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Uncertainty algorithms for MERIS / OLCI case 2 water products

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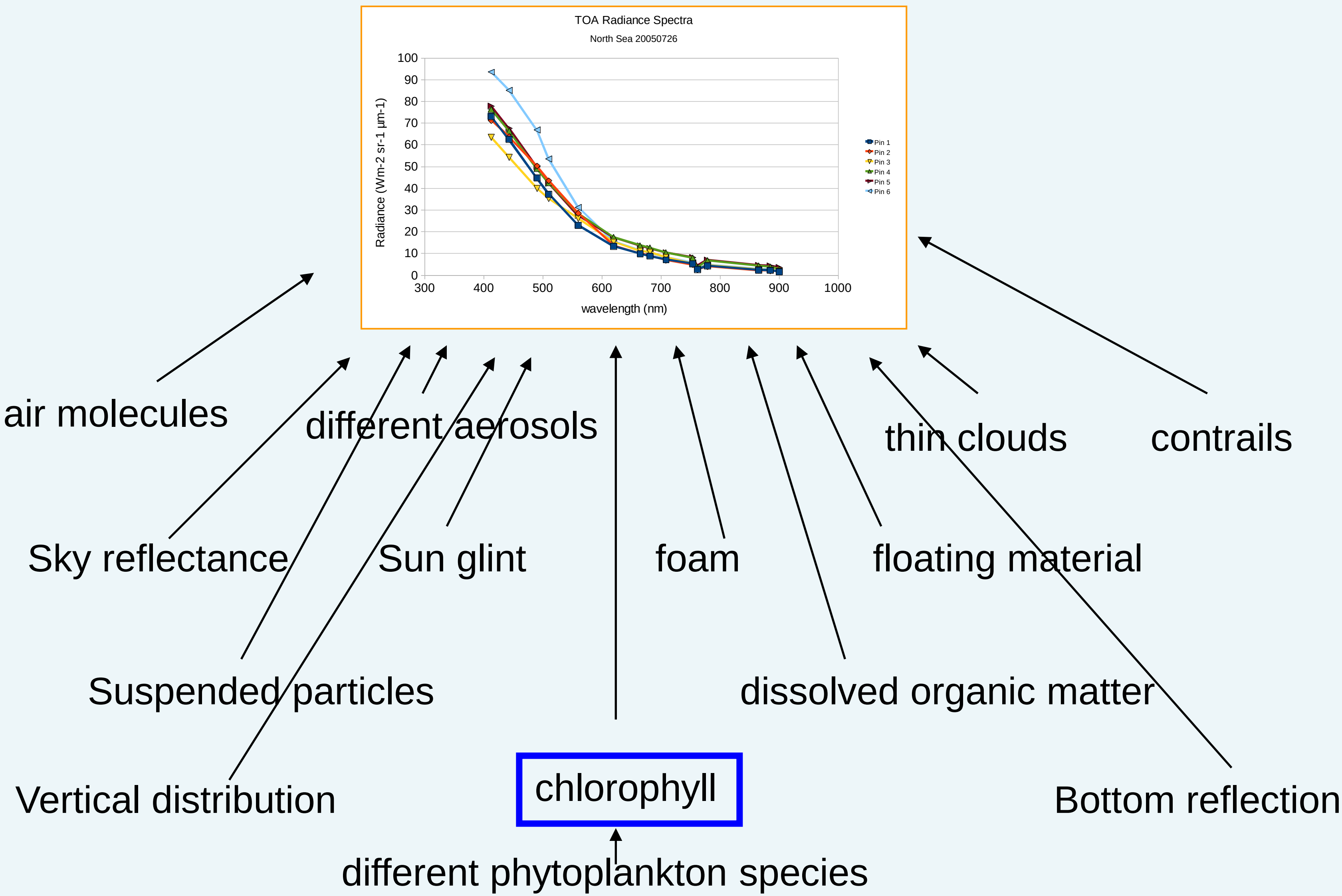
The problem of optically complex water

- high variability of optical properties of water constituents
- more factors which determine top of atmosphere reflectances than can be inversely retrieved
- the model behind the retrieval algorithm can represent only a fraction of the actual conditions
- *thus:*
  - the conditions and corresponding reflectance spectrum can be out of scope of the model
- *and even when in scope*
  - ambiguities and masking effects can lead to significant uncertainties
- Requirement for MERIS / OLCI case 2 water algorithm:
  - *flags when NN inputs or outputs are at the limit of the training range*
  - *co-algorithm to determine spectra, which are out of scope*
  - *co-algorithm to determine uncertainties*

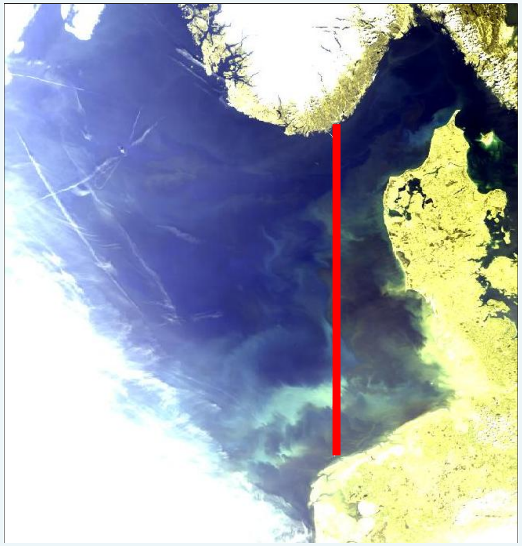
OLCI and MERIS case 2 water algorithms

- MERIS (4th reprocessing) and OLCI standard products of case 2 water are based on 2 neural network algorithm systems
  - atmosphere NN: Rtosa -> Rw (MERIS 12 / OLCI 14 spectral bands)
  - water NN: Rw (9 / 11 bands) -> 5 IOPs (apig, ad, ag, bp, bw)
  - the bio-optical model for water is based on parameters derived from the NOMAD data set (which has been extended to case 2 waters) concerning: IOPs, frequency distributions, co-variances.
  - atmosphere model is based on aerosol optical properties derived from coastal stations of the AERONET
  - large training data set of > 1 Mio. cases, simulation with a SOS atmosphere model (Zagolski, F., Santer R., Aznay O., 2007), and Hydrolight (Mobley, 1994) for water
- procedures for 3 types of checks:
  - flag if inputs or outputs of the NNs are at the lower or upper limit of the traning data set
  - flag if input spectrum is out of scope: test with auto-associative NN for atmosphere and a combination of an inverse and forward NN for water
  - determination of IOP uncertainties of the output of the NN with respect to the training data set

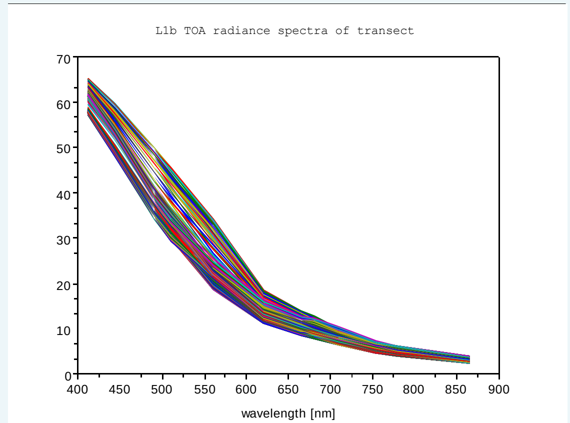
A manifold of factors determine the radiance spectrum at top of atmosphere



