Uncertainties in ocean colour remote sensing
Lecture 2: algorithms, validation

Roland Doerffer
Retired from Helmholtz Zentrum Geesthacht
Institute of Coastal Research
Now: Brockmann Consult
roland.doerffer@hzg.de
Algorithms and uncertainties

- Inversion schemes
- Saturation and masking effects
- Out of scope conditions
- Verification
- Validation
- Strategies for validation
- The OC-CCI approach
- Summary and conclusions
Case 1 water algorithm based on reflectance ratio model R445 / R555

\[ \text{Chl} = a [R(445) / R(555)]^b \]

Case 1 water:

Morel / Antoine MERIS Case 1 water ATBD
Water leaving radiance reflectance spectra in coastal water
Variability of water leaving reflectance spectra

Water leaving radiance reflectance spectra
MERIS North Sea 20060726

RLw (sr-1)
wavelength (nm)
The inverse problem

- Matrix inversion
- Inversion by optimization
- Inversion by neural network

Success depends on:
- Bio-optical model
- Ambiguities
Inverse Modellierung using Optimization Procedures

start values
model parameters
IOP / conc.

radiative
transfer
modell

reflectance-
spectra
simulated

do spectra agree?

parameters
are the
IOPs / conc.

change
parameters

determine
search direction
downhill in cost function

test = \sum (R_{sim}(i) - R_{sat}(i))^2

Satellite
Simplified scheme of NN Algorithm

\[
y_l = s(-d_l + \sum_{k=1}^{3} w_{kl} \cdot s(-c_k + \sum_{j=1}^{5} v_{jk} \cdot s(-b_j + \sum_{i=1}^{4} u_{ij} \cdot x_i)))
\]
Sensitivity at different concentration ranges and spectral bands

RLw for MERIS bands 1 (412 nm), 6 (560 nm), 10 (708 nm)

Sensitivity of the reflectance at a spectral band depends on the concentration.

To cover a large concentration range, many bands from the blue to NIR range are necessary.
Sensitivity at different concentration ranges and spectral bands

Chl. 5/10 mg m$^{-3}$
TSM 1 g m$^{-3}$
aYS(443) 0.1 m$^{-1}$

Chl. 5/10 mg m$^{-3}$
TSM 100 g m$^{-3}$
aYS(443) 0.1 m$^{-1}$
Searching for minimum: principle, 1D case

Search for minimum: Deviation between measured and simulated spectrum

Width can be estimated from the 2nd order derivative (Hessian matrix)
Error due to masking and ambiguities

- True spectrum simulated
- "measured“ spectrum = true * random error
- Retrieved spectrum when LM has found solution
## Results and errors of retrieval

<table>
<thead>
<tr>
<th>Variable</th>
<th>conc true</th>
<th>conc retr.</th>
<th>std dev of log conc</th>
<th>err. estimated %</th>
<th>err true %</th>
</tr>
</thead>
<tbody>
<tr>
<td>chlorophyll [mg m⁻³]</td>
<td>1</td>
<td>0.8337</td>
<td>0.09191</td>
<td>9.626</td>
<td>-19.94</td>
</tr>
<tr>
<td>detritus [g m⁻³]</td>
<td>1</td>
<td>1.152</td>
<td>0.1684</td>
<td>18.34</td>
<td>13.19</td>
</tr>
<tr>
<td>gelbstoff a443 [m⁻¹]</td>
<td>0.1</td>
<td>0.1005</td>
<td>0.03566</td>
<td>3.63</td>
<td>0.4842</td>
</tr>
<tr>
<td>min. SPM [g m⁻³]</td>
<td>1</td>
<td>0.9948</td>
<td>0.006498</td>
<td>0.6519</td>
<td>-0.5238</td>
</tr>
</tbody>
</table>

kdmin_true: 0.2096  kd490_true: 0.2636  
kdmin_ret: 0.2089   kd490_ret: 0.2609  
error: -0.33%       error: -1.04%
Uncertainties due to ambiguities for different concentration mixtures

