Copernicus FRM4SOC FICE 2025

Training on
In Situ Ocean Colour Radiometry

Quantification of uncertainties in satellite data products

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7-19 July 2025
Venice, Italy

The direct method

The comparison of satellite versus in situ data provides only general indications on the accuracy affecting data products: none of the statistical quantities associated to the comparison is a direct expression of the uncertainties.

Accuracy requirements for satellite radiometric products are commonly summarized by a spectrally and water-type independent *5% uncertainty*. This generic *5% uncertainty* requirement, however, should only apply to oligotrophic/mesotrophic waters in the blue-green spectral region. To assess the fulfilment of such a requirement, radiometric data products can be evaluated applying the so-called consistency principle: *independent measurements of the same quantity should agree within their individual uncertainties* (Immler *et al.* 2010).

Matchups construction

Matchups are constructed applying satellite extraction protocols, which may be different and naturally lead to appreciable differences in matchups results.

As an example, matchups can be confidently constructed using the median of the 3×3 satellite pixels centred at various measurement sites and applying criteria to maximize the *comparability* of *satellite* and *in situ* data.

Again, as an example, matchups can be retained for successive analysis when:

i. the time difference Δt between *in situ* measurement and satellite overpass is less than ±2 hr (only holding the *in situ* data closest in time to the satellite overpass);
ii. none of the 3×3 pixels is affected by the standard processing flags;
iii. the coefficient of variation (*i.e.*, the ratio of standard deviation to mean) of $L_{WN}(\lambda)$ is lower than 20% at 560 nm for the nine pixels (the 560 nm centre-wavelength is expected to exhibit a lower dependence on optically significant constituents and surface perturbations with respect to the other centre-wavelengths in the visible portion of the spectrum);
iv. the viewing angle is lower than 60°;
v. the sun zenith angle is lower than 70°; and
vi. the aerosol optical depth τ_a determined at a near-infrared centre-wavelength (*i.e.*, 865 nm) is lower than an extreme value such as 0.5 to avoid data affected by cloud perturbations.

Matchups statistics

Satellite data products can be evaluated through statistical indices for the *N* matchups of satellite (*SAT*) and *in situ* (*PRS*) data $[(\mathfrak{I}_1^{SAT}, \mathfrak{I}_2^{SAT}, \ldots, \mathfrak{I}_N^{SAT}), (\mathfrak{I}_1^{PRS}, \mathfrak{I}_2^{PRS}, \ldots, \mathfrak{I}_N^{PRS})]$ where $\mathfrak{I}$ is the compared quantity (*i.e.*, $L_{WN}(\lambda)$), and the subscripts 1, 2 …, *N* indicate the matchup index.

Statistical indices that can be considered are:

i. the median of differences Δ_m and the median of absolute (unsigned) differences $|\Delta|_m$;

ii. the median of relative differences ψ_m and the median of absolute (unsigned) relative differences $|\psi|_m$, both determined with respect to the *in situ* reference data;

iii. the root mean square of differences *rmsd*; and the determination coefficient r^2 from data regression.

The indices $|\Delta|_m$ and $|\psi|_m$ provide hints on the dispersion of data, conversely Δ_m and ψ_m provide information on biases. The quantities $|\psi|_m$ and ψ_m are expressed in percent and provide an immediate view on the comparison. On the contrary, $|\Delta|_m$, and *rmsd* are in physical units (*e.g., mW cm*$^{-2}$ *μm*$^{-1}$ *sr*$^{-1}$) and complement the comparison with statistical indices strictly related to the values and range of the assessed $L_{WN}(\lambda)$.

When considering that the $L_{WN}(\lambda)$ values may not exhibit normal distribution, the use of the median with respect to the mean allows to better determine the centrality of the comparison results.

