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<td>13/12/2019</td>
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<td>Craig Donlon (Technical Officer)</td>
<td>Digitally signed by Craig Donlon  Date: 2020.01.13 09:57:44 +01'00'</td>
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**Diffusion List**

- Sea Surface Salinity Team Members
- ESA (Craig Donlon, Paolo Cipollini)
## Amendment Record Sheet

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<td>Add Definitions (new section 2) terms relevant to this document</td>
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<td>Added Figure 1</td>
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1 Introduction

1.1 Executive Summary

This document holds the Product Validation and Algorithm Selection Report (PVASR) prepared by CCI+SSS team, as part of the activities included in the [WP200] of the Proposal (Task 2 from SoW ref. ESA-CCI-PRGM-EOPS-SW-17-0032).

1.2 Purpose and Scope

This document collects the information of the 1st Round Robin algorithm comparison exercise, intended to verify the performances of the CCI+SSS v1.7 products.

The objective of the first round robin (RR) CCI+SSS tests was to establish a method of algorithm selection for SSS estimation and to make an initial choice.

Future RR will serve to check improvements and/or degradation of future CCI+SSS versions and eventually improve RR methodologies.

1.3 References

1.3.1 Applicable Documents

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1.3.2 Reference Documents

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1.3.3 Structure of the document

The PVASR is structured as follows:

Section 2 there is a definition of terms used in this document

This document is composed of a description of Round Robin (RR) methodology (section 4), where we describe in-situ data used in the RR tests (ship tracks and PIRATA moorings) in section 3.1, the colocation methodology between in-situ and satellites for moorings and ship tracks in section 3.2, and metrics and plots used in RR tests (section 3.3).

We then present the satellite datasets used in comparison to CCI+SSS dataset in section 5.
In section 6 we explain the algorithm selection, show some results of RR exercise results (section 5.1), rationale for the algorithm selection (section 5.2) and open issues (section 5.3). We enumerate some perspectives for future RR in section 7.
2 Definitions

We provide below definitions, taken from [RD 05], and considerations adapted to the round robin exercise for determining the ‘best’ algorithm for satellite SSS products, that have been adopted throughout this document:

**Measurand:** particular quantity subject to measurement (in our case, the salinity, defined as the relative amount of salt dissolved in sea water (corresponding to gram of salt per kilogram of sea water) at the sea surface).

**Error:** result of a measurement minus a true value of the measurand. Since the ‘true’ value of the measurand is not known, the ‘true’ value of the error is unreachable.

**Uncertainty:** parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurand. Uncertainty of measurement comprises, in general, many components. In the case of RR, since measurements are validated by comparisons with measurements in the fields, ‘experimental standard deviations’ classically evaluated from the statistical distribution of the results of series of measurements realized in the same conditions, cannot be estimated. Hence, in the case of RR, the uncertainty is evaluated from assumed probability distributions of the measurand derived, with some uncertainty, from in situ measurements.

In [RD 05], ‘it is understood that the result of the measurement is the best estimate of the value of the measurand, and that all components of uncertainty, including those arising from systematic effects, such as components associated with corrections and reference standards, contribute to the dispersion’. In the case of satellite radiometric measurements, the absolute calibration of the SSS is not well known and important differences between the various satellite SSS come from the different systematic corrections that are applied. As a consequence, we will distinguish between ‘uncertainties associated with systematic effects’ (that can be quantified by a bias (see below)), from the ‘uncertainties associated with random errors’ coming from the noise of the measurements (linked to the radiometric resolution), from errors that are not well characterized given the present knowledge of the sources of errors.

**Discrepancy:** The difference between the data product and the validation value.

**(Relative) Bias:** The mean value of the discrepancy.

**Validation:** The process of assessing by independent means the quality of the data products derived from the system outputs.
**Precision**: The difference between one result and the mean of several results obtained by the same method, i.e. reproducibility (includes non-systematic errors only).

**Observational errors**: Observational errors are the ones corresponding to the precision of the instruments, plus when available, the ones due to inaccurate absolute calibration. The precision of in situ SSS is generally considered to be less than 0.01 for an individual measurement but absolute calibration of merchant ships TSG can be as large as 0.1 for a given transect. For satellite SSS, the absolute calibration error is usually unknown, the precision is on the order of 0.4 - 0.6 for individual SSS in warm regions as retrieved from Aquarius, or from SMOS and SMAP respectively. These observational errors are reduced at level 3 and level 4 according to the number of satellite passes occurring in the same pixel over one week, by roughly a factor $\sqrt{2}$ for Aquarius, and a factor 2 to 3 for SMOS and SMAP (see E3UB report).

**Sampling errors**: According to [RD 07], sampling errors arise when one data type does not represent a process (or scale) that the other does, e.g., due to the differences in their spatial and/or temporal samplings. Sampling errors are the “expected” differences, the low bound at which two estimates are allowed to differ.

**Satellite SSS**: Sea Surface Salinity within the first centimetre of the sea surface, by nature integrated over a surface that depends on the radiometer characteristics and on the data processing.

