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Acronyms

AD	Applicable document
ADB	Actions database
ADS	Analysis Dataset
ATBD	Algorithm theoretical basis documents
BEC	Barcelona Expert Center
CSIC	Consejo Superior de Investigaciones Científicas
CTC	Correlated Triple Collocation
DIR	Directory
DNB	Debiased Non-Bayesian
DS	Dataset availability
DUM	Dataset user manual
DVP	Development and validation plan
EO	Earth Observation
EOEP	Earth Observation Envelope Program
ESA	European Space Agency
ESL	Expert Support Laboratory
FR	Final review
FWF	Freshwater fluxes
GCOS	Global Climate Observing System
GNSS	Global Navigation Satellite System
IAR	Impact assessment report
IASC	International Arctic Science Committee
ICES	International Council for the Exploration of the Sea
ICM	Institute of Marine Sciences
IEEC	Institut d'Estudis Espacials de Catalunya
IPCC	Intergovernmental Panel on Climate Change
ISC	Ice-Sea Contamination
ITT	Invitation to tender
KO	Kick-off
L2OS	Level 2 Ocean Salinity
LSC	Land-Sea Contamination
MFF	Multifractal Fusion
MTR	Mid-term review
PAR	Preliminary analysis report
PGICs	Peripheral glaciers and ice caps
PM	Progress meeting
PMP	Project Management Plan
p.s.u.	Practical Salinity Unit
PDS	Power Density Spectra
PVR	Product Validation Report
RB	Requirements baseline
RD	Reference document

RFI	Radio Frequency Interference
SAR	Synthetic Aperture Radar
SIAR	Scientific and impact assessment report
SMAP	Soil Moisture Active and Passive
SMOS	Soil Moisture and Ocean Salinity
SoW	Statement of work
SR	Scientific roadmap
SSS	Sea Surface Salinity
SST	Sea Surface Temperature
TC	Triple Collocation
TDP	Technical data package
TN	Technical note
UPC	Universitat Politècnica de Catalunya
VIR	Validation and intercomparison report
VR	Validation report
WP	Work package

1 Introduction

1.1 Scope of this document

This document holds the Product Validation Report (PVR) prepared by Arctic+ Salinity team, as part of the activities included in the [WP301] of the Proposal (Task 3 from SoW ref. **EOP-SDR/SOW/084-17/DFP**).

The objective of this document is to present the results of the validation vs in-situ data of the Arctic+ SSS product v3.1, main output of the project.

1.2 Structure of the document

The PVR is structured as follows:

Section 1 covers the introduction and the description of this document.

Section 2 provides a brief description of all datasets used for the validation of the product. This includes a description of the first regional SSS product followed by the method to validate the new regional SSS product using in-situ observations. This sections also incorporates a description of the utilization of the Pi-MEP as a potential validation tool to be used in EO science.

Section 3 describes the collocation strategy and methods followed according to the type of in-situ data. It also includes the collocation criteria, as well as some specific considerations required by this project.

Section 4 refers to a brief description of the main areas considered during the validation exercises.

Section 5 describes the validation metrics to measure the quality of satellite SSS retrievals against in-situ (or reference) salinity measurements. Further this section introduces Correlated Triple Collocation (CTC) and the Wavenumber Spectral Analysis (WSA), which facilitated the quality assessment of SSS over regions with little to none in-situ observations.

Section 6 describes and analyses the results of the validation for each dataset.

Section 7 closes the report with a Summary and Conclusion of the new regional Arctic+ Salinity product.

1.3 Applicable documents

ATBD	Algorithm Theoretical Baseline Document	Arctic+Salinity_D1.3_ATBD_v2r0
DUM	Data User Manual	Arctic+Salinity_D1.2__v3r0
RBD	Requirement Baseline Document	Arctic+SSS_RBD_D1.2_v1r6
SoW	Statement of Work	EOP-SDR/SOW/084-17/DFP

2 Sea Surface Salinity validation for the Arctic region

The Arctic+ Salinity project is an effort from European Space Agency (ESA) to aid the international science polar research. In particular this project responded to the need to produce SSS product to be used to enhance the understanding of on-going international research projects. The regional SSS product produced was fully described within the terms of this project (ref. ATBDv2.0) and it was validated and discussed in different progress meetings. The outcomes from different internal meeting, were implemented in the Algorithm development document (ref. ATBD v2.0) to produce final Arctic+ Salinity product (v3.1).

This PVR presents the validation results of the SSS product (v3.1). Following sections contain the description of the satellite SSS product (see section 2.1). Next, there is a description of the reference in-situ datasets used as ground truth of salinity value at the surface (section 2.2).

2.1 Sea Surface Salinity satellite products

At the time of writing this PVR, there were 3 SSS products including the Arctic+ Salinity, which were especially designed to retrieve SSS in the Arctic region (Table 1). Hence, this PVR mainly focused on the validation of the Arctic+ Salinity product and other satellite products were only a reference to better understand the quality of the production of the regional product. Following there is a brief description of the main specification of the Arctic+ Salinity product (section 2.1.1). The technical analyses of the other satellite products were outside of the scope of this document. Thus, this PVR does not make an extensive description of those other products other than referring to its technical documentation (Section 1.3).

Table 1: List of satellite-based SSS Arctic-dedicated products.

PRODUCT NAME	ENTITY
BEC SSS V2.0	ICM/CSIC
ARCTIC+ SSS V3.1	ICM/CSIC
CEC-LOCEAN L3 ARCTIC)	CATDS

2.1.1 Arctic+ Salinity product

For this project, BEC developed a regional specific enhanced Arctic SSS product (Table 2, next page). This PVR shows the most up to date validation results obtained by comparing the satellite product against an in-situ data base (i.e., reference or ground truth).

Table 2: Arctic+ Salinity SSS product specifications. Notice that DOI was not provided because the dataset was distributed internally, only.

Specification	*Description*
Time period	2011 to 2019
Spatial resolution	0.25˚ by 0.25˚(EASE grid 2.0)
Temporal resolution	9-day maps generated daily
Version	3.1
Source	FTP hosted by BEC, sftp://becftp.icm.csic.es
DOI	N/A
Filename	BEC-L3-SSS-ARCTIC-025km-YYYYMMDD_YYYYMMDD_301.nc.

Some general information about the products is provided hereinafter:

- The product will be freely distributed and served at the BEC webpage (http://bec.icm.csic.es/) and at the project webpage (https://arcticsalinity.argans.co.uk).
- The product is distributed in the standard grid EASE-Grid 2.0 (ref. ATBD), which has a spatial resolution of 25Km. The product provides centred daily maps of SMOS-based SSS maps for the Arctic region, computed using a sliding window of 9 days.
- Product spans over the period 2011-2019.
- The product contains the following data:
    - Sea Surface Salinity (p.s.u.)
    - Sea Surface Salinity uncertainty (p.s.u.)
    - Sea Surface Salinity anomaly (p.s.u.): Difference between sea surface salinity provided by SSS field and SSS climatology provided by WOA 2018 A5B7.
    - Flags code:
        - HRE (high_radiometric_error): larger than 1.200000 p.s.u. for points closer than 150.000000 km to the ice edge or coast line;
        - LNM (low_number_of_L2B_measures): less than 4 L2B orbits;
        - LNMCORR (low_number_of_L2B_measures_in_spatial_correction_field): less than 50 L2B orbits flagged as good_quality.
        - (GQ): None of the above.

2.1.2 BEC Artic product v2.0

In addition to the validation for Arctic+ Salinity v3.1, the initial BEC product for the Arctic labelled as v2.0 has also been assessed. This product was developed in 2017 by BEC and is described in Olmedo et al., 2018. That product is out of the scope of this Arctic+ Salinity project. However, it has been considered as the benchmark to understand the evolution of the SMOS-based SSS products for the region developed in this initiative. Thus, it has been used.

The BEC Arctic v2.0 is a product that has some differences respect the new product. To start with, the old product uses a regular grid of 25km of spatial resolution, which does not match with EASE v2.0 grid. In addition, the retrieval algorithm is substantially different. In addition, the old product was produced using a variant of Optimal Interpolation, which introduces a non-natural smoothness into the product. This translates usually with a less noise level than the binned products, where no smoothing is applied. In addition, BEC Arctic v2.0 has a general bias correction computed by regressing the fields to an ARGO-derived climatology. This method substantially reduces the bias and centres the dataset vs the in-situ observation. This adjustment may have impact in the absolute bias associated to this older product.

Despite some of those fundamental differences, it was expected that Arctic+ Salinity initiative would yield data of better quality and capacities than the existing one.

2.2 Validation with in-situ data

The Arctic+ Salinity project has identified and described some of the most common in-situ observations available within the region (ref DUM and RBD). This section aims to present a summary description of those datasets used for the validation of the new regional SSS product.

2.2.1 ARGO buoys network

The ARGO project provides temperature and salinity in-situ observations over the global ocean. ARGO consists of almost 4000 floaters distributed over the world ocean. Since 2005, ARGO provides regular measurements of temperature and salinity with a typical sampling cycle from the surface (typically 5 to 10 m depth) down to 2000 m every ten days with a spatial resolution of about 3 degrees (this is roughly a profile every 300 km) *(Ninove et al.*, 2016). This sampling frequency is an advantage over other in-situ based measurements (i.e., ship-based measurements, gliders, moorings), which have such neither spatial nor temporal sampling frequency.

The accuracy of the sensors of temperature, salinity and pressure mounted in the ARGO platforms are ±0.005˚C, ±0.01 p.s.u. and ±2.4 dbar, respectively (ARGO quality control manual, 2011). Each sensor is subject to different quality control checks. This work considered all ARGO floats available from 2011 to 2019. The data was subject to real time and the delayed mode checks to ensure that all the data was classified as ‘good data’ (i.e., QC = 1, see ARGO quality control manual 2011). The process of quality control of the delayed mode can take up to eighteen months from the moment when the profile was recorded. This processing time depends on the Global Data Assembly Centres (GDACs) and it ensures the best quality of the data for analysis with any sensor drift adjustment needed (Wong, et al 2011). Furthermore, following the recommendations in ARGO user's manual, floats were checked against the so-called 'grey list' (downloaded on 19th February 2016). Floats included in this list were not included in the analysis, as they have been reported to have problems in one of the sensors during the real time quality checks. ARGO data is freely available at the GDAC IFREMER:

GDAC ftp://ftp.IFREMER.fr/IFREMER/ARGO/

The resulting ARGO dataset is also available at BEC ftp server. Table 3 below details the list of preliminary control checks done by BEC in the ARGO used later on the validation.

Table 3: Quality control checks for all the ARGO floats included in this study.

Terms	Criteria
QC flag	QC = 1; keep 'good' data only
ARGO Grey list	Platforms ID number were not in the grey list (download September 2019)
Profiles	Both temperature and salinity
Missing value at a given level	Exclude all parameters at the same level
Negative pressure value	Exclude all parameters at the same level

ARGO profiles that waived the quality control checks, had to pass an additional control check to make sure that all floats were 'OK', meaning that all the platforms were providing information on the three parameters with equal quality (Table 3). There were floats with no information of one of the three sensors (i.e., float with temperature information and pressure and missing salinity). There are reports of some floats (i.e., APEX) which can be related to a micro leak fault in the pressure pump (see ARGO data management 2011). Hence, there is the need to make an additional manual check to remove potential spurious pressure readings. The resulting ARGO dataset with all profiles was gridded in a homogeneous 1/2˚ horizontal grid and the depth were approximated to standard depth levels from surface down to 400 m in 5 m depth intervals. The recorded dataset stored in netCDF format in 9-day files containing the profiles within those nine days, centred the middle date (i.e., file content equivalent to the SSS products generated in this project).

As seen in previous works (Olmedo et al., 2018, Olmedo et al. 2020), this PVR used the cut of depth of 10 m, but no measurements shallower than 0.5 m are used due to the formation of bubbles and foam. In some ARGO floats (i.e., SOLO and PROVOR types) sensors measuring the physical properties of the water column (i.e., conductivity, temperature, and depth) stop pumping water at about 5 m depth (ref ARGO user manual).

This PVR used World Ocean Atlas (WOA) 2013 as climatological reference to compute long term anomalies at each profile location. Thus, this PVR discarded ARGO profiles with anomalies larger than 10˚C in temperature or 5 p.s.u. in salinity. A final profile filtering included profiles having temperature close to surface between −2.5˚C and 40˚C and salinity between 2 and 41 p.s.u

2.2.2 Mooring

This PVR found the upper most northern mooring station was PAPA (50˚ 2.5'N, 144˚ 51.9'W), which is part of the NOAA's Ocean Climate Station Project (OCS). This data resulted to be of good quality and expands from 2007 to 2020. However, mooring's latitude is below the minimum latitude (i.e., lat_{min} = 60˚ºN) set for the validation purpose of this PVR. Thus, this PVR did not use mooring data.

2.2.3 Ocean Melting Greenland

The Oceans Melting Greenland (OMG) has the objective to improve the estimates of sea level rise. Over a five-year (starting in 2016) campaign, OMG will observe changing water temperatures on the continental shelf surrounding Greenland, and how marine glaciers react to the presence of warm, saline Atlantic Water. Each year in the summer they have deployed 250 expendable temperature and salinity probes along the continental shelf. This data is public in the webpage and is very useful for validation in the Greenland region.

The colocation of the AXCTD profiles with Arctic+ data is the following: for spatial collocation measurements in a distance less than 12.5kms from the centre of Arctic+ grid point is considered. For the temporal collocation, all profiles within the 9-day product. The salinity values are obtained by doing the mean value in the range [0, 10] meters depth of the AXCTD.

2.2.4 EN4

The EN4 dataset is produced by MetOffice and consists of two products:

- Observed subsurface ocean temperature and salinity profiles with data quality information.
- Objective analyses formed from the profile data with uncertainty estimates. Data are available from 1900 to the present and there are separate files for each month (Good et al 2013).

2.2.5 TARA ship tracks

The Tara Polar Circle Expedition dataset (hereafter, TARA SSS) [28] contains data collected on board of research vessels operating in the Arctic Ocean from June to October 2013. Measuring instruments included thermosalinograph (TSG) Seabird SB45 and a temperature sensor (SBE38) recorded sea surface temperature and salinity at 3 m depth during the whole cruise.

TARA salinity data presented a large range of spatial variability of salinity S[26:35]) in the Arctic Ocean. This dataset was of great value for assessing the annual SSS reference used for the generation of the SMOS SSS product.