The direct method: application

By:

i. applying the consistency principle to satellite $L_{WN,\,i}^{SAT}(\lambda)$ and *in situ* $L_{WN,\,i}^{PRS}(\lambda)$ matchups with *i* indicating the matchup index; and

iii. assuming negligible correlations between uncertainties, the following relationship is statistically satisfied:

$$\left[L_{WN,\,i}^{SAT}(\lambda) - L_{WN,\,i}^{PRS}(\lambda)\right]^2 < k\times\left[u_{SAT,\,i}^2(\lambda) + u_{PRS,\,i}^2(\lambda) + v_{SAT,\,i}^2(\lambda) + v_{PRS,\,i}^2(\lambda)\right]$$

where $u_{SAT,\,i}(\lambda)$ indicates the expected uncertainty of satellite data, $u_{PRS,\,i}(\lambda)$ the quantified uncertainty for the *in situ* data and, $v_{SAT,\,i}(\lambda)$ and $v_{PRS,\,i}(\lambda)$ the spatio-temporal variabilities affecting satellite and *in situ* data, respectively.

Assuming k=1 and that most of the major contributions to radiance differences are accounted for

$$\varepsilon_i(\lambda) = \frac{L_{WN,\,i}^{SAT}(\lambda) - L_{WN,\,i}^{PRS}(\lambda)}{\sqrt{u_{SAT,\,i}^2(\lambda) + u_{PRS,\,i}^2(\lambda) + v_{SAT,\,i}^2(\lambda) + v_{PRS,\,i}^2(\lambda)}}$$

Zibordi, G., Talone, M., & Mélin, F. (2021). Uncertainty estimate of satellite-derived normalized water-leaving radiance. IEEE Geoscience and Remote Sensing Letters, 19, 1-5.

Interpretation of comparison results

$$\varepsilon_i(\lambda) = \frac{L^{SAT}_{WN,\,i}(\lambda) - L^{PRS}_{WN,\,i}(\lambda)}{\sqrt{u^2_{SAT,\,i}(\lambda) + u^2_{PRS,\,i}(\lambda) + \nu^2_{SAT,\,i}(\lambda) + \nu^2_{PRS,\,i}(\lambda)}}$$

