Inversion of Satellite Ocean-Color Data

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<u>Collaborators</u>

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Linear combination of TOA reflectance

Principle of the Method

-The top-of-atmosphere reflectance in selected spectral bands is combined linearly, after correction for molecular scattering and sun glint contributions.

-The coefficients of the linear combination minimize the perturbing effects, due to scattering and absorption by aerosols, and reflection by the surface. These effects are decomposed into a polynomial or principal components.

-The spectral bands are selected so that the linear combination is sensitive to chlorophyll-a concentration.

Minimization of Perturbing Effects

-TOA reflectance

$$\begin{split} R_{TOA}(\lambda) &= R_m(\lambda) + R_a(\lambda) + R_{ma}(\lambda) + T_m(\lambda)T_a(\lambda)R_w(\lambda) \\ R_c(\lambda) &= R_{TOA}(\lambda) - R_m(\lambda) = R_a(\lambda) + R_{ma}(\lambda) + T_m(\lambda)T_a(\lambda)R_w(\lambda) \\ &= R'(\lambda) + T_m(\lambda)T_a(\lambda)R_w(\lambda) \end{split}$$

-Linearly combining the corrected reflectance R_c in spectral bands centered at λ_i yields the index

 $I = \sum_{i} [a_{i}R_{c}(\lambda_{i})] = \sum_{i} [a_{i}R'(\lambda_{i})] + \sum_{i} [a_{i}T_{m}(\lambda_{i})T_{a}(\lambda_{i})R_{w}(\lambda_{i})]$

-To eliminate most of the atmospheric influence on I, one has to find coefficients a_i that fulfill

 $\boldsymbol{\Sigma}_{i}\left[a_{i} R'(\lambda_{i})\right] = 0$

-For this, $R'(\lambda_i)$ is decomposed in a polynomial or principal components, i.e.,

 $R'(\lambda_i) \approx \sum_j [b_j e_{ji}]$

-In general, a satisfactory representation can be obtained with only a few eigenvectors, e_j , since R' is a smooth function of wavelength.

-Substituting R' by its linear expression, we obtain

$$\boldsymbol{\Sigma}_{i} \{ [a_{i} \boldsymbol{\Sigma}_{j}[b_{j}e_{ji}] \} = \boldsymbol{\Sigma}_{j} \{ [b_{j} \boldsymbol{\Sigma}_{i} a_{i}e_{ji}] \} = 0$$

-To satisfy this equation, it is sufficient to have, for each e_i

 $\boldsymbol{\Sigma}_{i}\left[a_{i}e_{ji}\right]=0$

-This system of linear equations is solved using p wavelengths, $n = p \cdot 1$ eigenvectors, and $a_1 = 1$.

-Note that the coefficients b_j , which vary with geometry and geophysical conditions do not need to be known.



Figure 1. Application of the linear combination method to simulated GLI imagery. Perturbing effects are expressed as a polynomial.



Figure 2. Application of the linear combination method to global GLI data. (Courtesy of H. Murakami, JAXA.)



Figure 3. GLI Version 2 chlorophyll-a concentration product. (Courtesy of H.Murakami, JAXA.)



Figure 4. Application of the linear combination method to SeaWiFS imagery. The perturbing effects are decomposed into principal components.

Retrieval of the Ocean Signal

-First, a set of spectral bands is selected in the red and near infrared, for which the water body can be considered black, except in one of the spectral bands.

-Second, other sets of spectral bands are selected, that progressively include shorter wavelengths. At each step, only marine reflectance in one spectral band is unknown and therefore estimated.

$$[\lambda_i, i = 1, 2, ..., 8] = [412, 443, 490, 510, 555, 670, 765, 865]$$

1:
$$T_m(\lambda_6)T_a(\lambda_6)R_w(\lambda_6) \approx \sum_i [a_iR_c(\lambda_i)]$$
, $i = 6, 7, 8$

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2:
$$T_m(\lambda_5)T_a(\lambda_5)R_w(\lambda_5) \approx -a_6T_m(\lambda_6)T_a(\lambda_6)R_w(\lambda_6)$$

+ $\sum_i [a_iR_c(\lambda_i)], i = 5, 6, 7$

6: $T_m(\lambda_1)T_a(\lambda_1)R_w(\lambda) \approx -a_2T_m(\lambda_2)T_a(\lambda_2)R_w(\lambda_2) - a_3T_m(\lambda_3)T_a(\lambda_3)R_w(\lambda_3)$ $+ \sum_i [a_iR_c(\lambda_i)], i = 1, 2, 3$



Figure 5. Residual perturbing effects of the atmosphere and surface, i.e., $\sum_{i} [a_i R'(\lambda_i)]$, as a function of aerosol optical thickness at 555 nm.