**In-situ SSS**: Near Surface Salinity measured at several cm to several meter depth (see Figure 1).
Figure 1: Scale portraying the typical depth at which near-surface salinity is measured by various sensors/platforms. The small squares show the average measurement depth and the capped lines show the range for that average. For profiling platforms (ASIP, Bow Bridle, STS-Argo, Argo) the range represents the variability of the top-most point in the profile. For platforms with standardized configurations that measure at fixed depths (Salinity Snake, SSP, Wave Glider) the mean and range of each sensor at a particular depth are shown. For platforms where there are multiple sensor configurations (drifters, mooring, shipborne TSG) or that sample at different depths depending on the specifics of the platform, the range of measurement depths across all platforms is shown. Radiometric penetration depths were calculated using the Stogryn (1997) relationship and show penetration depths at 1.43 GHz over the salinity range of 20 pss to 38 pss and temperature range of −2 ºC to 35 ºC (where the “mean” value shown in the figure is for 20 ºC and 35 pss). (Figure taken from [RD 06])
3 Overview

We use three metrics for assessing the performances of the algorithms. They are designed to characterize uncertainties coming from three different types of errors that are handled differently in the various satellite processing:

**M1: The standard deviation between satellite SSS and in situ SSS:** it characterizes random errors that are expected from measurements noise, from errors that are not well characterized given the present knowledge of the sources of errors...

**M2: The bias between satellite SSS and in situ SSS:** it characterizes systematic errors that are expected from e.g. radiometer calibration issues, land-sea contamination, sun contamination...

**M3: The coefficient of determination (square of correlation coefficient) between satellite SSS and in situ SSS:** it is indicative of the signal to noise ratio and is very sensitive to too stringent filtering or smoothing of extrema values (e.g. low SSS in river plumes).

The significance of the difference between metrics derived from different products is evaluated using classical statistical tests as described in section 6.1. These significance tests take into account estimates of ‘observational errors’ and ‘sampling errors’.

The RR tests of year 1 (June 2018 to June 2019) of the CCI+SSS project include comparisons of salinity retrievals against in-situ observations in the Atlantic Ocean. We use two in situ data sets, PIRATA moorings and two repetitive ship tracks across the Atlantic Ocean.

We compute metrics between CCI+SSS data and in-situ SSS over several periods of time, in order to compare the same metrics over the same period, between in-situ and original salinity products used for generating CCI products (Aquarius, SMOS, and SMAP SSS).

We co-locate satellite and in-situ data with a satellite centred methodology.

Results of this RR exercise clearly show that CCI+SSS gives better results globally in comparison to all original products, for all the periods (Table 4). There are several exceptions, especially near Congo and Amazon rivers. These issues will be discussed at the end of this document.
4 Round robin methodology

Below is the description of the methodology of RR tests. The aim of these tests is to provide few metrics to compare and validate different satellite products. In this first version, we did not prioritize some metrics for algorithm selection, as almost all metrics have been improved, but it may be necessary to refine the strategy for ‘best algorithm selection’ in future RR versions.

We decided to focus on Atlantic Ocean, because it is an area of contrasted SSS regimes with very high and stable SSS in the subtropics and very low SSS near the Amazon and Congo plumes, with some regions strongly affected by RFIs, independent of the SMOS Ocean Target Transformation region (RD04: Yin et al. 2013) where SMOS Tbs are a posteriori calibrated.

This region is well monitored by numerous in-situ measurements along repetitive ship tracks crossing maxima and minima SSS regions or moorings allowing a monitoring of the data quality over the whole satellite period.

4.1 Insitu data

4.1.1 Ship tracks

We use regular merchant ship tracks along AX20 and AX11 lines between Europe and South America, from ORE SSS data base (http://sss.sedoo.fr/). Results presented in this report come from files downloaded on 1st June 2019.

AX20 salinity measurements come mainly from Toucan and Colibri merchant ships. AX11 measurements come from Cap San Lorenzo, Rio Blanco and Santa Cruz merchant ships (RD01).
AX20 and AX11 areas are delimited using linear boundaries, defined as $Lat = a \cdot Lon + b$, with $a$ and $b$ coefficients shown in Table 1.

A transect is considered as AX20 if the majority of its points below 45°N are between lines 1 and 2 (Figure 2).

A transect is considered as AX11 if the majority of its points below 45°N are between lines 2 and 3.

We consider only points below 45°N to determine if a transect is AX20 or AX11, because these two lines overlap in northern latitudes.

Only points included in these areas, more than 40 km away from coasts and below 45° north, and only if there are at least 100 points for one transect in one of these areas, are taken into account in the statistics.

We only use ship tracks that go at least from 20°N to 35°N.

The quality check is used to keep only good and probably good data.

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Considering all these measurements, we get between 6 and 9 good quality ship transect for AX11 and AX20 per year, except for 2018 (Figure 3).

Salinity measurements are collected at 5 meters depth for all AX20 tracks and at 10 meter depth for AX11 transects.

Figure 3: Histogram of ship transects

4.1.2 PIRATA

The second dataset we use is the Prediction and Research Moored Array in the Tropical Atlantic (PIRATA). PIRATA is composed of 18 moorings in tropical Atlantic, between 20°S and 20°N (Figure 4). These moorings provide daily measurements of salinity. We use a dataset from 2010 to 2016.

We use delayed mode data from PMEL (http://www.pmel.noaa.gov/gtmba/pmel-theme/atlantic-ocean-PIRATA), corrected from biases and drifts by Gilles Reverdin (LOCEAN) and Elodie Kestenare (LEGOS) (personal communication). This dataset is available from 2010 to 2016.

For our tests, we only use data collected at a depth smaller than five meters.
4.2 Colocation methodology

Our colocation methodology is centred on satellite measurements. We adapt the in-situ measurements in order to get an equivalent representativity of data to the satellite product we study.