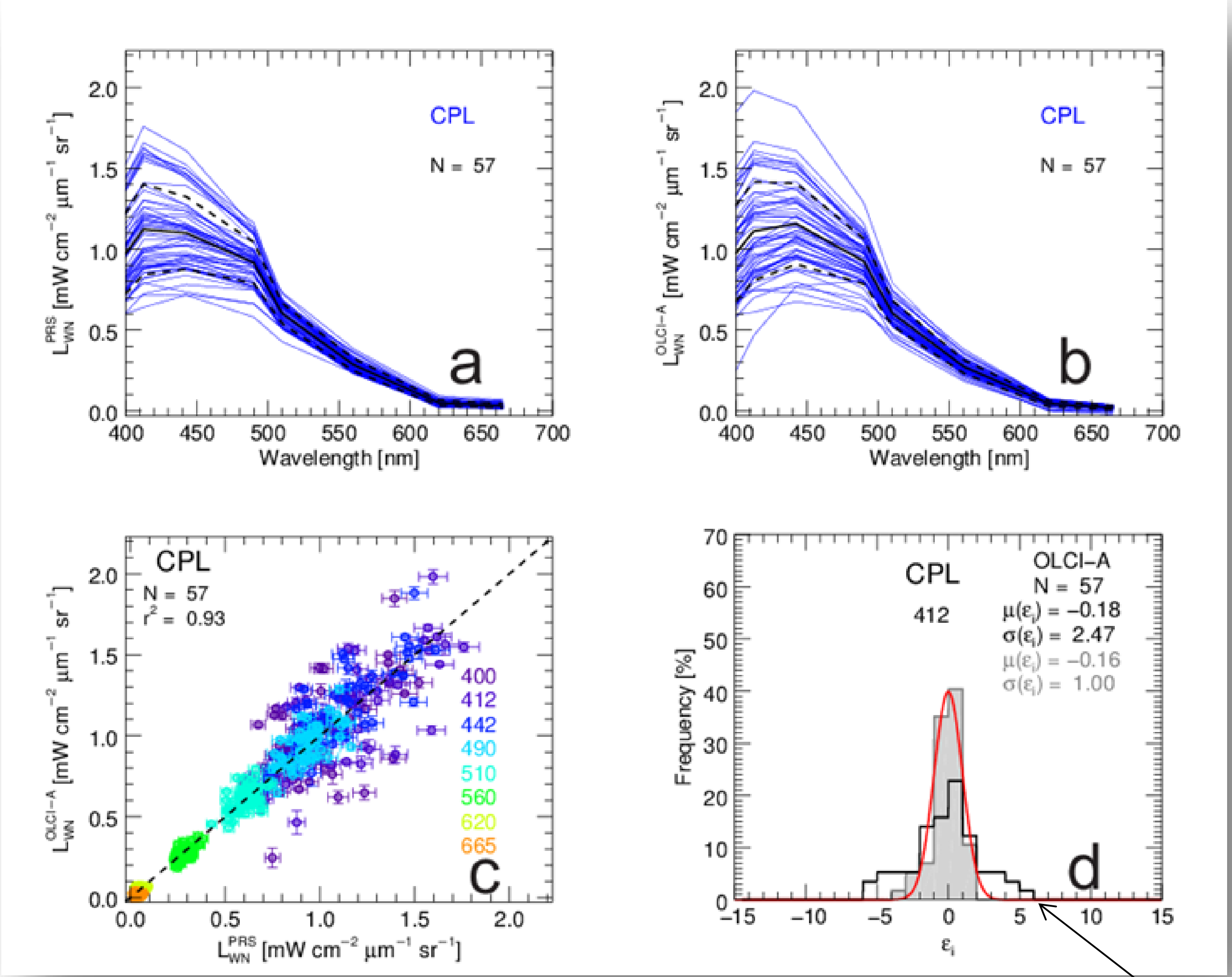
In agreement with Hunt *et al*. (2020) and following Zibordi *et al*. (2022):

if $u_{SAT,\,i}(\lambda)$, $u_{PRS,\,i}(\lambda)$, $\nu_{SAT,\,i}(\lambda), \nu_{PRS,\,i}(\lambda)$ *well describe the variance of the differences* $L^{SAT}_{WN,\,i}(\lambda) - L^{PRS}_{WN,\,i}(\lambda)$, *then the probability distribution of the* $\varepsilon_i(\lambda)$ *values would be standard normal and consequently centred at 0 with standard deviation* $\sigma(\varepsilon_i(\lambda))$ *equal to 1*.

In the case the uncertainty values are underestimated, the distribution of $\varepsilon_i(\lambda)$ would exhibit a standard deviation $\sigma(\varepsilon_i) > 1$.

On the contrary, if the uncertainty values are overestimated, the distribution of $\varepsilon_i(\lambda)$ would lead to $\sigma(\varepsilon_i) < 1$ (*see the equation for* ε_i).

Application



$$\varepsilon_i(\lambda) = \frac{L_{WN,\,i}^{SAT}(\lambda) - L_{WN,\,i}^{PRS}(\lambda)}{\sqrt{u_{SAT,\,i}^2(\lambda) + u_{PRS,\,i}^2(\lambda) + v_{SAT,\,i}^2(\lambda) + v_{PRS,\,i}^2(\lambda)}}$$

(a) AERONET-OC $L_{WN}^{PRS}(\lambda)$

(b) OLCI-A $L_{WN}^{OLCI-A}(\lambda)$

(c) scatter plot of $L_{WN}^{OLCI-A}(\lambda)$ versus $L_{WN}^{PRS}(\lambda)$

(d) distributions of the uncertainty-normalized difference ε_i at the 412 nm imposing

i. $u_{OLCI-A,\,i}(\lambda) = 0.05 \cdot L_{WN,\,i}^{OLCI-A}(\lambda)$ (*black line*) or

ii. a constant value for $u_{OLCI-A,\,i}(\lambda)$ so that

$\sigma(\varepsilon_i(\lambda)) = 1$ (*grey line and shaded background*)

compared to an ideal normal distribution (*red line*).