2.2.6 Validation against model output dataset

Results comparing the SSS satellite product to assimilating system TOPAZ are included in the Impact Assessment Report (IAR) delivered within this project.

2.3 Pi-MEP

The Pilot Mission Exploitation Mission (Pi-MEP) is an online platform dedicated to the systematic validation of different satellite SSS products. Pi-MEP releases periodic validation reports based in a rich in-situ database. For this report, the platform's latest outputs dated 15th May 2020 have been used.

The Marine Mammals Exploring the Oceans Pole to Pole (MEOP) brings together several national programmes to produce a comprehensive quality-controlled database of oceanographic data obtained in Polar Regions from instrumented marine mammals. This data is already being used in the Pi-MEP system [RD03].

This PVR referred to validation reports produced by Pi-MEP. These reports are in Appendix A of this PVR. It is expected that Pi-MEP will publish the results on its website upon final confirmation of this PVR.

It is worth mentioning that Pi-MEP relies heavily in the computation of metrics by means of a database of collocations between in-situ data and products. In this sense, a few aspects shall be considered, as explained below.

2.3.1 In-situ vs satellite centric collocations

The platform uses an in-situ-centric approach in the collocations. This is an important difference vs satellite-centric collocation, as it relies on identifying matching satellite data within certain distance and time window from the in-situ acquisition.

This approach works well for collocations made with instruments that offer "punctual" measurements, but not much with the "trace" measurements. Thus, collocations with ARGO are fine if done in this way, as one can assume that the measurement represents only one point, i.e., finding the optimal measurement matching the in-situ observation is possible.

However, this is no longer the case when using information from surface drifters or TSG. These instruments offer a semi-continuous set of measurements as they move in the surface of the ocean. This yields lines of multiples observations, many of which would result in collocations over the same satellite data point, due to the different spatial sampling. The consequence is that an in-situ-centric approach to these types of data would yield different values on the metrics, just purely because of the intra-pixel variability observed by the in-situ that is integral in an area of the satellite. Aiming to obtain a more representative value, usually is better to aggregate the "trace" type measurements to obtain statistical values under the satellite pixel.

2.3.2 Temporal collocation

The second point to have in mind is the way the temporal collocation is done. In the Arctic+ project, the daily product is obtained by merging 9 days of observations from SMOS. Thus, it was considered more reasonable to collocate the satellite product with all of the in-situ observations within the 9-day window used to generate the product.

However, Pi-MEP selects the central time of the product as reference and collocates according to that, which essentially leads towards a reduced number of collocations. In some cases, this makes sense, particularly if any type of temporal weighting has been applied to the product when merging data from several observational days, but when there is no weighting, just collocating with the central date may bias the metrics.

On the other hand, the use of the full 9-day period for the collocations means that same in-situ points may be used several times, as the 9-day window slides over the time series. This means that absolute number of collocations are much larger than the actual number of in-situ points, as they will be accounted for multiple times. This means that, if sparse in-situ data is available, particularly dispersed in-situ points will have a larger effect in the resulting metrics.

The specific weight these aspects have in the metrics themselves has not been studied in this project, nor it was an objective part of this activity. However, it is important to have this in mind when comparing the results from Pi-MEP vs the metrics delivered within this PVR, as criteria used for the collocation process is different.

2.3.3 Various grids

The third aspect to consider also is the difference in the result of the metrics according to the grids for each product contained in Pi-MEP. Re-gridding and reprojection has not been applied to the hosted datasets, which essentially means that resulting matchups will be different between products.

For global products, with global in-situ datasets, this is of little relevance, as one can expect that global statistics of the metrics will be similar for products with approximated grids. The different in-situ data points used have not much impact in the results as data points are accumulated thanks to the large size of the data in time and space.

However, when considering regional products and/or shorter time series, this assumption will not hold, and results of metrics may vary. Users of Pi-MEP shall consider this aspect when using the platform to compare products between them, as they may be being compared against different data clouds.

3 Collocation strategy

As also introduced in this document, the collocation strategy may have impact in the outcome of the validation. Different strategies obey to different approaches according to each problem, and whilst those may affect when inter-comparing products validated differently, they remain as the "rule of measuring" for a set of tests when considered.

The collocation procedures followed in the results of this PVR is described in the following sections.

3.1 Collocations with punctual measurements

In the case of in-situ of punctual nature (ARGO, OMG, EN4), the strategy followed is in-situ centric with the following strategy.

For a given in-situ point, the closest satellite point is searched, both in time and in space, with a limit of 25kms from the in-situ measurement and maximum period of 9-days off in time.

The two limits aim the following:

a. Associate the in-situ data point to a valid and existing satellite grid point, within the natural spatial resolution of the satellite product.
b. To account for the fact that the daily satellite products validated in this activity are produced using 9 days of SMOS passes, without any specific temporal weighting.

As stated previously, this strategy leads to some repetition in the use of the in-situ data points, but never over the same daily product. This has been deemed as the most solid strategy to enable validation of the product, as it maximizes the quantity of in-situ information to check the satellite products. Considering the shortage of in-situ observations in the area, it seems sensible to have into account this factor.

On the other hand, it forces for a stricter QC of the input in-situ measurements used, as "bad" data or wrongly referenced to the common observational layer will lead to a larger impact in the metrics of dispersed observations. This has been considered, and a strict QC has been applied to data to minimize this problem.

The reason why this in-situ centric approach has been selected in this case is because the following reasons:

a. Generally, it is more intuitive to use and do, as in-situ measurements can be identified as "independent" measurements that can be individually matched against satellite data, if representativeness issues are tackled/considered properly.

b. Because of the different “footprint” equivalence, it is far more common that one satellite data point matches with more than one in-situ data point than the other way around. Being in-situ centric enables to have multiple collocations of in-situ points with the satellite point under which they are, what enables to improve representativity of the statistical results.

Besides those two points, both approaches have been tested and yield equivalent results in the metrics. The reason why this happens is associated to the sparsity of the data, and not much as the collocation method. Indeed, if in-situ data points are separated between them by a distance larger than half the inter-grid point distance (i.e., a radius equivalent to half the spatial resolution), satellite centric or in-situ centric produce the same set of matchups. It is only when in-situ data is somewhat aggregated in space respect to the spatial resolution of the product that selecting one method or the other has impact in the metrics.

By using the in-situ centric approach for the aforementioned datasets, the following steps have been taken:

1. For each SSS L3 product, a sub-set of in-situ data is created using the 9-day time window associated to the product (therefore selecting the data within the period of SMOS observations used for that particular L3 products);
2. For each of the points inside the subset, all distances are computed between the geographical coordinates of the in-situ point and the L3 grid, by using the maximum circle distance formulae for a spheroid.
3. Then, the matching satellite point is selected as the one yielding the minor of the distances, whenever such distance is less than the spatial resolution of the satellite data (in our case, less than 25 kms).
4. If the minimum obtained distance is larger than 25 kms, the in-situ point is then rejected.

The so-generated matchups are used then to compare the salinity values and extract the statistics for the metrics explained in section 5 .

3.2 Collocations with trace measurements

For semi-continuous datasets (TARA) a satellite-centric strategy has been followed for the sake of representativeness of the data. Semi-continuous measurements may accumulate significant amounts of data points under the corresponding L3 grid cell, which, if in-situ centric is considered, would yields from dozens to hundreds of collocations with the same satellite point. This is very ineffective to bring metrics forward because of the individual in-situ measurements are not representative from the satellite data, which could be observing fine spatial variability, impossible to see from the satellite’s point of view.

To overcome this limitation, the best strategy is to group the in-situ data in spatial and temporal clusters matching the spatial and time resolution of the satellite product.

The way in which this has been done for this project is as follows:

1. For each SSS L3 product, a sub-set of in-situ data is created using the 9-day time window associated to the product (therefore selecting the data within the period of SMOS observations used for that particular L3 products).
2. The resulting sub-set is now split again in groups of points fitting within a given grid cell of the satellite product. As grid point coordinates refer to the centre point of the grid cell, a radius equal to half the spatial resolution has been selected to split the in-situ data in spatial clusters (i.e., 12.5 km radius, i.e., 25 kms diameter, matching the spatial resolution of the satellite-based product).
3. Each of the resulting groups is now averaged to produce a representative salinity value under the satellite-based product pixel. Additional parameters were also retained for QC of the metrics: number of in-situ points used in the average and the dispersion of their values (standard deviation) as indicator of sub-pixel high spatial variability.
4. The matchups are then set as the pairs of salinity values formed by the satellite-based grid point value, and the resulting in-situ average data point computed as explained before.

The so-generated matchups are used then to compare the salinity values and extract the statistics for the metrics explained in section 5 .

3.3 Additional considerations

A few additional aspects have been considered during the elaboration of the matchups.

3.3.1 Depth of reference for the in-situ data

This project used in-situ measurements acquired between [1-5m] considering that down to this depth the upper ocean is homogeneously mixed. For datasets providing more than one measurement within this depth range, we keep the shallowest measurement only to be compared with the satellite SSS.

3.3.2 Geographical constraints

Both Artic+ Salinity v3.1 and BEC v2.0 products extend below the Arctic Circle. Because of the product is meant to support Arctic research and operations, the relevant quality information for the users are the metrics within the circle. Therefore, just data over 60º˚N have been used, both from in-situ and satellite-based products.

3.3.3 Data for the metrics

All the parameters for the metrics are based in the differential of salinity values between the satellite-based product (SSS_{sat}) and the in-situ data (SSS_{ref}):

$$dSSS = SSS_{sat} - SSS_{ref}.$$

The statistical parameters are thus referred to the residuals and not to the data population, which is rather standard in this type of exercise.

3.3.4 Grid re-projection

As assessed already in section 2.3.3 , when performing metrics over multiple satellite-based products, there is need to consider the grids they use. Different grids may yield different matchups, in the sense that not the same in-situ points will be related to equivalent grid points in the various satellite-based product. This may not be as much relevant for global products, due to laws of big numbers, but in regional products and/or with scarce in-situ observations, the results may be highly impacted.

In this project, the team did a first run of metrics over Arctic+ Salinity v3.1 and BEC v2.0 without specific consideration to this, what turned out as unclear results when performing the inter-comparison.

Analysis of the results also helped to understand that, actually, the inter-comparison was not fair because each product had different grid and effective spatial coverage (one product was not measuring in some areas due to bad data, whereas the other does).

To circumvent this problem, metrics should be performed only over matching satellite data points for the products within the inter-comparison. When products have the same grid and temporal validity, this is straight forward as it is just a matter of selecting the matchups associated to the same grid points. But when this is not the case, resolution of the problem may result complex.

Indeed, if the time window covered by each product becomes different, then other ways to match the products in time with in-situ must be used (e.g., looking at the central time as reference, for example, as done in Pi-MEP). Luckily, both Arctic+ V3.1 and BEC v2.0 have matching time windows, so this problem is not present in this case.

However, what both satellite-based products lack of is of a common grid, being one of the evolutive aspects of the Arctic+ Salinity v3.1 product, which is computed using EASE v2.0, so that it uses a standard grid well known by the science and operational community working in the Arctic.

In this case, a reprojection of the dataset had to be done. To ensure that the reprojection was not bringing artifacts in the inter-comparison, it was decided to perform it in the two-ways:

a. Reprojecting Arctic+ Salinity v3.1 into BEC v2.0.
b. Reprojecting BEC v2.0 into Arctic+ Salinity v3.1.

Matchups and metrics were computed for both cases, as discrepancies in the results could point towards specific problems in this exercise and had to be considered.

4 Description of the main relevant Arctic regions

This PVR conducted the quality assessment of the satellite product in the whole Arctic circle and there were especial attention to three sub-regional regions representing specific processes or with particularities that may impact the results of the validation, which were: [1] Beaufort Sea in the Canadian basin; [2] Nordic Seas in North Atlantic face of the Arctic ocean (i.e., from the Greenland-to-Scottish Ridge to about 80˚N); and [3] the northern North Atlantic Sea (50˚N to the GSR). Each of this sub-study regions were selected due to its relevance to the climate community (e.g., studies of Freshwater fluxes or changes in ice sheet concentrations due to climate change).

Furthermore, the selected regions were also regions where in-situ observations are especially limited (ref. RBD). For more information and to learn about scientific relevance of the selected study region the reader must refer to IAR, where this project deepens into difference scientific questions.

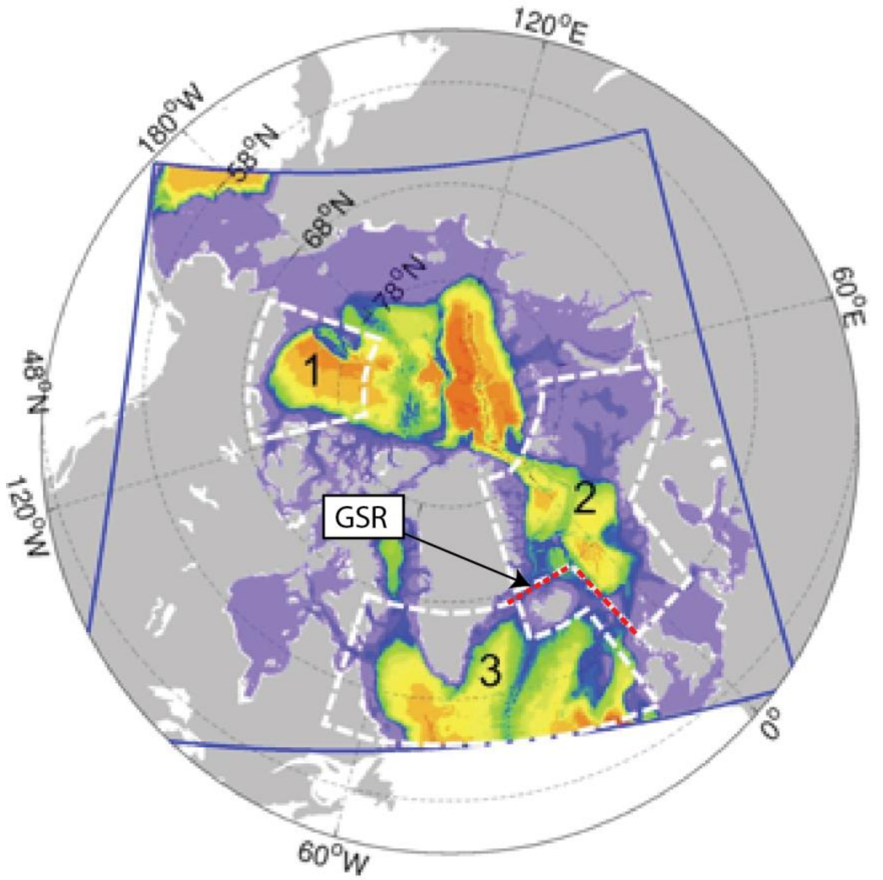


Figure 1: Arctic circle with delimited study regions (broken-white line) as: [1] Beauford Sea in the Canadian Basin; [2] Nordic Seas from Greenland-Scotland Ridge (GSR) to about 80˚N and [3] the northern North Atlantic (50˚N to GSR).