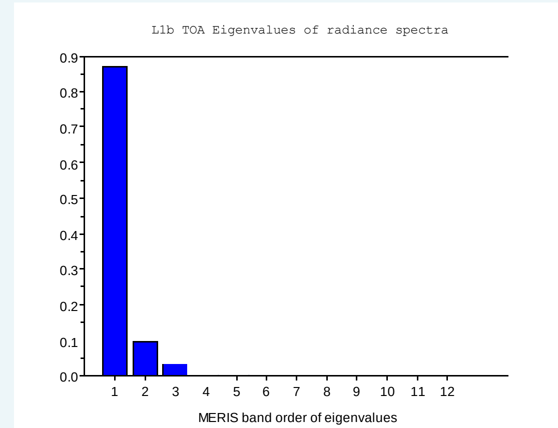
Information content of TOA radiances: PCA and aaNN



Transect North Sea TOA radiance

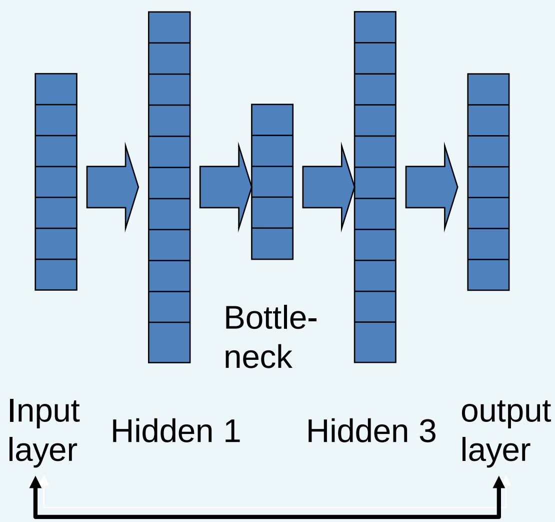


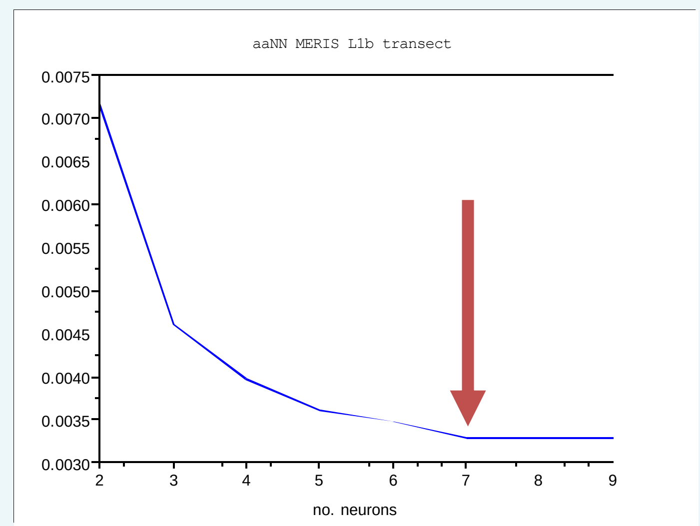
TOA radiance spectra along transect



Principle Component Analysis: only 3 significant factors

Auto-associative NN using a bottle-neck layer functions as a non-linear PCA
For this transect 7 neurons are sufficient to represent the variability of TOA radiances

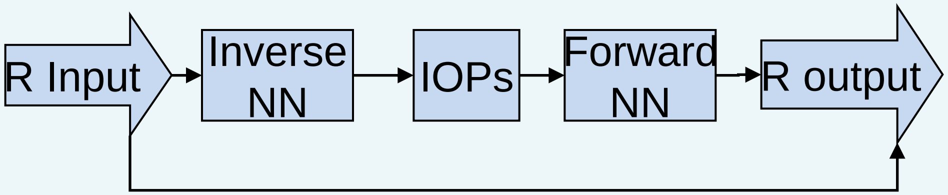




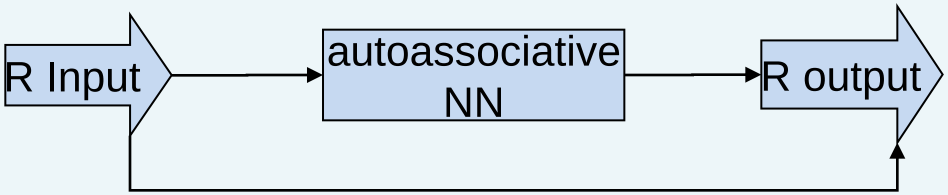
Detection of out of scope conditions

- 2 Procedures have been developed for MERIS / OLCI:
  - **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 chi2
- A threshold can be used to trigger an out of scope warning flag