Figure 6. Comparison of estimated and actual ocean signal, i.e., $T_m(\lambda)T_a(\lambda)R_w(\lambda)$, when the optical thickness at 550 nm is between 0.1 and 0.2.



Figure 7. Performance statistics for the retrieval of $T_m(\lambda)T_a(\lambda)R_w(\lambda)$. Bias (solid circles) and standard deviation (open circles) are given as a function of aerosol optical thickness at 550 nm.

<u>Conclusions</u>

-The perturbing influence of the atmosphere and surface is minimized adequately for each set of wavelengths, except when aerosol loading is large. The residual effects exhibit a bias increasing with aerosol optical thickness. The bias can be reduced by taking into account the last eigenvector of the decomposition into principal components, but just globally.

-Errors in the estimated ocean signal, i.e., $T_m(\lambda)T_a(\lambda)R_w(\lambda)$, increase with decreasing wavelength (residual effects at longer wavelengths propagate) and with increasing aerosol optical thickness. They become unacceptable when the optical thickness at 550 nm is above 0.3.

-Performance can be improved by optimizing the sets of selected wavelengths, or by using a knowledge of the aerosol optical thickness, which can be estimated from the satellite data.

Fields of Nonlinear Regression Models

Problem

To estimate marine reflectance ρ_w from top-of-atmosphere reflectance ρ_{TOA} and angular variables t without knowing the other variables x that influence the radiative transfer in the ocean-atmosphere system

<u>Methodology</u>

-Explanatory variables (ρ_{TOA}) are considered separately from the conditioning variables (*t*).

-An inverse model is attached to each t, and the attachment is continuous, i.e., the solution is represented by a continuum of parameterized statistical models (a field of non-linear regression models) indexed by t.

$$\rho_w = \zeta_t(\rho_{TOA}) + \varepsilon$$

where ε is the residual of the modeling.

<u>Methodology (cont.)</u>

Ridge functions, selected for their approximation properties, especially density, are used to define the statistical models explaining ρ_w from ρ_{TOA} and t.

$$\begin{aligned} \zeta_{tj}(\rho_{TOA}) &= \Sigma_{i=1, \dots, n} c_{ij} h(\mathbf{a}_{i}, \rho_{TOA} + b_{i}) \\ \rho_{wj} &= \zeta_{tj}(\rho_{TOA}) + \varepsilon_{j} \end{aligned}$$

where $a_i(t)$, $b_i(t)$, and $c_{ij}(t)$ are the model parameters.

Simulated Data Sets

62,000 joint samples of ρ_{TOA} and ρ_w split in two data sets, D_e^o and D_v^o , for construction and validation. Noisy versions D_e^1 , D_v^1 , D_e^2 , and D_v^2 , generated, by adding 1 and 2% of noise to ρ_{TOA} . The noise is defined by:

$$\rho_{TOAj}' = \rho_{TOAj} + v^c \rho_{TOAj} + v^{uc} \rho_{TOAj}$$

where v^c and v^{uc} are random variables uniformly distributed on the interval [-v/200, v/200], where v is the total amount of noise in percent.

Function Field Construction

-The free parameters of the field, i.e., the maps $a_i(t)$, $b_i(t)$, and $c_{ij}(t)$, are estimated by multi-linear interpolation on a regular grid covering the range of t.

-The adjustment is considered in the least-square sense, and minimization of the mean squared error is carried out using a stochastic gradient descent algorithm.

Function Field Construction (cont.)

-A sufficient number of n = 15 basis functions was selected via simulations, and three fields of this kind, ζ^0 , ζ^1 , and ζ^2 were constructed for 0, 1, and 2% of noise.

-Since the components ζ_{tj} take their values in the same vector space (the vector space spanned by the linear combinations of ridge functions), the approach is not equivalent to separate retrievals on a component-by-component basis.