It is important to note that these regions have been used to gauge the potential spatial heterogeneity of the product. However, most of the in-situ data sets have strong spatial limitations (e.g., ARGO buoys are not present in the Beaufort Sea), so strictly splitting data by regions systematically was not efficient.

The only data offering a reasonable spatial coverage representing the Arctic region at once is TARA dataset. In this case, and due to the richness of measurements, it was decided to provide metrics for each of the seas associated to the Arctic domain, separately.

5 Description of the validation metrics

5.1 Qualitative statistical moments of SSS against a reference dataset

The statistical assessment of the quality of the SSS satellite retrievals resulted of the comparison against the ground truth. Hence, the validation metrics based on statistical measurements of the difference between the two quantities at the collocations (dSSS):

1. Mean of dSSS: estimation of precision (also referred as bias)
2. Standard Deviation (std) of dSSS: Estimation of accuracy
3. Root Mean Squared Distance (RMSD), which basically is a linear combination of the previous two quantities.
4. Correlation coefficients of SSS_{sat} vs SSS_{ref}.
5. Maps of the spatial distribution of errors: the mean of the dSSS and the standard deviation of the dSSS are computed per each grid point in the map. This kind of metric allows us to understand the origin of the errors (higher errors close to land, at higher latitudes due to ice-sea contamination, etc).

The regional SSS validation in the Arctic encountered some challenges which included seasonal variation of the sea ice, and scarcity of in-situ data. The limitation of reference ground truth data was foreseen at the preparation of the Arctic+ Salinity project (ref. RBD). However, this PVR paid special attention in finding alternative reference datasets, other than ARGO floats, which is one of the most limited in-situ datasets in the Arctic.

5.2 Correlated Triple Collocation

Triple Collocation (TC) is a method originally introduced in [Stoffelen, 1998] to provide estimates of the measurement error variances of three systems measuring the same variable at the same time. TC is based on the statistical relations among the measurement variances and covariances to deduce the error variances for each measurement. TC requires to have a series long enough of collocated triples of measurements, to obtain reasonable estimates of the order-2 moments of the measurements. Besides, it is usually required that the three measurement systems be completely independent, but they have different space-time acquisition scales, and thus the so-called representativity error must be properly accounted for.

Recently [González-Gambau, 2020], a variant of TC, especially adapted to deal with remote sensing measurements, has been introduced: The Correlated Triple Collocation (CTC). When applying CTC, the data are assumed to have the same space-time sampling, that is, they represent the same spatial and time scales. In contrast with standard TC, it is assumed that two of the datasets can have correlated errors (for instance, they are derived from the same basic measurement system). Besides, and considering that remote sensing series are typically not too long or maybe we are interested in assessing the evolution of the error of the systems as time passes, CTC is optimized to provide reasonably good estimates of the error variances even with a limited number of samples. With those conditions, CTC can be used to obtain maps of error variances of triples of remote sensing SSS maps and obtain a different map for every year.

The formulas for obtaining CTC estimates of the error variances are a bit lengthy and we will not copy them here; we refer the interested reader to the original paper (see section 8).

5.3 Wavenumber spectral analysis

The analysis of spectral slopes permitted to obtain information about the effective spatial resolution of the remote sensing data. Theoretical studies have reported that PDS (Power Density Spectra) slopes are expected to be in between -1 and -3 depending on the dynamical regime that drives the ocean (Blumen, 1978; Charney, 1971). Moreover, the presence of noise makes the straight curve of log PDS vs log wavenumber to bend and become horizontal at high wavenumbers. Another situation that can appear is when the data is over smoothened and then there is a systematic lack of energy at high wavenumbers, in this case, a faster-than-linear decay is observed for wavenumber larger than the resolution threshold.

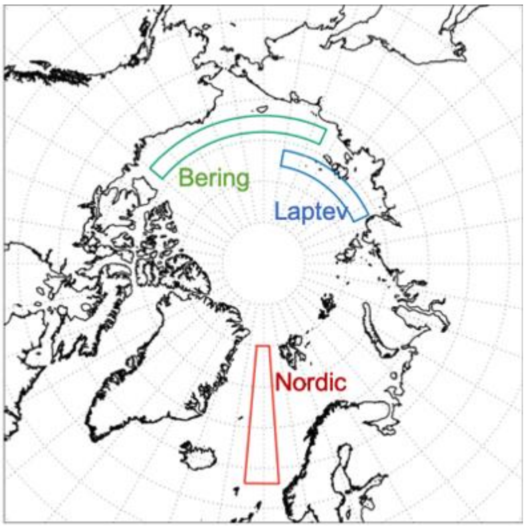


Figure 2: Selected areas to compute the PDS. Bering Strait is defined by 155ºE-130ºW & 70-72ºN (green box), Laptev Sea is defined by 115-170ºW & 76-78ºN (blue box) and Nordic Seas as defined by 4ºE-5ºW & 63-80ºN (red box).

This PVR applied the spectral analysis approach as in Hoareau et al. (2018) over three regions (Figure 2), which were contained within study regions described earlier:

- Bering Strait (155ºE-130ºW & 70-72ºN)
- Laptev Sea (115-170ºW & 76-78ºN)
- Nordic Seas (4ºE-5ºW & 63-80ºN)

For each region and product, the method computed the mean PDS over the full year 2016 and only for months from June to October (less ice-sea covered) (Figure 21) to reduce the fluctuations of each individual spectrum. PDS were given as a function of wavenumber values in degrees (latitude degrees for meridional regions, i.e., Nordic Sea, and longitude degrees for zonal regions, i.e., Laptev and Bering) and as wavelength values in kilometres. We use as a reference the slope k-2 (Blumen, 1978; Charney, 1971).

6 Results of the product validation

6.1 Re-gridding and reprojection

As explained previously, to do a fair comparison between the Arctic+ SSS v3.1 and BEC Arctic v2.0, there was need to perform metrics over common points. Because the different grids, the base of common points is too small, so re-gridding was required to achieve this comparison.

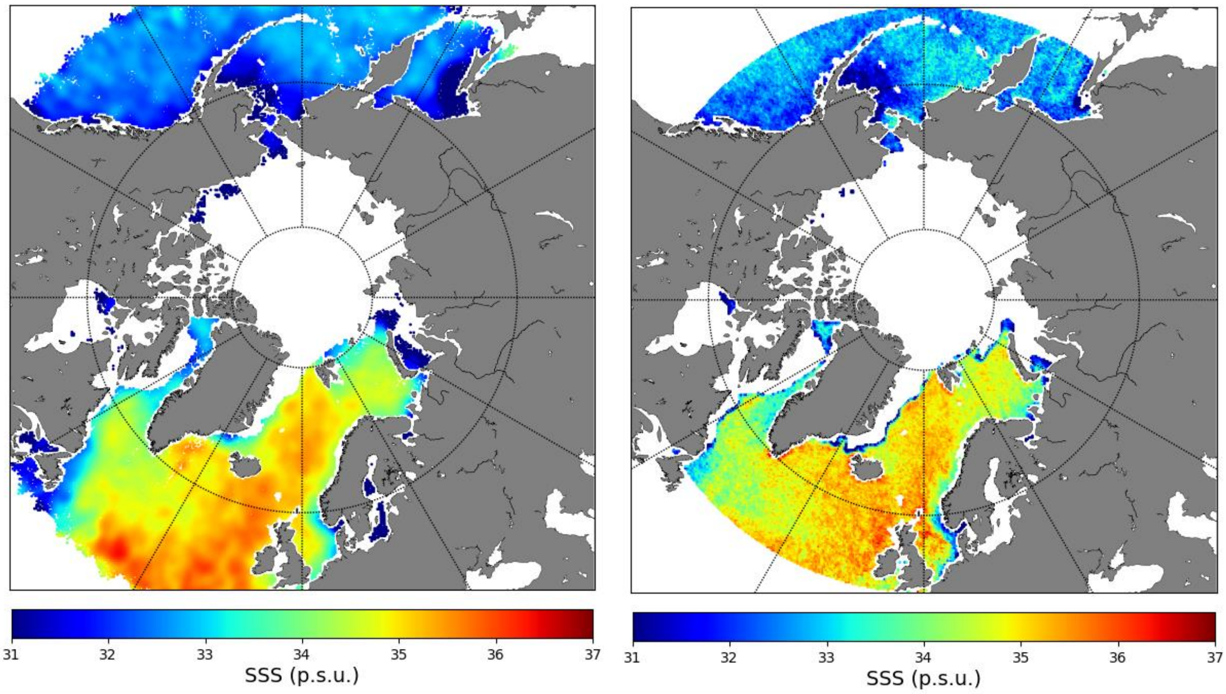


Figure 3: Examples of L3 products for BEC Arctic v2. (left) and for Arctic SSS v3.1 (right) for the 07/06/2016. It is possible to see that both products have some radical differences, with the Arctic+ product capturing more spatial variability than the BEC v2.0, where the spatial smoothing reduce them.

Examples of the native grids are included in Figure 3, above. Besides the geographical extension, the main difference between the two products is the resolution of horizontal gradients in SSS. In addition, Arctic+ SSS product has significantly less “holes” in the maps. Whilst holes can be expected due to presence of ice, others were associated to lack of good retrievals to fill them. This already informs that the new product can offer an improved spatial coverage and that retrieval method is more successful. The actual quality, though, relies in the metrics offered in the next sections of the document.

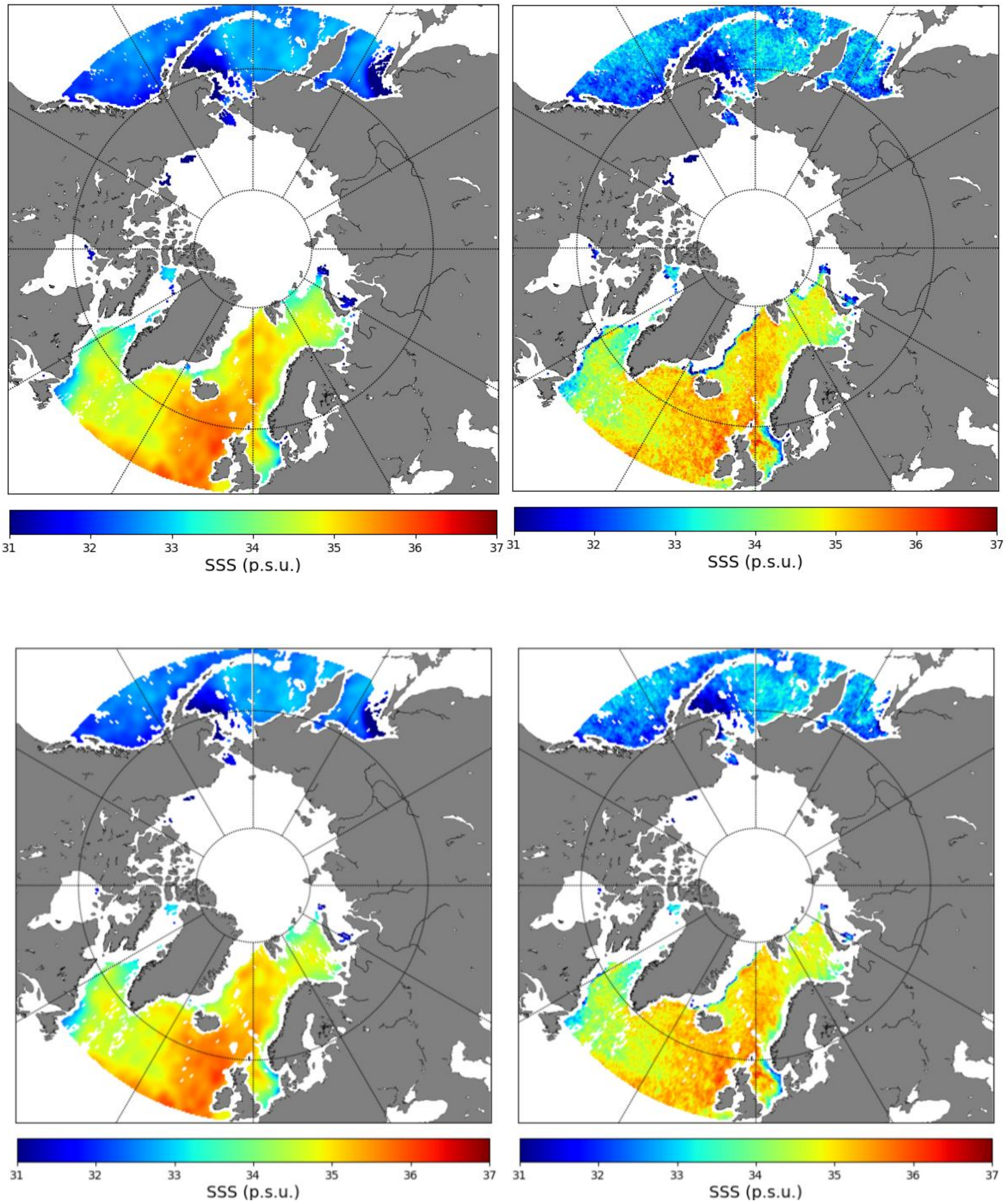


Figure 4: Example of re-projected L3 product for BEC Arctic v2. (top, left) into the Arctic+ SSS v3.1 (top, right), and of Arctic+ SSS product (bottom, right) into the BEC Arctic v2.0 (bottom left) for the 07/06/2016. Spatial coverage of the re-projected products is now identical for each way, as non-common points after re-projection and re-gridding have been excluded. Note that, however, those are not identical, depending on what direction data was reprojected.

The reprojection has been done in the two-way fashion. To ensure metrics were done only by common points, the re-gridding has included a data filtering removing data that was missing in any of the two datasets. This way, the resulting L3 grids for each product refer exactly to the same grid points, if well the set will be different when reprojecting BEC v2.0 into Arctic+ v3.1 or the other way around.