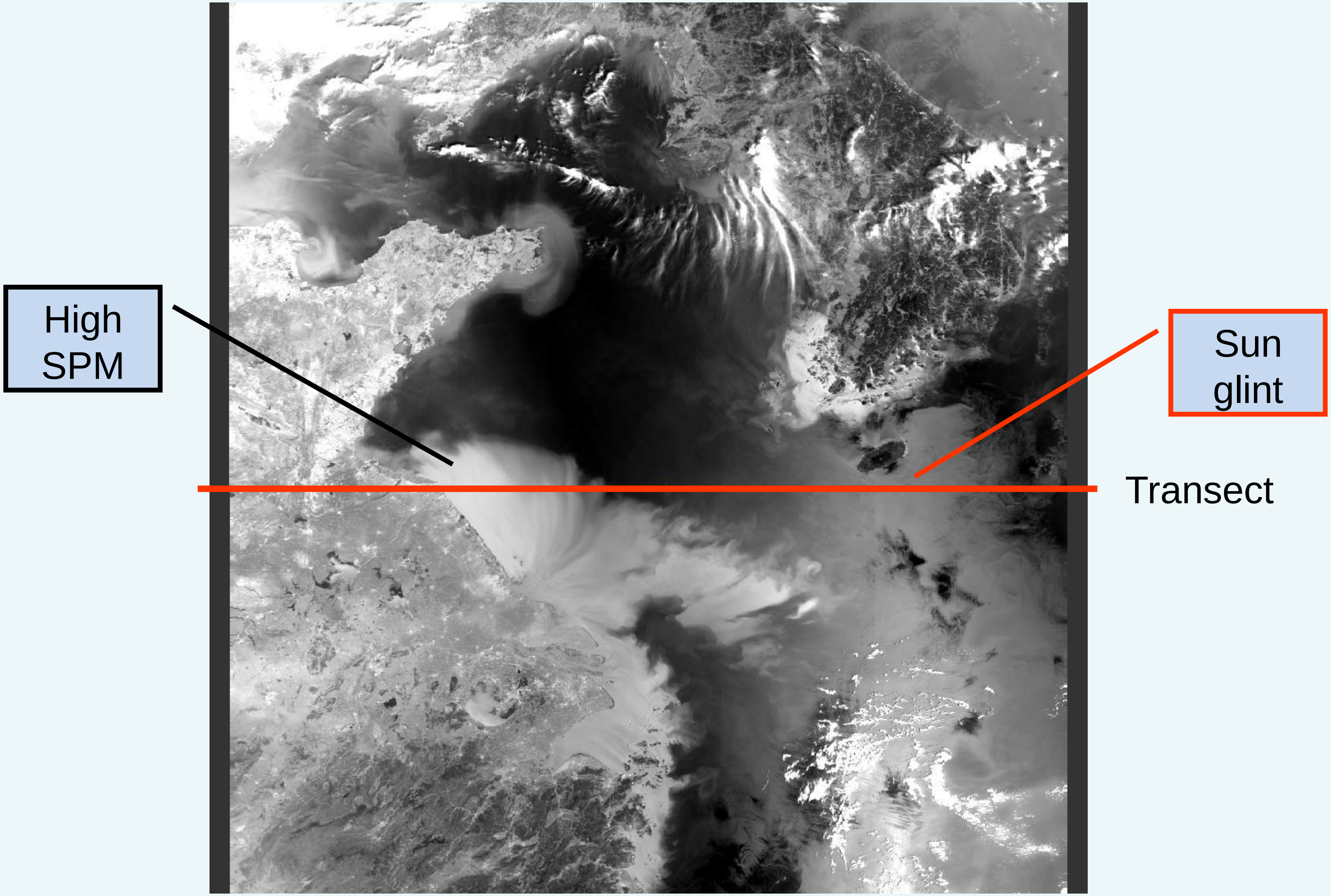
- Combination of inverse and forward NN



- Auto-associative NN

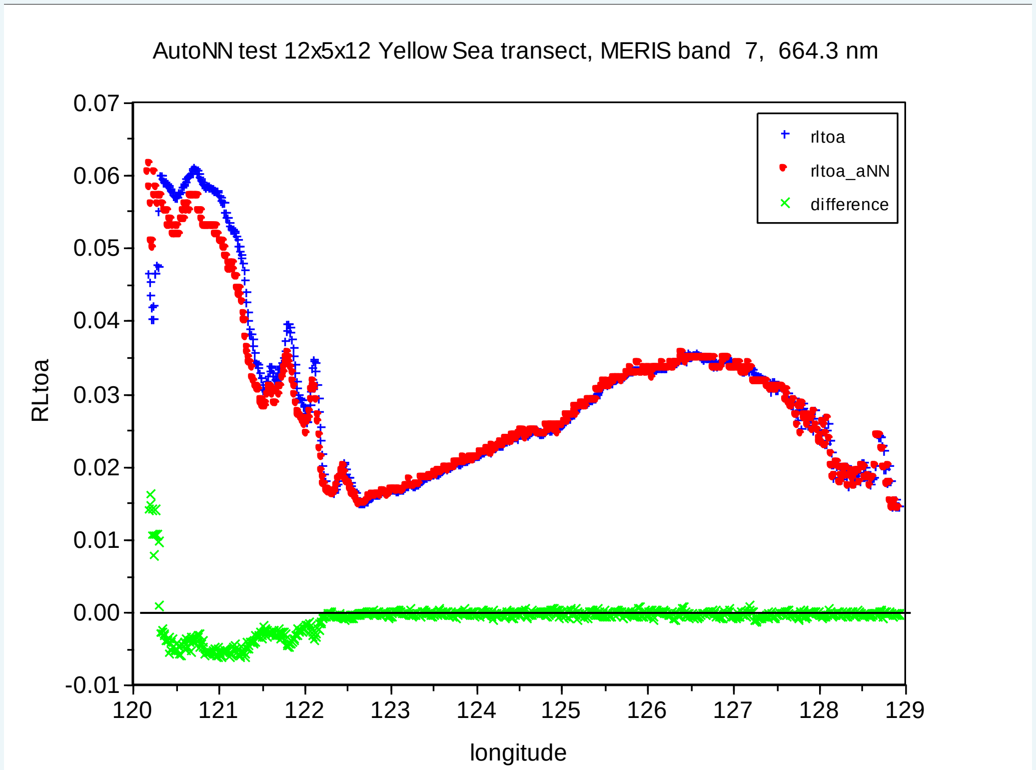


Detection of out of scope conditions aaNN: example for L1 (TOA) data

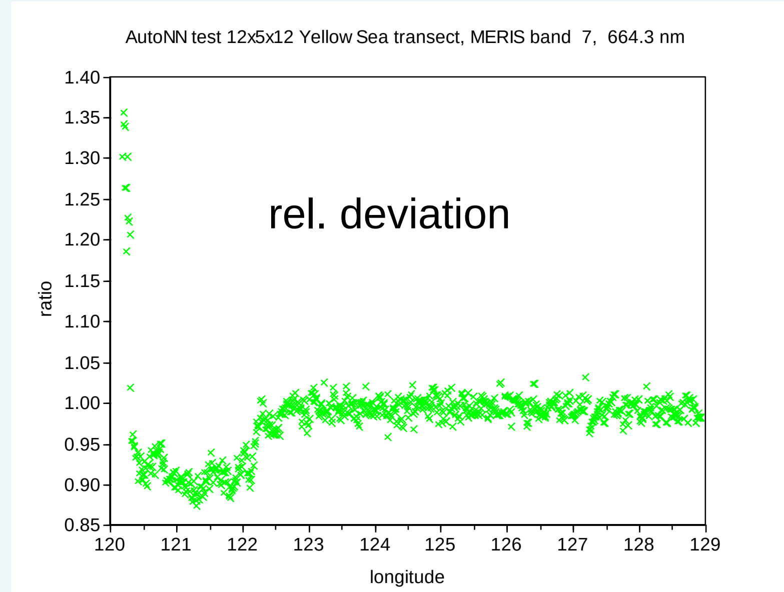