All cases of turbid water

2 mg m-3

model chlorophyll µg/l

nn-derived µg/l

case 2 water chlorophyll retrieval with NN
Ambiguities 2

Typical North Sea coastal water: ay_443: < 0.2 m-1, TSM < 5 mg/l
Determine uncertainties on a pixel by pixel basis II

conc_bp
0.05 - 0.5 - 5 - 45

conc_pig
0.005 - 0.03 - 0.15 - 1.0

conc_gelb
0.005 - 0.035 - 0.2 - 0.15

chl

tsm
Signal depth at different spectral bands

Multiband algorithms: the information for each band may come from a different water layer

$z_{90} = 1/k$

coastal:
TSM = 5 mg/l
Chlor. = 5 µg/l
Gelb = $a_{380} = 1 \text{m}^{-1}$

open ocean:
Chlor. = 1 µg/l
Detection of out of scope conditions

- 2 Procedures have been developed
  - **Combination of an inverse and forward Neural Network**
  - **Use of an autoassociative Neural Network**
- Both produce a reflection spectrum, which is compared with the input spectrum
- Deviation between input and output spectrum can be computed as a chi2
- A threshold can be used to trigger an out of scope warning flag

- **Combination of inverse and forward NN**

- **Auto-associative NN**
Detection of out of scope conditions (MERIS processor)

- $r, r'$ – log of reflectances
- $c$ – log of concentrations
- $g$ – geometry information
- $q$ – quality indicator

Comparator to trigger out of scope flag

If $RLw < 0.0009$, $RLw = 0.0009$ ($\rho \approx 0.003$)

Flag PCD1_16,17 $q$ true if $\sum (r(i) / r'(i)) > 4.0$
Detection of out of scope conditions (MERIS processor)

Top of atmosphere radiance spectra at normal and critical locations
Detection of out of scope conditions (MERIS processor)

Chi_square is computed by comparing
The input reflectance spectrum
with the output of the forward NN
Detection of out of scope conditions using an aaNN

- Important to detect toa radiance spectra which are not in the simulated training data set
- These are out of scope of the atmospheric correction algorithm
- Autoassociative neural network with a bottle neck layer

![Diagram of autoassociative neural network](image)

Functions also as nonlinear PCA
i.e. bottle neck number of neurons
Provide estimate of Independent components

For the GAC training data
Set of ~ 1Mio. Cases
Bottleneck minimum was 4-5
Detection of out of scope conditions aaNN: example for L1 (TOA) data

High SPM

Sun glint

Transect
Detection of out of scope conditions aaNN: example

significant deviation in area with high SPM concentrations, but not in sun glint area
Verification

- Using simulated test data
- You can detect ambiguities
- Non linear behaviour
- Concentration ranges with failures
- It might be necessary to change bio-optical model
- Or range and frequency distribution of the training data set
Test of NN I 1

- 443 nm
- 1020 nm
Test of NN I 3

Kd_min

Kd_490
Test of NN 17x27x17, training with 5% random noise on RLw
Validation

- NOMAD data set
  - Compiled, quality checked and maintained by OC group of NASA
  - In situ observations from different cruises, different teams, instruments, procedures, sky and wave conditions
  - Includes RLw at 6 MERIS bands (412, 443, 490, 510, 560, 665)
  - a_total, b_total / bb_total at 443
- Note: in situ data have their own variabilities and uncertainties!

