Inverse modeling of case-2 waters: Error sources and error propagation

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Overview

- Case 2 model
- Error sources
- Error propagation
- Error ranking
- Consequences for fit strategy

Model: Optically deep case-2 water

Irradiance reflectance $$R(\lambda) = f \cdot \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}.$$ Gordon et al. (1975)

Backscattering $$b_b(\lambda) = b_{b,W}(\lambda) + X \cdot b_{b,X}^* \cdot (\lambda/500)^n$$

Absorption $$a(\lambda) = a_W(\lambda) + Y \cdot \exp[-S \cdot (\lambda-440)] + C \cdot a_P^*(\lambda)$$

$b_{b,W}(\lambda) = 0.00111 \cdot (\lambda/500)^{-4.32}$ = backscattering coefficient of pure water (m^{-1})

$b_{b,X}^* = 0.0086\ m^2\ g^{-1}$ = specific backscattering coefficient of suspended matter at 500 nm

$a_W(\lambda)$ = absorption of pure water (from: H. Buiteveld, J. H. M. Hakvoort, M. Donze: The optical properties of pure water. *SPIE Vol. 2258, Ocean Optics XII, 1994, p. 174-183)*

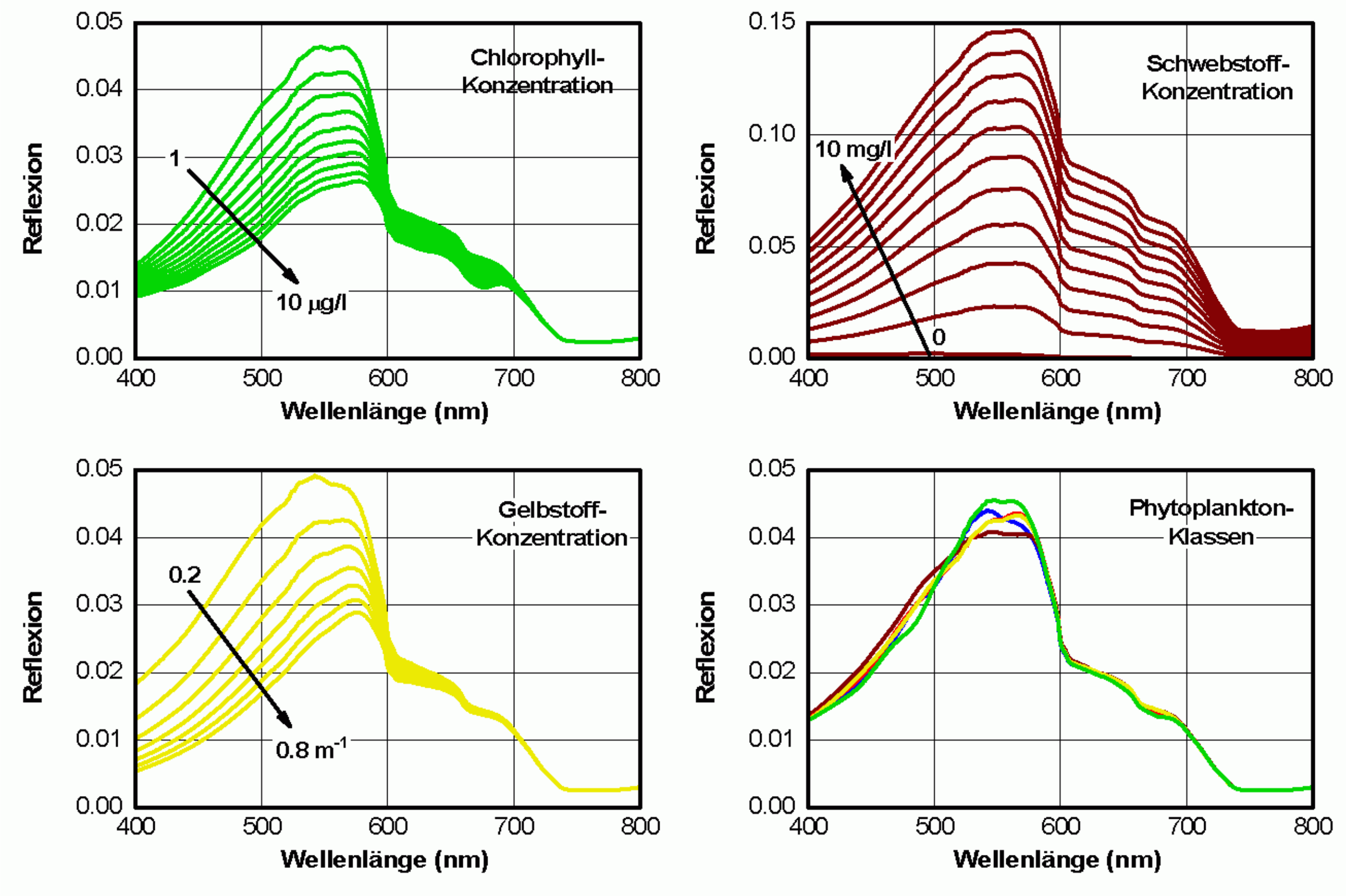
$a_P^*(\lambda)$ = specific absorption of phytoplankton