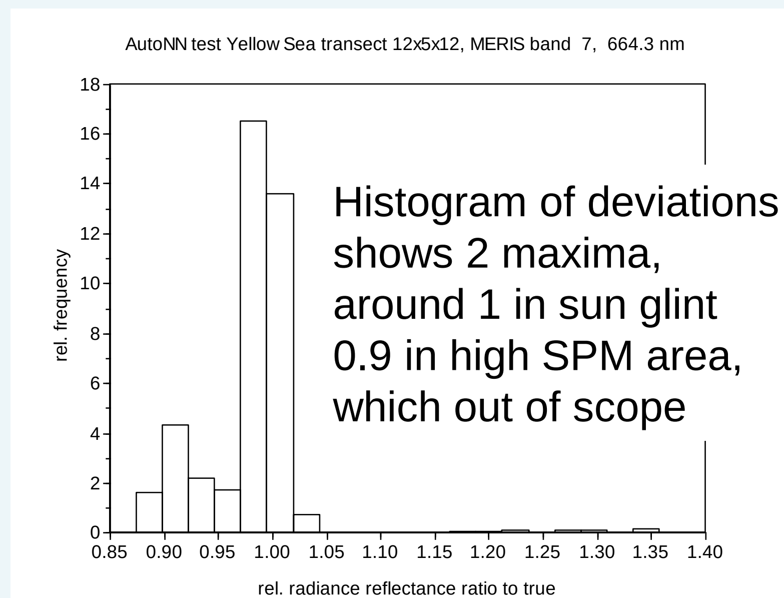
MERIS scene of the Yellow Sea

Detection of out of scope conditions aaNN: example

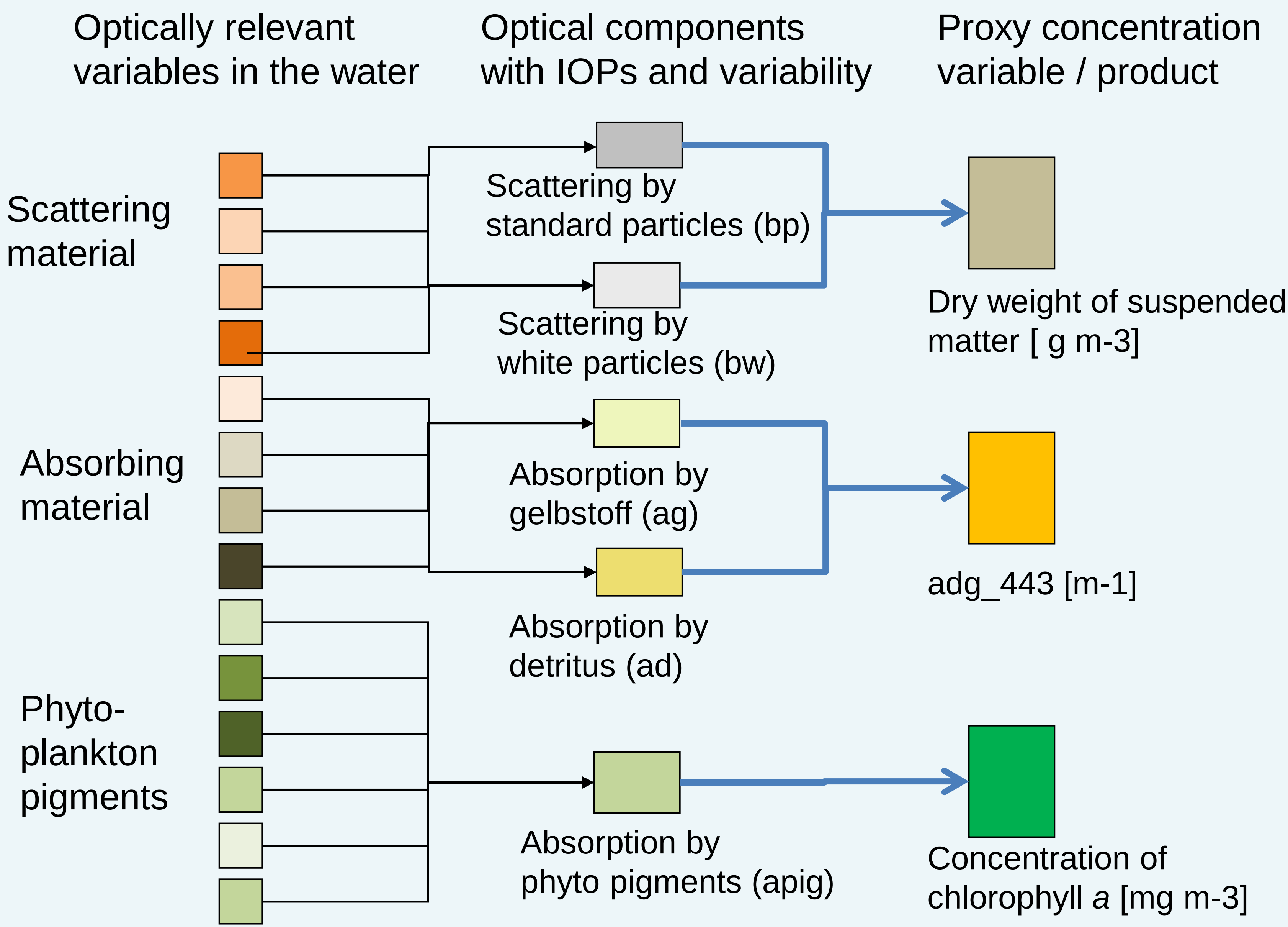


significant deviation in area with high SPM concentrations, but not in sun glint area