Relationship between chlorophyll a concentration and the absorption coefficient of phytoplankton pigments
Total absorption at 443 nm (water + constituents)
log10_a443_nn = log10_a443_measured * 0.977 - 0.0167, stdev = 0.141
Frequency distributions of measured and derived $a_{443}$ after removing outliers with $\text{sum}_\text{sq} > 1.0 \times 10^{-5}$
Measured and nn-derived a443 for all cases with sd <1.0e-5
Differences and rel. deviation

Log10 difference

Mean difference: 0.0086102 m\(^{-1}\), stdev: 0.129
Mean ratio: 0.9717098, stdev: 0.334

Log10 ratio
Sum\_sq of measured and nn derived reflectances
Test of NN based on measurements for chlorophyll

Log10 scale, red: 1 by 1 line
Comparison of histograms: measured, NN computed

Histogram of log chlorophyll measured (blue) and from NN algorithm (red)
Histogram kd489 measured and NN derived
Uncertainties related to comparison with in situ data

- Error in method and handling, e.g. HPLC for chlorophyll determination
- Sample not representative for water volume of pixel
- Vertical distribution: water comes from a certain depth, e.g. 4 m for FerryBox
- Temporal difference between sample and satellite overpass
- Sub-pixel patchiness
- Scatter in bio-optical data, e.g. relationship between concentration and IOPs
Uncertainties: Ocean Colour CCI Approach

- Definition of optical water classes from reflectance spectra (9 classes)
- Determination of the membership of in situ reflectance data
- Determination of the uncertainties from statistics of available in situ data for each class

- Determination of the membership of a pixel to different optical water classes
- Weighting of the uncertainties by Fuzzy Logic
Ocean Colour Climate Change Initiative

EO Science Team

European
- R. Brewin, PML, UK
- V. Brotas, FCUL, Portugal
- C. Brockmann, BC, Germany
- A.B. Couto, FCUL, Portugal
- R. Doerffer, BC, Germany
- S. Groom, PML, UK
- T. Jackson, PML, UK
- H. Krasemann, HZG, Germany
- F. Mélén, JRC, EU
- D. Müller, HZG, Germany
- M. Peters, BC, Germany
- D. Ramon, HYGEOS, France
- L. Santoleri, CNR, Italy
- T. Storm, BC, Germany
- T. Platt, PML, UK
- F. Steinmetz, HYGEOS, France
- P.Y. Deschamps, HYGEOS, France
- A. Valente, FCUL, Portugal

Non-European
- E. Devred, LU, Canada
- G. Feldman, NASA, USA
- B. Franz, NASA, USA
- Z.-P. Lee, BU, USA
- T. Hirata, HU, Japan
- T. Moore, UNH, USA
- M. Wang, NOAA, USA

Climate Research Group
- I. Allen, PML, UK
- L. Bertino, NERSC, Norway
- S. Clavatta, PML, UK
- W. Gregg, NASA, USA
- T. Hirata, HU, Japan
- C. Le Quéré, UEA, UK
- S. Saux-Picart, PML, UK
- E. Simon, NERSC, Norway
- H. Von Storch, HZG, Germany

System Engineering
- M. Boettcher, BC, Germany
- N. Formferra, BC, Germany
- M. Grant, PML, UK
- A. Chuprin, PML, UK
- J. Swinton, TPZ Vega, UK

Courtesy of PML
# GCOS Requirements: a Major Challenge

<table>
<thead>
<tr>
<th>Variable/Parameter</th>
<th>Horizontal Resolution</th>
<th>Vertical Resolution</th>
<th>Temporal Resolution</th>
<th>Accuracy</th>
<th>Stability</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water Leaving Radiance</td>
<td>4km</td>
<td>N/A</td>
<td>daily</td>
<td>5%</td>
<td>0.5%</td>
</tr>
<tr>
<td>Chlorophyll-a concentration</td>
<td>30km</td>
<td>N/A</td>
<td>weekly averages</td>
<td>30%</td>
<td>3%</td>
</tr>
</tbody>
</table>

A major challenge to meet all the GCOS requirements: extremely high requirements for the quality and long term stability of the data.

OC-CCI: Strong research component to quantify, and where possible, reduce errors.

Courtesy of PML
Band Shifting and Bias Correction

Each sensor has a different set of wave bands. These are 'shifted' to a common set of wave bands: the SeaWiFS bands were used as reference. It is an “interpolation” technique based on IOP algorithms (Mélín et al., 2011).

Data from the different sensors may have biases with respect to each other.

