NOWPAP - PICES Joint Training course
on Remote Sensing Data Analysis

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

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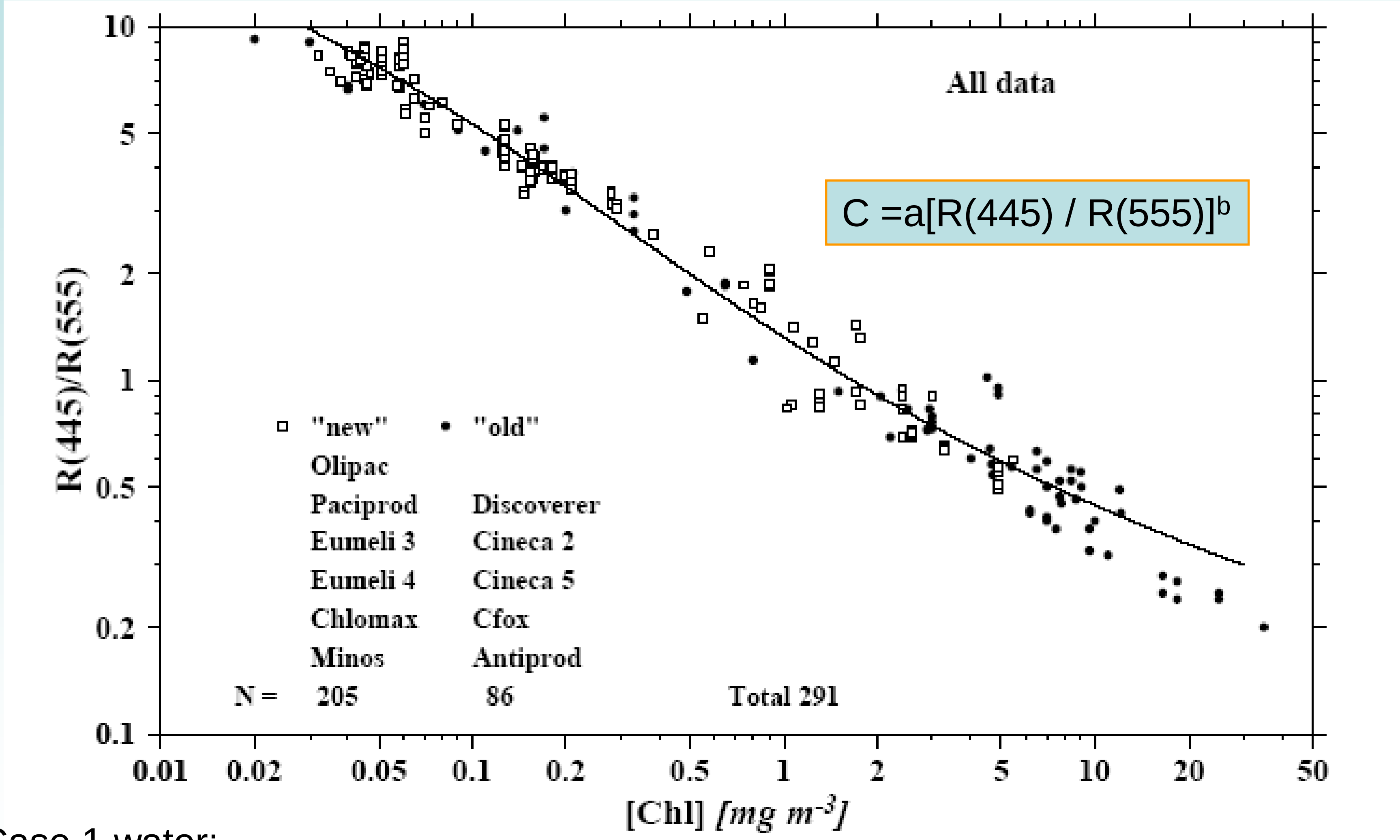
Algorithms and uncertainties

- Inversion schemes
- Saturation and masking effects
- Out of scope conditions
- Verification
- Validation
- Strategies for validation
- Summary and conclusions

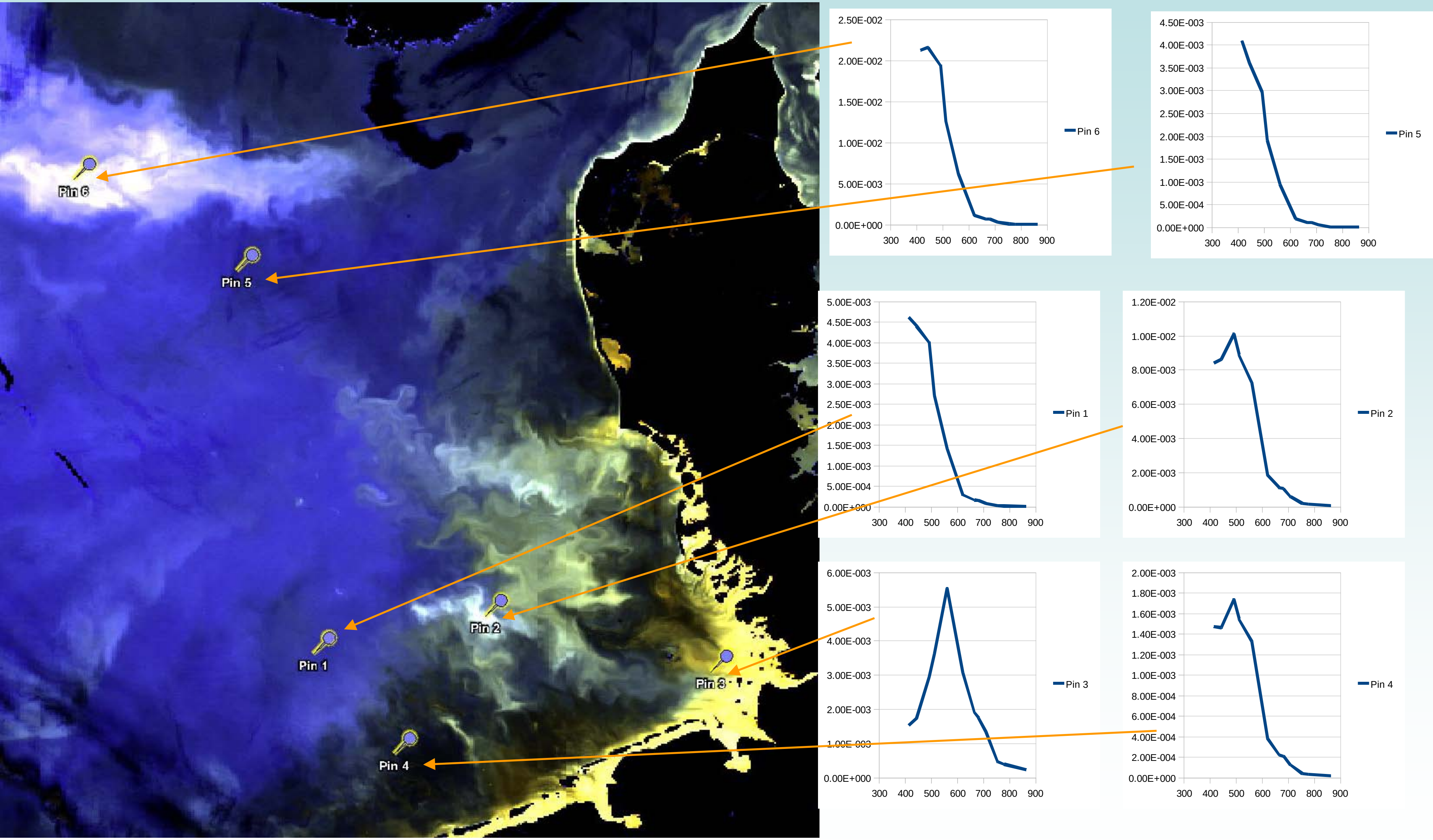
Case 1 water algorithm based on reflectance ratio model R445 / R555



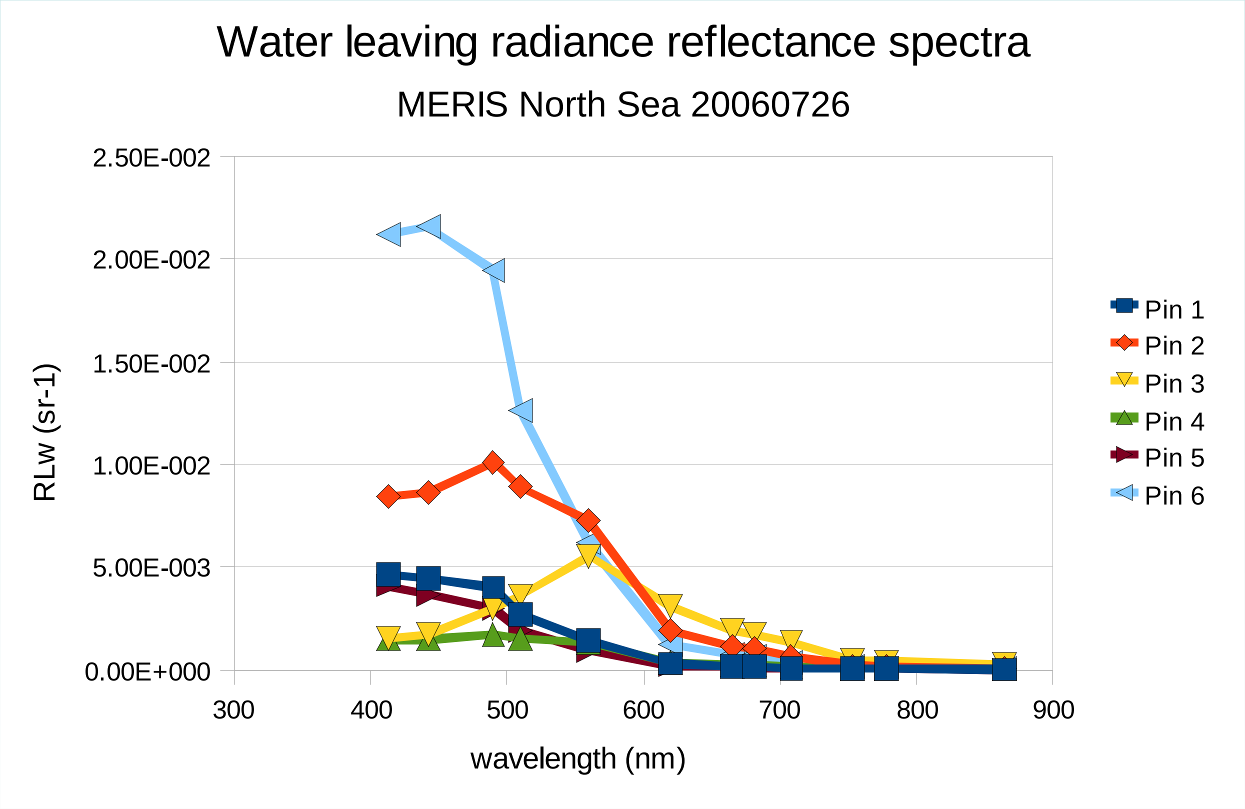
Case 1 water:

Morel / Antoine MERIS Case 1 water ATBD

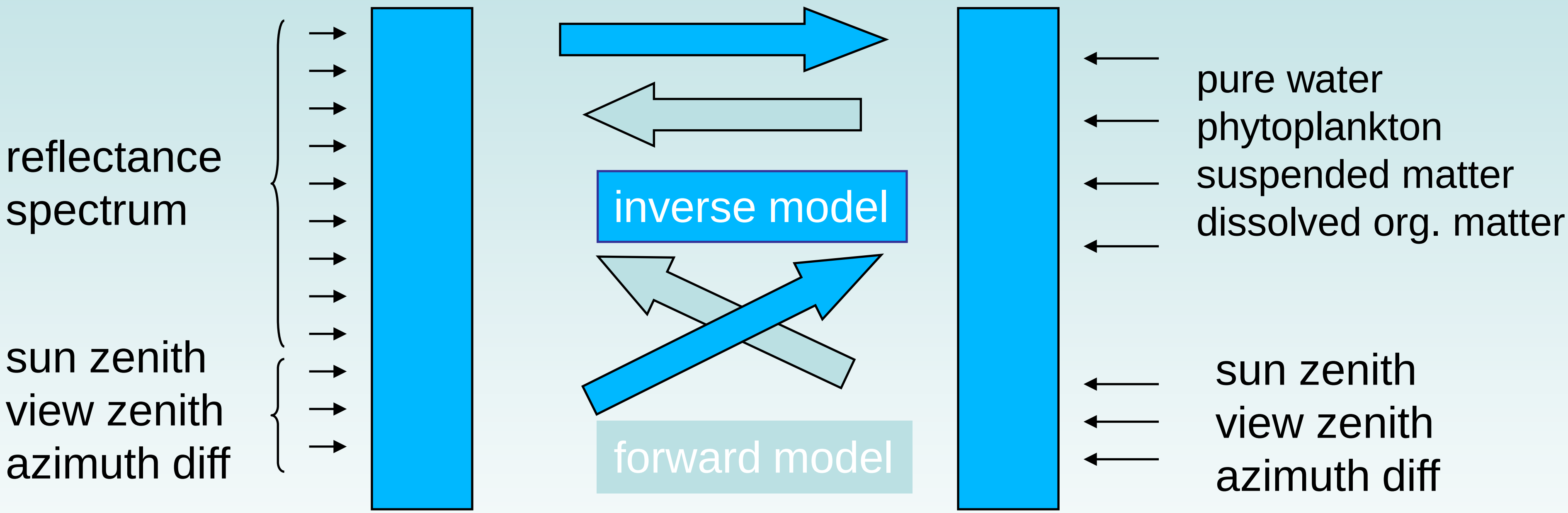
Water leaving radiance reflectance spectra in coastal water