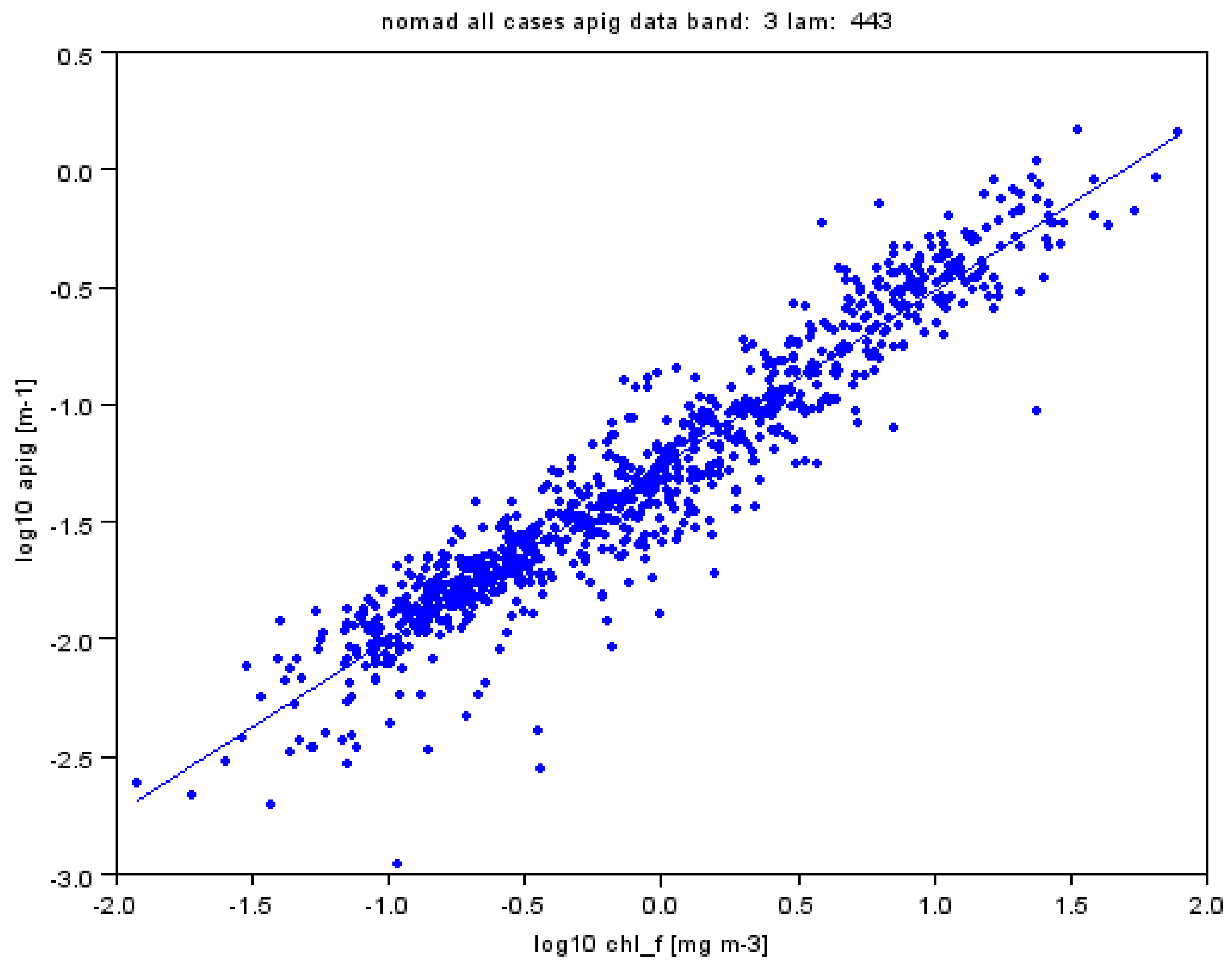




Uncertainties due to the bio-optical model

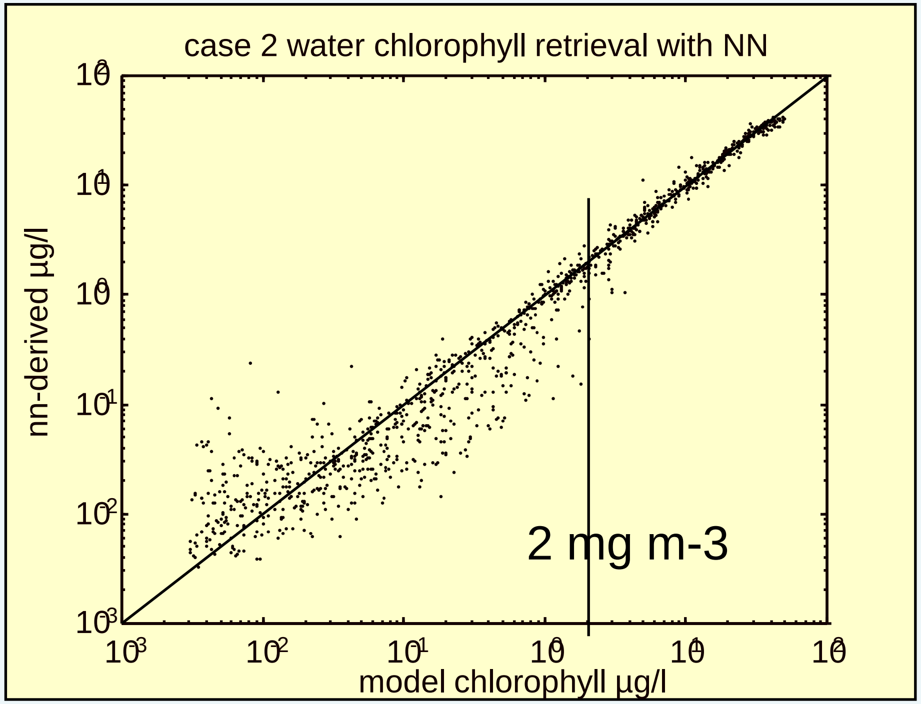


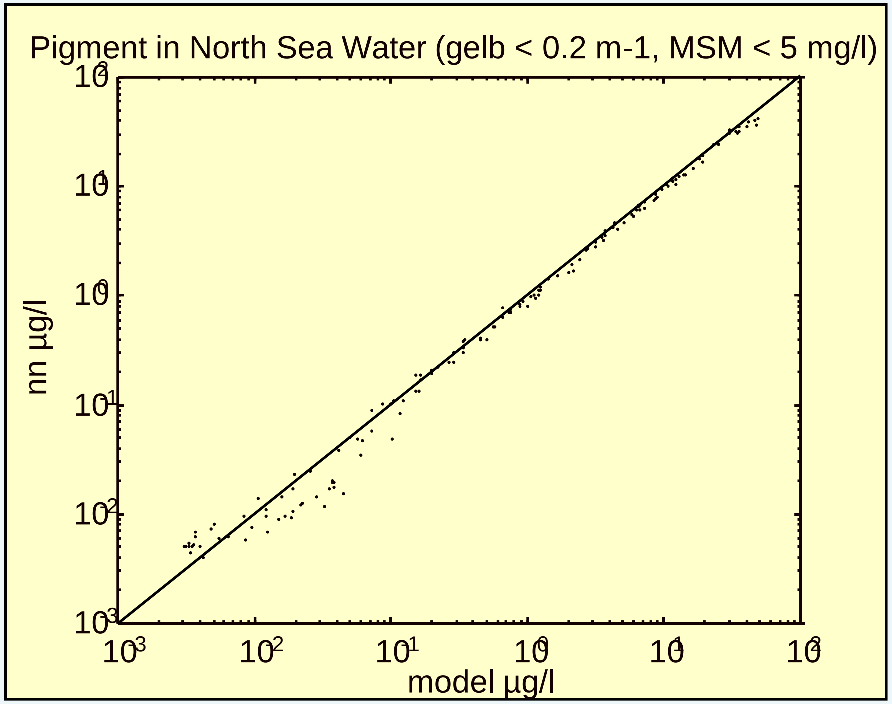
Uncertainties due to variable relationship between a_pig and chlorophyll