WASI

The model considers 3 water constituents (WCs): Phytoplankton, Gelbstoff, Suspended Matter.

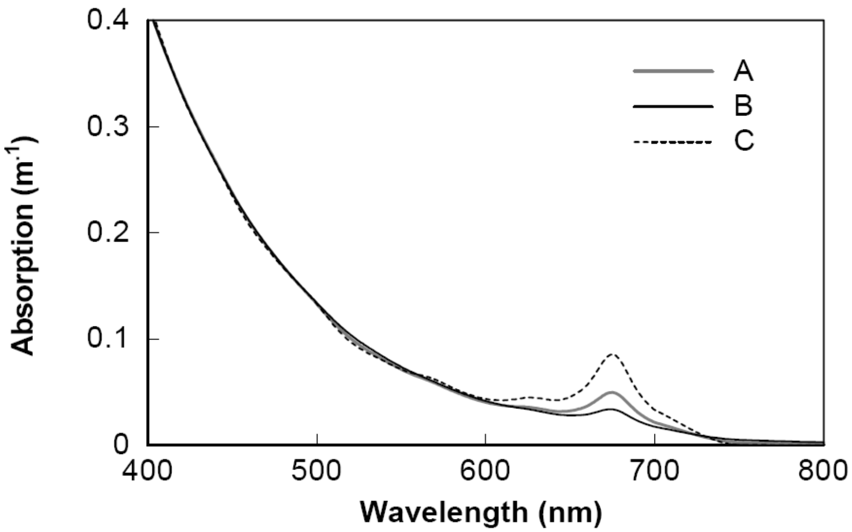
H. R. Gordon, O. B. Brown, M. M. Jacobs (1975): Computed Relationships between the Inherent and Apparent Optical Properties of a Flat Homogeneous Ocean. *Applied Optics 14, 417-427.*

Model: Variability of R(λ)



Error source: Ambiguities

- Ambiguity: different parameter combinations yield similar spectra
- Problem increases drastically with number of fit parameters
  - → keep it as low as possible



Example: Absorption of water constitutents

$a_{WC}(\lambda) = C \cdot a_P^*(\lambda) + Y \cdot \exp[-S \cdot (\lambda - 440)]$