4.2.1 Moorings

- spatial colocation: we compare mooring data to the nearest neighbour satellite pixel (i.e. given the spatial resolution of the satellite grids, at less than 0.125° for SMOS, 0.1° for SMAP and 0.5° for Aquarius measurements).

- temporal colocation: mooring data are averaged over satellite data temporal averaging period (T) (e.g. 7-days or one month for CCI comparisons depending on the product resolution) at each available day of the period. We use a mean weighted with a gaussian distribution (sigma=T/4).
4.2.2 Ship tracks

spatial colocation: Ship measurements are smoothed along the track, over the spatial resolution of the satellite, with a gaussian weight.

The standard deviation is set to one quarter of the spatial resolution (95% of the weight in a radius of half the spatial resolution).

This smoothing is limited to 2 hours before and 2 hours after the central point.

Then, we average ship measurements taken successively over the same satellite pixel.

Only pixels with more than 4 available in-situ measurements are used for the statistics.

The resulting colocations are compared to the nearest corresponding satellite pixel in time.
4.3 Metrics

For selecting the algorithm, the metrics defined in section 3 are computed as described below (horizontal bars indicate the mean over a set of measurements). The tests about the significance of the difference between metrics derived from different products are described in section 6.1.

- standard deviation of the differences (std diff)

\[
\text{std}_\text{diff} = \sqrt{\text{SSS}_{\text{in-situ}} - \text{SSS}_{\text{satellite}}}^2 - (\text{SSS}_{\text{in-situ}} - \text{SSS}_{\text{satellite}})^2
\]

- bias

\[
\text{bias} = \frac{\text{SSS}_{\text{in-situ}} - \text{SSS}_{\text{satellite}}}{\text{SSS}_{\text{in-situ}}}
\]

- coefficient of determination \( r^2 \) of the linear regression \( y \) between in-situ SSS and satellite SSS:

\[
r^2 = \max \left[ 0,1 - \frac{\sum (Y - y)^2}{\sum (Y - \bar{Y})^2} \right], \text{ with } Y = \text{SSS}_{\text{in-situ}} - \text{SSS}_{\text{satellite}}
\]

In these equations, \( \text{SSS}_{\text{in-situ}} \) corresponds to the salinity of the in-situ measurements, after the colocation processing described before.
$SSS_{satellite}$ corresponds to the salinity sensed by satellite.

$n$ is the number of measurements.

In addition, we compute the rmsd:

$$rmsd = \sqrt{(SSS_{in-situ} - SSS_{satellite})^2}$$

We do not use rmsd for selecting the algorithm as it is related to the bias and $std_{diff}$:

$$rmsd = \sqrt{std_{diff}^2 + bias^2}$$

### 4.4 Figures

We use three kinds of representations for displaying our RR tests.

- Maps

For moorings we compute these four metrics considering every colocation point during a given laps of time, at each mooring location.

Ship transects are divided into bands of three degrees of latitude. We compute statistics for each band, considering every colocation point during the studied time laps.

Maps are used to see in which areas strong differences between CCI product and reference are observed.

- Scatterplots

Statistics are computed for CCI products and for a reference satellite product. Results are analysed in the form of a scatterplot comparing results of CCI products vs the reference product.

In every scatterplot we plot the diagonal in blue and a linear fit in red (except for biases, where the red line corresponds to zero).

Scatterplot for AX20 and AX11 are in two separated figures.

For ship tracks, colours correspond to the mean latitude of the latitudinal bands we defined to calculate statistics.

Scatterplots show clearly how CCI products globally evolved in comparison to the reference.
- Time series

Scatterplots and maps show statistics computed during the entire period, and therefore do not give any information on the temporal evolution of the products. To look at it we used time series.

For PIRATA we simply plot the evolution of each mooring, in comparison to the corresponding collocated satellite data (CCI and reference).

For merchant ship data we compute global statistics for each available ship transect and we plot the evolution of the metrics in time.
5 Description of the algorithms & ancillary data tested during the round robin exercise

In this first RR tests, we tested 5 versions of CCI+SSS products which allow to identify flaws and bugs. The sixth and seventh versions are equivalent to the fifth, only the structure of NetCDF files have been modified. We report here comparisons between CCI+SSS v1.7 that we compare to the original SSS of each individual satellite. Only satellite pixels further than a satellite footprint are considered:

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<td>7 days</td>
<td>150km</td>
<td>1 day</td>
<td>2011/06/01 2015/05/01</td>
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Table 2: Original products compared to CCI in the RR tests

We consider SMOS products sampled over the same grid as CCI, without spatial averaging, so with a spatial resolution of about 50km, close to SMAP resolution.
6 Algorithms selection

6.1 Results of the round robin exercise

In order to highlight the differences between CCI and original satellite products, we report the summary of the comparison metrics in the tables below. We coloured the table cells to indicate in green improved statistics with respect to other products and in red degraded statistics. When products have equivalent statistics, they are set to white. See Table 3 for a more precise explanation of the colouring method.

<table>
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<tr>
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<td>+</td>
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</tr>
<tr>
<td>+</td>
<td>-</td>
<td>CCI better than Ref1 worse than Ref2: Ref1 red, Ref2 green, CCI white</td>
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<td>CCI equivalent to Ref1 and equivalent to Ref2: Ref1 white, Ref2 white, CCI white</td>
</tr>
</tbody>
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Table 3: Meaning of colours in result tables. Ref1=reference product 1; Ref2=reference product 2

To define the colours, we look at the level of significance of the differences between the metrics computed with various products. For the first RR, they are defined as follows; this definition could be refined in future RR.