Examples of the reprojection can be seen in Figure 4 (previous page). One important aspect is that, once set over the same grid, it is possible to verify also what are the differences between the two products before the validation with in-situ data.

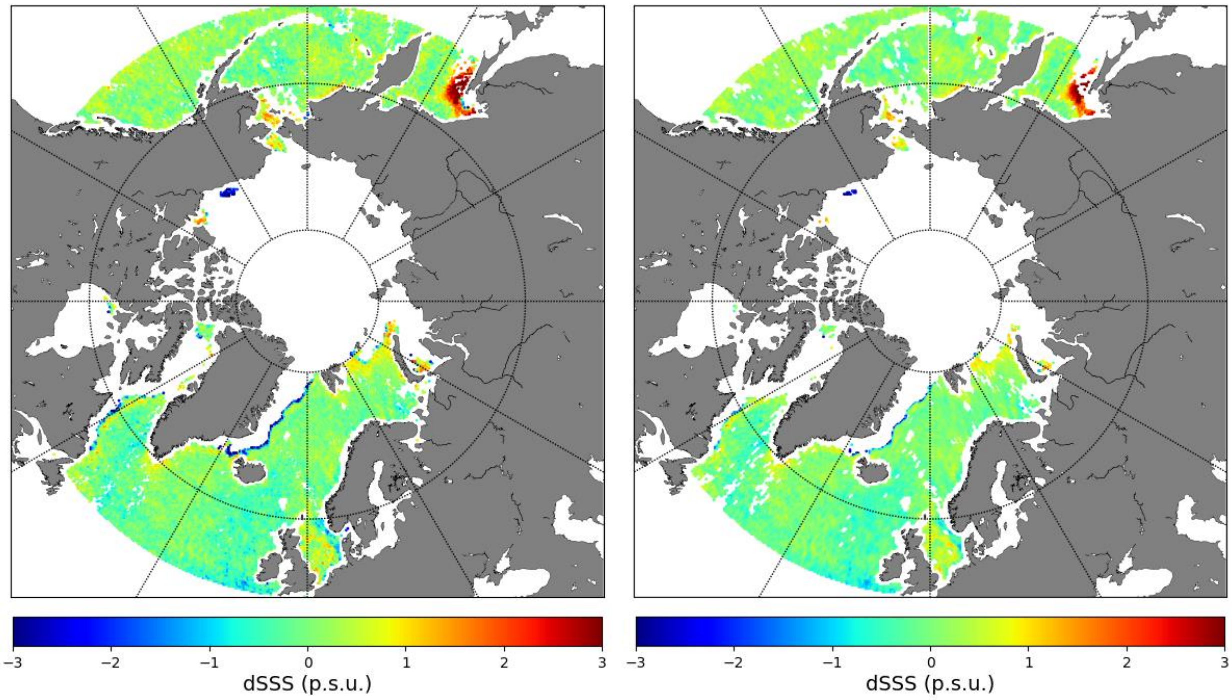


Figure 5: Example of SSS differences between BEC v2.0 and Arctic+ v3.1 product, obtained for the same day (07/06/20216), when reprojecting BEC v2.0 into Arctic+ v3.1 (left) and the other way around (right). The results already inform about the main differences between the two products.

The analysis of these maps show that they do not have substantially different overall SSS values (mean of dSSS is close to zero), but there are variations in spatial coverage (i.e., presence of holes) and on some spatial patterns.

6.2 SSS validation against ARGO

The first part of the validation related to the results with the ARGO buoys. Being a global system with a long time series, it is the only source of in-situ information available that systematically retrieves T and S data compatible with the satellite observations in a long period of time.

Unfortunately, validity of the metrics with ARGO for the Arctic region is rather limited, due to some shortcomings of the dataset explained below.

6.2.1 Additional details on ARGO dataset

The spatial distribution of ARGO buoys is the main issue when using ARGO in the Arctic region. Figure 6 shows the total number of ARGO collocations and their position for the period of the Arctic+ v3.1 time series (2011-2018).

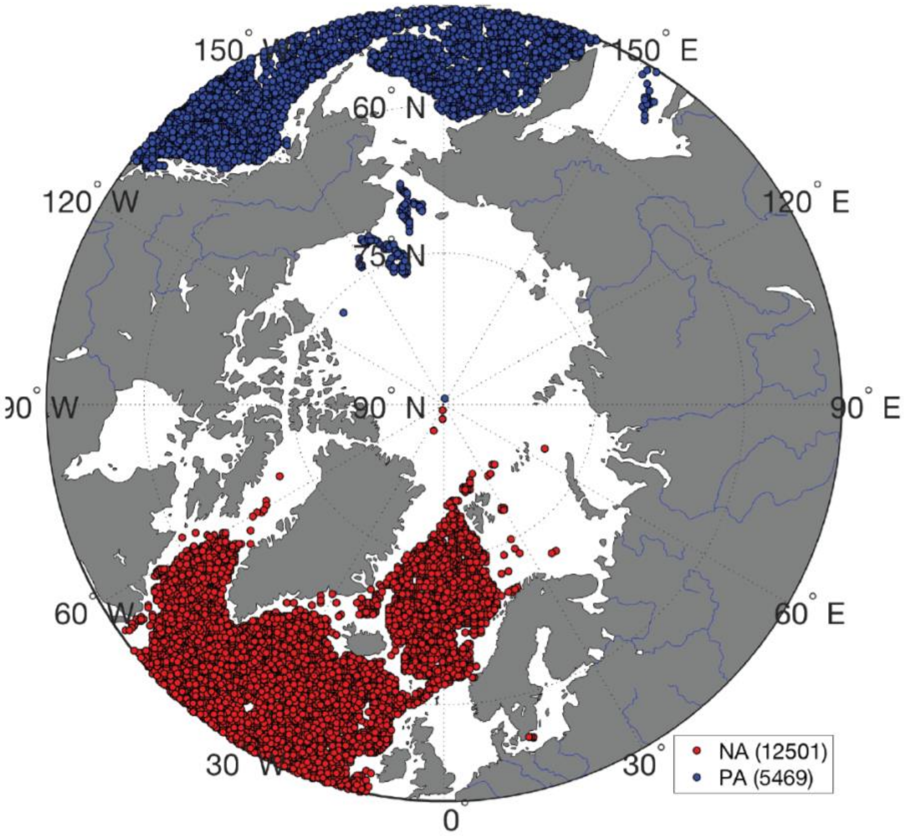


Figure 6: Spatial distribution of all resulting ARGO collocations for the Arctic+ v3.1 product, for the period 2011-2018. Red dots refer to the collocations found in the Atlantic arc, whereas blue dots are associated to the Pacific arc. Circle represents only the information over 55º N.

Whilst the number of collocations seems high, one should take note that these collocations are obtained with the daily product that uses 9 days of SMOS observations to produce one daily map. Thus, the number of collocations is increased because of the 9-day sliding window. Nevertheless, it is easy to see that 69% of all collocations correspond to the Atlantic arc, and that there are just a few points taking place within the internal seas of the Arctic region.

In addition, the number of collocations found for each satellite-based product is not great. In Figure 7 it is possible to see an example of the total of ARGO profiles found for a given day in the region for the Arctic+ v3.1. product. The figure also confirms the practically complete absence of ARGO profiles in the internal seas of the Arctic region.

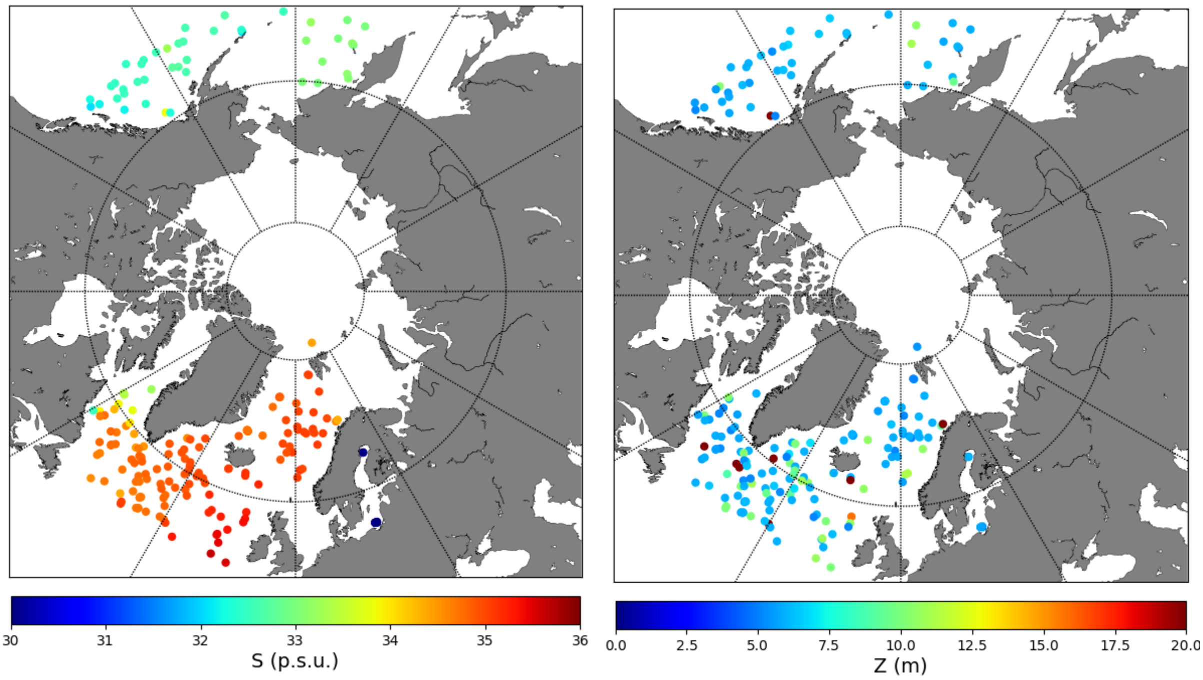


Figure 7: Example of total daily ARGO profiles matching the 9-day period associated to one Arctic+ v3.1 product (18/05/2018 to 27/05/2018). (Left) represents the salinity value of the uppermost ARGO measurement for each profile; (Right) contains the information about the depth of the uppermost ARGO measurement for each profile.

Whereas the number does not seem that bad, it dramatically reduces when ARGO profiles are filtered as indicated in section 2.2.1 . This is clear in the example showed in Figure 8, below, which also highlights the problem is not specific to the Arctic+ v3.1. product, but also for BEC v2.0 product. The issue with these results is that essentially limits the validation with ARGO to the Atlantic arc, and within the Greenland and Norwegian Seas.

From 2011 to 2018, maps of gridded matchups (Figure 9), show there is a range between 40-60 matchups in the North Atlantic face of the Arctic ocean. However, most of the other Arctic regions have a low number of ARGO collocations (below 20), as in the Beaufort Sea, or there were no ARGO observations directly (e.g., Laptev Sea).

The collocations with ARGO have been made using the procedure described in section 3.1. Because of the different grid, re-projection and re-gridding was carried out over the two satellite-based products. As explained before, this task involved the reconstruction of BEC v2.0 fields into the projection and grid of Arctic+ v3.1 and vice versa.

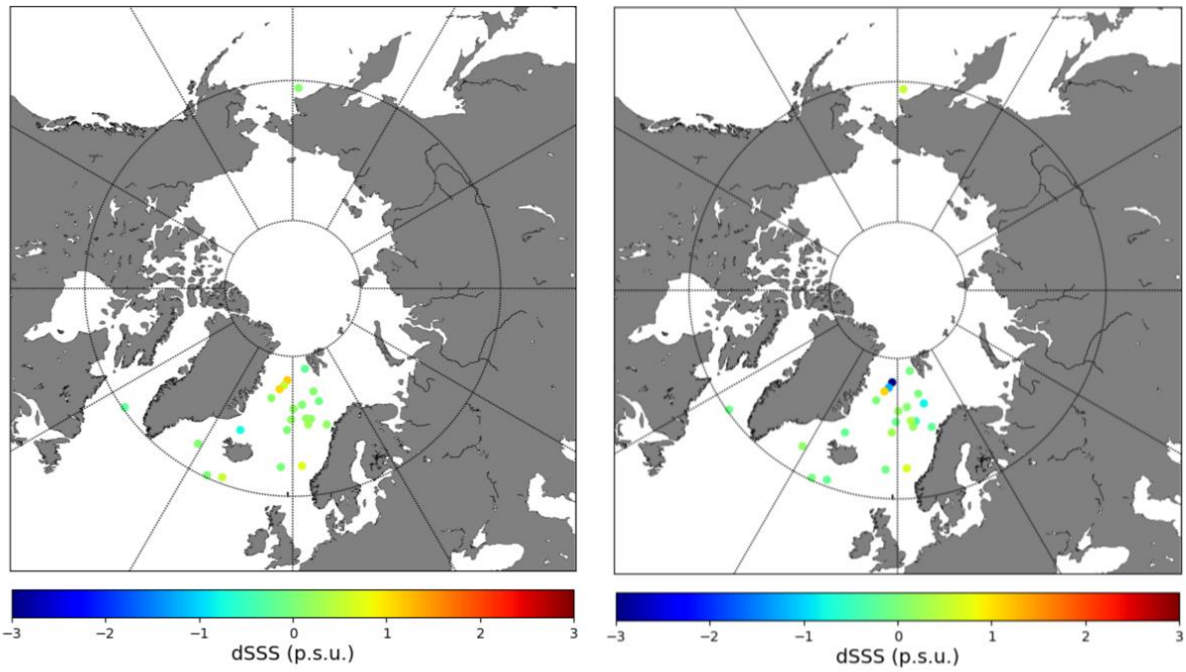


Figure 8: Example of total daily ARGO filtered matchups matching the 9-day period associated to a BEC v2.0 product (left) and an Arctic+ v3.1 product (right) (15/06/2018).