443 nm, log10 scale, 920-956 samples for chl_f, NOMAD data set

Uncertainties due to ambiguities for different concentration mixtures

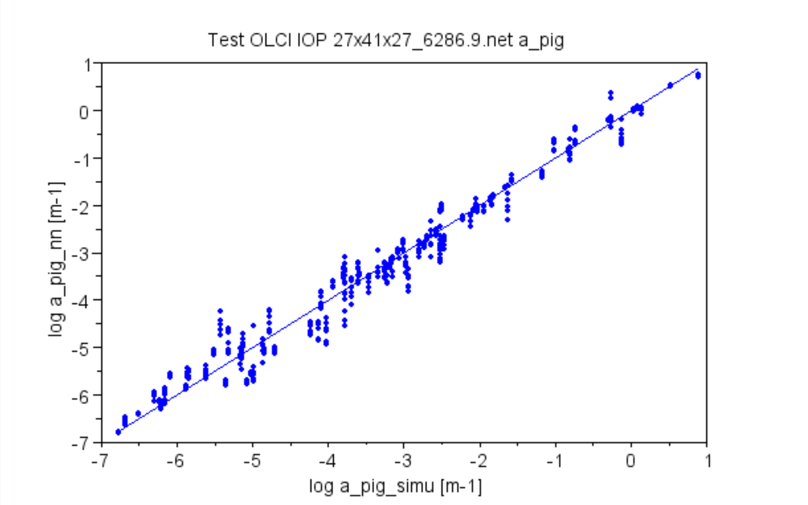




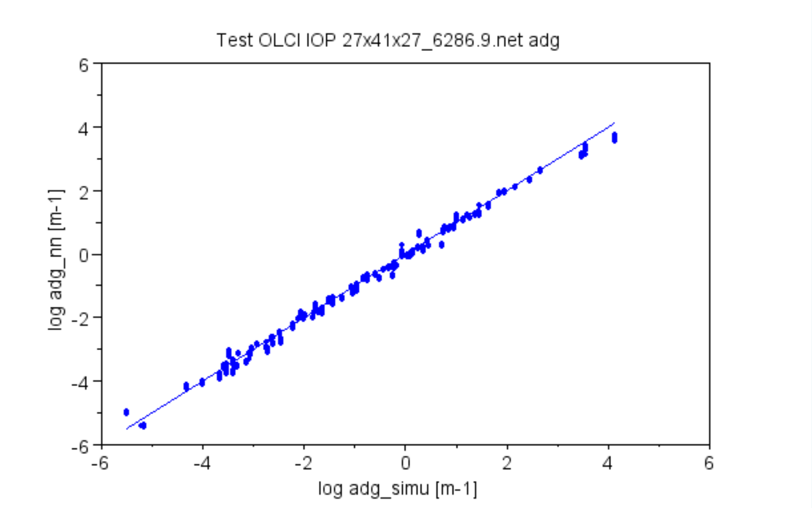
All cases of turbid water

Typical North Sea coastal water:
ay_443: < 0.2 m-1, TSM < 5 mg /l

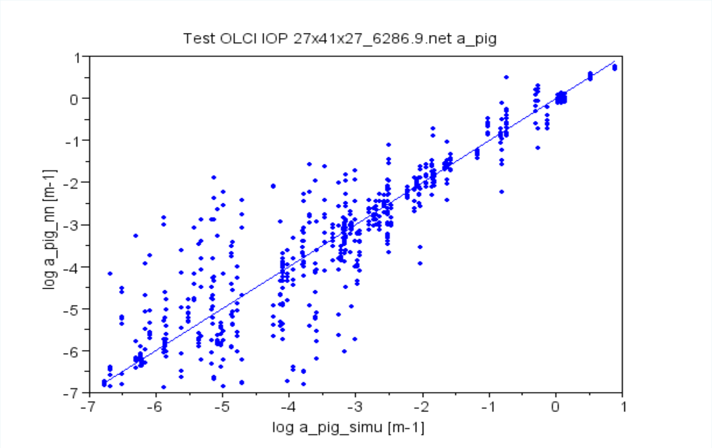
Tests of NNs with different assumed uncertainties of reflectances



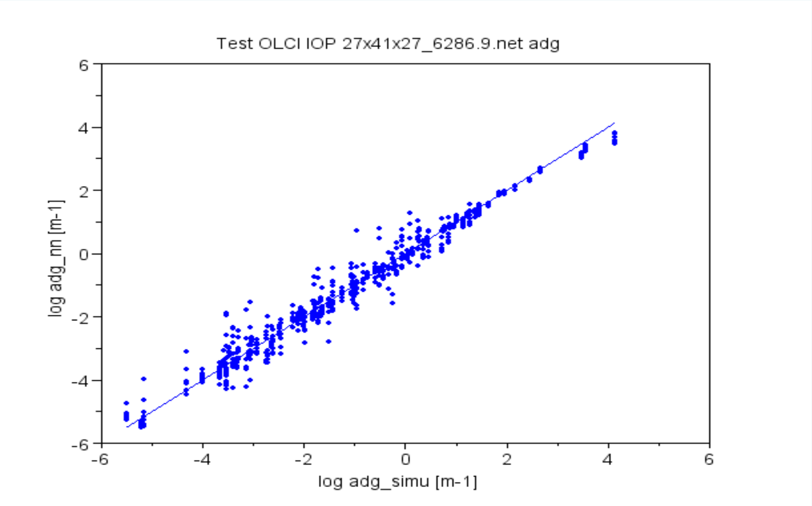
Test of a_pig, no additional error



Test of adg, no additional error



Test of a_pig with an extra random error with a standard deviation of 3%



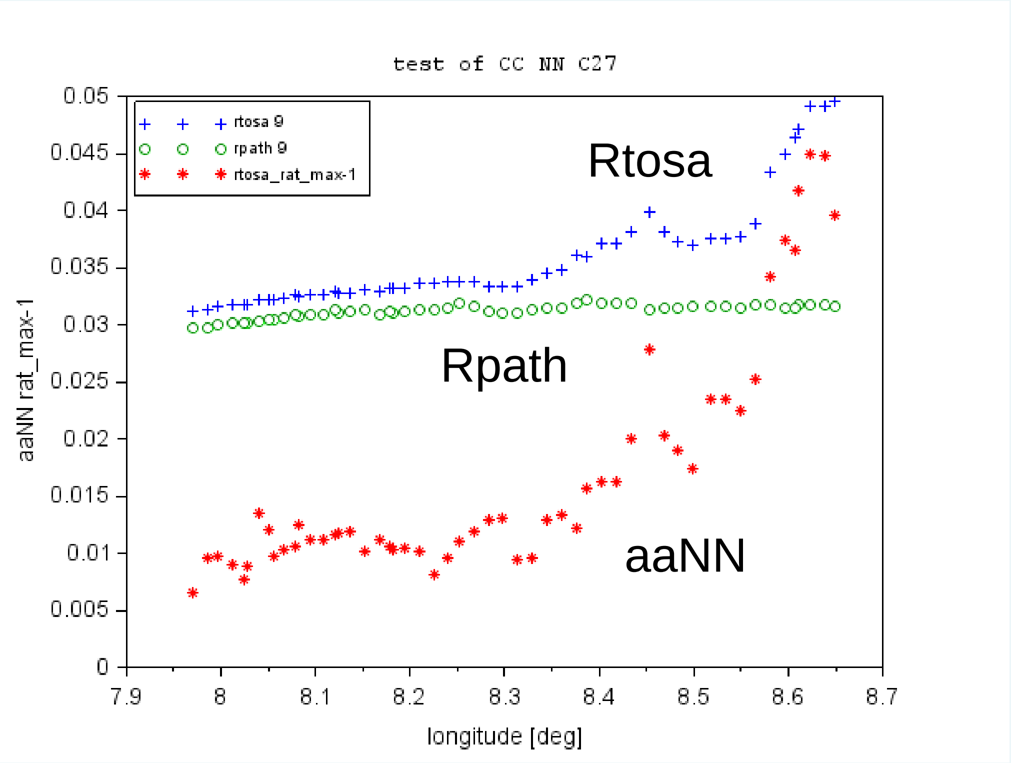
Test of adg with an extra random error with a standard deviation of 3%