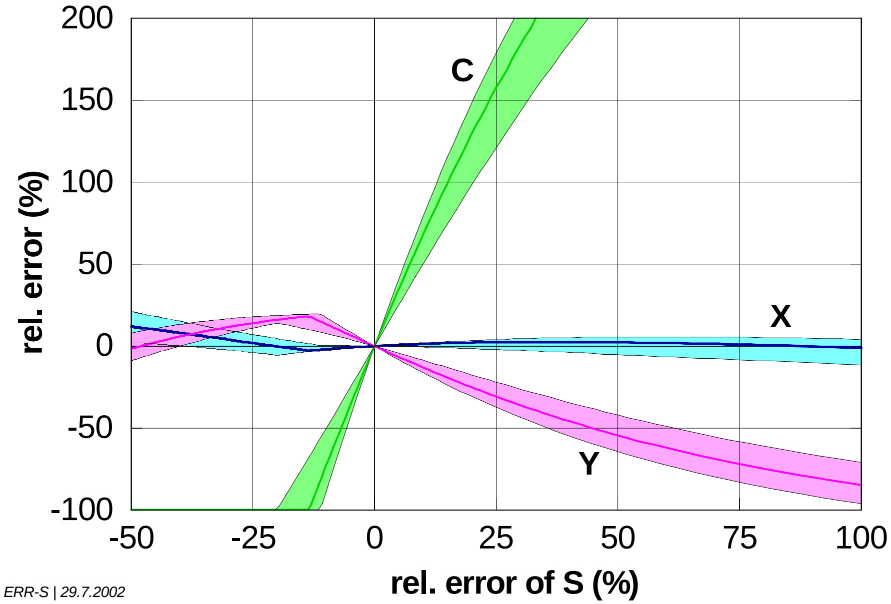
Curve	C	Y	S
A	2 µg/l	0.200 m^{-1}	0.0140 nm^{-1}
B	1 µg/l	0.232 m^{-1}	0.0124 nm^{-1}
C	4 µg/l	0.132 m^{-1}	0.0200 nm^{-1}

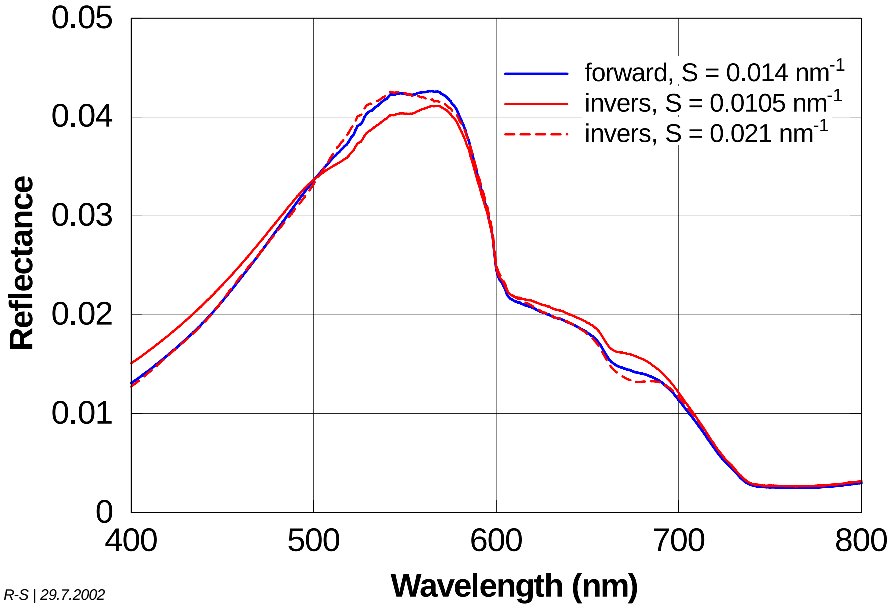
P. Gege, A. Albert (2006): A tool for inverse modeling of spectral measurements in deep and shallow waters. *In: L.L. Richardson and E.F. LeDrew (Eds): "Remote Sensing of Aquatic Coastal Ecosystem Processes: Science and Management Applications", Kluwer book series: Remote Sensing and Digital Image Processing, Springer, ISBN 1-4020-3967-0, pp. 81-109.*