- **Bias:**

We first consider a systematic observational error on each ship transect equal to the one specified in ship files, Ship-transect. We also consider the sampling error coming from the natural variability of SSS within a satellite pixel and within one week, $Enat$; we derive an order of magnitude of $Enat$ from the standard deviation of in situ SSS within 50km (Figure 7).

The resulting uncertainty on the ship-satellite SSS coming from ship SSS systematic observational error and sampling error is roughly estimated as:

$$E_{bias} = \sqrt{\frac{E_{ship\_transect}^2}{N_{transect}} + \frac{E_{nat}^2}{N_{ind}}}$$
With $E_{\text{ship\_transect}}$ the systematic observational error over each transect,

$N_{\text{transect}}$ the number of transects

$E_{\text{nat}}$ the sampling error related to SSS natural variability

$N_{\text{ind}}$ the number of independent colocation points.

Far from coast, according to Figure 7, the sampling error due to natural variability is smaller than 0.1 so that $E_{\text{ship\_transect}}$ dominates the total error. It is on the order of 0.1 pss for each transect; considering the number of averaged transects $N_{\text{transect}}$, we use as threshold for significant bias:

$$B_{\text{thresh}} = \sqrt{\frac{0.1^2}{N_{\text{transect}}}}$$

It varies in the range 0.009 pss for the total period to 0.016 pss for the SMAP period.

On another hand, at less than 100km from coast, $B_{\text{thresh}}$ is dominated by the sampling error. Considering Figure 7, a natural variability of 0.5 pss seems a reasonable order of magnitude for $B_{\text{thresh}}$. 
For PIRATA moorings, we consider an error of the order of 0.1pss, so $B_{\text{thresh}} = \sqrt{\frac{0.1^2}{N_{\text{moorings}}}}$, with $N_{\text{moorings}}$ the number of moorings.

- **Std diff**: We test the significance of the differences between std diff of CCI and original products by using a Fisher-Snedecor test, with a threshold of 5% of significance.

  - We test the significance between correlation coefficients of CCI ($r_{CCI}$) and original products ($r_{orig}$). If $r_{orig}$ is near 0, we can use a t-test; if not, we have to pass the correlation coefficients through Fisher transformation, and we use the test described in Biometry (RD03) page 585. We use a threshold of 5% of significance.

We define ‘better’, ‘worse’ and ‘equivalent’ statistics using following criteria:

- **Bias**
  - Product A better than product B if $|\text{bias}_A| \leq |\text{bias}_B| - B_{\text{thresh}}$
  - Product A equivalent to product B if $|\text{bias}_A - \text{bias}_B| < B_{\text{thresh}}$
  - Product A worse than product B if $|\text{bias}_A| \geq |\text{bias}_B| + B_{\text{thresh}}$

- **Std diff**
  - Products A and B are equivalent if the difference of Std diff is not significant
  - Product A better than product B if the difference of Std diff is significant, and $\text{std}\_\text{diff}_A \leq \text{std}\_\text{diff}_B$
  - Product A worse than product B if the difference of Std diff is significant, and $\text{std}\_\text{diff}_A \geq \text{std}\_\text{diff}_B$

- **$r^2$**
  - Products A and B are equivalent if the difference of $r^2$ is not significant
  - Product A better than product B if the difference of $r^2$ is significant, and $r^2_A \geq r^2_B$
Product A worse than product B if the difference of $r^2$ is significant, and $r^2_A \leq r^2_B$

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Table 4: Results of RR tests over total period (NB the number of points corresponds to the number of points over the EASE grid that is oversampled at 25km resolution; the number of independent pixels is roughly 1/2 this number of points). CCI Better in 11 cases; worse in 0 case; equivalent in 1 case.
### Table 5: Results of RR tests over SMOS period; CCI Better in 11 cases; worse in 0 cases; equivalent in 1 cases

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### Table 6: Results of RR tests over SMAP period; CCI Better in 8 cases; worse in 3 cases; equivalent in 1 case.

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Table 7: Results of RR tests over Aquarius period; CCI Better in 11 cases; worse in 0 case; equivalent in 1 case. Note that spatial resolution of Aquarius differs from the one of SMOS and of CCI products.

Figure 8: Comparisons with PIRATA moorings, SMAP period. (a) $r^2$ SMAP, (b) $r^2$ SMOS, (c) $r^2$ CCI, (d) bias SMAP, (e) bias SMOS, (f) bias CCI

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Table 4 to Table 7 summarize the results of RR tests. The number of collocated points differs because our colocation methodology takes into account the dimensions of the grid of satellite products, and because products do not have exactly the same criteria to eliminate RFI, land or sea ice contaminated areas.

With respect to original processing, CCI products are globally in a better accordance with in-situ data. Improvement is particularly clear over the total period (from 2010 to 2018) and the SMOS-only period: comparing to SMOS product, the \( r^2 \) with respect to ships measurements increased from 0.68 to 0.81, \( std\_diff \) decreased from 0.7 to 0.49 and bias from -0.1 to -0.03 over the entire period; \( r^2 \) increased from 0.59 to 0.82, \( std\_diff \) decreased from 0.87 to 0.41 and biases from -0.28 to -0.12 during SMOS-only period.