Variability of water leaving reflectance spectra



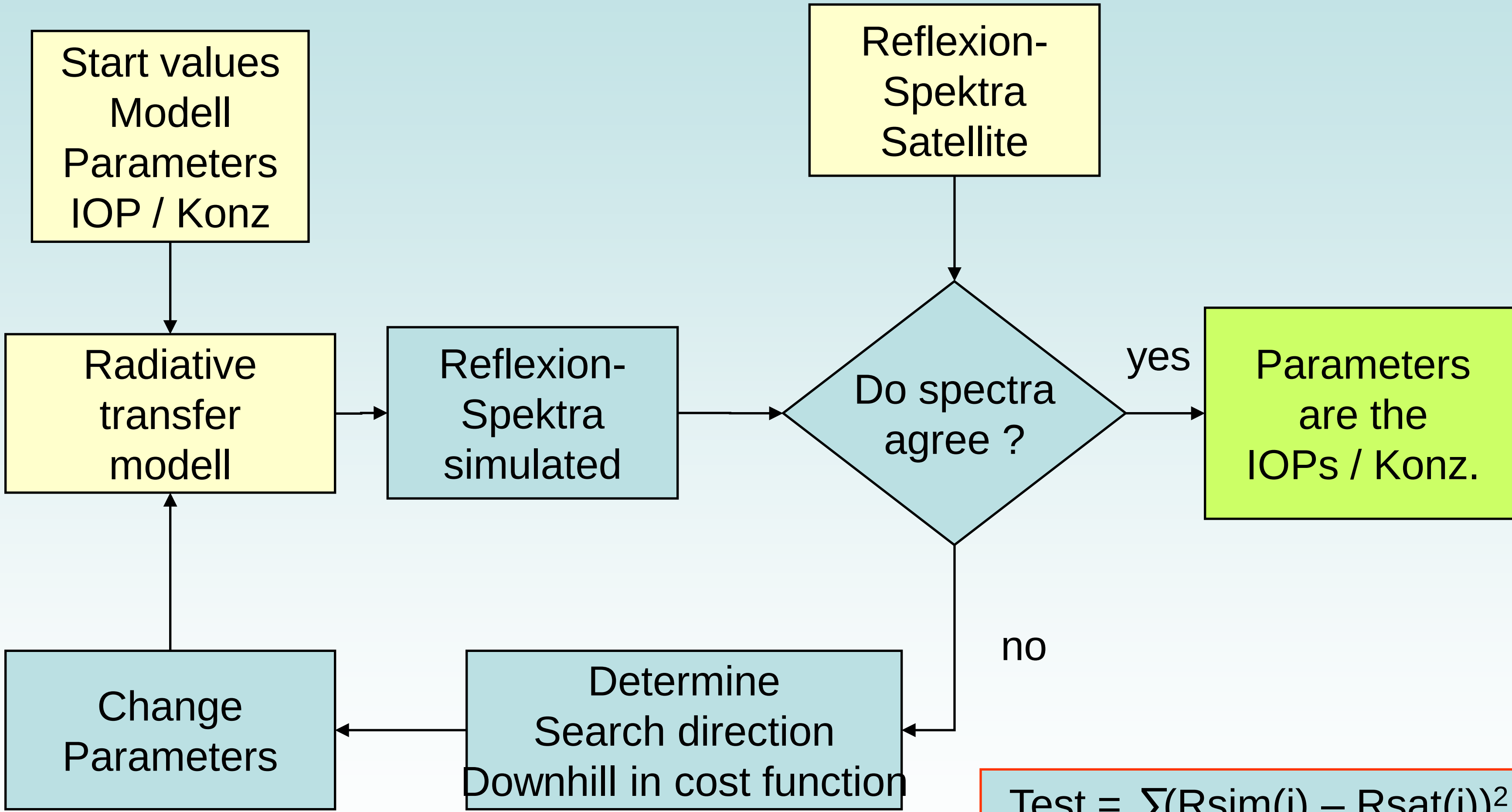
The inverse problem



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

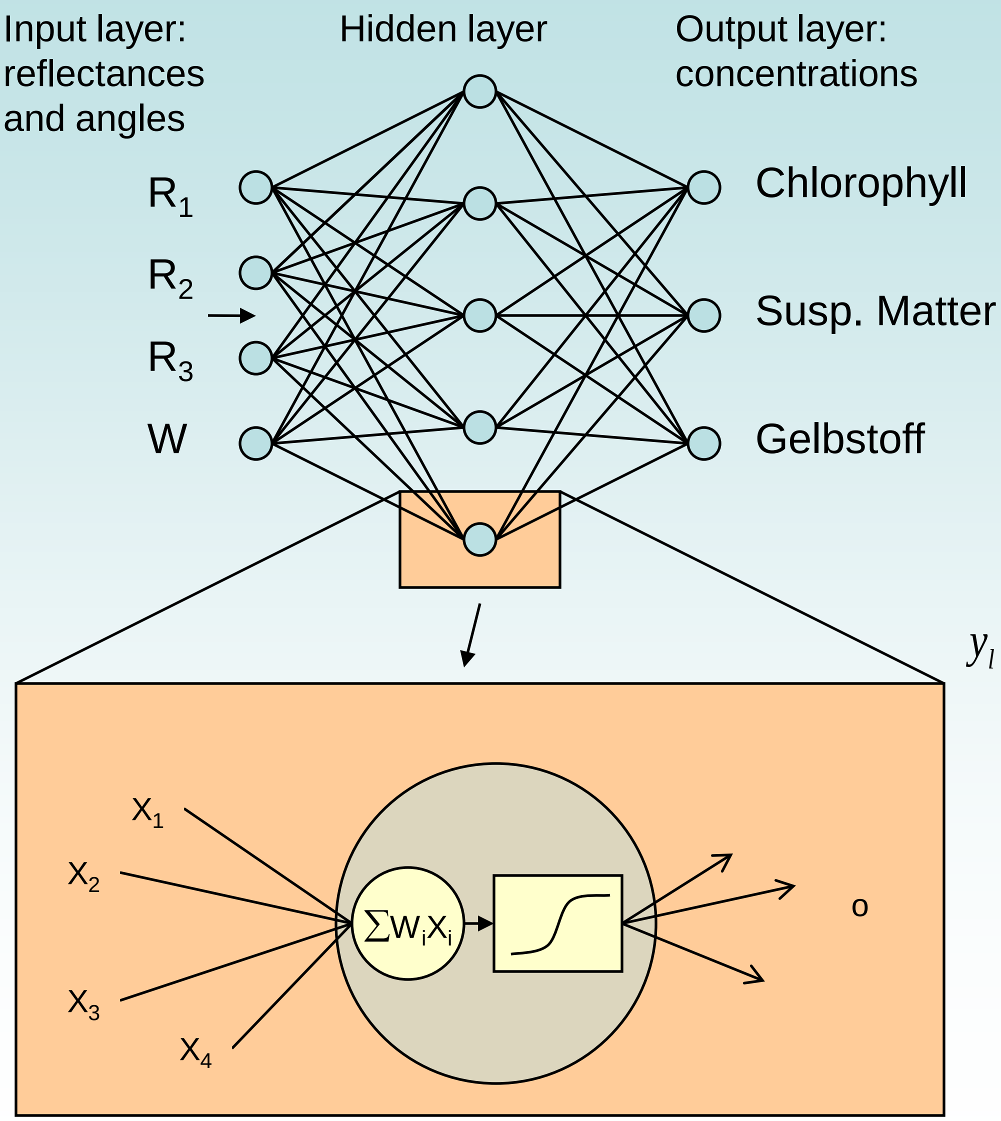
Success depends on:
- Bio-optical model
- ambiguities

Inverse Modellierung using Optimization Procedures



$$Test = \sum(Rsim(i) - Rsat(i))^2$$

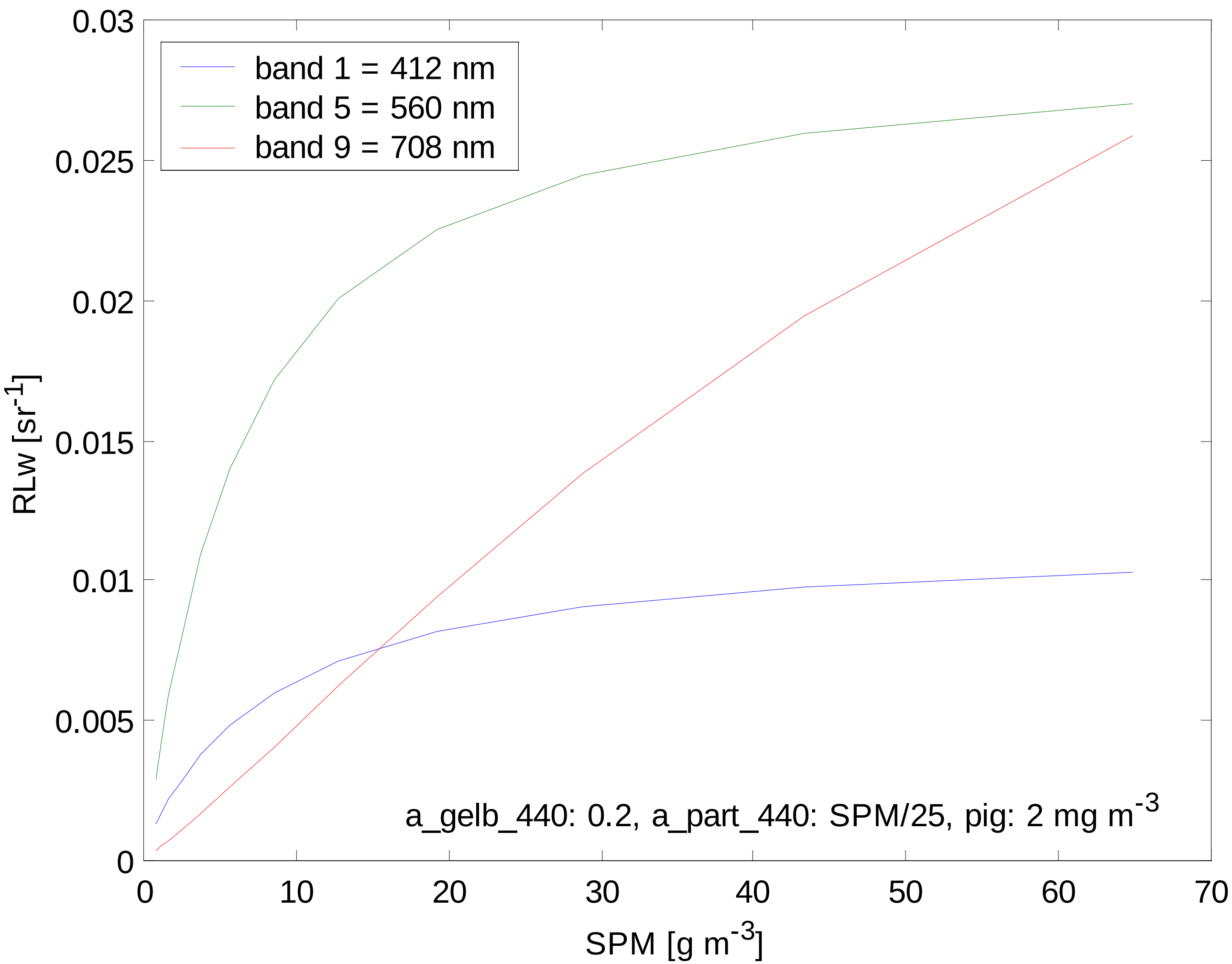
Simplified scheme of NN Algorithm



$$y_l = s(-d_l + \sum_{k=1}^{3} w_{kl} \cdot s(-c_k + \sum_{j=1}^{5} v_{jk} \cdot s(-b_j + \sum_{i=1}^{4} u_{ij} x_i)))$$

Sensitivity at different concentration ranges and spectral bands

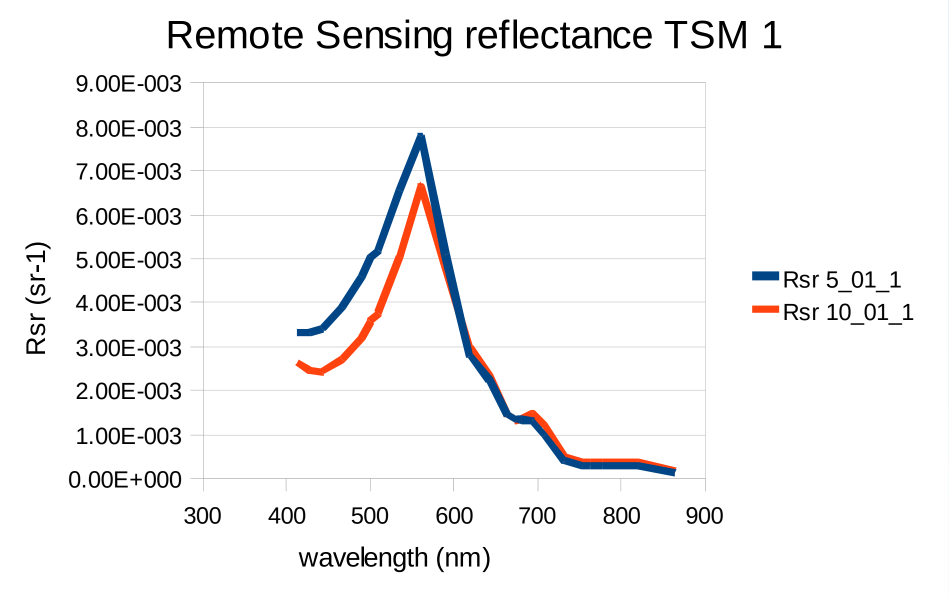
RLw for MERIS bands 1 (412 nm), 6 (560 nm), 10 (708 nm)

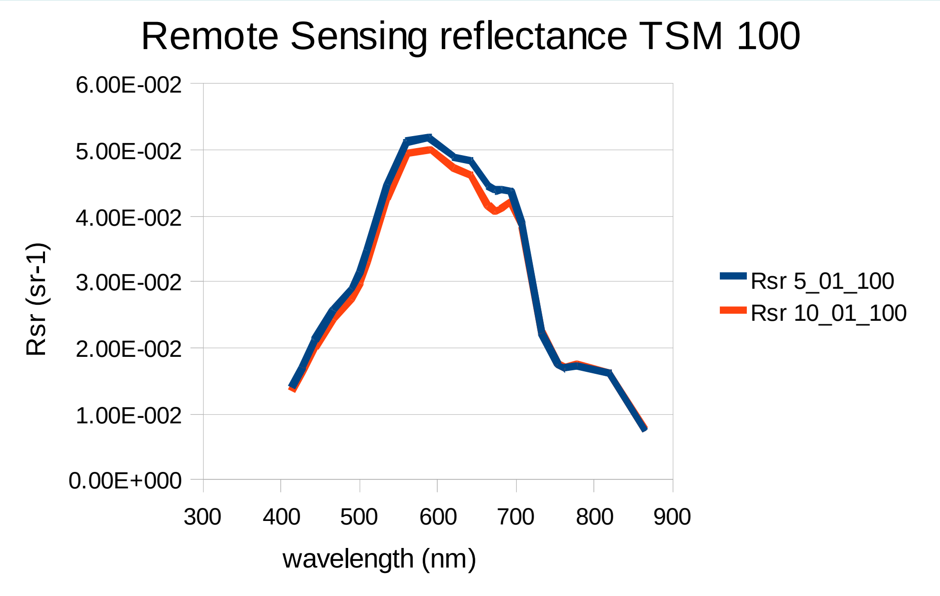


Sensitivity of the reflectance at a spectral band depends on the concentration

To cover a large concentration range many bands from the blue to NIR range are necessary