Determination of uncertainties

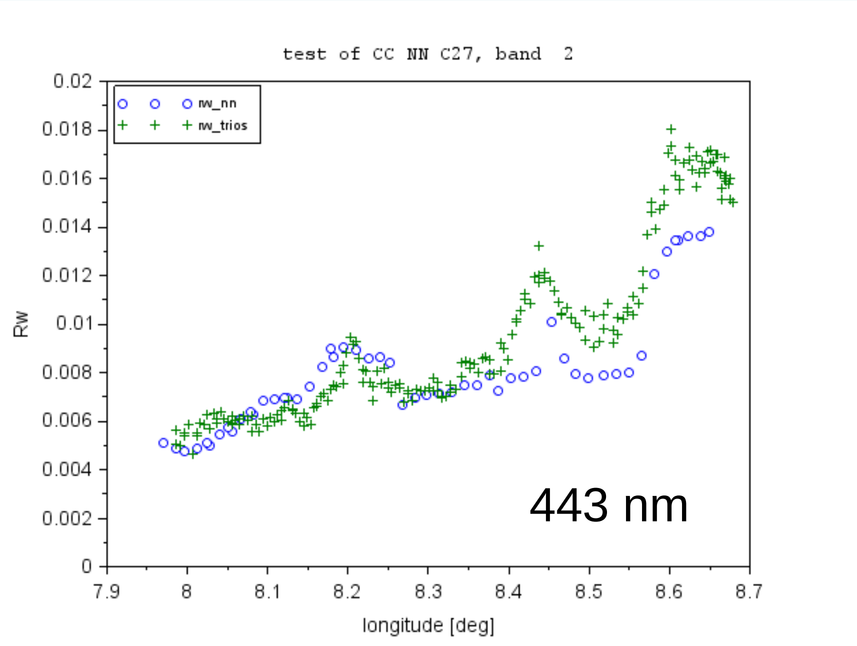
This procedure determines uncertainties – if the data are within the scope of the model – due to ambiguities and masking effects

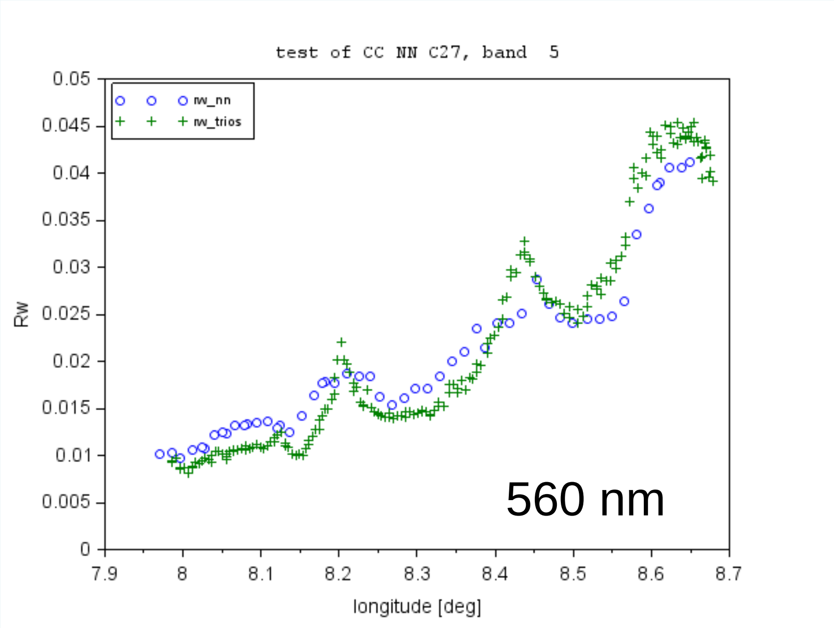
- test of simulated with the inverse neural network
- test with different assumed uncertainties of reflectances
- compute deviations between output of the NN and the corresponding data of the model are included in look-up table
- train a NN with the 5 IOPs as input and the deviations of the 5 IOPs as output: apig, ag, ad, bp, bw
- further NNs are trained with the 5 IOPs as input and the combined 3 products as output:
  - absorption by phytoplankton pigments (apig / chlorophyll),
  - absorption by yellow substance / gelbstoff and detritus (agd) ,
  - scattering by standard and white particles (btsm / TSM)