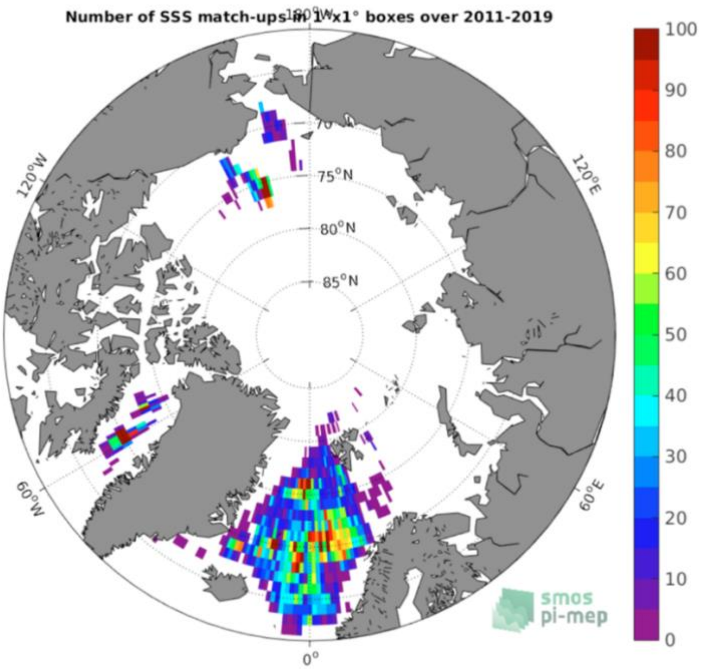


Figure 9: 2011 to 2018 Spatial distribution of the number of ARGO-to-satellite matchups (image courtesy of Pi-MEP).

As further explained in section 6.3, there is a limitation in the resulting matchups when moving from one grid to the other, resulting in much less matchups when doing the reprojection of Arctic+ v3.1 into BEC v2.0 than in the other way around. Because of that, results hereinafter are just limited to the two products common points on the grid for Arctic+ v3.1, which yields larger number of collocations.

6.2.2 Global results

Using the described procedures, two datasets of collocations with ARGO were made for both BEC v2.0 and Arctic+ v3.1 product. The results are shown in Figure 10 and Table 4.

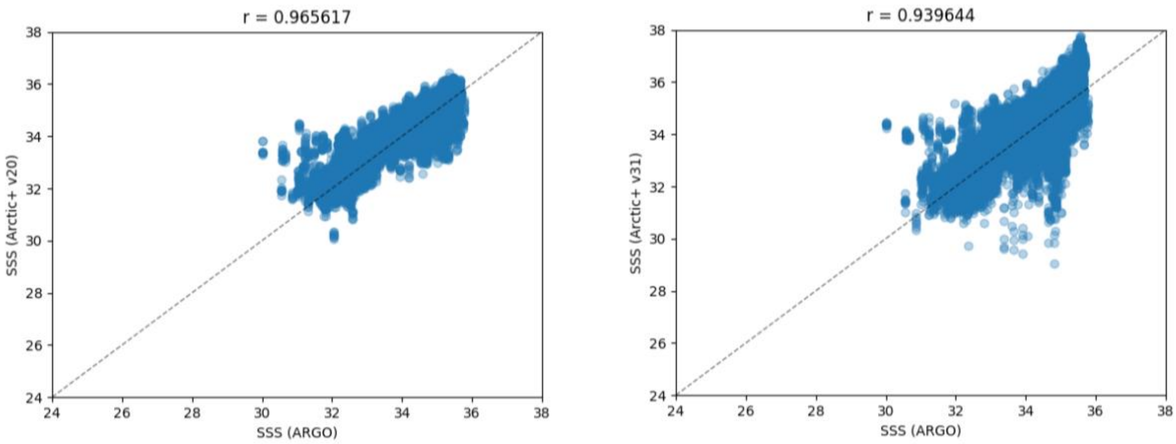


Figure 10: Scattergrams for the matchups for ARGO vs BEC v2.0 (left) and Arctic+ v3.1 (right), respectively) using points for the entire period 2011-2018. Only common points in the two products after reprojection are being used In the metrics.

Figure 10 informs about the behaviour of the SSS from satellite-based products respect to ARGO data. It is clear in the plots that BEC v2.0 is closer to ARGO in the sense that vertical dispersion of the data is significantly less (shown as the thickness of the cloud in the y-axis). This is expected, because as introduced already in this document, the BEC v2.0 products have both a spatial smoothing and are corrected from systematic bias by calibrating with ARGO. Thus, it is not surprising that bias is very close to zero (Table 4).

Table 4: Summary of the global metrics for the matchups for ARGO vs BEC v2.0 and Arctic+ v3.1 using points for the entire period 2011-2018. Only common points in the two products after reprojection are being used In the metrics.

Product	Mean	Std	RMSD	R
BEC v2.0	-0.01	0.28	0.29	0.97
Arctic+ v3.1	0.02	0.39	0.39	0.94

The information yielded by the other statistical parameters enhances this point of view, with the level of noise seen in Arctic+ v3.1 product around 0.1 p.s.u. higher than in BEC v2.0. Correlation is slightly better for BEC v2.0, due to the same reasons. Nevertheless, the metrics between the two products are not much conclusive about what product is best, if one attends only to the global statistics.

One aspect that is visible in Figure 10 is that BEC v2.0 product does not seem to behave as well in low salinity regimes than in the higher range of them. Salinity regimes are connected also to spatial locations in the area, thus, pointing towards the fact that BEC v2.0 product could be less useful for certain studies or applications. The scatter plot for Arctic+ v3.1 (right, in the figure) seems to correct this issue, giving a more homogeneous output along all the salinity regimes, but at the price of an increased dispersion in the data that manifests in the computed metrics.

All in all, conclusion of the global analysis with ARGO is that, for the specific region of the product where ARGO collocations exist, BEC v2.0 has slightly better results, even if the internal behaviour of the cloud points indicates that Arctic+ v3.1 maps better potential dynamics at low salinity regimes.

6.2.3 Time series results

The solely advantage of ARGO data for the validation of the Arctic salinity products relies in that can offer a time series matching the life span of the satellite-based data products. This is not available by means of other in-situ datasets.

The team has extracted metrics based also in the time series, which outputs appear in Figure 11 (next page) for the common points between the two satellite-based products. The analysis of the biases (top panel in the figure) shows that both sets of collocations for BEC v2.0 (blue line) and Arctic+ v3.1 are close to zero. The most striking difference, though, is the larger interannual variability observed in the case of Arctic+ v3.1 which seems not visible in BEC v2.0. This is likely to be connected to the retrieval method for the new product that seems not to cope with some of the limitations in SMOS. For instance, negative biases are appearing towards mid-October in almost every year, which is a known issue in SMOS observations. The fact that BEC v2.0 does not manifest this issue can be connected to the fact that the Arctic+ v3.1 tries to become as much independent of external data as possible. The building of a Tb climatology using SMOS data could inherit this type of limitations in the dataset.

One way to circumvent this seasonality native to SMOS is to introduce the climatology information as a 12-month map rather than a single annual map.

The other aspect the biases talked about is the issues at the start of the mission. It is clear that in 2011 the quality of the Arctic+ v3.1 product is not consistent with the rest of the year. This can be connected to the higher incidence of RFI in the region during this period, that was substantially mitigated lately by means of international cooperation and effort of the mission.

Figure 11: Results of time series of metrics for bias, noise, correlation, and number of matchups. The series has a data point per daily product of the satellite-based products. Blue line corresponds to BEC v2.0 and orange line to Arctic+ v3.1.

The impact of the RFI in this period is made clear by the behaviour of the standard deviation of dSSS as seen in Figure 11 (second panel). The results for Arctic+ v3.1 are much noisier than for BEC v2.0 in this period, whereas for the rest of the time series seems that there is a consistent difference of 0.1 p.s.u. in the levels of noise, matching what has been observed in the global stats. Nevertheless, even if the levels of noise are consistently higher in the Arctic+ v3.1 product, those are not generally deploying a different behaviour, which points again towards the impact of the smoothing and adjustment against ARGO present in the BEC v2.0 product and non-existent in the Arctic+ v3.1 product.

The fact that the new product is noisier against ARGO is only an artefact coming from the different choices done when creating the two products. As BEC v2.0 uses directly in-situ ground information to create the SSS field of reference, and thus, filtering the data points not compliant with the criterion used in the debiased non-Bayesian method, in Arctic+ v3.1 dataset is not relying in such information to create the reference on TB. As result, filtering is significantly less strict. In this sense, BEC v2.0 tends to be better against ARGO because the filtering impose in the SMOS data during the retrieval process will push the results towards the climatologic value represented by ARGO, whereas the new Arctic+ v3.1 has not such limitation, and thus, containing more dynamic information. On the other hand, the implemented algorithm has the risk that more spurious data can be accepted, which manifests with the difference values in the average level of noise.

The third panel of Figure 11 refers to the behaviour of the correlation of the matchups between ARGO and the satellite-based products. These results shall be taken with some “spice”, as these correlations are obtained in daily basis, i.e., using the available collocations within a daily product. As explained before, the number of matchups in each daily product cannot be very high (bottom panel on Figure 11 details this number per each data point) and the representativity of the parameter computed with a low number of points may be not reliable. Nevertheless, typically at least 50 points are required to have a consistent estimation of the correlation coefficient, so the results are helpful for the interpretation. As indicated also in the global results, it is possible to see that the two products are very close in this regard, even if Arctic+ v3.1 is consistently below BEC v2.0. As also explained before, the quality is significantly degraded for 2011 vs the other years.

As a final note, it is also important to consider that the degraded quality during 2011 may be of regional nature and not general for the product. This could require specific investigation or assessment of the product by other means so that to confirm the nature of the problem and decide of data over this period should be released or not to the community. As said, this seems to be connected to the way in which the TB climatology is produced, so there could be room for improvement of the product in this regard.

6.3 SSS validation against TARA

One of the most useful datasets of in-situ observations used in the project is the TARA dataset, resulting of a cruise campaign between June and October 2013 (TARA expedition). The information consists of TSG observations, as indicated above. Being closer to the surface and as a semi-continuous track, the number of points is ideal to assess the capabilities of satellite-based datasets in monitoring natural spatial variability of SSS. In addition, it is the only in-situ dataset accessible to the team that yields SSS measurements over all the Arctic sub-basins.

6.3.1 Additional details on TARA dataset

The advantage of TARA is also that informs about a variety of salinity regimes associated to the Arctic, whilst its main inconvenient is that is not a temporal synoptic dataset, as measurements were taken over a relatively long period of time (Figure 12). This lack of synopticity means that validation against TARA is not fully representative of the true nature of the data quality, as quality of the satellite-based products is known to depend on the month of the year and the spatial location. As TARA only covers a few months of one year, it cannot be considered alone to understand the resulting quality.

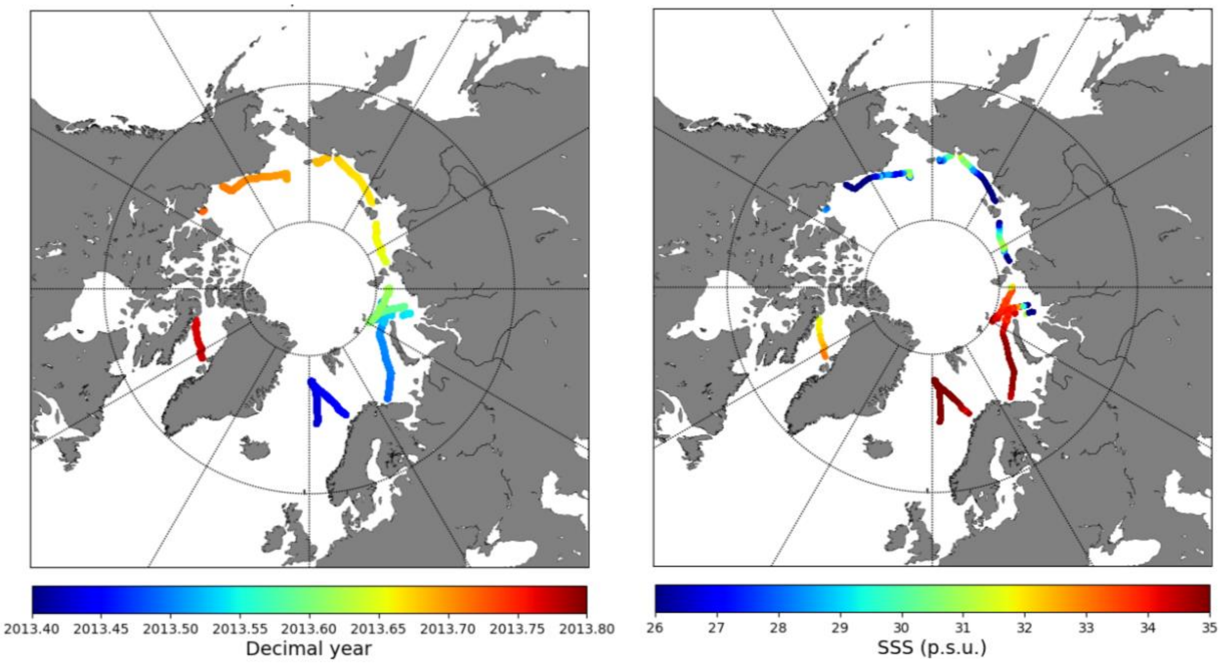


Figure 12: TARA expedition TSG information. (Left) Dates of acquisition (in decimal year) and (right) measured SSS values. TARA expedition circumnavigated the Arctic between June and October 2013 following a counterclockwise path. SSS data reveals the high spatial variability of SSS in the Arctic, as result of the multiple sources of SSS variability (river tributaries, ice melting).

6.3.2 General metric results

As discussed in the earlier sections of this document, mean, standard deviation, RSMD and correlation were computed for all the residuals of the collocated points between TARA and the BEC v2.0 and Arctic+ v3.1. Collocation procedure appears described in section 3.2.

To ensure fair comparison, this was done over the re-projected datasets. The results show below correspond to the matchups obtained when BEC v2.0 product was re-projected into Arctic+ v3.1. Metrics for the other reprojection were also produced. However, the number of matchups highly reduces due to a reduced number of matching points in the resulting grids, as consequence of the different spatial resolution of the products. Some examples are given to visualize this problem.

6.3.2.1 Spatial distribution of dSSS

Figure 13 (next page) shows the resulting dSSS values for all the matchups between TARA and SMOS-based data products. The results already show that Arctic+ v3.1 product behaves differently in each Arctic sub-basin. These differences per each basin are related to various factors, including but not limited to presence of RFI, or lack of climatologic data, which is required for the retrieval process (ref. ATBD).

The plots already show that there is a significant difference in the number of resulting matchups between TARA and the satellite-based product, according to the reprojection done. In particular, a total of 225 collocation points is found when reprojecting BEC v2.0 into Arctic+ v3.1 product, but only 71 points are found when doing it the other way around. This difference comes from the different spatial resolution of the two products, which causes many grid points being filtered out when retaining only common points.