Bias correction removes consistent biases between the datasets and is carried out by generating climatologies of temporally overlapping data and deriving per-pixel maps of bias between the sensors.

Courtesy of PML
Criteria Considered include:
Use metrics that have been commonly used in the literature;
Separate random and systematic components of errors;
Map errors and uncertainties on a pixel-by-pixel basis;
Serve the modelling community as well as the Earth Observation community;
Select metrics that are appropriate for the algorithms; and
Base uncertainty estimates on comparison with in situ data.

Selected Metrics
Root-Mean Square Errors
Bias
Standard Deviation

<table>
<thead>
<tr>
<th>Product</th>
<th>In-situ data match ups</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chl-a</td>
<td>≈6000</td>
</tr>
<tr>
<td>Rrs(412)</td>
<td>≈14500</td>
</tr>
<tr>
<td>Rrs(443)</td>
<td>≈12700</td>
</tr>
<tr>
<td>Rrs(490)</td>
<td>≈15100</td>
</tr>
<tr>
<td>Rrs(510)</td>
<td>≈3300</td>
</tr>
<tr>
<td>Rrs(555)</td>
<td>≈7500</td>
</tr>
<tr>
<td>Rrs(670)</td>
<td>≈6000</td>
</tr>
</tbody>
</table>

Courtesy of PML
Error Specification by Optical Water Type

Spectral Radiance Values Per Pixel

Fuzzy Logic Membership in Optical Water Type

Biogeochemical and Bio-optical Products

Advantages:
- Not limited by geographic region, provided all possible optical water types are classified
- Error assignment on basis of overall optical signal, and not on a single variable, e.g., chlorophyll, and hence consistent across products
- Total number of water types is small, so number of observations per class would be greater than if we were to use a large number of class intervals
- Optical classification provides a way to distinguish case-1 and case-2 waters
- No sharp boundaries across types

Weighted uncertainties, by Optical Type and by Product

Uncertainties per pixel and per product

Fuzzy classification uses fuzzy c-means (FCM) clustering algorithm (Moore et al. 2009)

Type 1

Type 2

... ...

Type N

Courtesy of PML
Error Specification by Optical Water Type

July 2003 dominant water class

July 2003 RMSD $\log_{10}$ Chl-a

July 2003 Bias $\log_{10}$ Chl-a

Chl-a July 2003

Courtesy of PML
Comparison to GCOS Requirements

Relative % difference wrt in-situ data

Match-ups distributed across bins of equal size

±30 % GCOS requirement

Courtesy of PML
Future Work

The distribution of data used in the creation and validation of the remote sensing products is still not representative of the global oceans.

We are looking to incorporate more data into our in situ database.

Analysis of additional missions (already started in phase 1):
OCM2, VIIRS OLCI.

Frequency distribution of chlorophyll-a in the OC-CCI monthly composite for July 2003 and the in situ chlorophyll concentrations from the match-up database. Each distribution is normalised to its maximum value.

Courtesy of PML
Uncertainty Characterisation

(c) Equal class interval

(d) Equal bin count

Courtesy of PML
Uncertainty Characterisation

Chlorophyll-a match-up comparison and dominant optical water class

Satellite estimated Chlorophyll-a (mg m^{-3})

In situ Chlorophyll-a (mg m^{-3})

Class 1
Class 2
Class 3
Class 4
Class 5
Class 6
Class 7
Class 8

Courtesy of PML
Comparison to GCOS Requirements

Histograms of relative error in \( R_{rs} \) at various blue and green SeaWiFS wavebands, based on the bias computed using optical classification.

Example shown is for OC-CCI monthly composite \( R_{rs} \) fields for July 2003.

GCOS requirement (5%) is shown as a vertical red line in each plot.

Only the magnitude (modulus) of the relative error is shown, not the sign.
Future Work

More emphasis on inter-mission consistency (atmospheric correction, vicarious calibration, ... ) to create a more harmonised product.

Use POLYMER atmospheric correction for all sensors?