Theoretical Results for GLI

				Field ζ^0			
	λ (nm)	380	412	443	460	520	545
\mathcal{D}_e^0	RMS	0.000357	0.000362	0.000221	0.000165	5.33e - 05	6.64e - 05
	RMSR	0.027290	0.025008	0.019108	0.016000	6.19e - 03	7.69e - 03
\mathcal{D}_v^0	RMS	0.000357	0.000363	0.000221	0.000165	5.36e - 05	6.63e - 05
	RMSR	0.028168	0.025763	0.019607	0.016372	6.23e - 03	7.65e - 03
\mathcal{D}_e^1	RMS	0.000901	0.000846	0.00055	0.000422	0.000150	0.000187
	RMSR	0.055998	0.049971	0.04171	0.036165	0.016896	0.021906
\mathcal{D}_v^1	RMS	0.000888	0.000833	0.000543	0.000417	0.000152	0.000186
	RMSR	0.056408	0.049936	0.041885	0.036508	0.017140	0.021722
Field ζ^1							
\mathcal{D}_e^0	RMS	0.000434	0.000431	0.000267	0.000202	6.96e - 05	8.48e - 05
	RMSR	0.028771	0.025905	0.021234	0.018443	8.02e - 03	9.91e - 03
\mathcal{D}_v^0	RMS	0.000433	0.000433	0.000267	0.000202	7.18e - 05	8.56e - 05
	RMSR	0.029120	0.026096	0.021457	0.018729	8.30e - 03	9.95e - 03
\mathcal{D}_e^1	RMS	0.000654	0.000631	0.000402	0.000309	9.76e - 05	0.000132
	RMSR	0.041901	0.037426	0.031563	0.027655	1.12e - 02	0.015271
\mathcal{D}_v^1	RMS	0.000646	0.000624	0.000397	0.000305	0.000100	0.000131
	RMSR	0.041971	0.037267	0.031546	0.027777	0.011457	0.015066

Field ζ^0

Table 1. Root Mean Squared error (RMS) and Root Mean Squared Relative error (RMSR) for the models ζ^0 and ζ^1 evaluated on the construction and validation data sets (D_e^0 and D_v^0) and on 1% noisy versions of them (D_e^1 and D_v^1).



Figure 8. Estimated versus expected marine reflectance for model ζ^{1} adjusted on 1% noisy data.



Figure 9. Conditional quantiles (of order 0.1, 0.25, 0.5, 0.75, and 0.9) of the residual ρ_w error distributions as a function of aerosol optical thickness at 550nm for model ζ^1 applied to 1% noisy data.



Figure 10. Conditional quantiles (of order 0.1, 0.25, 0.5, 0.75, and 0.9) of the residual ρ_w error distributions as a function of scattering angle for model ζ^1 applied to 1% noisy data.



Figure 11. $\rho_w(443)/\rho_w(545)$ as a function of [Chl-a] for theoretical ρ_w and for ρ_w estimated by ζ^1 from 1% noisy data.

Application to SeaWiFS Imagery

-Function field methodology tested on SeaWiFS imagery acquired on day 323 of year 2002 over Southern California.

 $-\zeta_{f}^{2}$ gives large differences in ρ_{w} compared with SeaDAS values, resulting in 78% difference in chlorophyll-a concentration on average.

-Differences may be explained by large noise level on ρ_{TOA} (e.g., 14% at 412 nm), due to RT modeling uncertainties.

-Noise distribution estimated on 2,000 randomly selected pixels of the imagery, and introduced during the execution of the stochastic fitting algorithm, yielding function field ζ_t^* .



Figure 12. Marine reflectance ρ_w estimated by ζ^* for SeaWiFS imagery acquired on day 323 of year 2002 over Southern California.



->0.026

- <0.000

- <0.001

->0.002





Figure 14. Histograms of marine reflectance ρ_w retrieved by SeaDAS and ζ^* .



Figure 15. Marine reflectance spectra retrieved by SeaDAS and ζ^* .



Figure 16. *[Chl-a]* retrieved by SeaDAS and ζ^* , fractional difference, and histograms for SeaWiFS imagery acquired on day 323 of year 2002 over Southern California. Average difference is 19.6%.

<u>Conclusions</u>

Fields of non-linear regression models emerge as solutions to a continuum of similar statistical inverse problems. They match well the characteristics of the remote sensing problem, allowing separation of the explanatory variables (ρ_{TOA}) from the conditioning variables (t).

The inversion is robust, with good generalization, and computationally efficient. The retrievals of ρ_w are accurate, with an error uniform over the entire range of ρ_w values. Situations of absorbing aerosols are handled well.

For noise levels up to a few percent, a general noise scheme may be appropriate, but for large noise levels, the noise distribution needs to be estimated. A plug-in approach may be reasonable.