Over SMAP or Aquarius periods, the improvement is also clear on \( std\_diff \) and \( r^2 \): \( r^2 \) still rise from 0.77/0.79 (for SMOS only/SMAP only) or 0.70/0.74 (for SMOS only/Aquarius only) to 0.82. \( Std\_diff \) is also reduced, from 0.61/0.57 (for SMOS only/SMAP only) to 0.52 for SMAP period, and from 0.67/0.52 (for SMOS only/Aquarius only) to 0.47 for Aquarius period. Biases remain equivalents over these periods. It is also remarkable that for global Atlantic Ocean, CCI product give always better results than all the original products. This indicates that CCI product is more efficient than a simple average of input satellite products, and brings a real improvement on salinity fields. Figure 8 shows an example for \( r^2 \) and bias over SMAP period, compared to PIRATA moorings. (e.g.: at 0N35W, CCI bias is smaller than SMOS bias and SMAP bias; at 4N38W, \( r^2 \) of CCI is better than \( r^2 \) for SMOS and \( r^2 \) for SMAP).

Statistics with PIRATA moorings give similar information: a better performance of CCI globally, particularly for the entire period, and with exception of biases during SMAP and Aquarius periods. However, when looking to maps, we can notice moorings where CCI give worse results than input products. This is particularly the case for the mooring near Congo river (6S8E).

Finally, we observe that this improvement occurs mainly further than 100km from coasts. At less than 100km from coast, statistical metrics do not systematically indicate an improvement; however, due to large SSS natural variability in these regions and the fact that SSS distribution in variable regions is far from gaussian, the results of our tests need to be kept cautiously. In particular the reduction of \( std\_diff \) during the Aquarius period with Aquarius products is likely an artefact of a larger smoothing of Aquarius SSS relatively to SMOS/SMAP SSS. Except for total period and SMOS period, where we observe a clear improvement of statistics over 45°N due to important RFI in 2012, statistics in high latitudes remains nearly unchanged.

### 6.2 Rationale for the algorithm’s selection

The debiasing method used in CCI+SSS algorithm allows an adjustment of all satellite salinity measurements. The bias, \( std\_diff \) and \( r^2 \), are improved almost everywhere with respect to...
original products. According to the comparisons in Table 4 to Table 7, we observe that CCI products improve significantly around 78% of the statistics with respect to in-situ data (47 cases over 60), and degrades only 6.6% of the statistics (4 cases): these degradations concern relatively small bias differences (less than 0.02) or std_diff at less than 100km from coast, region characterized with large natural variability leading to uncertainties in the absolute calibration, and possibly affected by RFIs. 15% (9 cases over 60) of the statistics remain equivalent or intermediate between reference products and CCI.

This shows that the self-consistency debiasing method reduce systematic biases and provide a less biased product than a simple average of the input products

6.3 Open issues and discussion

In section 6.1, we noticed bad results of CCI+SSS with respect to PIRATA mooring near Congo river. This can be due to the proximity of the corresponding mooring to a very strong gradient of variability in salinity (see Figure 9). The variability field used in CCI algorithm, which is a climatology, could be too low in this area.

Figure 9: Time series of PIRATA mooring at 6S8E, near Congo river. (a) Total period, (b) Aquarius period, (c) SMAP period, (d) Example of salinity gradients near Congo river (SSS SMOS, 2017/08/27)

On the first version of CCI+SSS products, emphasis has been put on tropical and subtropical regions. In the future, more attention will be paid to high latitudes.
7 Conclusion and future work

The first version of the RR tests applied to v1.6 of CCI+SSS products show that statistics relative to in-situ measurements do not really improve in river plumes areas (Amazon (AX20 close to American coast) and Congo (PIRATA mooring at 6S 8E)) with respect to original SSS from each satellite mission. In these areas, CCI+SSS have sometimes a more important bias than original products (see bias figures in the annexes), likely due to an absolute calibration issue. This may also be a consequence of a too weak variability in 7 days products. One perspective for the generation of next version of CCI+SSS products will be to increase the variability allowed in the generation of the weekly products.

In the next version of RR we plan to:

- prioritize the metrics for selecting the ‘best’ algorithm. Actually, in this first version of CCI+SSS products the improvement with respect to original products is very clear, but it is expected to be less clear in future versions.

- Add a class of distance to coast equal to 400km in the metrics calculation, as land-sea contamination remains large within this distance to coast

- Add a validation of the errors in the products, for instance by comparing statistical distributions of the satellite minus in situ SSS differences normalized by the theoretical errors with gaussian distribution having a standard deviation equal to one.

- Ensure that comparisons between several CCI+SSS versions are made over the same grid points

- Extend the verification toward the North Atlantic subpolar gyre e.g., by integrating comparisons with monthly binned SSS from ships of opportunity up to 2017 (RD03: Reverdin et al. 2018)
Figure 10: In-situ data at high latitude
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**CCI Better in 11 cases; worst in 0 cases; equivalent in 1 case.**

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CCI Better in 11 cases; worst in 0 cases; equivalent in 1 case.
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CCI Better in 8 cases; worst in 3 cases; equivalent in 1 case.

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CCI Better in 11 cases; worst in 0 cases; equivalent in 1 case.