Error sources

- Ambiguities (mainly between phytoplankton and Gelbstoff)
- WC optical properties are variable and only approximately known for actual measurement (enhances ambiguity problem between phytoplankton and Gelbstoff)
- Conversion from optical to gravimetrical units
- Sensor properties (λ range, λ resolution, radiometric resolution, noise, calibration errors)
- Measurement errors (illumination, shadow …)
- Model errors
    - Gordon equation is approximation
    - Parameterisation of WC spectra is approximation
    - Some effects are ignored, e.g. fluorescence
- Set-up of retrieval algorithm (initial values, parameter increments, accepted residual)

Error propagation: Example of S



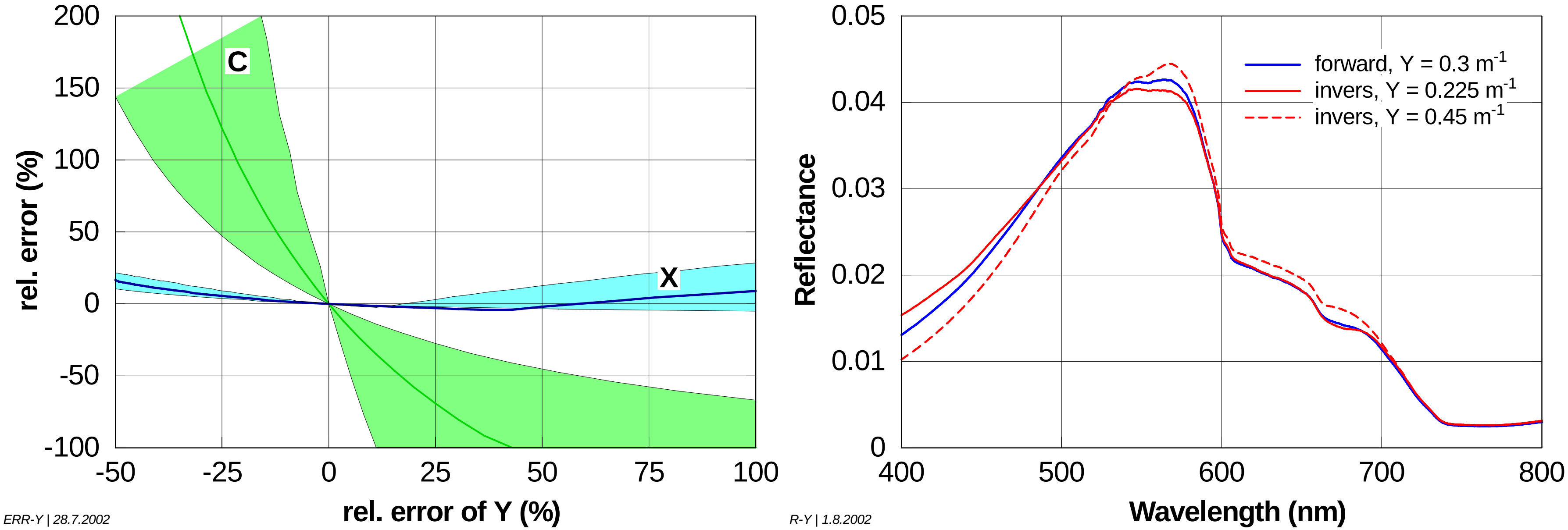


S error of 25 % (0.0140 nm^{-1} → 0.0175 nm^{-1}) causes

- C error of 150 %
- Y error of -30%
- X error of 3 %

P. Gege (2002). Error propagation at inversion of irradiance reflectance spectra in case-2 waters. *Ocean Optics XVI Conference, November 18-22, 2002, Santa Fe, USA.*