One critical aspect that is extracted from Figure 13 is that global metrics derived with TARA will not tell the true story of the quality of the product. Local assessment is necessary to enable a proper assessment. This was done and results are shown later in this document.

The assessment for BEC v2.0 and Arctic+ v3.1 shows some communalities between them: both products are generally better over the Atlantic arc of the Arctic region; both products also show a significant negative bias over the Barents Sea that becomes in a significantly positive bias on the Chukchi and Beaufort Seas. The most striking difference is the results on the Baffin Bay, where it seems BEC v2.0 performs very well and Arctic+ v3.1 product does not do as well. This last point, however, has been further investigated by the team, finding one aspect that requires consideration when using TARA, and is that the ship did not sustain a constant speed all along the campaign, resulting in a varying number of valid TSG measurements falling within a given satellite-based product grid cell. In particular, the speed seems to be minor at the first half of the campaign (June to August 2013) and progressively increasing towards the second half (September to October 2013).

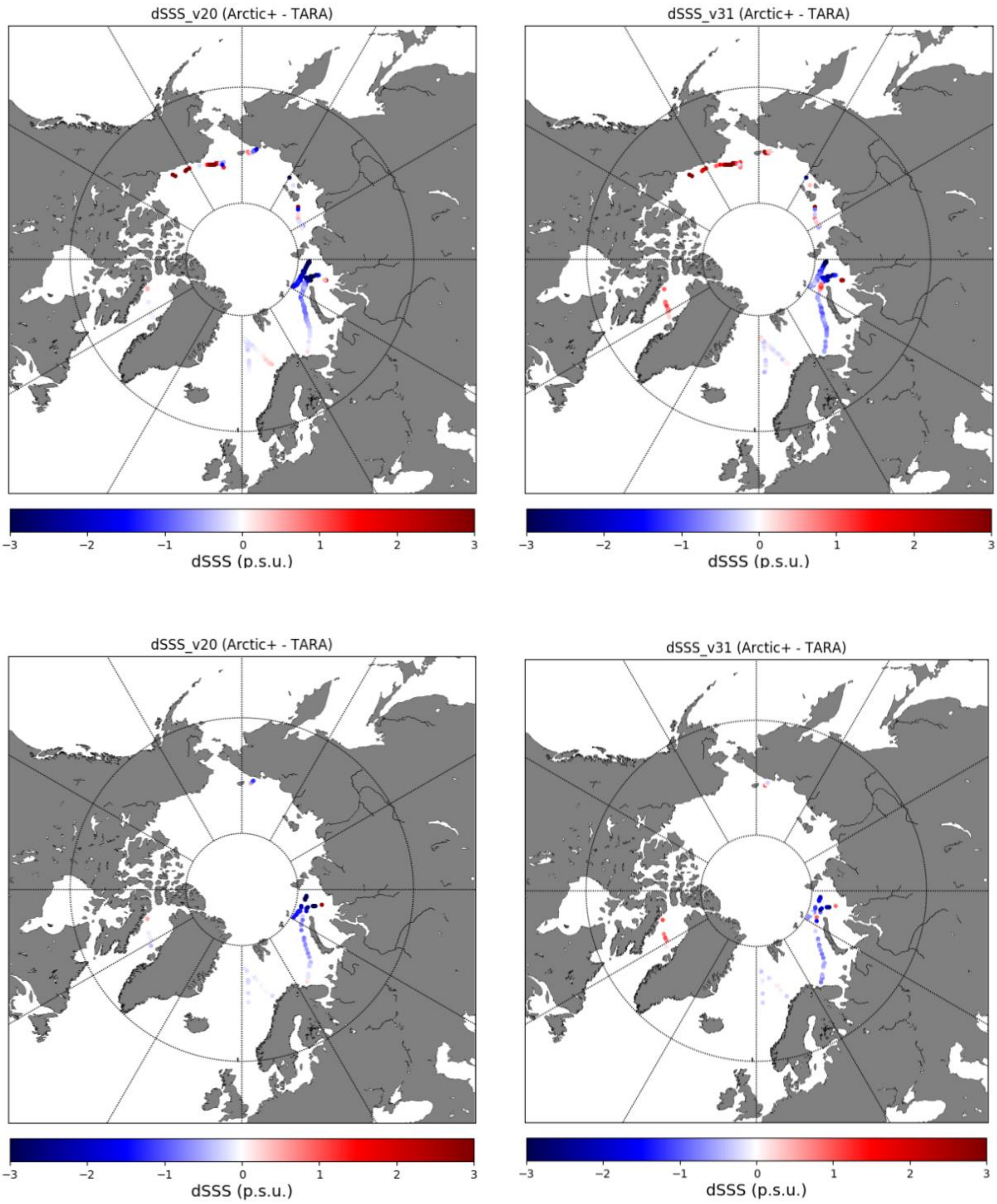


Figure 13: delta SSS between satellite-based SSS products and TARA TSG SSS measurements, for BEC v2.0 (left column) and Arctic+ v3.1 (right column). The matchups were obtained after reprojecting BEC v2.0 in the same grid than Arctic+ v3.1 product (top row) and after reprojecting Arctic+ v3.1 into BEC v2.0 (bottom row). Whilst dSSS values are not dramatically differently, there is a significant number of differences in the number and position of the matchup, as expected.

As consequence, the last segment of the campaign provides sometimes less than 5 TSG data points per grid cell, in comparison to the more than 100 found in the earlier stages. This temporal change in the spatial resolution of TARA is expected to have impact, and metrics done over Baffin Bay cannot be considered as much representative as the ones at start of the campaign.

Nevertheless, such limitation applies to both BEC v2.0 and Arctic+ v3.1 so the fact that values there are better in the former than in the later points towards a kind of limitation in the Arctic+ v3.1 product. This has been verified with the team at BEC in charge of the development of the retrieval algorithm and there is an agreement that the cause of this is likely the procedure followed to produce the climatology required in the algorithm. Lack of observations in the area are thus limiting such climatology, and hence introducing a bias that does not appear in BEC v2.0 over this region of the Arctic.

6.3.2.2 Global correlation

Using all the output collocations for each case, it is possible to produce scattergrams and derive some basic statistical parameters. Figure 14 (next page) summarizes these outcomes, resulting that the highest correlation value is reached with the collocations for Arctic+ v3.1. The novel product yields the best outcome despite the way the reprojection is done.

However, as already introduced, reprojecting Arctic+ v3.1 into BEC v2.0 leads towards much less collocations (71 vs 225, which means roughly 1/3 of the collocations done when reprojecting in the other direction).

The improvement of Arctic+ SSS v3.1 vs BEC v2.0 manifests as better quality in the retrieved salinities at lower values, which get closer to the 1:1 line in the scattergrams. This is less unclear for the higher end, yet another reason why splitting the metrics by areas is relevant. Because of the splitting in areas will reduce number of useful matchups even further, it makes no sense to produce such metrics for the case of reprojecting Arctic+ v3.1 into BEC v2.0.

Further on the results, it is also possible to check that the segments of TARA showing higher spatial variability intra-pixel are mainly found in the low salinity regime of the scatterplot. The fact that Arctic+ v3.1 manages to get closer to TARA is, thus, an important outcome, as it points towards a better representativity of the natural variability as compared to BEC v2.0. This result could be expected, as BEC v2.0 has some implicit smoothing on the L3 maps, which would penalize this possibility.

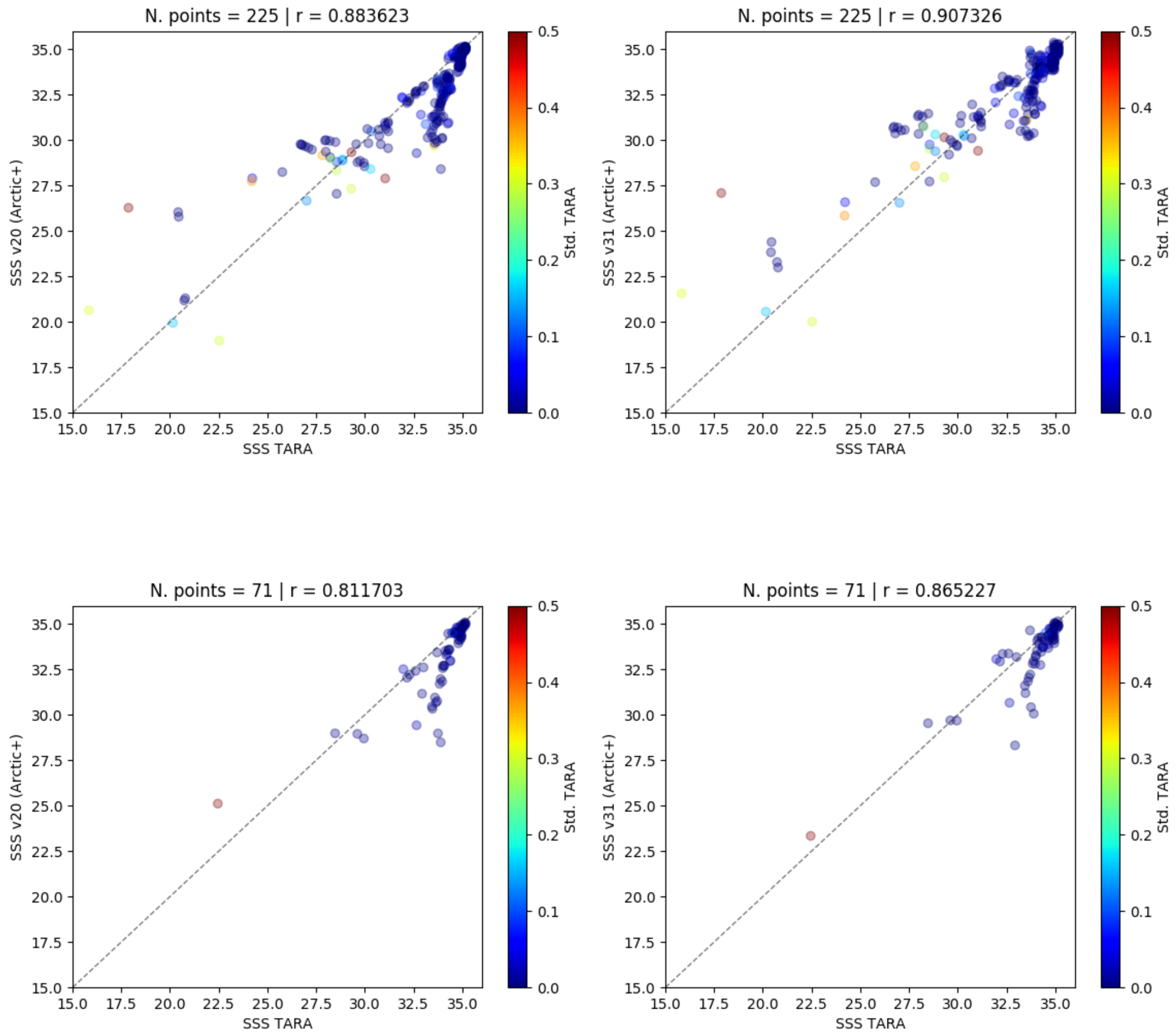


Figure 14: Scattergrams for the various satellite-based product types with respect to TARA. (Left) results for BEC v2.0 product; (right) results for Arctic+ v3.1 product. (Top row) results with BEC v2.0 product reprojected into Arctic+ v3.1; (bottom row) results with Arctic+ v3.1 reprojected into BEC v2.0 product. All resulting match ups are considered. Vertical colour bar indicates the standard deviation found within the set of TARA measurements integrated in each satellite-based grid cell.

6.3.3 Regional metric results

To assess the quality of the Arctic+ v3.1 product over a specific region, a splitting of the TARA transect was done, grouping data by the natural sub-basins, as seen in Figure 15.

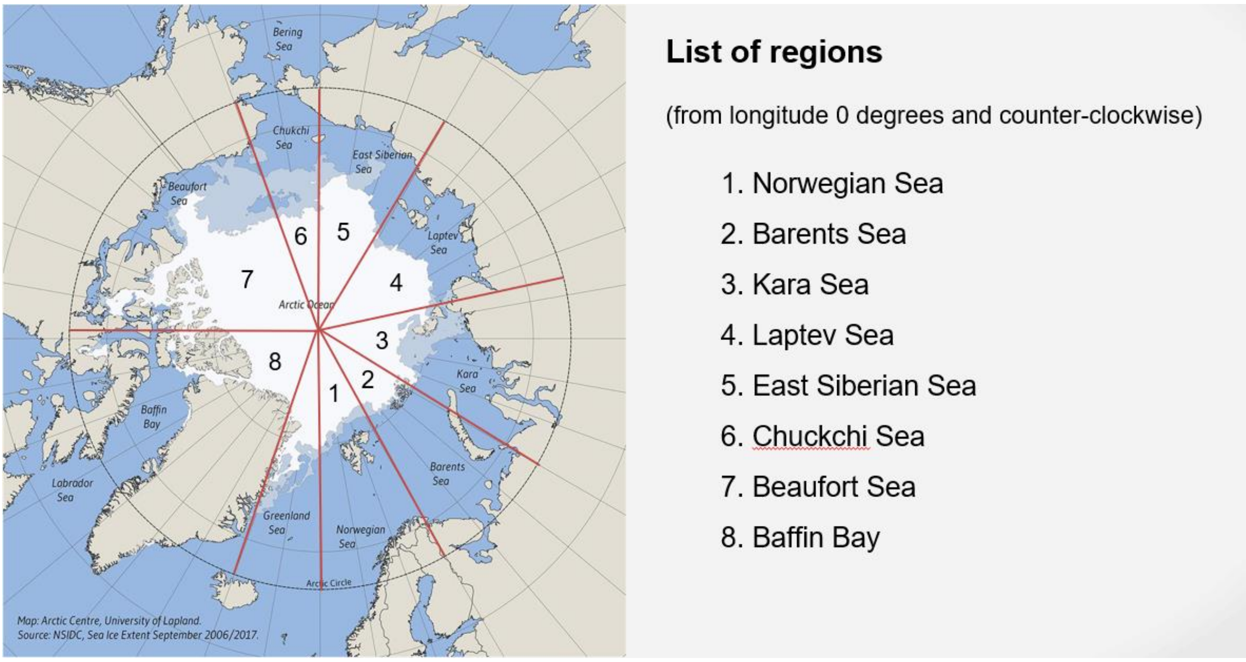


Figure 15: Geographical splitting of the Arctic region to produce metrics separately for each segment of the TARA expedition.