For all comparisons and all stats: CCI Better in 41 cases; worst in 3 cases; equivalent in 4 cases.
2.1 summary

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Ref2: CCI better than Ref1 worst than Ref2: Ref1 red, Ref2 green, CCI white
Ref1 and equivalent to Ref2: Ref1 red, Ref2 white, CCI green
CCI worst than Ref1 and worst than Ref2: Ref1 green, Ref2 green, CCI red
CCI worst than Ref1 equivalent to Ref2: Ref1 green, Ref2 white, CCI white
CCI equivalent to Ref1 and better than Ref2: Ref1 white, Ref2 red, CCI green
CCI equivalent to Ref1 and worst than Ref2: Ref1 white, Ref2 green, CCI red
CCI equivalent to Ref1 and equivalent to Ref2: Ref1 white, Ref2 white, CCI white

For all comparisons and all stats: CCI Better in 11 cases; worst in 0 cases; equivalent in 1 case.
2.2 Atlantic

2.2.1 PIRATA

2.2.1.1 Tracks examples

![Salinities at 6S10W](image1)

Figure 1: Example of PIRATA moorings, weekly

2.2.1.2 bias

![Bias maps](image2)

(a) bias, CCIv2019 7 7, SMOS period (b) bias, SMOS L3QA 317, SMOS period

Figure 2: PIRATA, bias maps, SMOS period
2.2.1.3 $r^2$

(a) $r^2$, CCI v2019 7 7, SMOS period (b) $r^2$, SMOS L3QA 317, SMOS period

Figure 4: PIRATA, $r^2$ maps, SMOS period

2.2.1.4 $\text{rmsd}$

Figure 5: $r^2$, CCI v2019 7 7 vs SMOS L3QA 317, SMOS period
2.2.1.5 \textit{std diff}

Figure 6: PIRATA, rmsd maps, SMOS period

Figure 7: rmsd, CCI v2019 7 7 vs SMOS L3QA 317, SMOS period

Figure 8: PIRATA, std diff maps, SMOS period
Figure 9: std diff, CCI v2019 7 7 vs SMOS L3QA 317, SMOS period

2.2.2 Ship tracks
2.2.2.1 Time series
Figure 10: Statistics over Ship tracks, SMOS period
2.2.2.2 bias

Figure 11: Statistics over Ship tracks, by 3 degrees of latitude

Figure 12: bias SMOS L3QA 317 vs CCI v2019 7 7, SMOS period

2.2.3 r2
2.2.2.4 **rmsd**

Figure 13: Statistics over Ship tracks, by 3 degrees of latitude

(a) \( r^2 \), CCI v2019 7 7, SMOS period
(b) \( r^2 \), SMOS L3QA 317, SMOS period

Figure 14: \( r^2 \) SMOS L3QA 317 vs CCI v2019 7 7, SMOS period

(a) Scatterplot 2, SMOS period, AX20
(b) Scatterplot \( r^2 \), SMOS period, AX11
2.2.2.5 std diff
Figure 17: Statistics over Ship tracks, by 3 degrees of latitude

Figure 18: std_diff SMOS L3QA 317 vs CCI v2019 7 7, SMOS period

3.1 summary

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CCI Better in 8 cases; worst in 0 cases; equivalent in 4 cases.

For all comparisons and all stats: CCI Better in 8 cases; worst in 0 cases; equivalent in 4 cases.
3.2 Atlantic
3.2.1 PIRATA
3.2.1.1 Tracks examples
Figure 19: Example of PIRATA moorings, weekly
3.2.1.2 bias

(a) bias, CCl v2019 7 7, SMAP period (b) bias, SMOS L3QA 317, SMAP period

Figure 20: PIRATA, bias maps, SMAP period

3.2.1.3 r2

(a) r2, CCl v2019 7 7, SMAP period (b) r2, SMOS L3QA 317, SMAP period

Figure 22: PIRATA, r2 maps, SMAP period
3.2.14 **rmsd**

(a) rmsd, CCI v2019 7 7, SMAP period
(b) rmsd, SMOS L3QA 317, SMAP period

Figure 24: PIRATA, rmsd maps, SMAP period

3.2.15 **std diff**

Figure 25: rmsd, CCI v2019 7 7 vs SMOS L3QA 317, SMAP period
3.2.2 Ship tracks

3.2.2.1 Time series
Figure 28: Statistics over Ship tracks, SMAP period
### 3.2.2.2 bias

![Figure 29](image_url1)

(a) bias, CCI v2019 7 7, SMAP (b) bias, SMOS L3QA 317, SMAP period

Figure 29: Statistics over Ship tracks, by 3 degrees of latitude

![Figure 30](image_url2)

(a) Scatterplot bias, SMAP period, AX20 (b) Scatterplot bias, SMAP period, AX11

Figure 30: bias SMOS L3QA 317 vs CCI v2019 7 7, SMAP period

### 3.2.3 r2
3.2.2.4 \textit{rmsd}
3.2.2.5 \textit{std diff}

Figure 33: Statistics over Ship tracks, by 3 degrees of latitude

Figure 34: rmsd SMOS L3QA 317 vs CCI v2019 7 7, SMAP period
Round Robin tests: Report 27-Aug-2019

Figure 35: Statistics over Ship tracks, by 3 degrees of latitude

(a) \( \text{std diff, CCI v2019 7 7, SMAP} \)
(b) \( \text{std diff, SMOS L3QA 317, SMAP period} \)

Figure 36: \( \text{std diff SMOS L3QA 317 vs CCI v2019 7 7, SMAP period} \)
4 Annex 3: SMOS L3QA 317 vs CCI v2019 7 7, SMOSTotal period.

4.1 summary

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CCI Better in 11 cases; worst in 0 cases; equivalent in 1 case.