Sensitivity at different concentration ranges and spectral bands



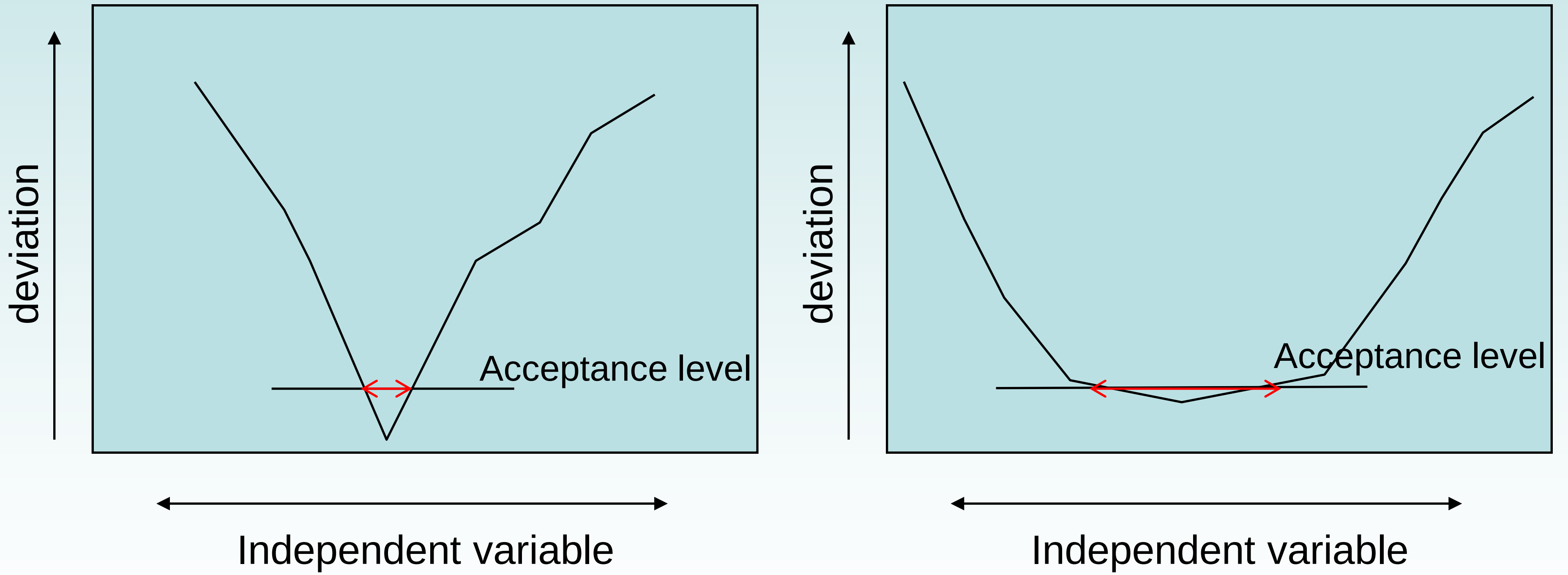


Chl. 5/10 mg m-3
TSM 1 g m-3
aYS(443) 0.1 m-1

Chl. 5/10 mg m-3
TSM 100 g m-3
aYS(443) 0.1 m-1

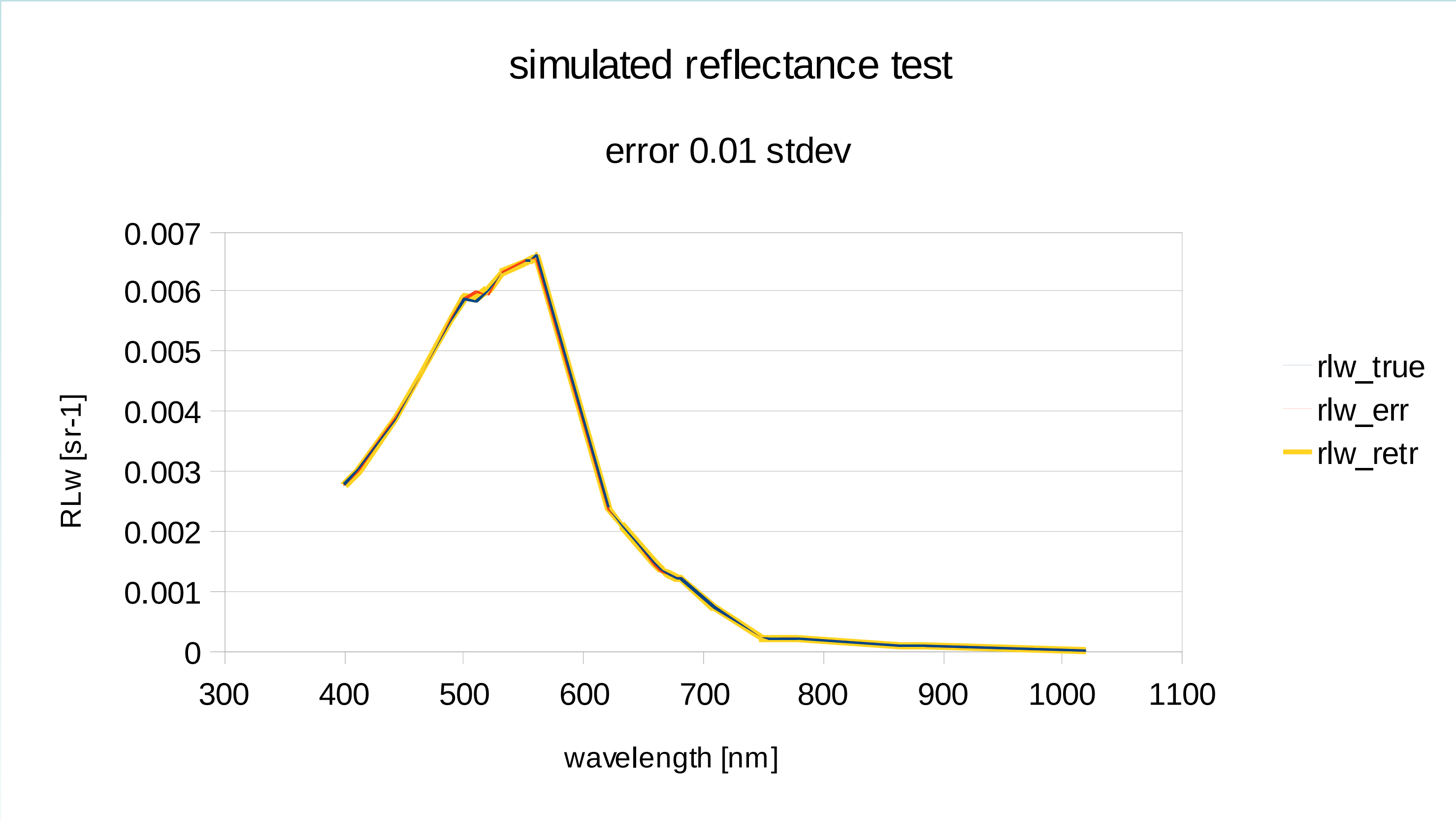
Searching for minimum: principle, 1D case

Search for minimum: Deviation between measured and simulated spectrum



Width can be estimated from the 2nd order derivative (Hessean matrix)

Error due to masking and ambiguities



- True spectrum simulated
- „measured“ spectrum = true * random error
- Retrieved spectrum when LM has found solution

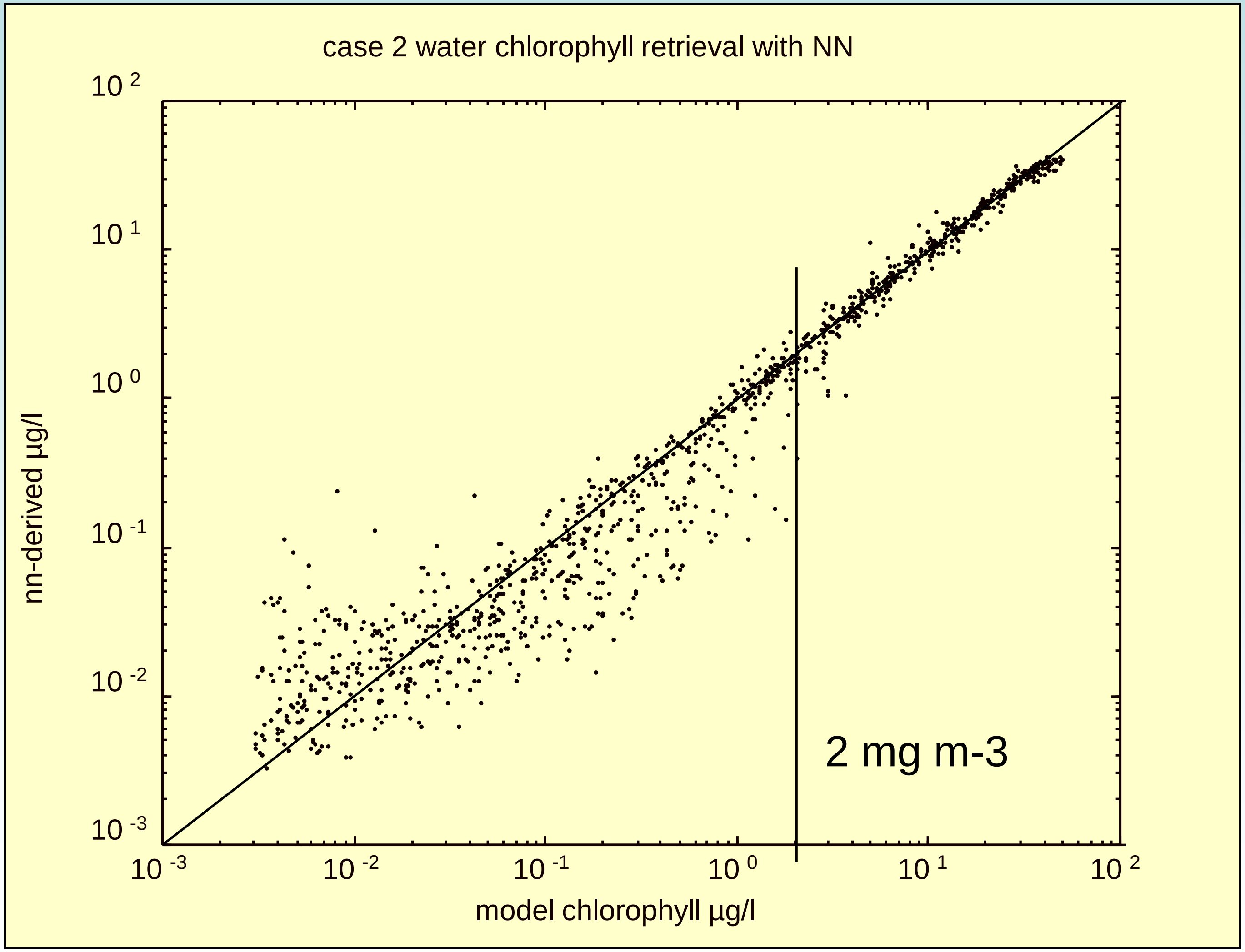
Results and errors of retrieval

Variable	conc true	conc retr.	stdev of log_conc	err. estimated %	err true %
chlorophyll [mg m-3]	1	0.8337	0.09191	9.626	-19.94
detritus [g m-3]	1	1.152	0.1684	18.34	13.19
gelbstoff a443 [m-1]	0.1	0.1005	0.03566	3.63	0.4842
min. SPM [g m-3]	1	0.9948	0.006498	0.6519	-0.5238

kdmin_true: 0.2096
kdmin_ret: 0.2089
error: - 0.33%

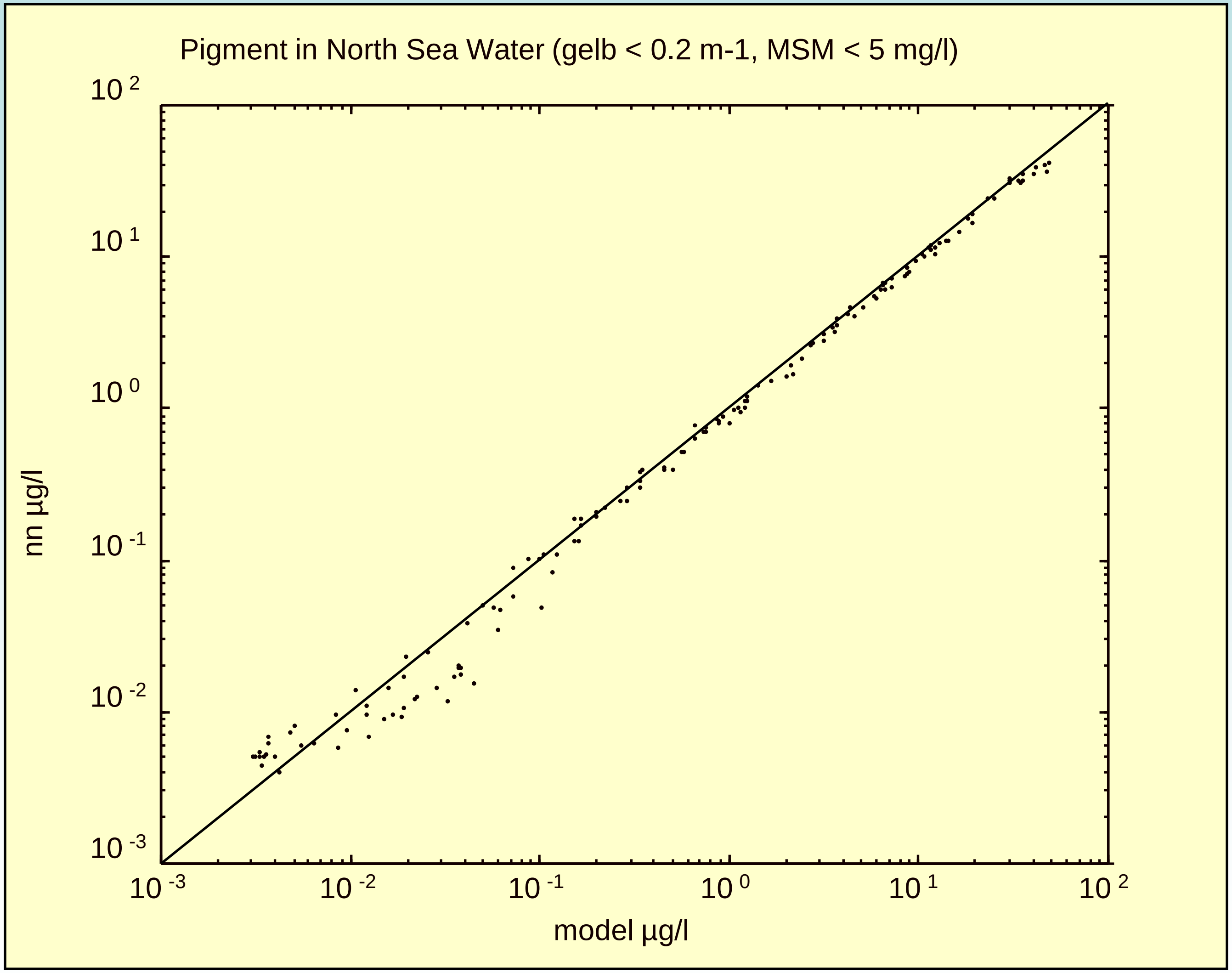
kd490_true: 0.2636
kd490_ret: 0.2609
error: -1.04%