N indicates the number of matchups, *r*^{2} the determination coefficient and, $\mu(\varepsilon_i)$ and $\sigma(\varepsilon_i)$ the mean and standard deviation of the ε_i values, respectively.

$\sigma(\varepsilon_i) > 1$. *Thus the 5% uncertainty is underestimated!*

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Details

$$\varepsilon_i(\lambda) = \frac{L_{WN,\,i}^{SAT}(\lambda) - L_{WN,\,i}^{PRS}(\lambda)}{\sqrt{u_{SAT,\,i}^2(\lambda) + u_{PRS,\,i}^2(\lambda) + v_{SAT,\,i}^2(\lambda) + v_{PRS,\,i}^2(\lambda)}}$$

λ [nm]	400	412	442	490	560	665
$\mu(L_{WN,i}^{PRS}) \pm \sigma(L_{WN,i}^{PRS})$ [mW cm^{-2} μm^{-1} sr $^{-1}$]	0.972±0.248	1.123±0.279	1.100±0.224	0.916±0.128	0.285±0.038	0.030±0.014
$\mu(u_{PRS,i}/L_{WN,i}^{PRS}) \pm \sigma(u_{PRS,i}/L_{WN,i}^{PRS})$	0.050±0.002	0.049±0.002	0.049±0.002	0.051±0.002	0.073±0.004	0.404±0.163
$\mu(v_{SAT,i}/L_{WN,\,i}^{SAT}) \pm \sigma(v_{SAT,i}/L_{WN,\,i}^{SAT})$	0.035±0.036	0.031±0.024	0.025±0.016	0.020±0.012	0.039±0.021	0.469±0.988
|ψ|	0.144	**0.130**	0.088	0.070	0.104	0.434
ψ	–0.002	–0.007	+0.026	+0.005	–0.037	–0.227
$\mu\left(\varepsilon_i(u_{SAT,\,i} = 0.05 \cdot L_{WN,\,i}^{SAT})\right) \pm \sigma(\varepsilon_i)$	–0.06±2.90	–0.18±2.47	+0.66±1.67	+0.12±1.31	–0.41±1.32	–0.88±1.47
$\mu(\varepsilon_i(\sigma(\varepsilon_i) = 1)) \pm \sigma(\varepsilon_i(\sigma(\varepsilon_i) = 1))$	–0.15±1.00	–0.16±1.00	+0.36±1.00	+0.07±1.00	–0.35±1.00	–0.66±1.00
$\mu(u_{SAT,i}(\varepsilon_i(\sigma(\varepsilon_i) = 1))/L_{WN,\,i}^{SAT})$	0.302	**0.203**	0.107	0.080	0.100	0.920

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End

Impact of Δ_t on PRS uncertainties

Site	Δ_t [hours]	400	412	443	490	510	560	620	667	*N*
CPL	1	3.5	3.3	3.0	2.8	3.0	4.1	11.3	14.4	366
	2	3.9	3.7	3.2	3.1	3.2	4.4	12.1	15.1	188
AAOT	1	3.9	3.7	3.3	3.1	3.2	4.1	9.9	12.5	483
	2	6.3	5.6	4.9	4.7	4.7	5.6	7.9	9.0	260

Pairs of triplets within the interval Δ_t were used to estimate the spatio-temporal uncertainties characterizing the in situ data: $u_{mu}(L_{WN}^{Chla})/L_{WN}^{Chla}$ (in %) indicates the median relative uncertainty of AERONET-OC situ data contributing to matchups constructed with diverse Δ_t, for $\tau_a(412) \leq 0.2$ and $\theta_0 \leq 45°$ (N is the number of pairs of triplets considered for Δ_t).