The performance of the metrics has been done in the same way as before and for both the BEC v2.0 and the Arctic+ v3.1 product. The results are summarized in Table 5, below. Note that table only refers to the metrics obtained when reprojecting BEC v2.0 into Arctic+ v3.1. Results are not shown for the other case, as discussed.

Table 5: Summary of results of metrics for TARA expedition over common points, split by regions defined in Figure 15.

Product		Full	Norg. Sea	Barents Sea	Kara Sea	Laptev Sea	East Siberia	Chukchi Sea	Beaufort Sea	Baffin Bay
BEC v2.0	Mean	-0.54	-0.06	-0.49	-1.78	0.48	-0.74	1.34	2.74	0.03
	Std	1.63	0.16	0.31	1.32	2.44	1.22	1.50	2.07	0.18
	RMSD	1.71	0.17	0.58	2.21	2.49	1.43	2.01	3.43	0.19
	R	0.88	0.59	0.31	0.90	0.84	0.94	0.17	0.95	0.87
Arctic+ v3.1	Mean	-0.07	-0.09	-0.62	-0.8	0.72	0.42	2.44	2.26	0.61
	Std	1.52	0.22	0.21	1.40	2.60	1.32	1.40	0.93	0.31
	RMSD	1.52	0.23	0.66	1.62	2.70	1.39	2.82	2.44	0.68
	R	0.91	0.52	0.48	0.89	0.80	0.94	0.40	0.98	0.62

In this case, Arctic+ SSS v3.1 product performs generally better than BEC v2.0. This is reflected in the results of the metrics over the full area, showing a reduced bias and noise level. Bias has been globally improved by 0.5 p.s.u., noise level by 0.1 p.s.u. and RMSD by 0.2 p.s.u. Correlation is also slightly better. All indicators, thus, point towards a positive result in terms of quality improvement.

However, the global results shall always be considered with some spice, in the sense that regional biases of opposite sign may lead to a global bias of 0, which is not accurate with the reality of the product.

The table above shows that there are areas where Arctic+ v3.1 significantly reduces the bias with respect BEC v2.0, but there are also areas where this is the opposite. Two, aspects, however, drive these differences, including the availability of matchups (not all the areas have the same size nor number of matchups) and they are not acquired at the same time of the year, which may also impact the comparison between regions, as sea conditions and SMOS retrievals may have seasonal effects not captured by TARA, due to its short duration on time.

Attending to the RMSD, there are six regions where Arctic+ SSS v3.1. performs better or equal than BEC v2.0, and two where does worse. One was already reported previously, corresponding to Baffin Bay and the other Chukchi Sea. In both cases, TARA shows fewer average measurements, but in equal conditions, Arctic+ v3.1 shows larger biases than BEC v2.0, which drives the RMSD towards worse values.

Considering the correlation coefficient, it seems Arctic+ v3.1 is almost systematically equal or better than BEC v2.0. This informs that Arctic v3.1 captures better the SSS dynamics than BEC v2.0, even if the product may be occasionally more biased. This is encouraging as it means that Arctic+ SSS products may be indeed better for scientific research, even if it would require an improvement on the L3 mapping to reduce the existing biases. As indicated, the main difference in this regard is due to the way in which the retrieval process does use of the climatology and how this is generated. We estimate that the regional biases can be easily explained to a lack of in-situ information when building the climatology, which introduces the biases in such part of the retrieval and not in the manner the SSS dynamics is extracted from SMOS data with the method detailed in the ATBD.

This theory is duly supported by the results in Baffin Bay. It is true TARA has much less data in this area in comparison to others, but at the same time, the relative comparison between BEC v2.0 and Arctic v3.1 with the same in-situ data points show that BEC v2.0 performs better. The team has not found any other explanation to this anomaly in the metrics than the potential influence in the quality of the climatology field used.

6.4 SSS validation against OMG

The datasets of the Ocean Melting Greenland experiments were also used to perform the validation. The procedure to produce the matchups is described in section 3.1, and done similarly to ARGO. As also described in section 2.2.3 , OMG datasets consist of vertical profiles of areal delivery expendable CTDs (AXCTDs) thrown into multiple points of the coastal waters of Greenland, both in the side of the Greenland Sea and the Baffin Bay.

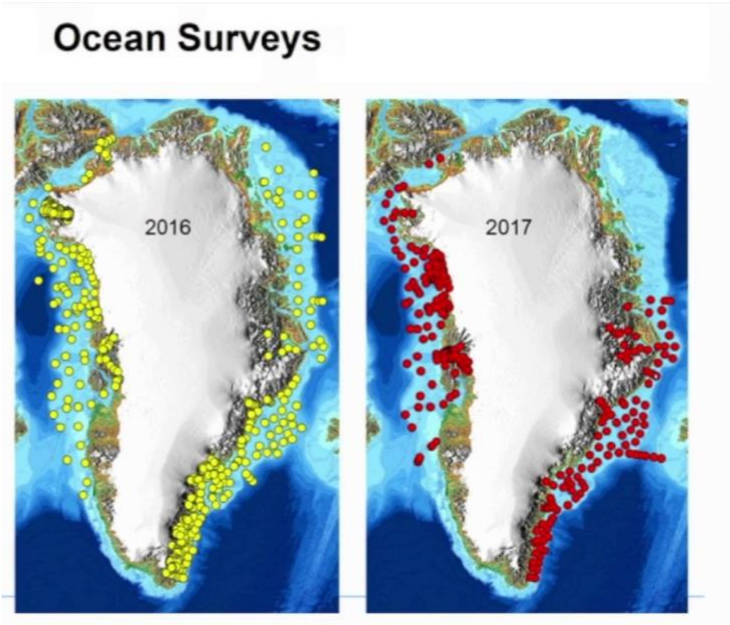


Figure 16: Spatial distribution of the AXCTDs obtained during the OMG campaign in 2016 (left plot) and 2017 (right plot. Vast majority of profiles were obtained in the areas closest to coast.

The main limitation of the dataset is that it is only limited to the times of the year where the coastal waters of Greenland are free of icesheet, and vast majority of the data points are rather close to coast (Figure 16). This was expected, as OMG experiment had as a goal to observe the impact of freshwater lenses as result of melting ice over land areas. Given that mixing of those lenses can be rather fast, proximity to coast was a requirement for the measurements.

This restricts substantially the number of valid collocations between the satellite-based products and OMG data. The problem is even worse if the metrics are tried using a common grid and only common points between Arctic+ v3.1 product and BEC v2.0 product. This additional restriction takes place because for performing metrics over common points, we remove any grid point not having information in any of the two versions of the products, thus, leading to larger gaps, especially in areas where retrieval is more difficult. This includes edges of the sea ice and proximities to coastal areas and land. Hence, OMG matchups are heavily penalized.

Because of that, for OMG data on common points metrics have not been produced. Instead, results are included separately for each dataset. However, readers shall not consider those metrics fully compatible, due to the huge scarcity of the collocations and the different matchups resulting of the different spatial coverage and resolution of the two products.

6.4.1.1 Results of the metrics

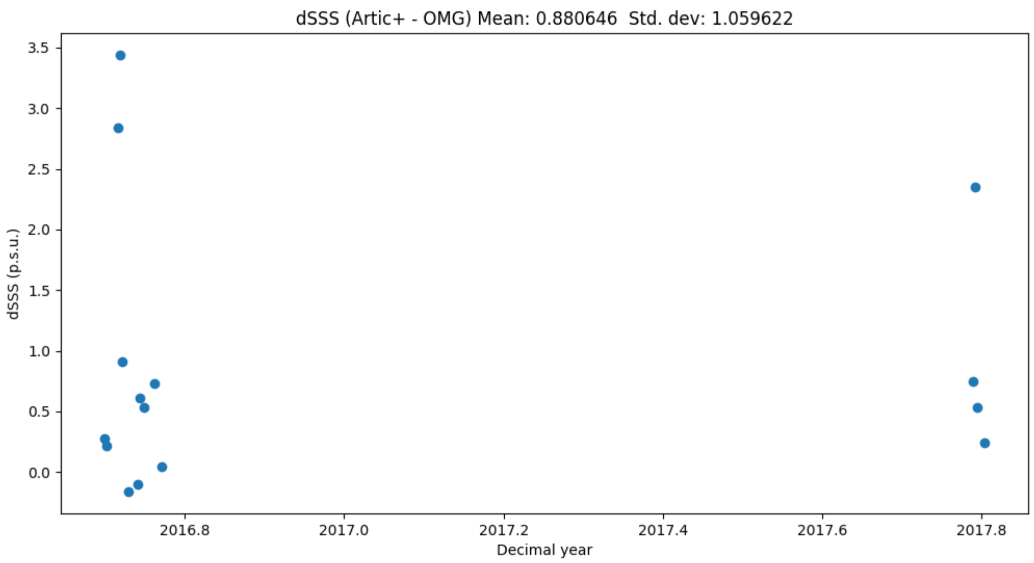
The summary of the metrics can be found in Figure 17, next page. Top row of the figure contains the output for BEC v2.0, whereas the bottom row shows the outcomes for Arctic+ v3.1. A summary of the metrics is presented in Table 6, below.

Table 6: Global metrics for OMG matchups vs the two satellite-based SSS products.

Product	Mean (psu)	Std (psu)	RMSD (psu)	R
BEC v2.0	0.88	1.06	1.38	0.09
Arctic+ v3.1	2.09	1.82	2.77	0.04

The results of the table cannot be understood without paying attention to the information appearing in Figure 17 (next page). One of the aspects that is most striking in the figure is that Arctic+ v3.1 yields far more collocations with OMG than BEC v2.0. BEC v2.0 only yields valid collocations for 2016 and 2017. This is worth mentioning because relates to the time span associated to both products. BEC v2.0 runs only till end of 2017, whereas Arctic+ v3.1 runs till end of 2020. As OMG started in 2016, it means only two years are available, vs the 4 years for Arctic+ v3.1.

Checking the output matchups in the time series plots (left plots for both products in figure), it is obvious why Arctic+ v3.1 is significantly penalized, as there is a strong bias by data selection in the comparison. For instance, if we narrow the comparison to the matchups for 2016 and 2017, the individual dSSS found in both products are rather similar, even if Arctic+ v3.1 bias seem somewhat larger. However, what really drives the metrics off are the data points distributions for the other years. Whereas in 2016 most matchups are showing a lower bias (around 0.5 p.s.u. for BEC v2.0 and 1 p.s.u. for Arctic+ v3.1), for the other years there are clusters of points at very high dSSS values. The high dispersion of the data points is also an indicator of the low representativity of the metrics obtained with this in-situ dataset, caused by the low number of resulting collocations.



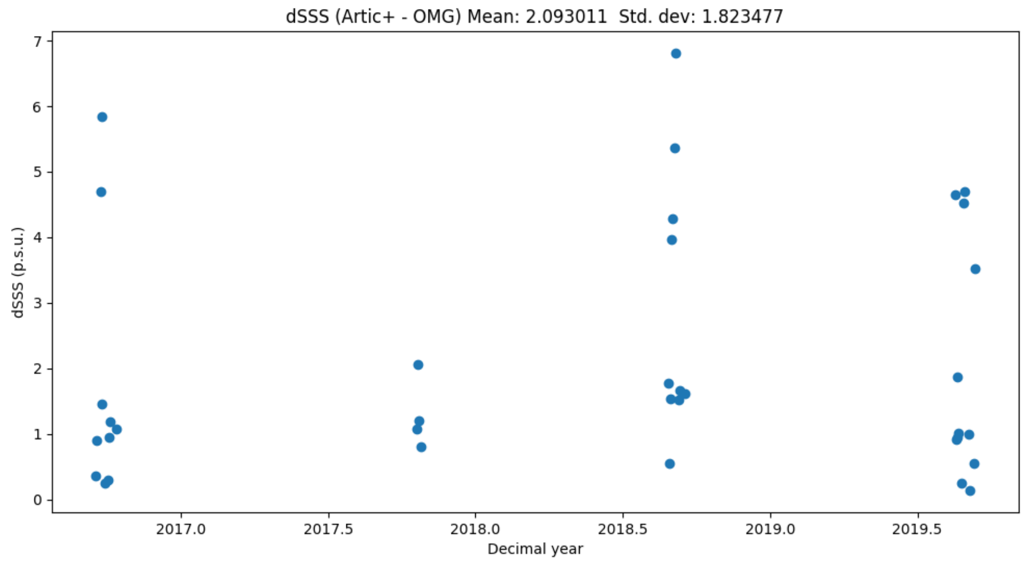


Figure 17: Results of matchups between OMG dataset and BEC v2.0 (top panel) and Arctic+ v3.1 (bottom panel). Note that x-axis is not the same in both figures.

6.4.1.2 Additional comments

The scattergrams computed for the OMG dataset matchups are shown in Figure 18, below. They clearly highlight the problem of the dSSS dispersion induced by the extra collocations available for Arctic+ v3.1 vs BEC v2.0 as result of the different time series spam. Whilst the correlation between the two datasets is very low and meaningless, the standard deviation of OMG measurements within the first 10 meters of the AXCTD profiles is interesting (colour bar in the plots of the figure).

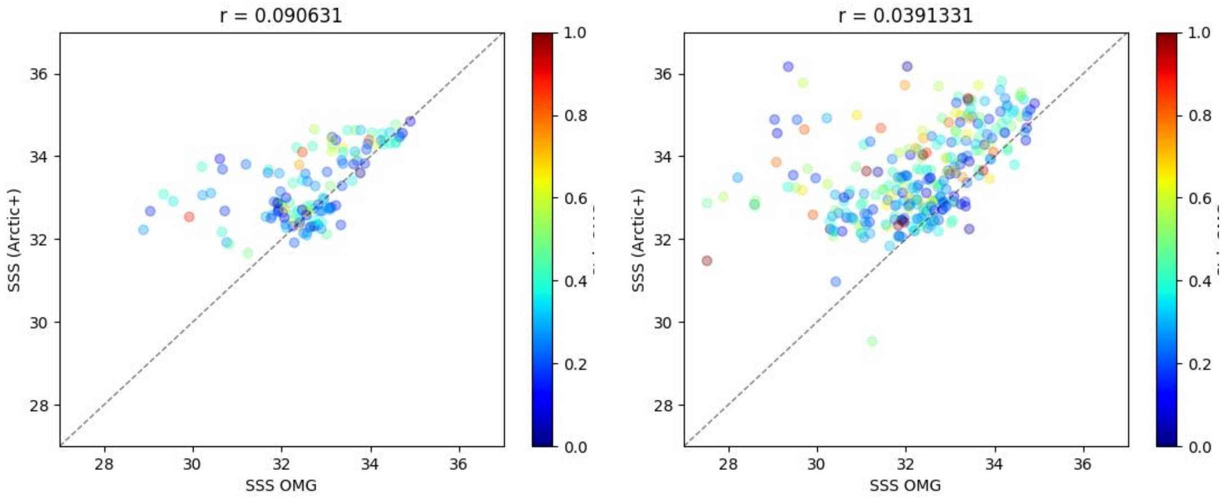


Figure 18: Scattergrams for the matchups between OMG and BEC v2.0 (left) and Arctic+ v3.1 (right). Colour bar refers to the standard deviation of the OMG measurements within the [0,10m] depth ranges of the AXCTD profiles.