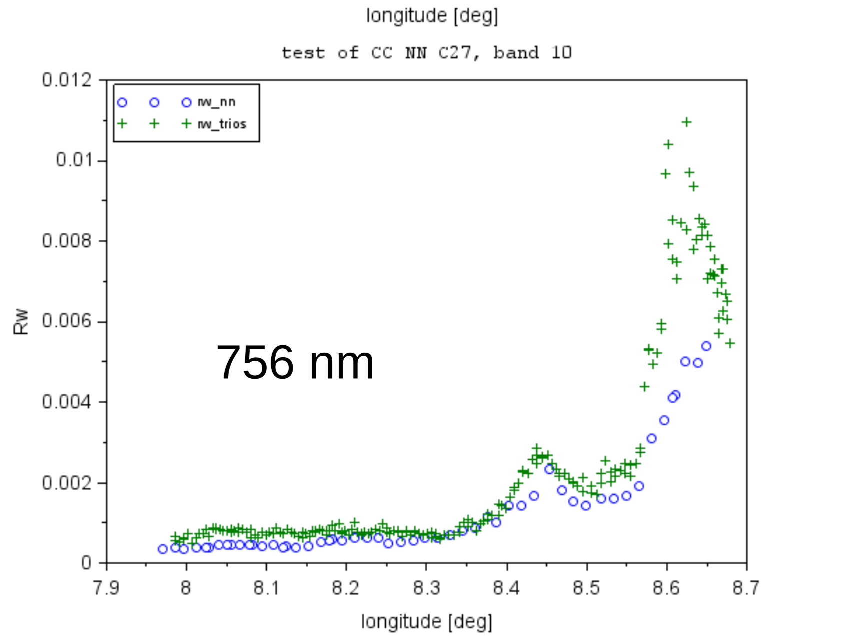
Helgoland transect C27



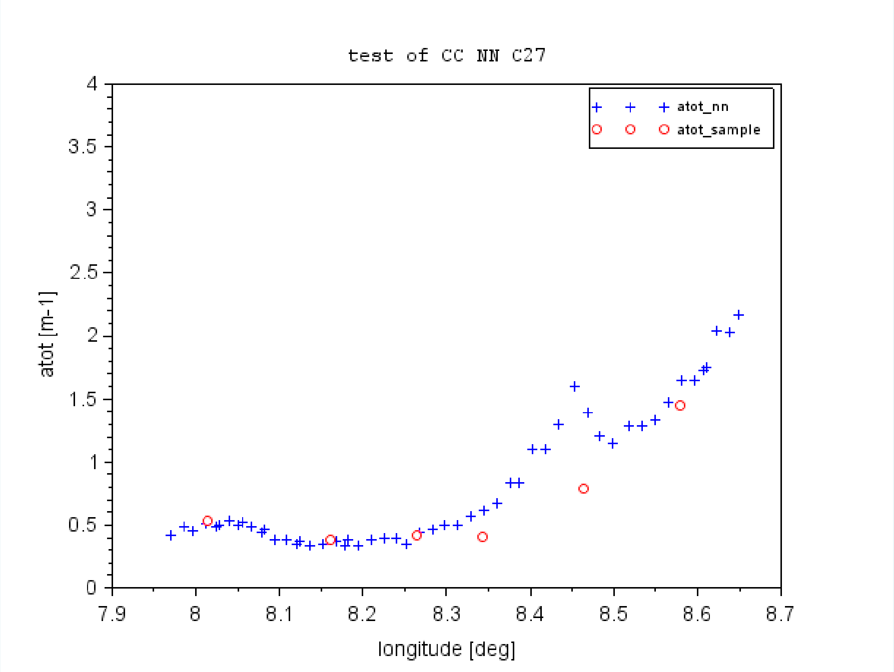
Rw water reflectance



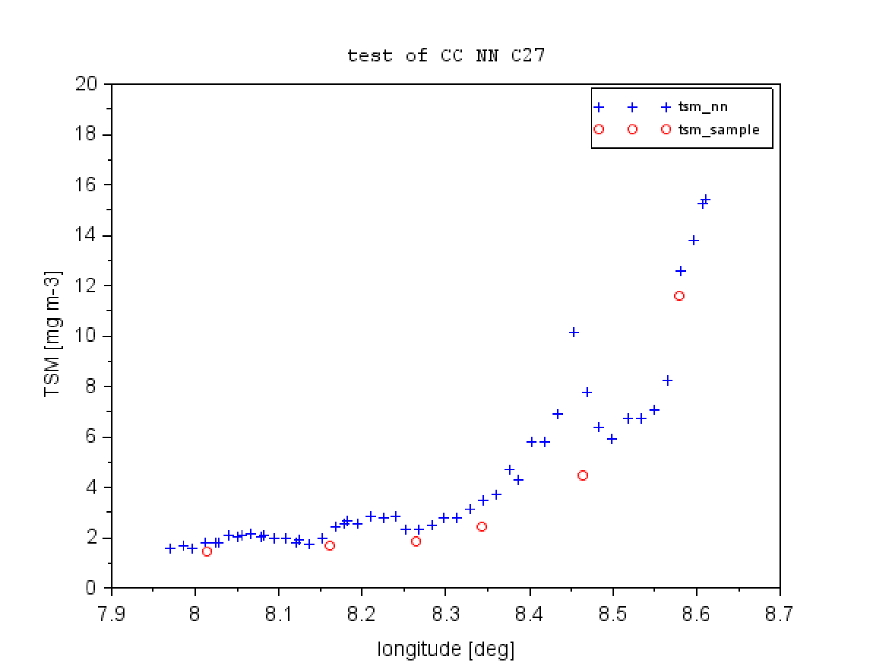




Helgoland transect C27



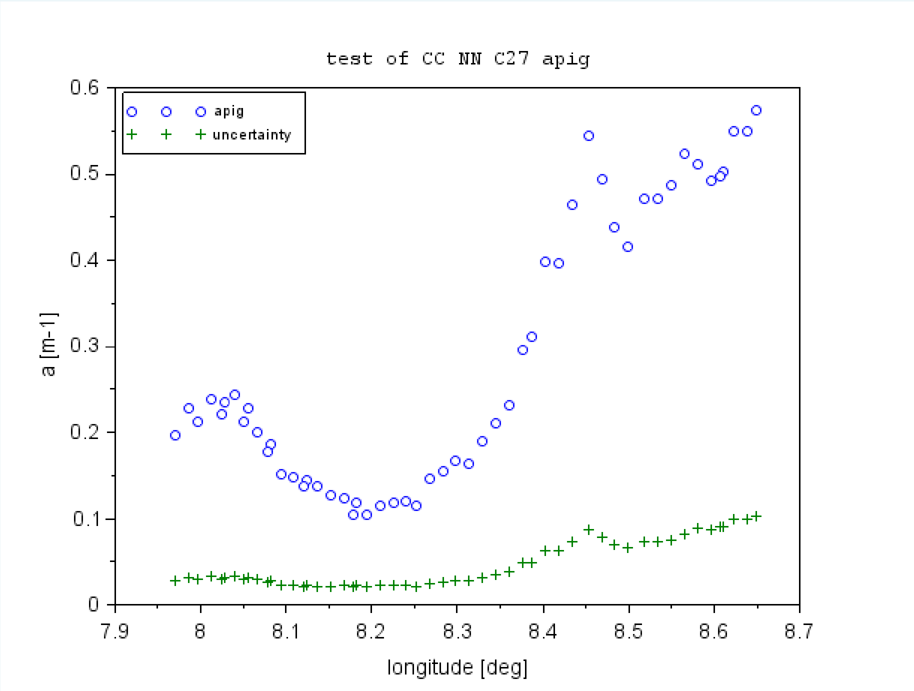
atotal_443

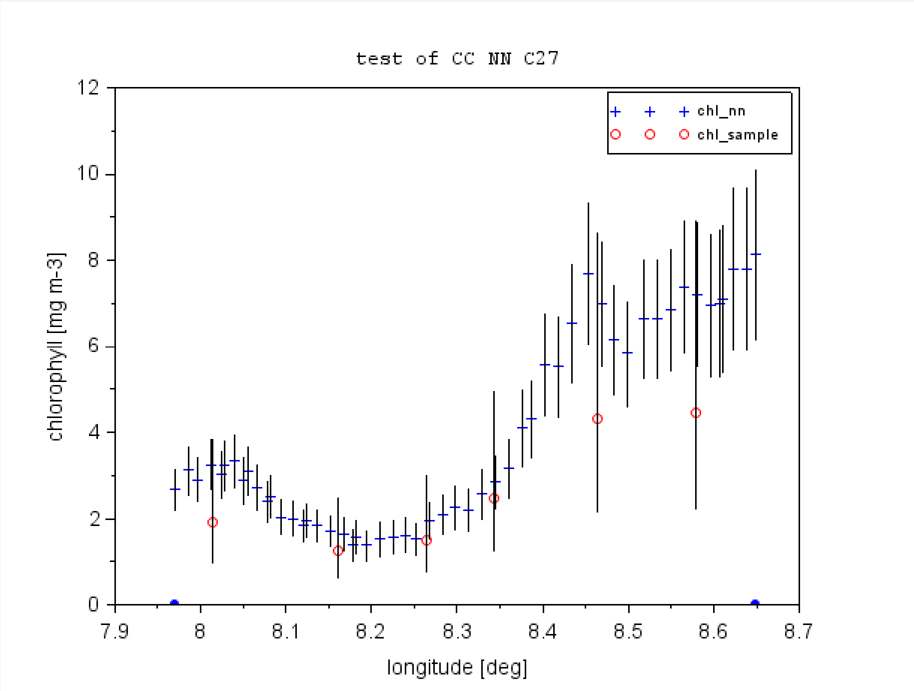


TSM

red dots: water samples, blue dots: MERIS data

Helgoland transect C27





apig_443 (blue dots) and
uncertainties (green dots)
MERIS data

chlorophyll and uncertainties
of water samples (red dots with bars)
and MERIS data (blue dots with bars)

Summary and conclusion

Problem

- In most case 2 waters we have more variables, which determine TOA radiances, than we can retrieve
- Importance of variables in water change with their concentrations and variables can mask each other and spectra might be ambiguous wrt. the IOPs or concentrations of water constituents
- The model behind a case 2 water algorithm is a simplification, reflectance spectra can occur, which are outside the scope of the model

Requirement

- Thus, we have to check if a TOA or water reflectance spectrum is in scope of the model used for the algorithm
- and we have to determine the uncertainty of the retrieved IOPs due to ambiguities and masking effects

Solution for MERIS / OLCI

- Co-algorithm to identify out of scope spectra by using an aaNN or combination of inverse and forward IOP-Rw NN
- uncertainty NN which is trained with the deviations between the IOPs of the simulated test data set and the IOPs as output of the inverse NN

Open problem

- validation of the uncertainty NN with field data