbf{x}_a] \]

  • Optimize the objective function given the forward model to estimate the state vector.
    \[ \rho_{TOA}(\lambda, \theta_0, \varphi, \theta_v) = \mathbf{F}(RH, O_3, Pr, WS, WV, fmf, \tau_a, a_{ph}, a_{dg}, b_{bp}, \gamma, Chl - a) \]

  • Estimate the error covariance matrix:
    \[ \mathbf{\hat{S}} = (\mathbf{\hat{R}}^T \mathbf{S}_e^{-1} \mathbf{\hat{K}} + \mathbf{S}_a^{-1})^{-1} \]

    \( \mathbf{S}_e \) is the error covariance matrix from measurements (random + correlated)

    \( \mathbf{S}_a \) is the error covariance matrix of the prior

    \( \mathbf{\hat{K}} \) is the Jacobian matrix

Ibrahim et al. (2022)
Another type of algorithm to estimate the uncertainty
Bayesian OE algorithm test on real data (MODIS Aqua)

\[ R_{rs}(443) \text{ (OE)} \]
\[ 76.5^\circ W 75^\circ W 73.5^\circ W 72^\circ W 70.5^\circ W 69^\circ W \]

\[ R_{rs}(443) \text{ (Oper.)} \]
\[ 76.5^\circ W 75^\circ W 73.5^\circ W 72^\circ W 70.5^\circ W 69^\circ W \]

\[ \text{Chl-a} = 0.11 \text{ mg m}^{-3}, \chi^2 = 0.60 \]

\[ \text{Chl-a} = 0.20 \text{ mg m}^{-3}, \chi^2 = 0.65 \]

Ibrahim et al (2022)
Validating pixel-level uncertainty for the Bayesian algorithm

Fig. 7. Top row is a histogram of the difference between the retrieved and in-situ $R_n$ at 443, 555, and 667 nm, respectively, for the OE algorithm in red, and the operational algorithm in black. The bottom row is the CDF of the absolute normalized error $\Delta_N$ for $R_n$ at the same three bands, where the red curve is estimated from the OE algorithm, and the black curve is the ideal case for a standard normal.
Questions?