Uncertainties due to ambiguities for different concentration mixtures



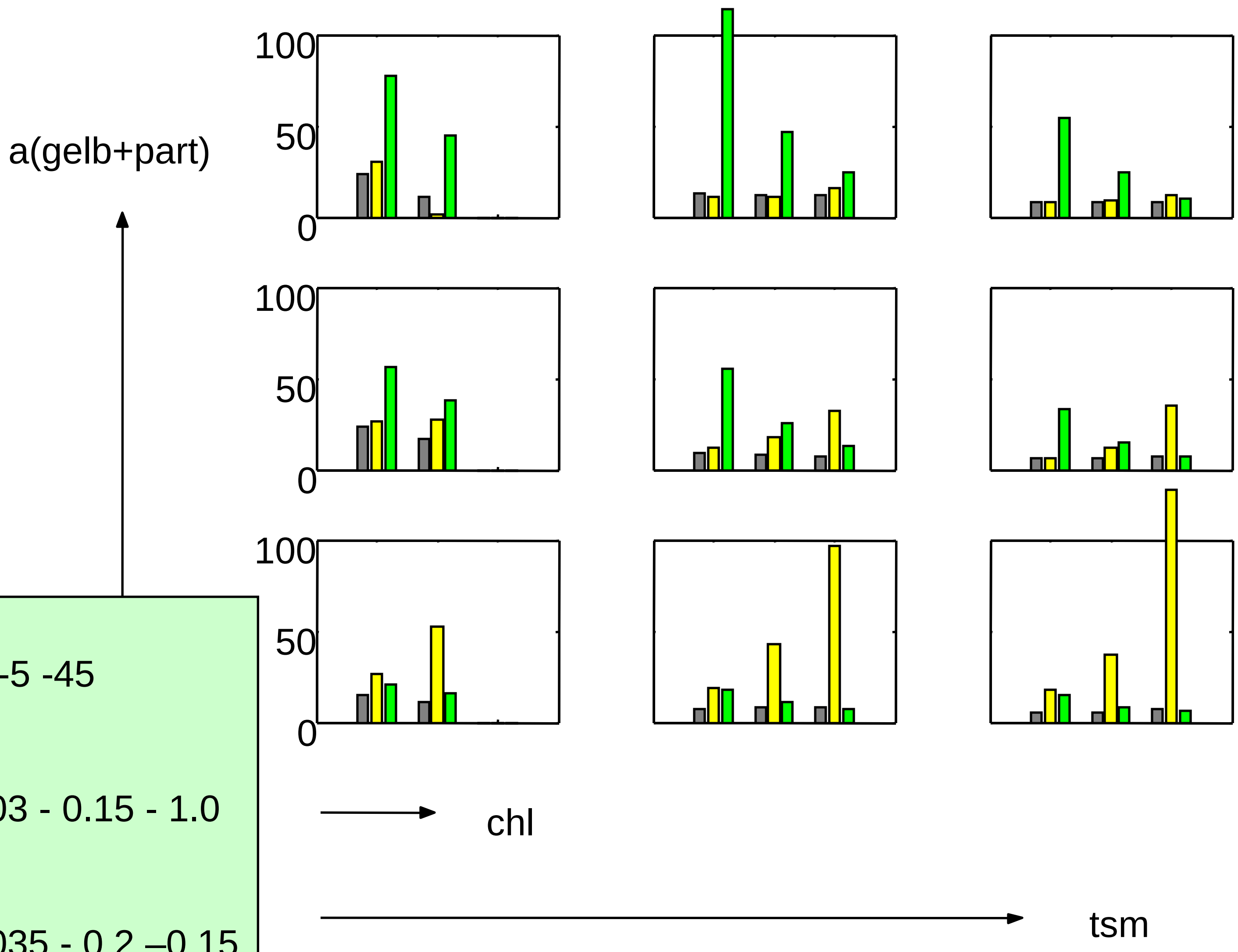
All cases of turbid water

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



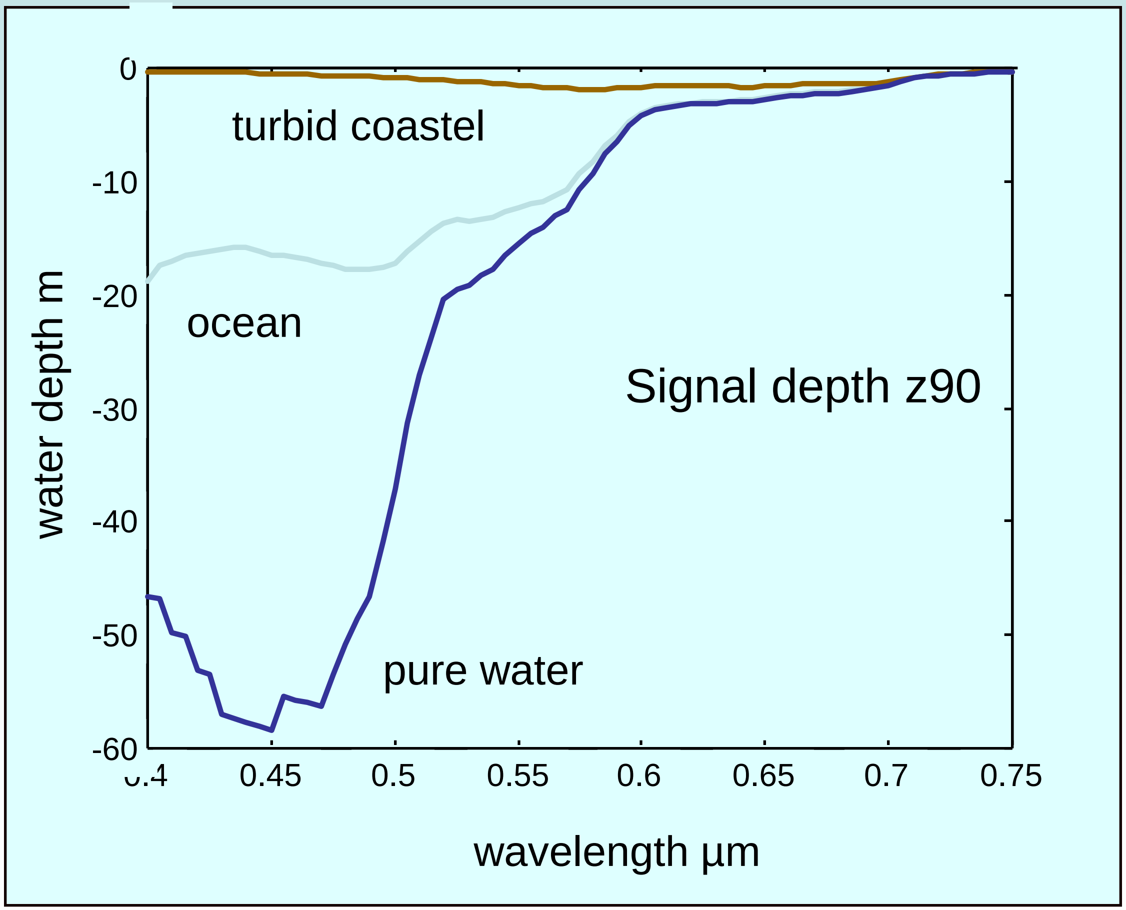
conc_bp
0.05 - 0.5 -5 -45

conc_pig
0.005 - 0.03 - 0.15 - 1.0

conc_gelb
0.005 - 0.035 - 0.2 –0.15

Signal depth at different spectral bands

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



$z_{90}=1/k$

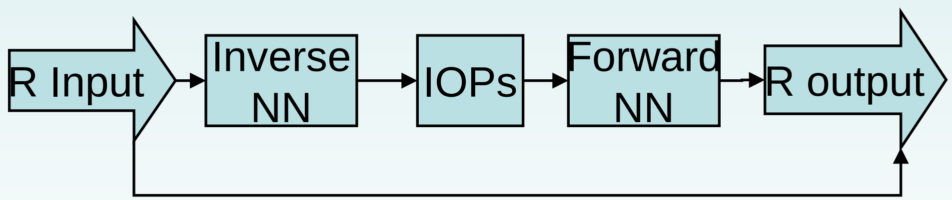
coastal:
TSM=5 mg/l
Chlor.=5µg/l
Gelb=a_{380}=$1m^{-1}$

open ocean:
Chlor.=1µg/l

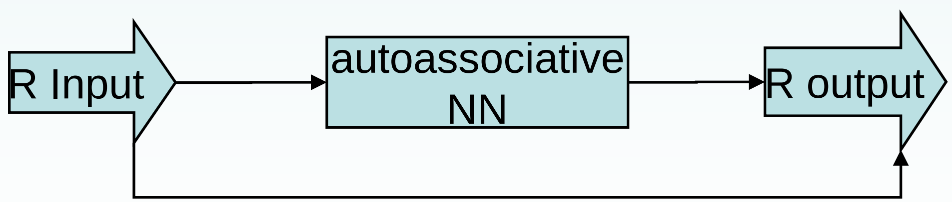
Detection of out of scope conditions

- 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

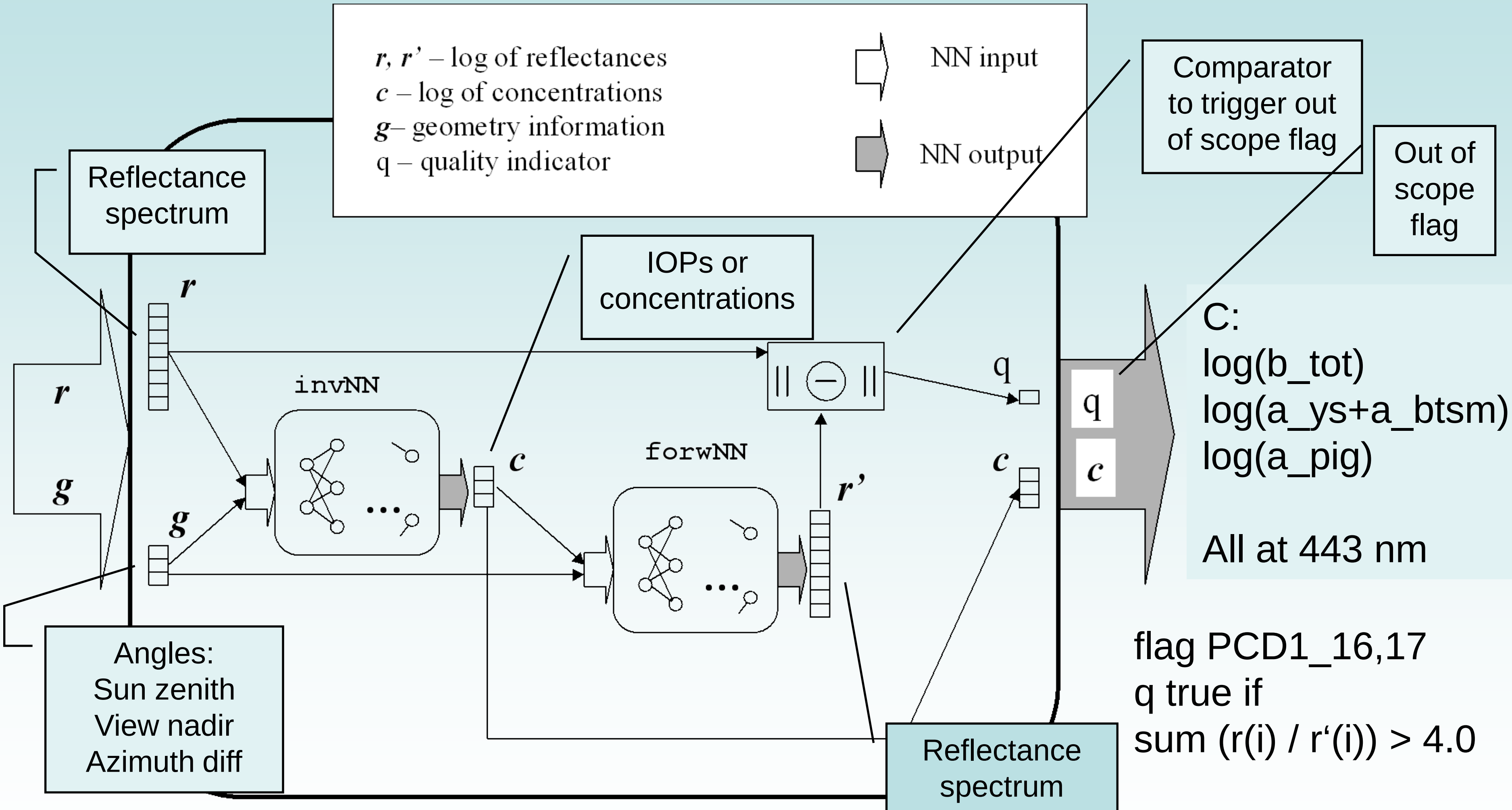
- Combination of inverse and forward NN



- Auto-associative NN

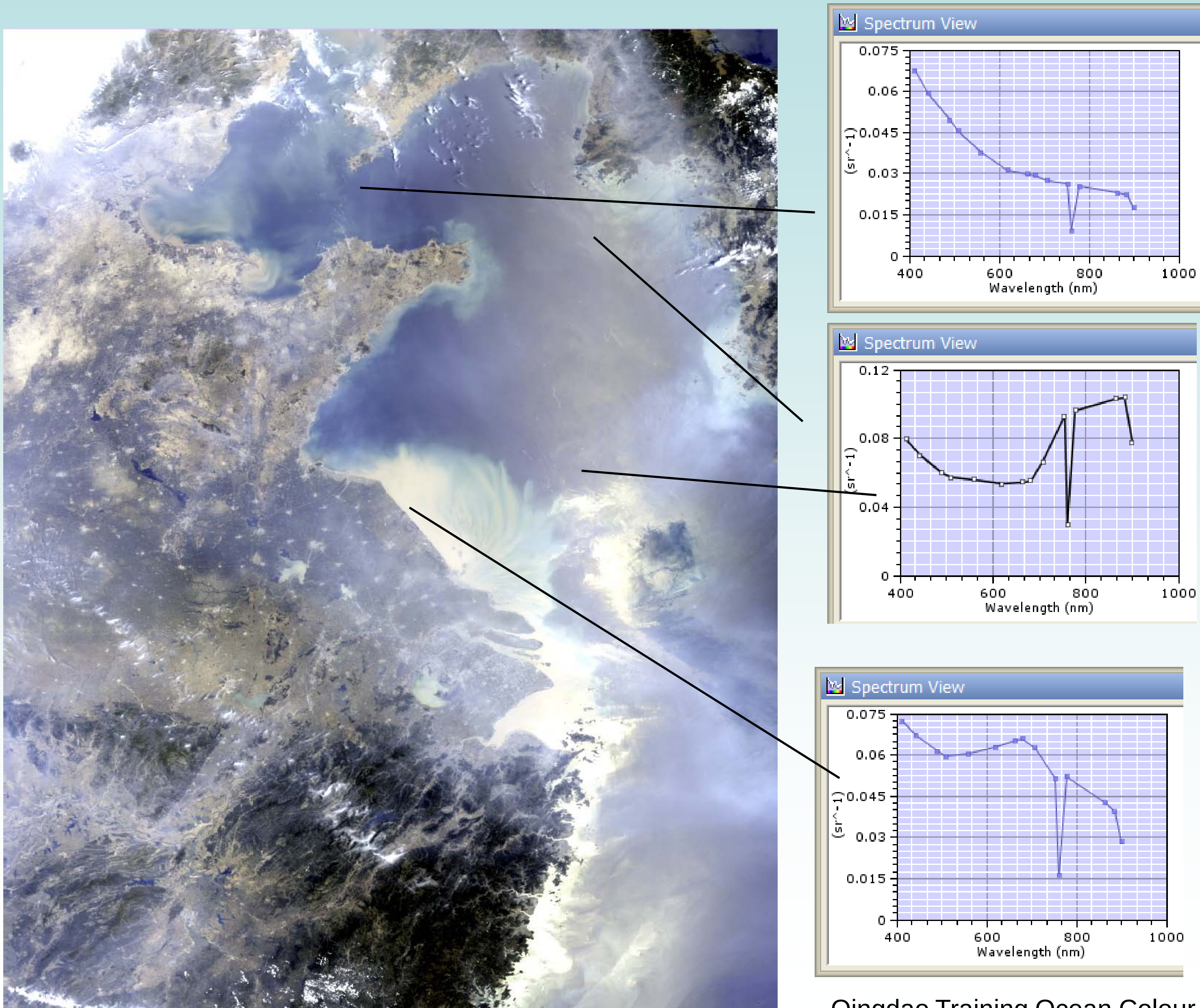


Detection of out of scope conditions (MERIS processor)



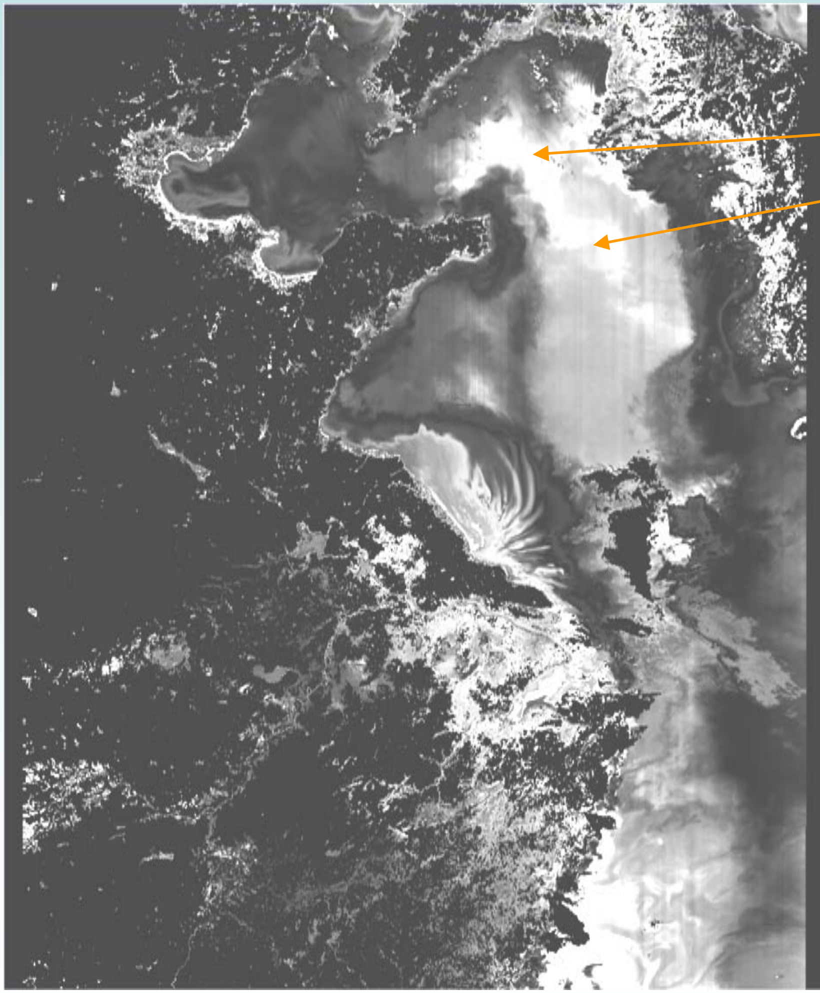
If RLw < 0.0009, RLw = 0.0009 (ρ ≈ 0.003)