For all comparisons and all stats: CCI Better in 11 cases; worst in 0 cases; equivalent in 1 case.
4.2 Atlantic
4.2.1 PIRATA
4.2.1.1 Tracks examples
Figure 37: Example of PIRATA moorings, weekly
4.2.1.2 bias

(a) bias, CCI v2019 7 7, SMOSTotal period  (b) bias, SMOS L3QA 317, SMOSTotal period

Figure 38: PIRATA, bias maps, SMOSTotal period

Figure 39: bias, CCI v2019 7 7 vs SMOS L3QA 317, SMOSTotal period

4.2.1.3 r²

(a) r², CCI v2019 7 7, SMOSTotal period  (b) r², SMOS L3QA 317, SMOSTotal period

Figure 40: PIRATA, r² maps, SMOSTotal period
2/PIRATA, SMOS_L3QA_317 vs CCI_v2019_7_7 SMOSTc

Figure 41: r2, CCI v2019 7 7 vs SMOS L3QA 317, SMOSTotal period

4.2.1.4 rmsd

(a) rmsd, CCI v2019 7 7, SMOSTotal period  
(b) rmsd, SMOS L3QA 317, SMOSTotal period

Figure 42: PIRATA, rmsd maps, SMOSTotal period

4.2.1.5 std diff

Figure 43: rmsd, CCI v2019 7 7 vs SMOS L3QA 317, SMOSTotal period
4.2.2 Ship tracks

4.2.2.1 Time series

Figure 44: PIRATA, std diff maps, SMOSTotal period

Figure 45: std diff, CCI v2019 7 7 vs SMOS L3QA 317, SMOSTotal period
Figure 46: Statistics over Ship tracks, SMOSTotal period
4.2.2.2 bias

Figure 47: Statistics over Ship tracks, by 3 degrees of latitude

(a) bias, CCI v2019 7 7, SMOSTotal period
(b) bias, SMOS L3QA 317, SMOSTotal period

Figure 48: bias SMOS L3QA 317 vs CCI v2019 7 7, SMOSTotal period

(a) Scatterplot bias, SMOSTotal period, AX20
(b) Scatterplot bias, SMOSTotal period, AX11

4.2.3 r2
4.2.2.4 rmsd
4.2.2.5 std diff

Figure 51: Statistics over Ship tracks, by 3 degrees of latitude

Figure 52: rmse SMOS L3QA 317 vs CCI v2019 7 7, SMOSTotal period
Figure 53: Statistics over Ship tracks, by 3 degrees of latitude

Figure 54: std diff SMOS L3QA 317 vs CCI v2019 7 7, SMOSTotal period

5.1 summary

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CCI better than Ref1 and Ref2: Ref1 red, Ref2 red, CCI green
CCI better than Ref1 worst than Ref2: Ref1 red, Ref2 green, CCI white
CCI better than Ref1 and equivalent to Ref2: Ref1 red, Ref2 white, CCI green CCI worst than Ref1 and better than Ref2: Ref1 green, Ref2 red, CCI white CCI worst than Ref1 and worst than Ref2: Ref1 red, CCI worst than Ref1 and equivalent to Ref2: Ref1 green, Ref2 white, CCI white CCI equivalent to Ref1 and worst than Ref2: Ref1 white, Ref2 green, CCI red
CCI equivalent to Ref1 and equivalent to Ref2: Ref1 white, Ref2 white, CCI white

$$Ref1 + Ref2 = Product$$

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<th>std diff</th>
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CCI Better in 11 cases; worst in 0 cases; equivalent in 1 case.

For all comparisons and all stats: CCI Better in 11 cases; worst in 0 cases; equivalent in 1 case.
5.2 Atlantic

5.2.1 PIRATA

5.2.1.1 Tracks examples
Figure 55: Example of PIRATA moorings, weekly
5.2.1.2 bias

Figure 56: PIRATA, bias maps, Aquarius period

Figure 57: bias, CCI v2019 7 7 vs SMOS L3QA 317, Aquarius period

5.2.1.3 r2

Figure 58: PIRATA, r2 maps, Aquarius period
Figure 59: r2, CCI v2019 7 7 vs SMOS L3QA 317, Aquarius period

5.2.1.4 rmsd

Figure 60: PIRATA, rmsd maps, Aquarius period

Figure 61: rmsd, CCI v2019 7 7 vs SMOS L3QA 317, Aquarius period

5.2.1.5 std diff
5.2.2 Ship tracks

5.2.2.1 Time series
Round Robin tests: Report 27-Aug-2019

Figure 64: Statistics over Ship tracks, Aquarius period
5.2.2.2 bias

Figure 65: Statistics over Ship tracks, by 3 degrees of latitude

Figure 66: bias SMOS L3QA 317 vs CCI v2019 7 7, Aquarius period

5.2.2.3 $r^2$
5.2.2.4 \textit{rmsd}
5.2.2.5 std diff
Round Robin tests: Report 27-Aug-2019

Figure 71: Statistics over Ship tracks, by 3 degrees of latitude

Figure 72: std diff SMOS L3QA 317 vs CCI v2019 7 7, Aquarius period
6 Annex 5: SMAP RSS3 40 vs CCI v2019 7 7, SMAP period.

6.1 summary

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<td>CCI v2019 7 7</td>
<td>50 km</td>
<td>7 days</td>
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For all comparisons and all stats: CCI Better in 8 cases; worst in 3 cases; equivalent in 1 case.