Reduce errors such that we completely meet GCOS requirements.

Listen to user feedback and provide support and updates to product.

Merge new datasets and sensors into the processing chain to increase product accuracy and coverage.

Courtesy of PML
Strategies to determine uncertainties for coastal water: Solutions

- **Out of scope detection**
  - Check of auxiliary variables, e.g. windspeed -> whitecaps
  - Check of reflectance in particular bands: NIR reflectance for floating material
  - Auto-associative neural network
  - Combination of backward and forward neural network (standard MERIS processing)
  - Convergence of optimization procedure on high deviation level

- **Ambiguities in bio-optical / reflectance model**
  - Analysis of simulated data using the bio-optical model

- **Uncertainties on a pixel by pixel basis**
  - Empirical from observations, optional for different optical water classes
  - Variations in optimization procedure
  - Determination using variations of simulated data set -> look up table, NN
Summary and Conclusion: uncertainties

- There are a lot of factors, which determine top of atmosphere radiance spectra
- Vice versa the information content of TOA spectra is much too low to determine all of these factors independently
- In complex water the signal can be very low in the blue spectral range
- Atmospheric correction then extremely critical
- In complex water the dominant component might mask the effect of all other components
- In this case the uncertainty range for the subdominant components increases significantly
- Saturation effects limit the accuracy and may cause a shift in the importance of bands
- There are constellations of atmosphere / water which leads to failure in the algorithms
- These out of scope conditions have to be detected and marked per pixel using flags and uncertainty indicators
- Expected errors can be determined by sensitivity studies
- Of high importance is a continuous validation using in situ observations of high quality
Colour Remote Sensing of complex water is possible!

But:

- Restrict to a small number of components with similar optical properties
- Detection of special cases such as red tides, cyanobacteria
  - Exclude or develop special algorithms
- General knowledge about vertical distribution at different seasons
- Bathymetry to estimate possible bottom effects
- Determine penetration depth / z90 depth
- Determine scope of algorithm
- Develop algorithm to determine / flag out of scope conditions
- Determine uncertainties for each product

**Atmospheric correction most challenging issue**

- Develop special procedures for atmospheric correction over complex waters
- Problems: adjacency effects, floating material
- Determine conditions when AC leads to too large uncertainties
MERIS 20070505
Top of atmosphere radiance reflectance RLtoa RGB

New York
Path radiance + Fresnel reflectance RLpath MERIS band 5 (560 nm)
Water leaving radiance reflectance $RL_w$ MERIS band 5 (560 nm)
Water leaving radiance reflectance $RL_w$ MERIS band 2 (443 nm)
Chlorophyll
Acknowledgements

• Supported by various projects
  – ESA Case 2 Water Regional Algorithm
  – ESA Glint correction
  – ESA Water radiance
  – ESA CoastColour
  – ESA Dragon
  – ESA Ocean Colour CCI
  – DLR DeMarine
• Neural Network Training software H. Schiller, GKSS
• MERIS data provided by ESA
• Implementation of C2R and Glint correction in BEAM: M. , Brockmann-Consult
Summary and conclusions

- Uncertainty in coastal water products can be large due to the large number of factors in atmosphere and water, which determine the reflectance spectrum.
- Conditions where algorithms (AC & water) fail.
- Prerequisite for a successful retrieval are optical models of the atmosphere and the water, which meet the actual conditions.
  - Regional models might be necessary.
- Reflectance spectra have to be tested if they are within the scope of these models.
  - Out of scope spectra have to be flagged, treated with special algorithms or excluded from further processing.
- Limited sensitivity of reflectance spectrum and ambiguities lead to an uncertainty even for spectra, which are in scope.
  - Uncertainties have to be quantified on a pixel-by-pixel basis.
- Validation in coastal waters by match up in situ samples can be difficult due to patchiness and fast changes.
  - Uncertainties in in situ match up data have to be quantified.
  - Validation should be complemented by statistical analysis of larger areas, transects and time series.