Detection of out of scope conditions (MERIS processor)



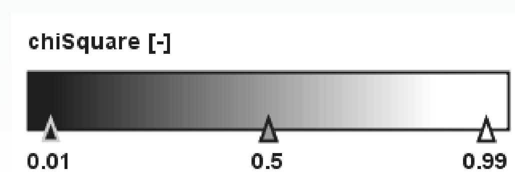
Top of atmosphere radiance spectra at normal and critical locations

Detection of out of scope conditions (MERIS processor)



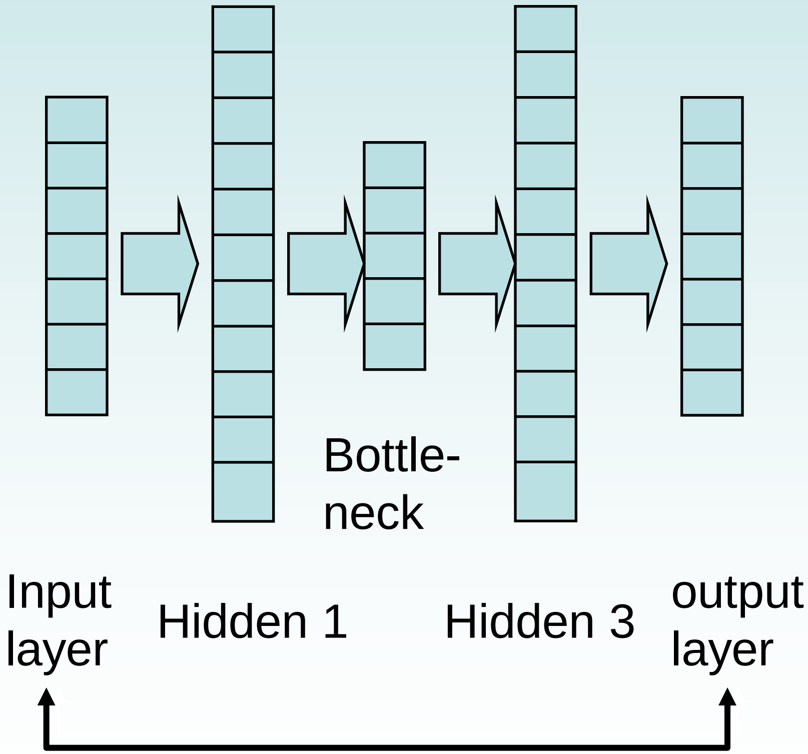
Exeptional bloom,
Indicated by high Chi_square value

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

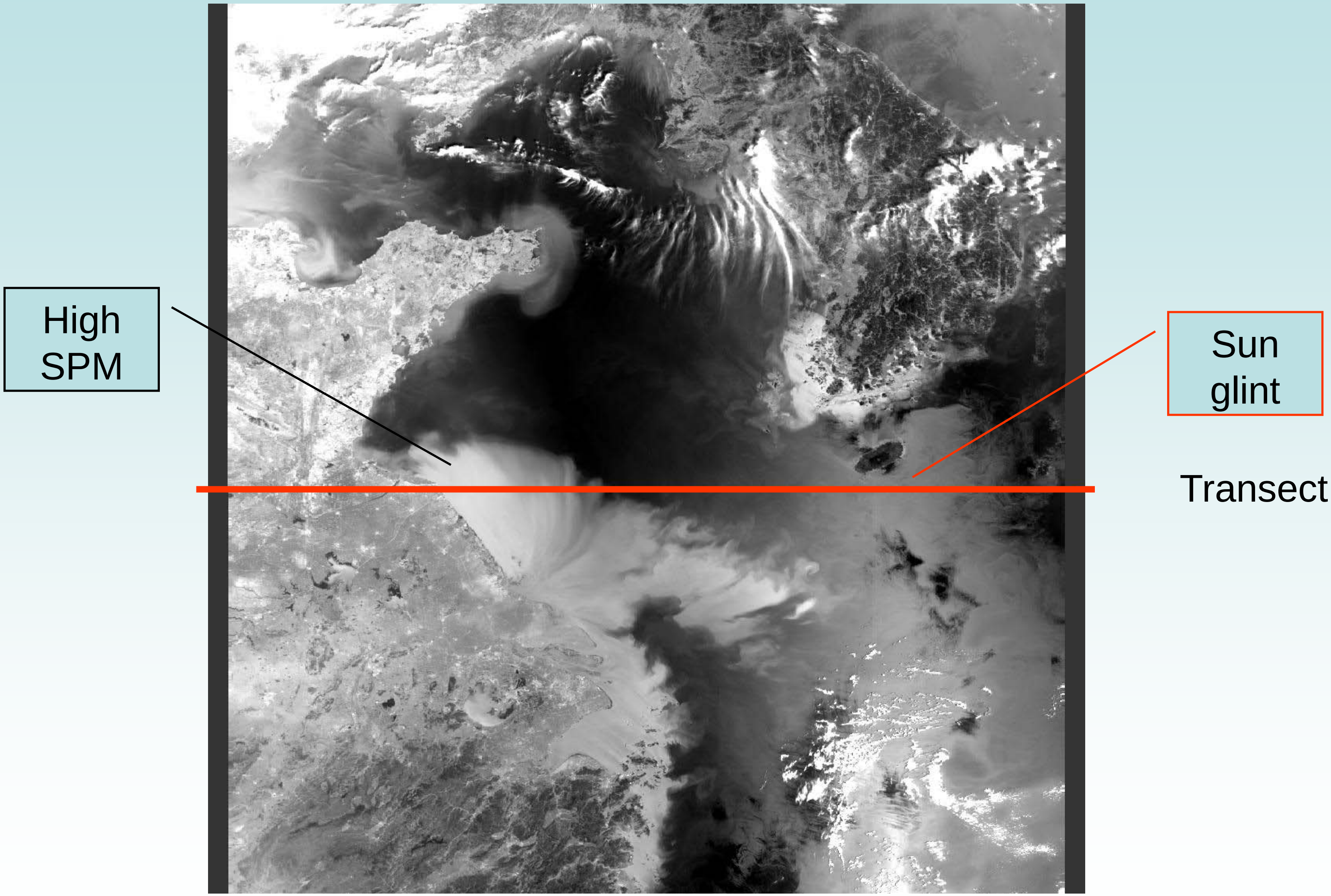
- Important to detect toa radiance specta which are not in the simulated training data set
- These are out of scope of the atmospheric correction algorithm
- Autoassociative neural network with a bottle neck layer



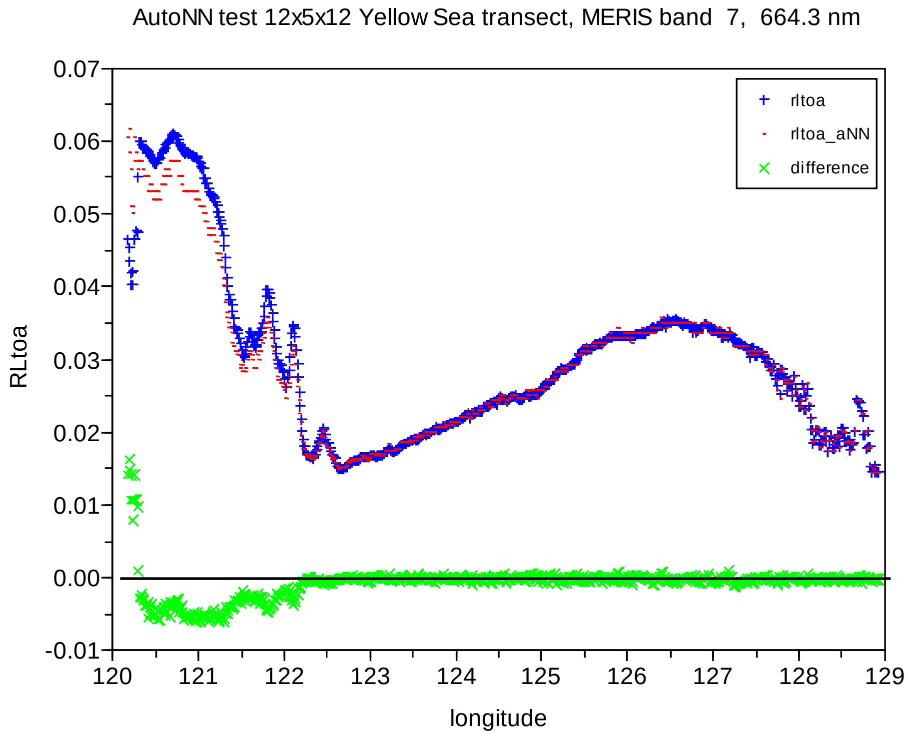
Functions also
as nonlinear PCA
i.e. bottle neck number of
neurons
Provide estimate of
Independent components

For the GAC training data
Set of ~ 1Mio. Cases
Bottleneck minimum was 4-5

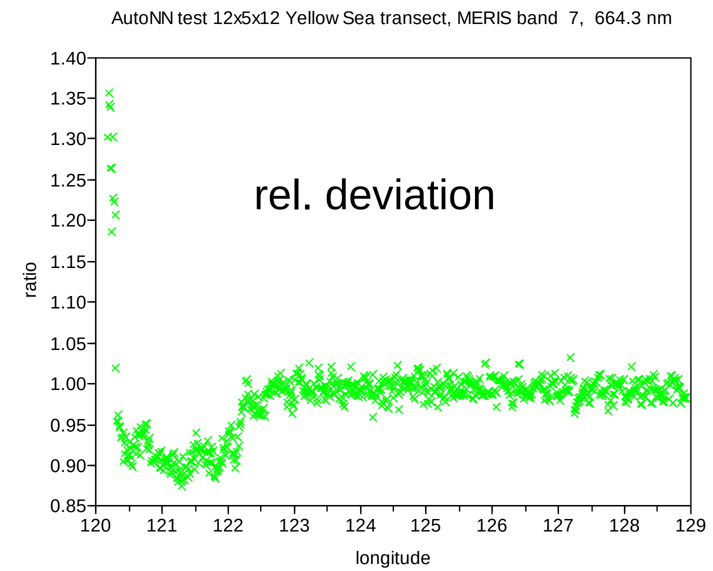
Detection of out of scope conditions aaNN: example for L1 (TOA) data

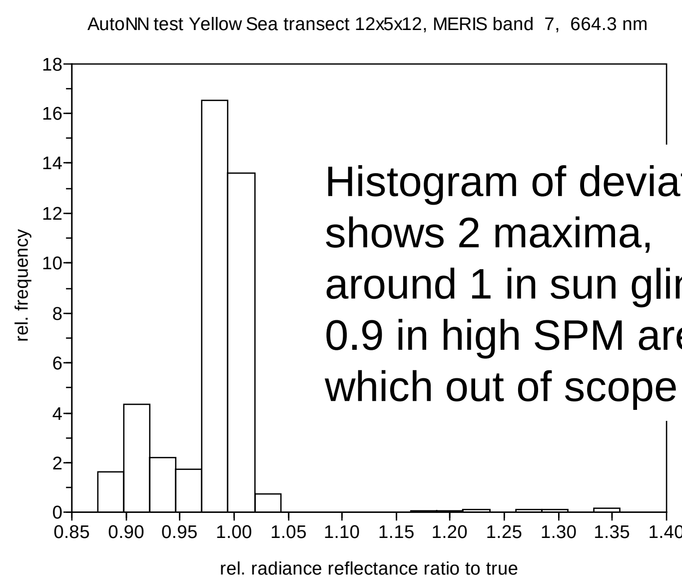


Detection of out of scope conditions aaNN: example



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



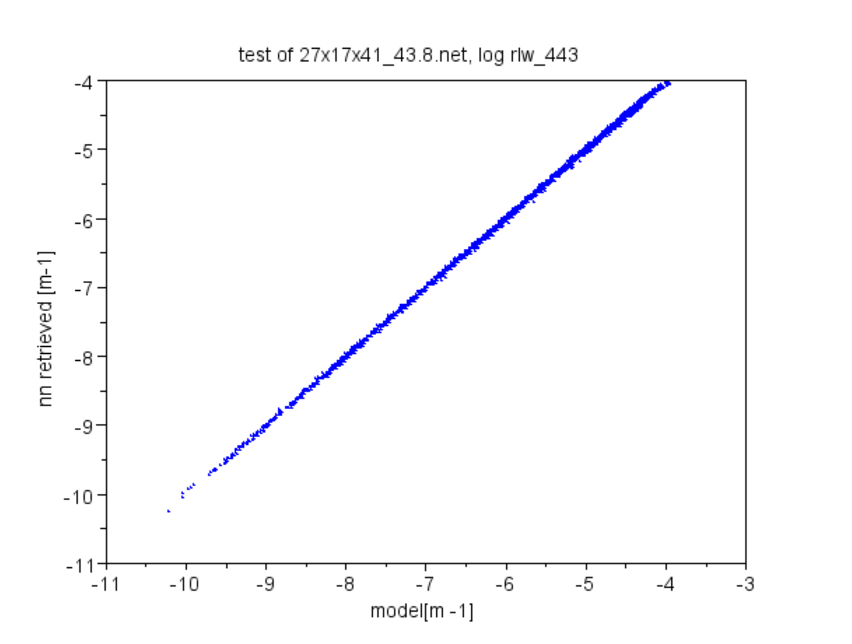


Histogram of deviations shows 2 maxima, around 1 in sun glint 0.9 in high SPM area, which out of scope