Error propagation: Example of Y

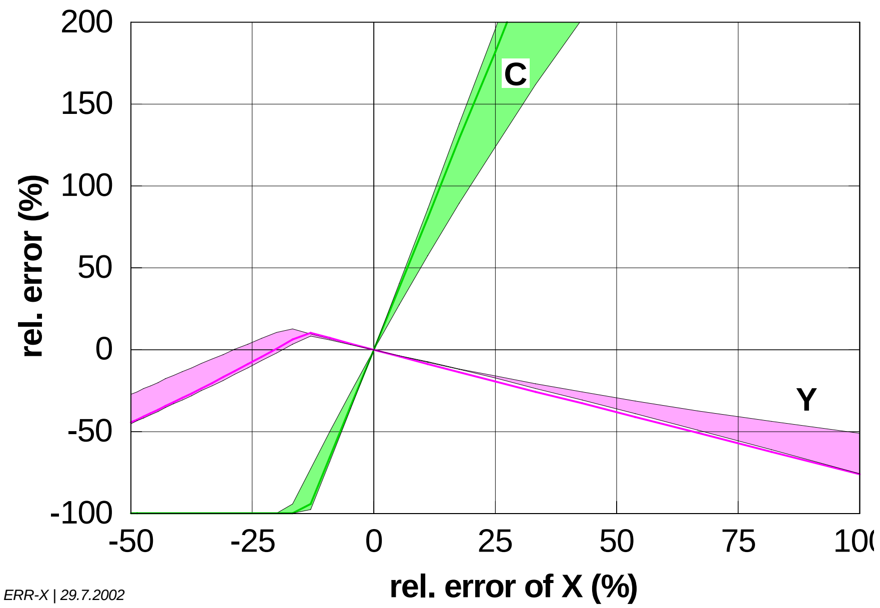


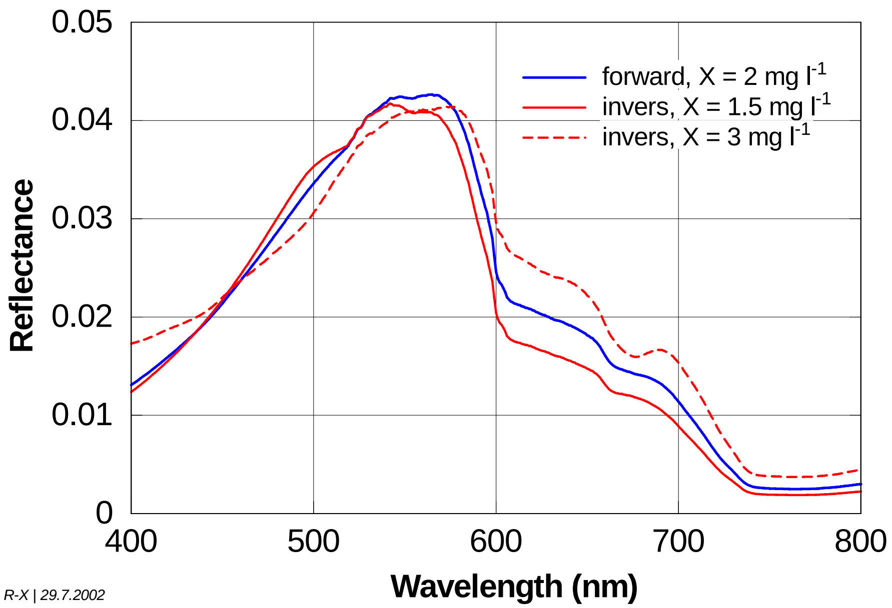
Y error of 25 % (0.3 m^{-1} → 0.375 m^{-1}) causes

- C error of -70 %
- X error of 2 %

P. Gege (2002). Error propagation at inversion of irradiance reflectance spectra in case-2 waters. *Ocean Optics XVI Conference, November 18-22, 2002, Santa Fe, USA.*

Error propagation: Example of X





X error of 25 % (2 mg/l → 2.5 mg/l) causes

- C error of 180 %
- Y error of -20%

P. Gege (2002). Error propagation at inversion of irradiance reflectance spectra in case-2 waters. *Ocean Optics XVI Conference, November 18-22, 2002, Santa Fe, USA.*