CCI Better in 8 cases; worst in 3 cases; equivalent in 1 case.
6.2 Atlantic

6.2.1 PIRATA

6.2.1.1 Tracks examples
Salinities at 6S10W

(a) 6S10W weekly

Salinities at 6S8E

(b) 6S8E weekly

Figure 73: Example of PIRATA moorings, weekly
6.2.1.2 bias

(a) bias, CCIv201977, SMAP period (b) bias, SMAP RSS3 40, SMAP period

Figure 74: PIRATA, bias maps, SMAP period

6.2.1.3 r2

(a) r2, CCIv201977, SMAP period (b) r2, SMAP RSS3 40, SMAP period

Figure 76: PIRATA, r2 maps, SMAP period
6.2.1.4 rmsd

(a) rmsd, CCI v2019 7 7 vs SMAP period (b) rmsd, SMAP RSS3 40, SMAP period

Figure 78: PIRATA, rmsd maps, SMAP period

Figure 79: rmsd, CCI v2019 7 7 vs SMAP RSS3 40, SMAP period

6.2.1.5 std diff
6.2.2 Ship tracks

6.2.2.1 Time series
Figure 82: Statistics over Ship tracks, SMAP period

(a) AX20

(b) AX11
6.2.2.2 bias

(a) bias, CCI v2019 7 7, SMAP (b) bias, SMAP RSS3 40, SMAP
period

Figure 83: Statistics over Ship tracks, by 3 degrees of latitude

(a) Scatterplot bias, SMAP period, AX20 (b) Scatterplot bias, SMAP period, AX11

Figure 84: bias SMAP RSS3 40 vs CCI v2019 7 7, SMAP period

6.2.2.3 \( r^2 \)
Figure 85: Statistics over Ship tracks, by 3 degrees of latitude

Figure 86: r² SMAP RSS3 40 vs CCI v2019 7 7, SMAP period

6.2.2.4 rmsd
6.2.2.5 std diff
Round Robin tests: Report 27-Aug-2019

Figure 89: Statistics over Ship tracks, by 3 degrees of latitude

Figure 90: std diff SMAP RSS3 40 vs CCI v2019 7 7, SMAP period

(a) Scatterplot std diff, SMAP period, AX20
(b) Scatterplot std diff, SMAP period, AX11

7.1 summary

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Ref1 Ref2 Product

+ + CCI better than Ref1 and Ref2: Ref1 red, Ref2 red, CCI green
+ - CCI better than Ref1 worst than Ref2: Ref1 red, Ref2 green, CCI white
+- CCI better than Ref1 and equivalent to Ref2: Ref1 red, Ref2 white, CCI green CClworstthanRef1 and betterthanRef2: Ref1 green, Ref2 red, CCI white CClworstthanRef1andworstthanRef2:
- - CClworstthanRef1 and worstthanRef2: Ref1 green, Ref2 green, CCI red CClworstthanRef1 and equivalenttoRef2: Ref1 green, Ref2 white, CCI red
= + CCI equivalent to Ref1 and worst than Ref2: Ref1 white, Ref2 red, CCI green CCI equivalent to Ref1 and equivalent to Ref2: Ref1 white, Ref2 white, CCI red
= - CCI equivalent to Ref1 and equivalent to Ref2: Ref1 white, Ref2 white, CCI white
= = CCI equivalent to Ref1 and equivalent to Ref2: Ref1 white, Ref2 white, CCI white

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CCI Better in 9 cases; worst in 0 cases; equivalent in 3 cases.

For all comparisons and all stats: CCI Better in 9 cases; worst in 0 cases; equivalent in 3 cases.
7.2 Atlantic
7.2.1 PIRATA
7.2.1.1 Tracks examples
Figure 91: Example of PIRATA moorings, weekly
7.2.1.2 **bias**

![Bias plots](image1)

(a) bias, AQUARIUS CAPv5, Aquarius period

(b) bias, CCI v2019 7 7, Aquarius period

**Figure 92:** PIRATA, bias maps, Aquarius period

![Correlation plots](image2)

**Figure 93:** bias, CCI v2019 7 7 vs AQUARIUS CAPv5, Aquarius period

7.2.1.3 **r²**

![R² plots](image3)

(a) r², AQUARIUS CAPv5, Aquarius period

(b) r², CCI v2019 7 7, Aquarius period

**Figure 94:** PIRATA, r² maps, Aquarius period
7.2.14 \( \text{rmsd} \)

```
(a) rmsd, AQUARIUS_CAPv5, Aquarius period
(b) rmsd, CCI_v2019_7_7, Aquarius period
```

Figure 96: PIRATA, rmsd maps, Aquarius period

7.2.15 \( \text{std diff} \)

```
Figure 97: rmsd, CCI_v2019_7_7 vs AQUARIUS_CAPv5, Aquarius period
```
7.2.2 Ship tracks

7.2.2.1 Time series
Figure 100: Statistics over Ship tracks, Aquarius period
7.2.2.2 bias

Figure 101: Statistics over Ship tracks, by 3 degrees of latitude

(a) Scatterplot bias, Aquarius period, AX20
(b) Scatterplot bias, Aquarius period, AX11

Figure 102: bias AQUARIUS CAPv5 vs CCI v2019 7 7, Aquarius period

7.2.2.3 r2
Figure 103: Statistics over Ship tracks, by 3 degrees of latitude

Figure 104: r² AQUARIUS CAPv5 vs CCI v2019 7 7, Aquarius period

7.2.2.4 rmsd
7.2.2.5 **std** diff
Figure 107: Statistics over Ship tracks, by 3 degrees of latitude

Figure 108: std diff AQUARIUS CAPv5 vs CCI v2019 7 7, Aquarius period