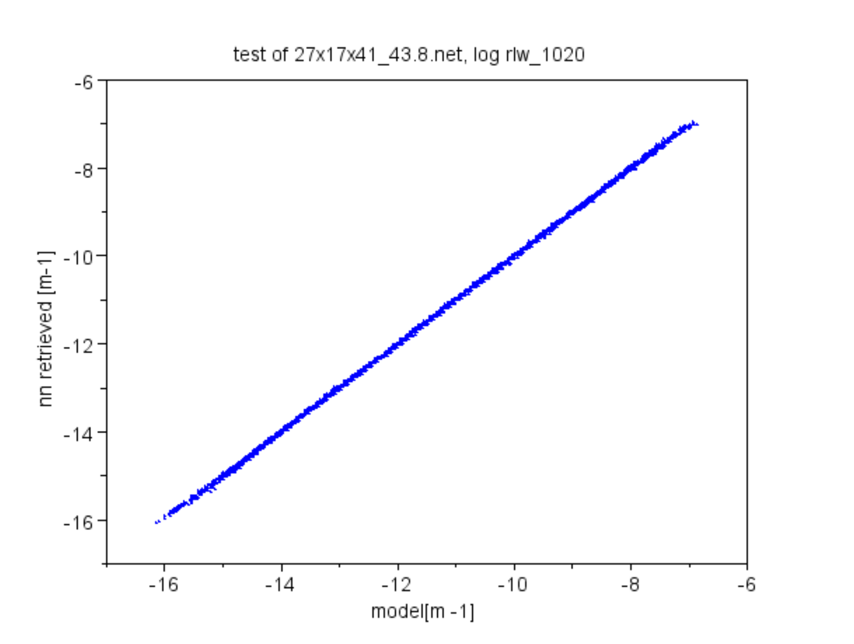
Verification

- 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

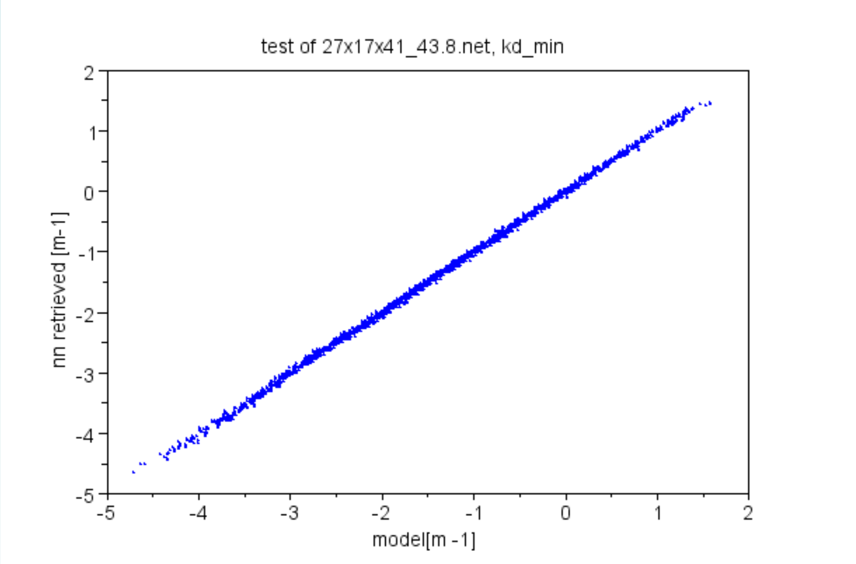


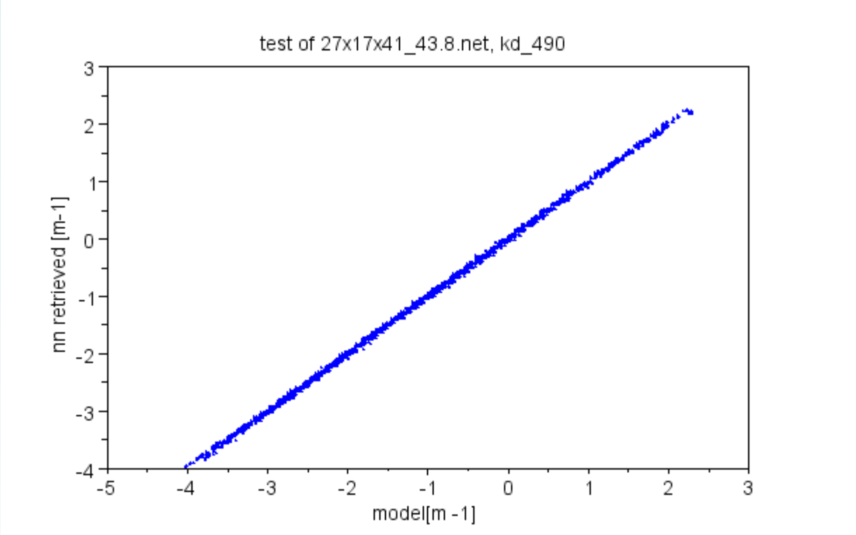
443 nm



1020 nm

Test of NN I 3

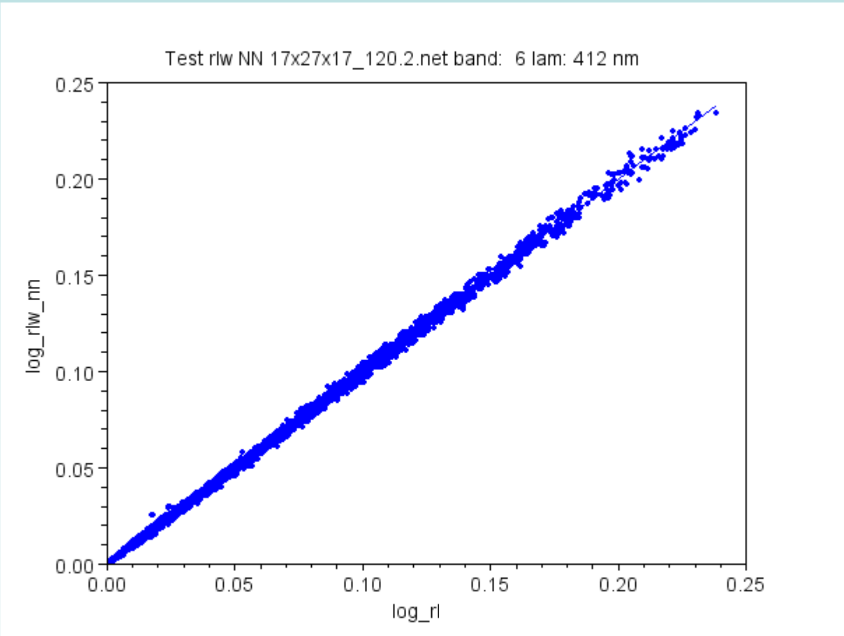


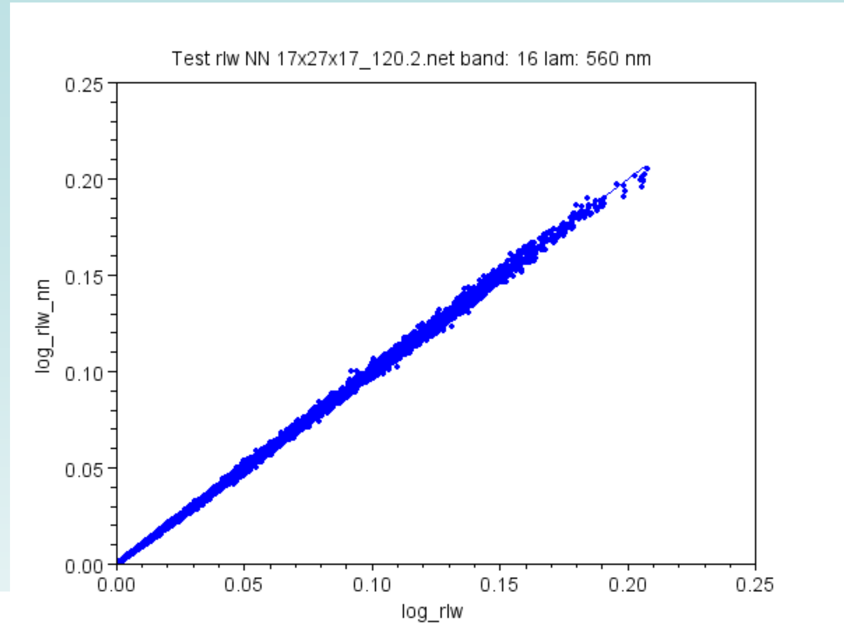


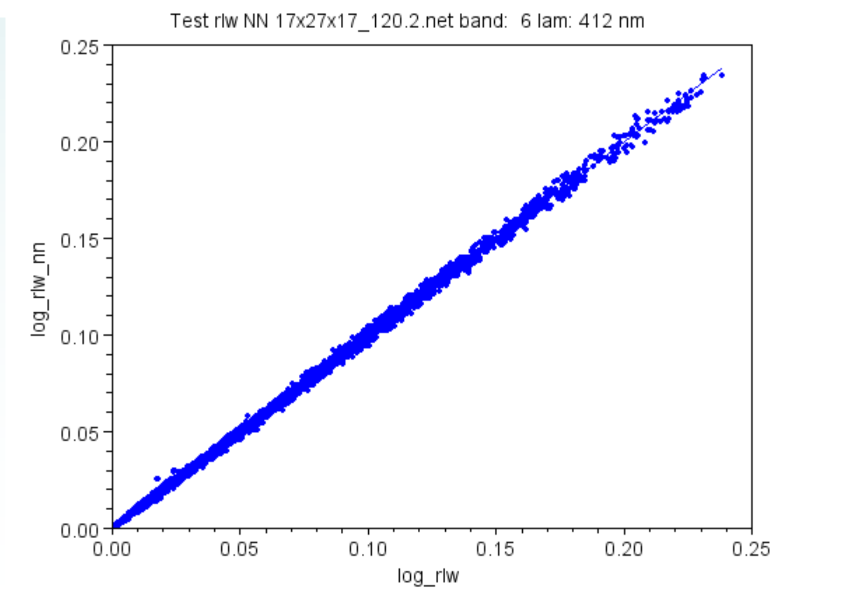
Kd_min

Kd_490

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

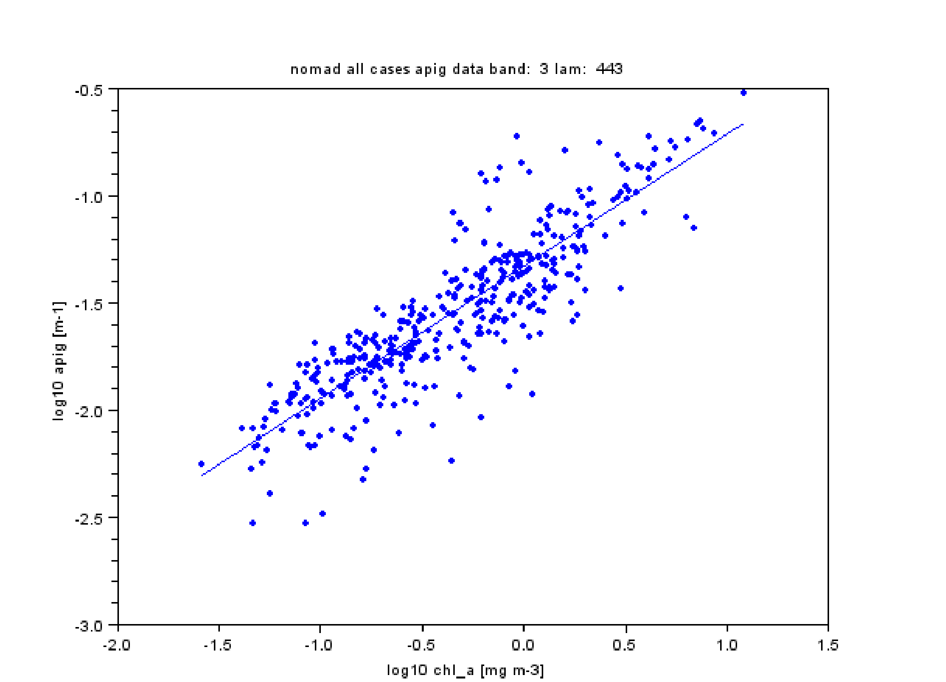






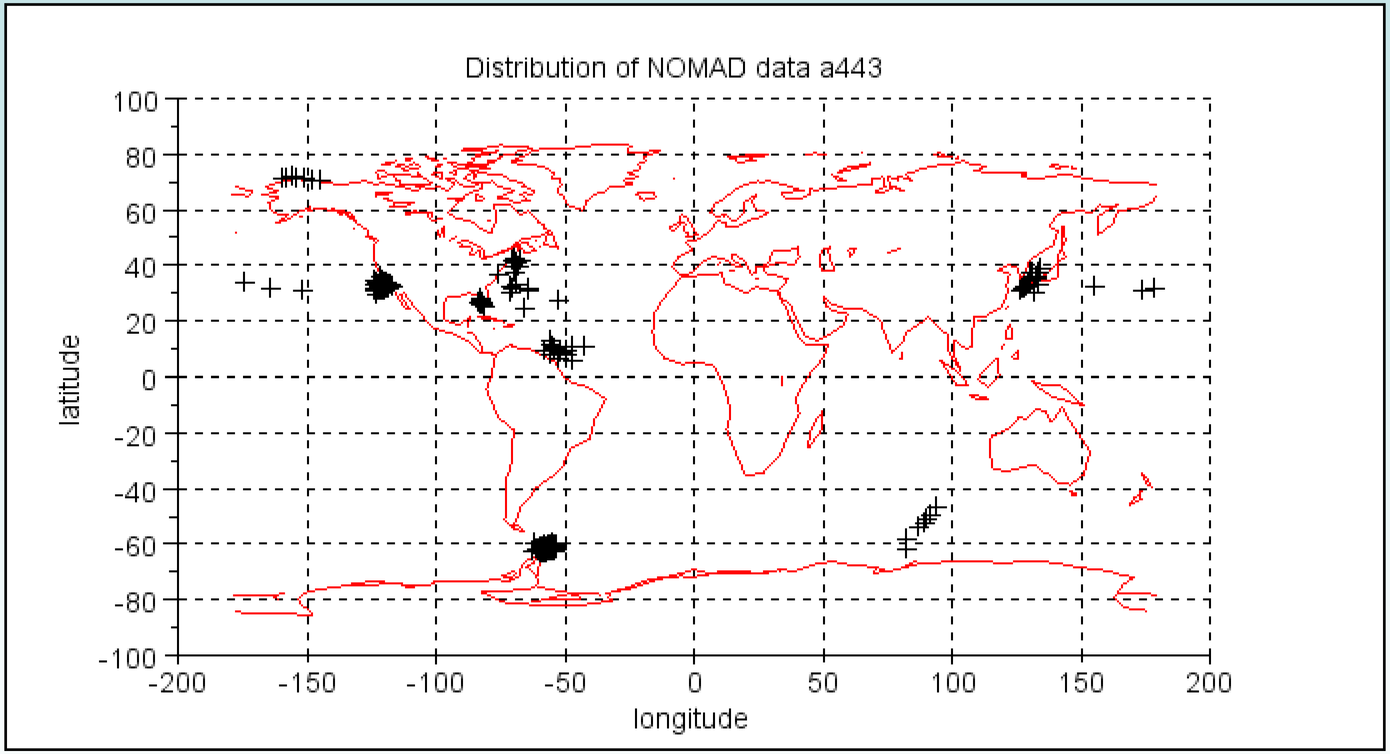
Validation

- 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 at443
- Note: in situ data have their own variabilities and uncertainties!

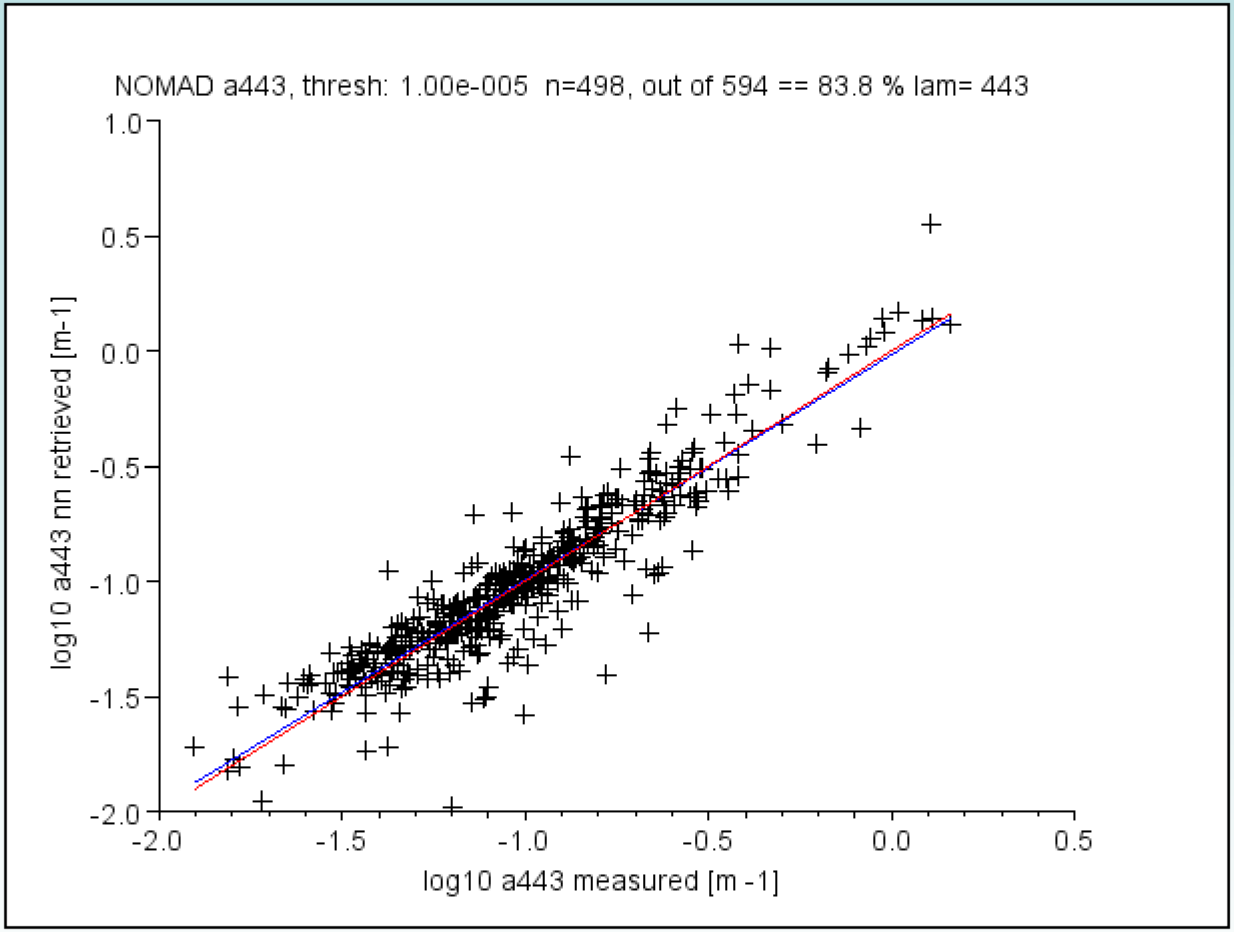


Relationship between chlorophyll a concentration and the absorption coefficient of phytoplankton pigments