Error propagation: Comparison of errors

Par.	Default value	Par. error	C error	X error	Y error	Par. error	C error	X error	Y error
f	0.4	-25%	17%	36%	1%	50%	10%	-35%	3%
n	0	-0.5	-17%	14%	26%	0.5	12%	-12%	-22%
S	0.014 nm^{-1}	-25%	158%	3%	-31%	50%	193%	7%	-35%
$a_P*(\lambda)$	spectrum	mean	56%	3%	9%	max	-100%	-8%	-21%
C	2 µg l^{-1}	-25%	–	-3%	7%	50%	–	5%	-10%
X	2 mg l^{-1}	-25%	-100%	–	-9%	50%	376%	–	-38%
Y	0.3 m^{-1}	-25%	49%	4%	–	50%	-100%	5%	–

f errors: affect mainly X, some influence on C.
n errors: affect mainly Y, some influence on C and X.
S errors: cause very large errors for C (easily > 100 %), large errors for Y, but almost no errors for X.
Wrong spectrum $a_P*(\lambda)$: affects mainly C. Errors are difficult to quantify since $a_P*(\lambda)$ is not parameterised.
C errors: cause only minor errors, except errors at high C cause high Y errors.
X errors: cause very large errors in C (easily > 100 %) and large errors of Y.
Y errors: cause very large errors in C (easily > 100 %), but have almost no influence on X.

P. Gege (2002). Error propagation at inversion of irradiance reflectance spectra in case-2 waters. *Ocean Optics XVI Conference, November 18-22, 2002, Santa Fe, USA.*

Error ranking

Rank	C		X		Y	
1	X	±3.4%	f	±19%	S	±20%
2	S	±3.5%	–	–	X	±33%
3	Y	±6.5%	–	–	n	±0.48
4	$a_P*(\lambda)$	±25%	–	–	–	–

Required accuracies for concentration errors below ±25 %

C determination: 3 parameters must be known very accurately: X, S, Y. Few percent error is critical. $a_P*(\lambda)$ represents a conversion factor from "optical" to gravimetric phytoplankton concentrations, which is highly variable in nature.

X determination: Retrieval of suspended matter is quite robust. The only notable error source, f, can be determined with little error from models. Main problem is the conversion from "optical" to gravimetric concentrations, since the conversion factor $b_{b,X}*$ is highly variable in nature.

Y determination: Not critically affected by errors. Main error source is S. For X and n relatively large errors are acceptable.

P. Gege (2002). Error propagation at inversion of irradiance reflectance spectra in case-2 waters. *Ocean Optics XVI Conference, November 18-22, 2002, Santa Fe, USA.*

Consequences for fit strategy

- Restrict fit parameters to reasonable interval
- Start fit using "reasonable" initial values
  - from analytic equations
  - from adjacent image pixels
- Use correlations between the parameters
  - may not be applicable to the concentrations. Case-2-waters are water types with low correlation between C, X, Y.
  - may be applicable to spectral shape parameters. For example, S is correlated to Y since exponential equation is no physical description of Gelbstoff absorption, but merely an empirical relationship. A model for the relationship between S and Y was developed by Gege (2000).
- Use a multi-step approach when fitting many parameters

P. Gege (2000): Gaussian model for yellow substance absorption spectra. *Ocean Optics XV Conference, October 16-20, 2000, Monaco.*

Example: Multi-step approach in WASI

1. Determine initial value of X using analytical equation
2. Determine initial values of C, Y using analytical equations
3. Fit X, Y; fix all other parameters
4. Fit C, Y, S; fix all other parameters
5. Fit all parameters

P. Gege (2005): The Water Colour Simulator WASI. User manual for version 3. *DLR Internal Report IB 564-01/05, 83 pp.*

Summary

- Determination of **Suspended matter** backscattering is reliable
- Determination of **Gelbstoff** absorption is reliable if S uncertainty is below 20 %
- Determination of **Phytoplankton** absorption is unreliable if errors of X, S, Y are above ~ 5 %
- Errors can be reduced using a fit strategy which accounts for error propagation

Phytoplankton retrieval requires fit strategy based on error modeling!