Total absorption at 443 nm (water + constituents)

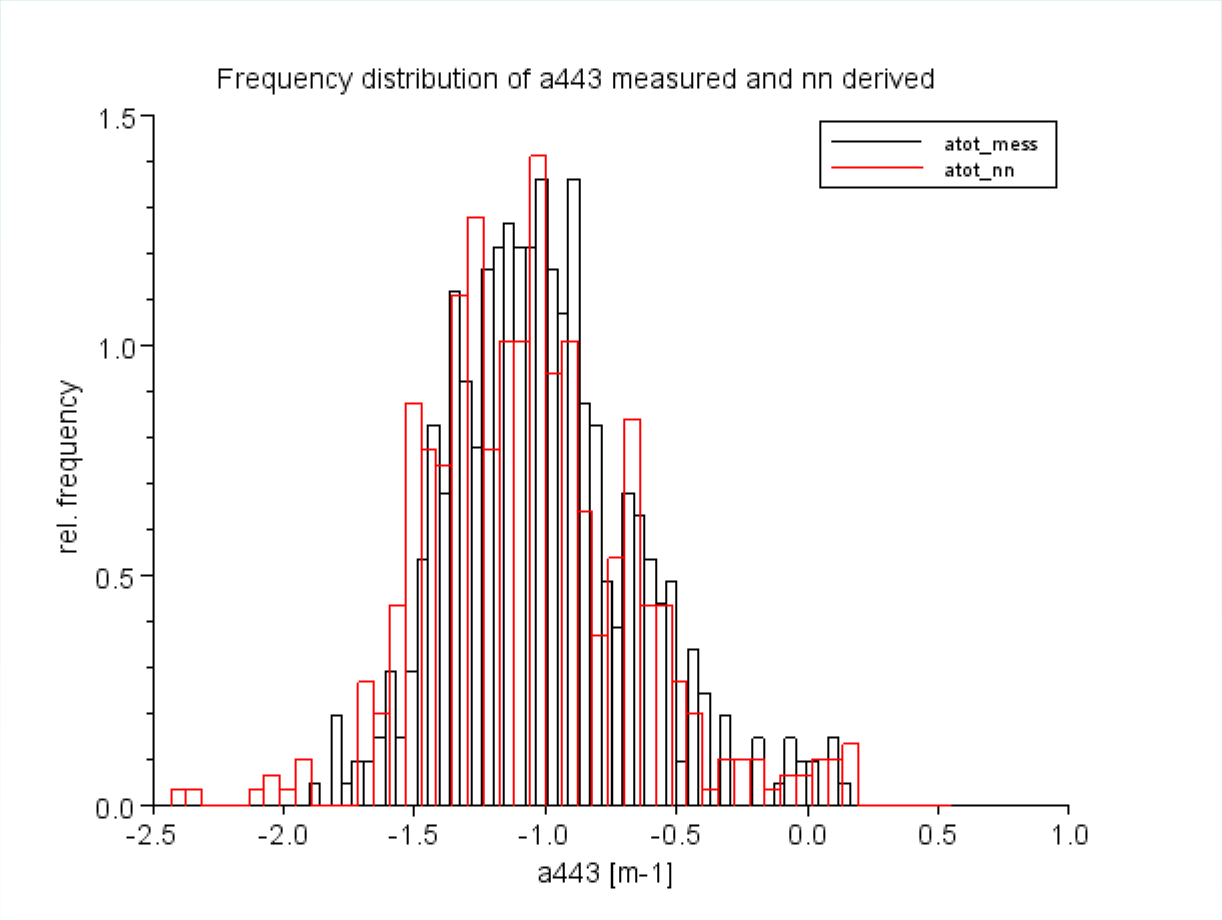


a443



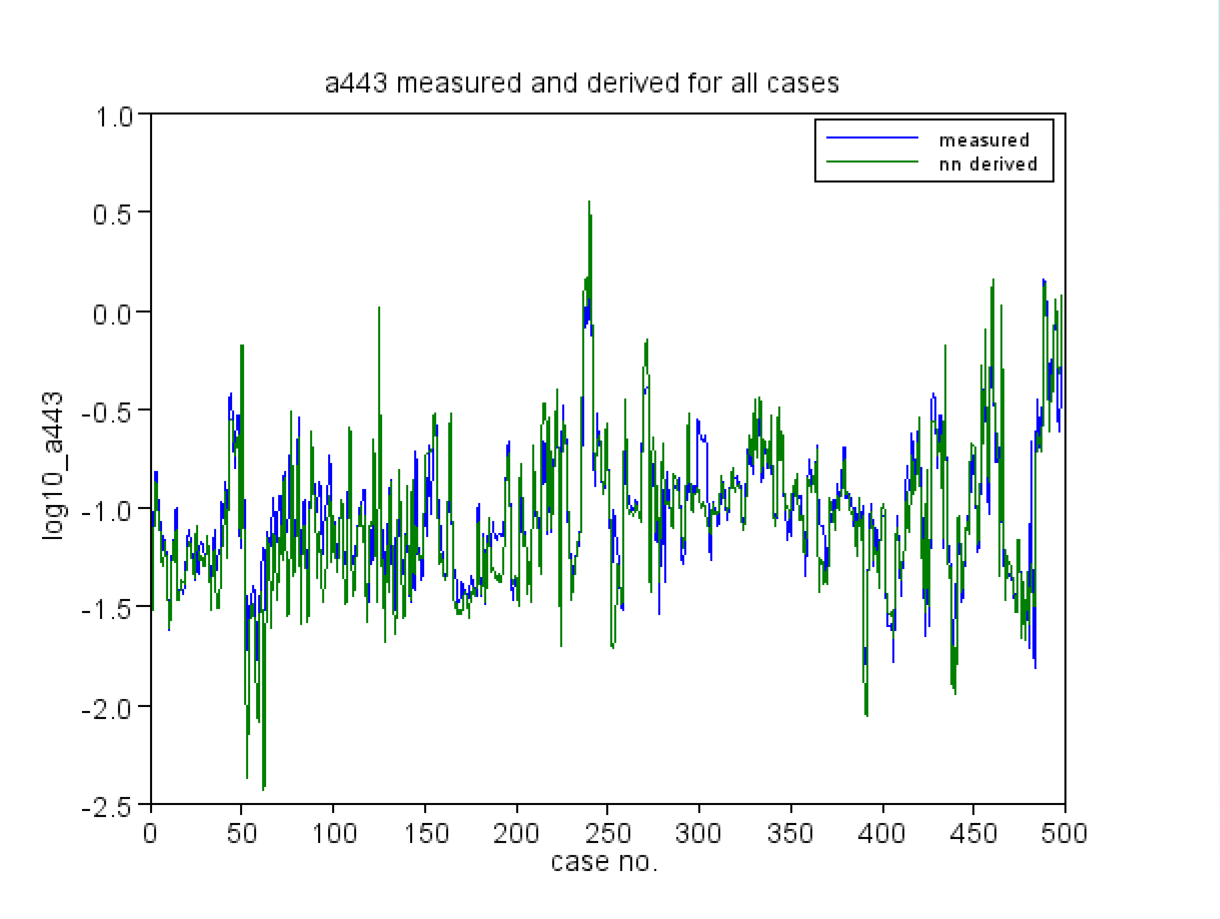
log10_a443_nn = log10_a443_measured * 0.977 - 0.0167, stdev = 0.141

Frequency distribution

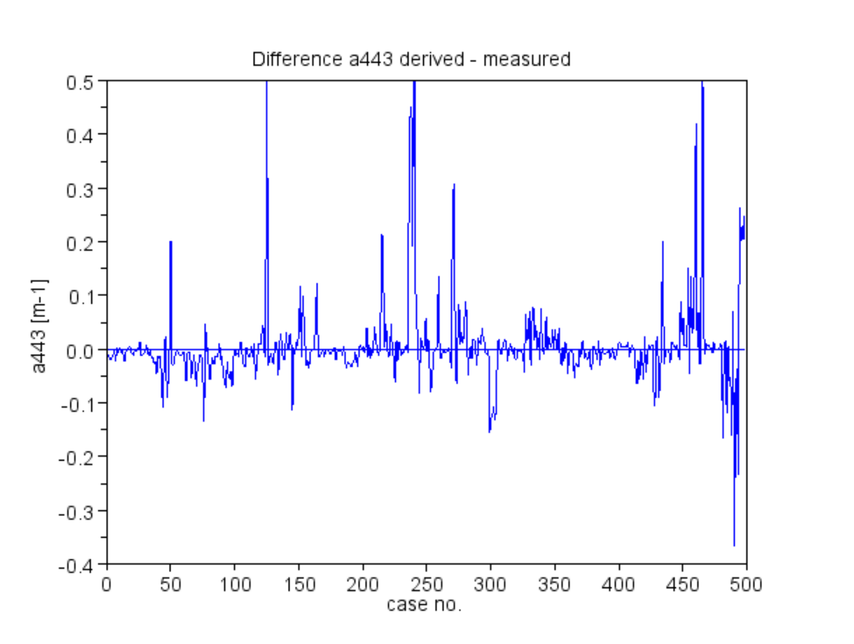


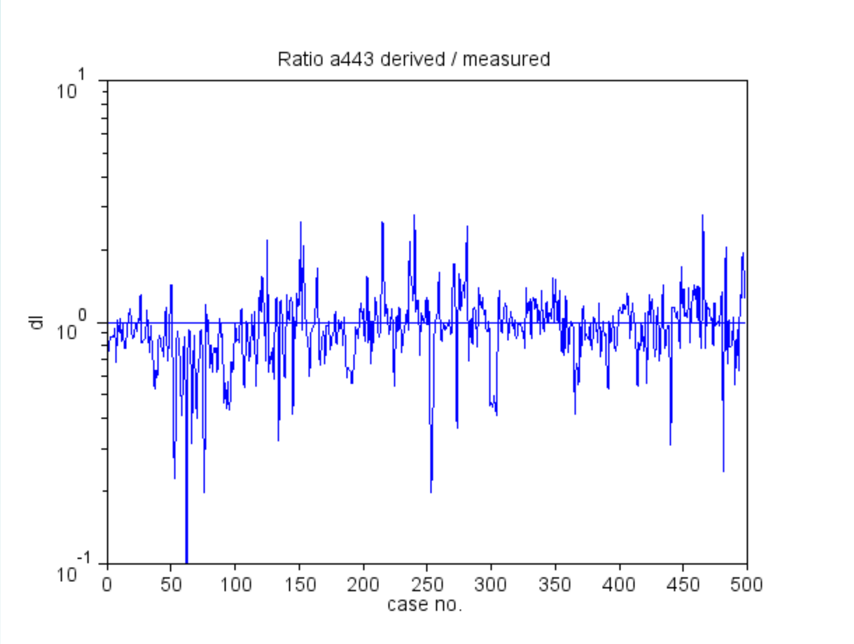
Frequency distributions of measured and derived a443 after removing outliers with sum_sq > 1.0 e-5

Measured and nn-derived a443 for all cases with sd <1.0e-5



Differences and rel.deviation



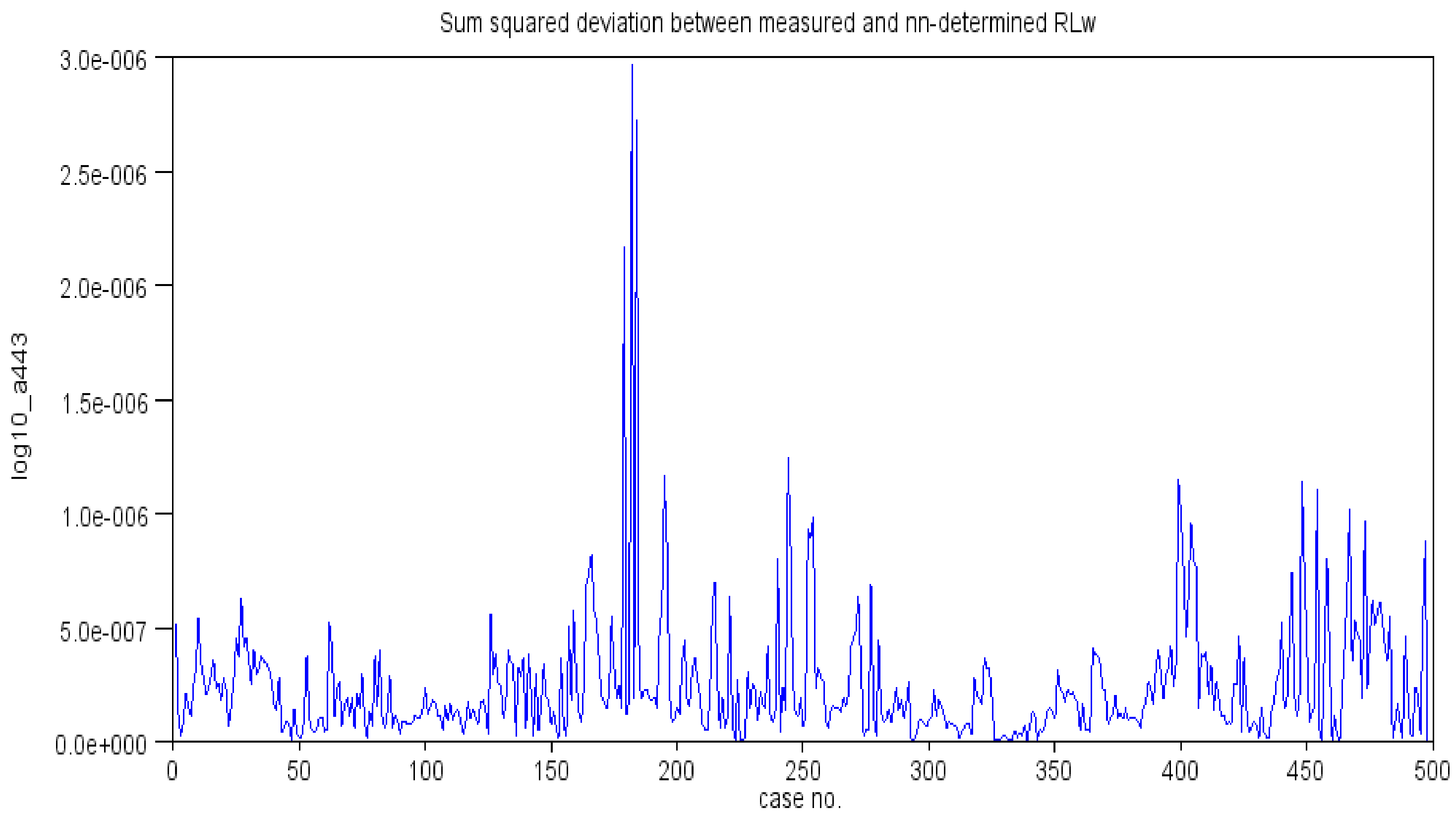


Log10 difference

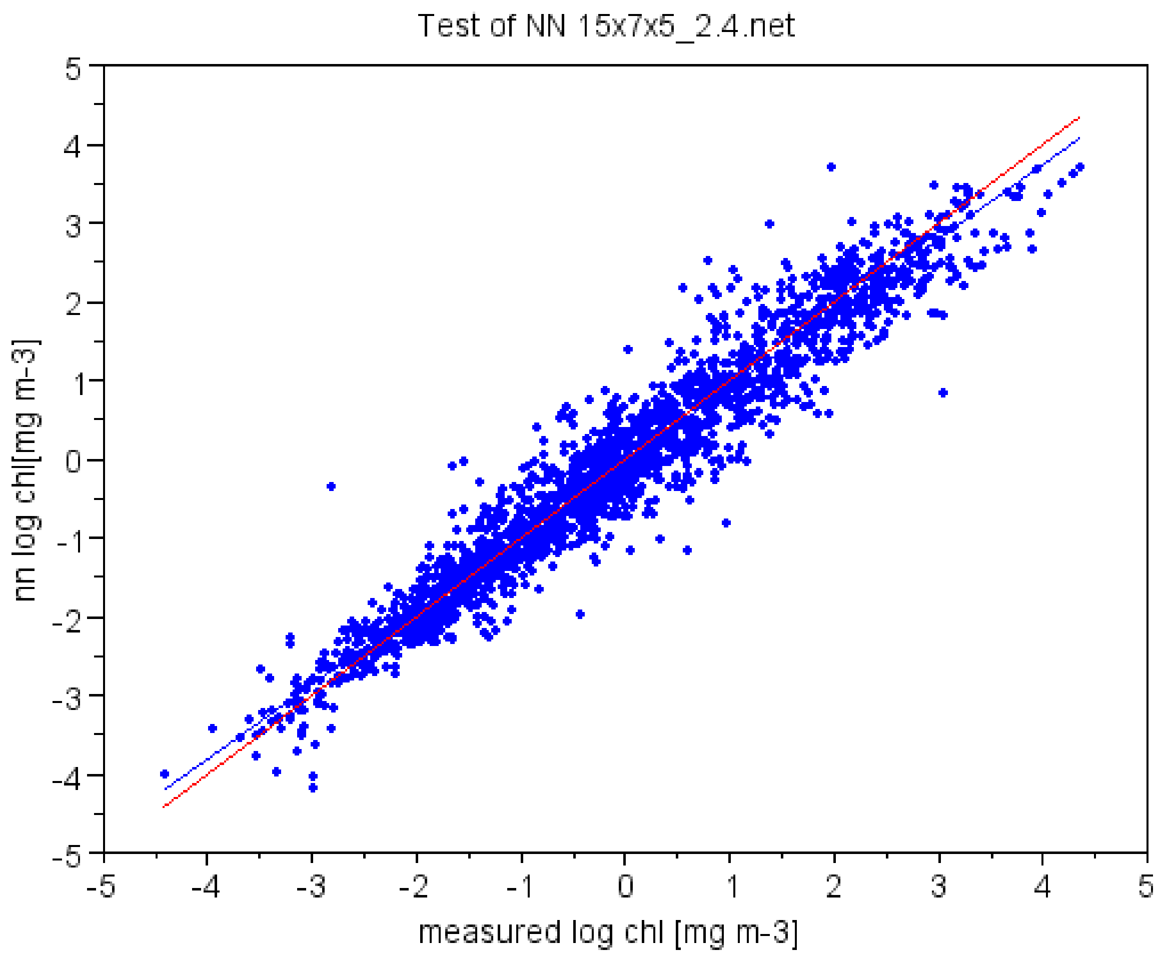
Log10 ratio

Mean difference: 0.0086102 m-1, stdev: 0.129
Mean ratio: 0.9717098, stdev: 0.334

Sum_sq of measured and nn derived reflectances

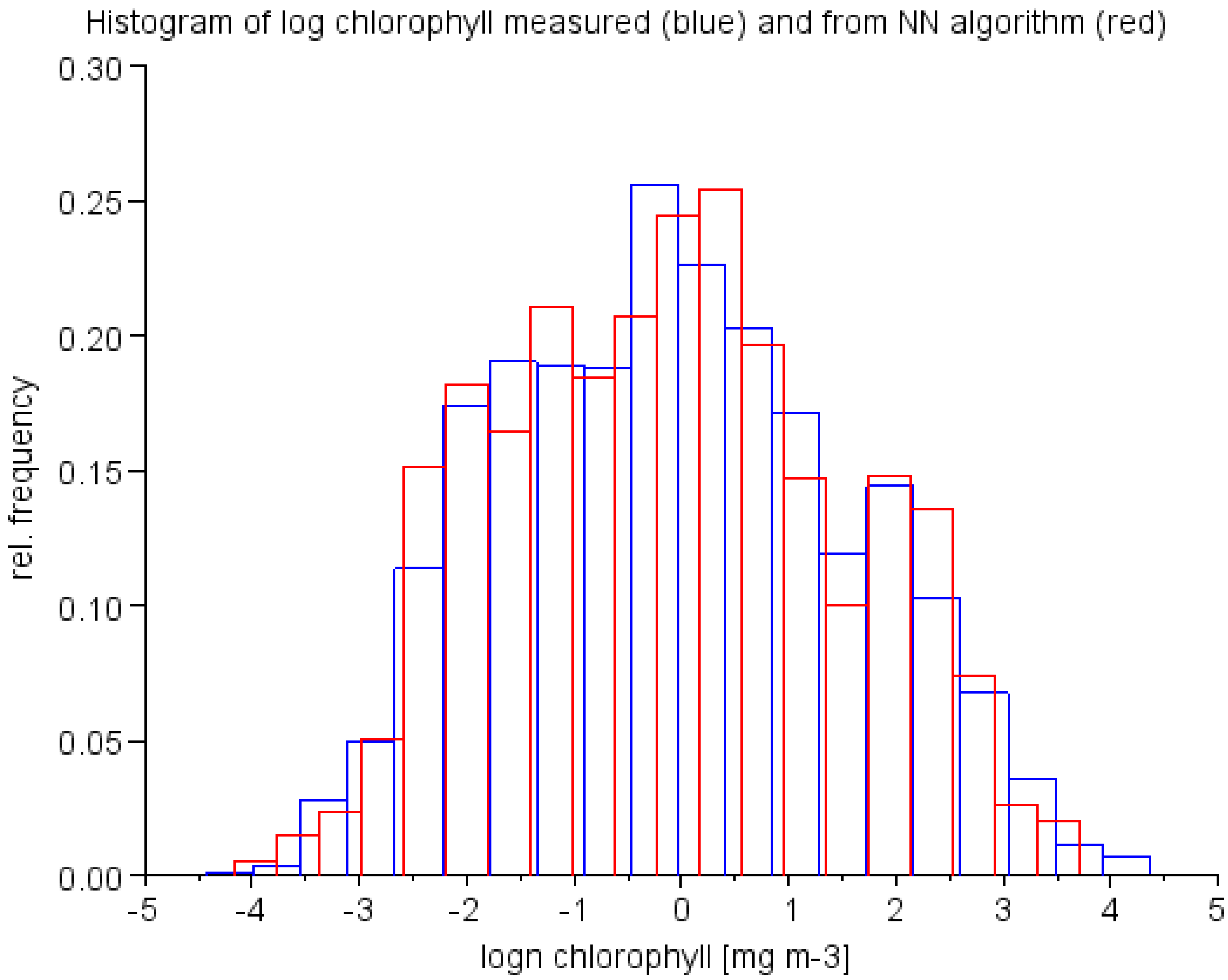


Test of NN based on measurements for chlorophyll

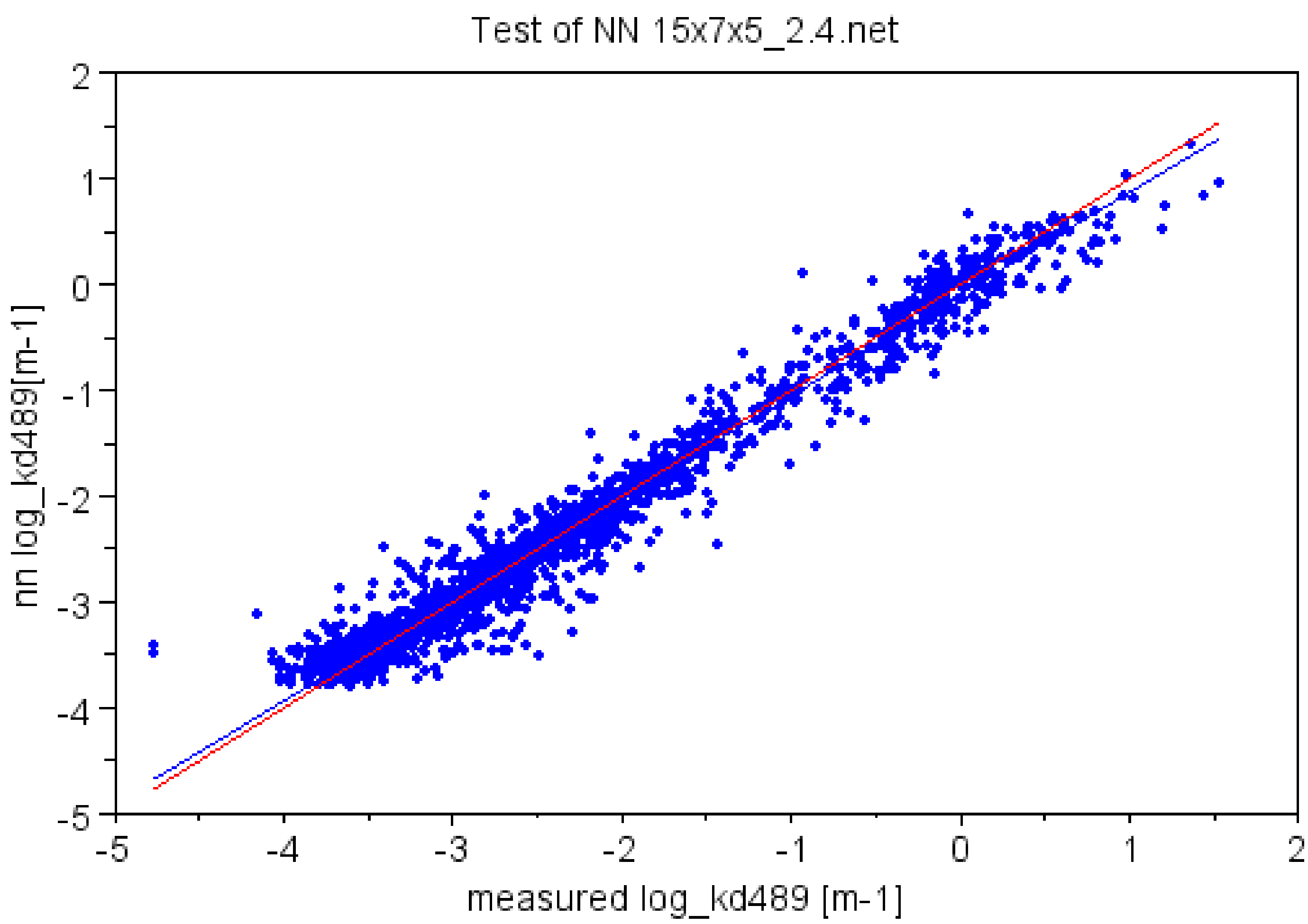


Log10 scale, red: 1 by 1 line

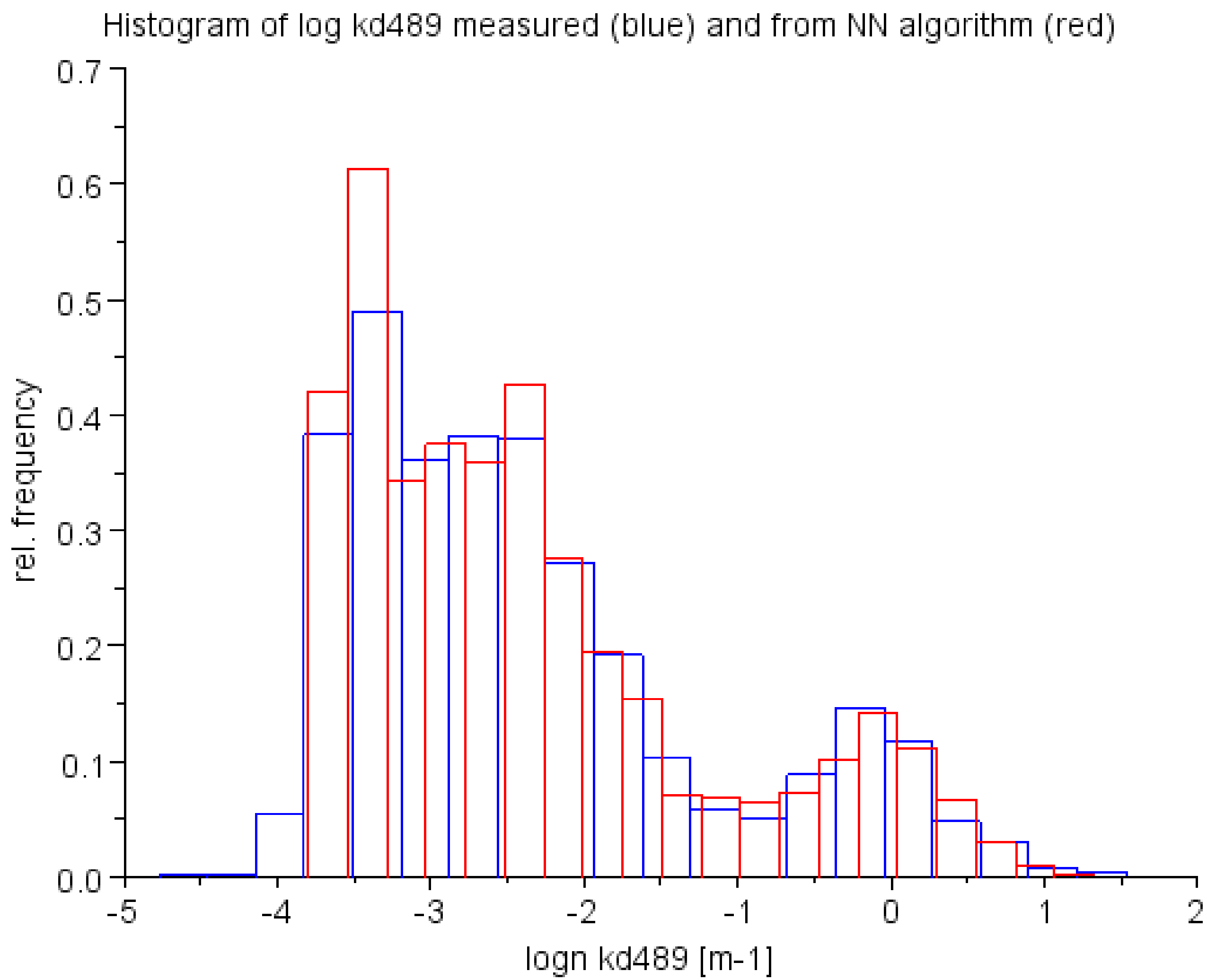
Comparison of histograms: measured, NN computed



NN for kd489


Test of NN 15x7x5_2.4.net
nn log_kd489[m-1]
measured log_kd489 [m-1]
2
1
0
-1
-2
-3
-4
-5
-5
-4
-3
-2
-1
0
1
2

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

Strategies to determine uncertainties for coastal water: Solutions

- **Out of scope detection**
  - Check of auxilary variabels, 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

Acknowledgemets

- Supported by various projects
  - ESA Case 2 Water Regional Algorithm
  - ESA Glint correction
  - ESA Water radiance
  - ESA CoastColour
  - ESA Dragon
  - 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