Indeed, it is possible to see that there is a significant fraction of the most-deviated points that also manifest a large standard deviation of S values within the first 10 meters layer. This information is relevant because talks about potential stratification effects not taken properly account when performing the metrics, if even possible.

Figure 19 (next page) shows an example of an AXCTD profile typically found within the OMG database. It is possible to see that salinity values can change more than 1.5 p.s.u. within the first 10 meters. This type of information is what OMG aimed to detect but implies that integrating salinity values within the first 10 meters of the water column to have a representative value may be too limiting for the metrics. However, according to the OMG information, this step is necessary to build a meaningful value of S for the uppermost layer, as AXCTDs have a splash effect in the first meters, when the probe lands over the water surface with a larger fall speed than once submersed in water. Inertial forces introduce a non-natural variability of S values in those first meters.

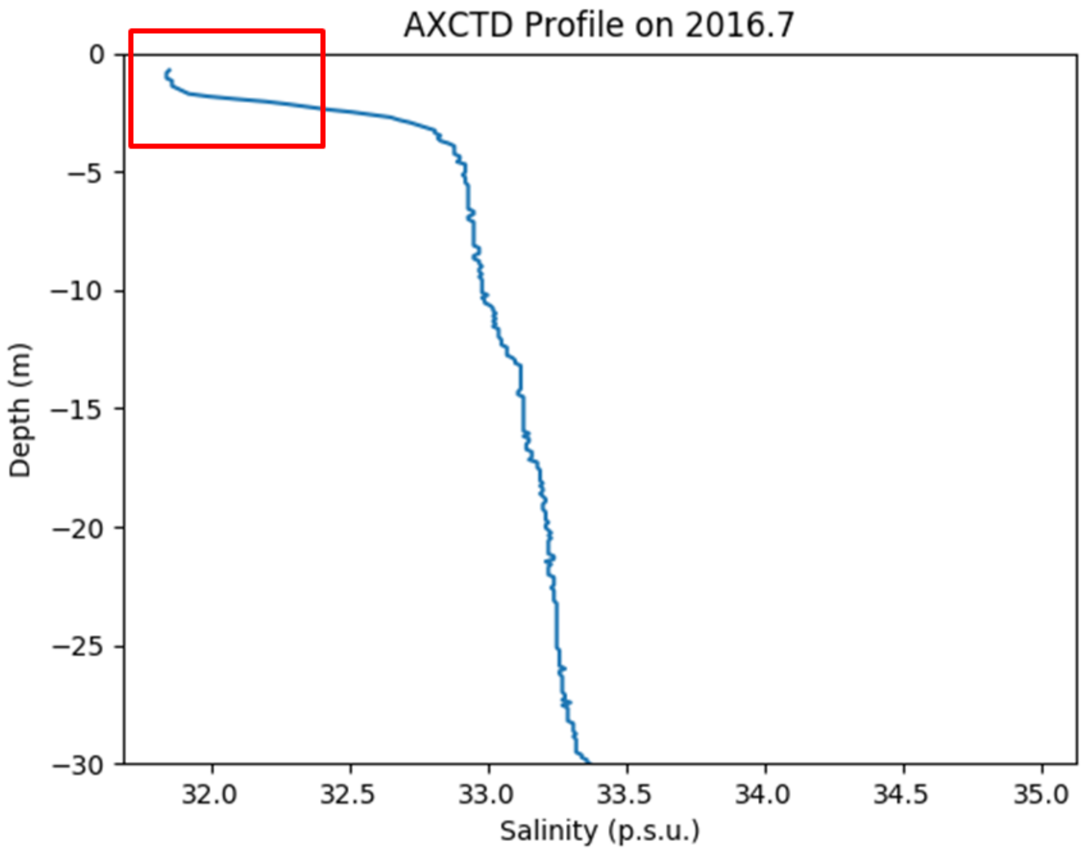


Figure 19: Example of vertical profile of salinity for an AXCTD delivered in the OMG experiment. Red box contains the uppermost segment (closest to surface) of the profile, which shows a slightly increase of S in the very first values vs the later points.

As seen here, however, the use of OMG is rather local to a very specific part of the Arctic region, and in addition, it operates in areas where SMOS datasets have the most difficult to obtain valid SSS values. Due also to the reduced number of points, validation with OMG dataset is not considered applicable for the general validation of Arctic+ v3.1 product. Results have bene included, however, to reflect the validation effort done by the team and enable discussion about difficulties in the validation found within the project that may be of help for the future.

6.5 SSS validation by intercomparison of three datasets (Triple Collocation)

For the application of Correlated Triple Collocation method, we have taken three sets of collocated SSS maps: JPL SMAP v4.2 SSS, 8-day maps; BEC SMOS Arctic SSSv 2.0, 9-day maps and BEC SMOS Arctic v3.1, 9-day maps.

The Level 3 SSS maps from SMAP, version 4.2 is provided by Jet Propulsion Laboratory (JPL) (Fore et al., 2016). They are available at:

https://podaac-opendap.jpl.nasa.gov/opendap/allData/smap/L3/JPL/V4.2/

Time collocation is done by identifying the first day of the three periods. As JPL SMAP maps are 1-day shorter time collocation is not perfect but considering the orbital gaps in a 9-day period we consider the difference to be negligible. As the three products use different grids, we have reprojected all of them on a cylindrical projection of 0.25º step in both longitude and latitude. This projection can cause some significant spatial distortions, but it is considered that the spatial structure of the error variances has typical scales much larger than the typical pixel size, so the evaluation of the error variances will not be very affected. Finally, considering that the effective resolution of BEC SMOS Arctic v2.0 is 12.5 km (due to the application of optimal interpolation), Gaussian filters with appropriate dispersion scale have been applied to both JPL SMAP v4.2 and BEC SMOS v3.1 to have products of comparable spatial scales. To decide the size of the dispersion scales of the Gaussian filters, the Power Spectral Densities (PDS) [Hoareau, 2018] of the products are calculated and compared. We have computed zonal PDS in the region delimited from 70º to 80º N in latitude, and from 0º to 50º W in longitude; the maps for the full year 2016 have been considered, as shown in Figure 23 (top).

With the products reduced to the common resolution (that of BEC v2.0), we have applied Correlated Triple Collocation (CTC), following [González-Gambau, 2020], to estimate the standard deviation of the errors of the three products. The results are shown in Figure 20 (next page).

As shown in the figure, over the majority of the Arctic BEC v3.1 has the smallest error, excepting some specific regions where BEC v2.0 is better. JPL 4.2 is in all cases the product with the greatest error. The differences between the products are evidenced in Figure 21.

As shown in the figures, BEC v3.1 has smaller error than BEC v2.0 except in the Hudson Bay, Eastern coast of Greenland and Kara sea.

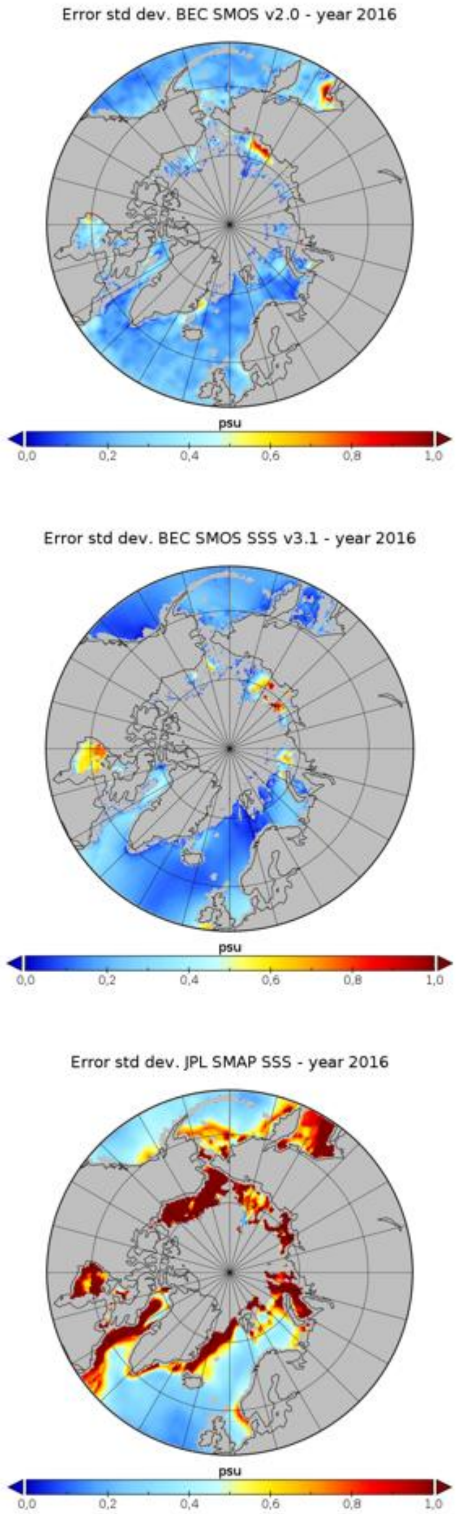


Figure 20: Error standard deviations computed via CTC for (from top to bottom) BEC SMOS Arctic SSS v2.0, BEC SMOS Arctic SSS v3.1 and JPL SMAP SSS v4.2, for all the collocated maps in the year 2016.

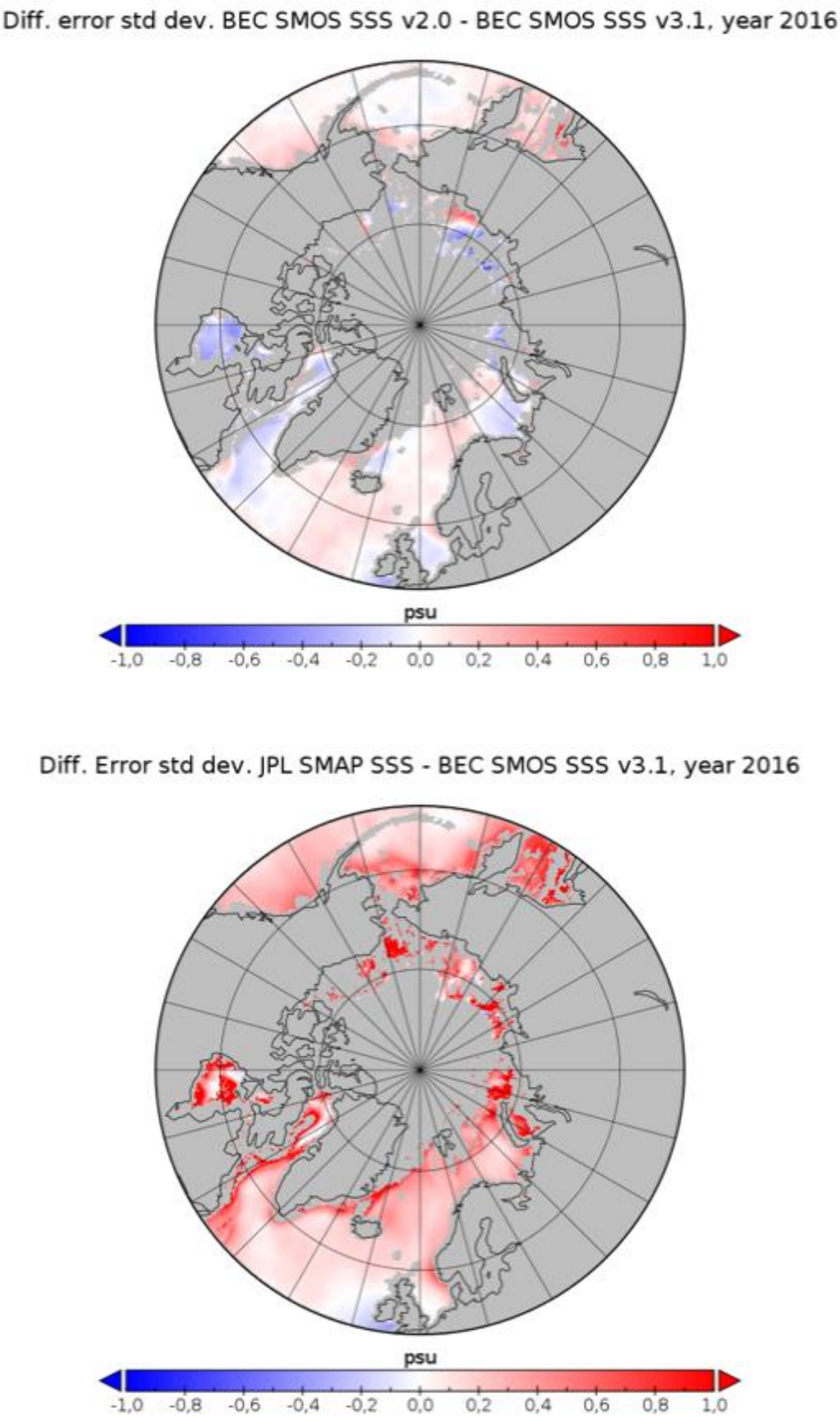


Figure 21: Difference between the error standard deviations of BEC SMOS SSS v2.0 (top) and of JPL SMAP SSS v4.2 (bottom) with BEC SMOS SSS v3.1 for the year 2016.

6.6 SSS validation: wavenumber spectral analysis

First of all, note that the PDS shape of the data in all regions are similar when averaging the spectra over all the year (Figure 22) or only over the ice-free months, i.e., from June to October (Figure 23). The results indicate that, despite the level of noise of each remote sensed product that produce small fluctuations in the otherwise PDS straight shape, the geophysical structures of the SSS data are consistent until a 50 km wavelength for the case of BEC SSS v3.1 (blue) in all regions and for SMAP JPL (red) which corresponds to a spatial resolution of 25 km, as they follow the slope of -2.

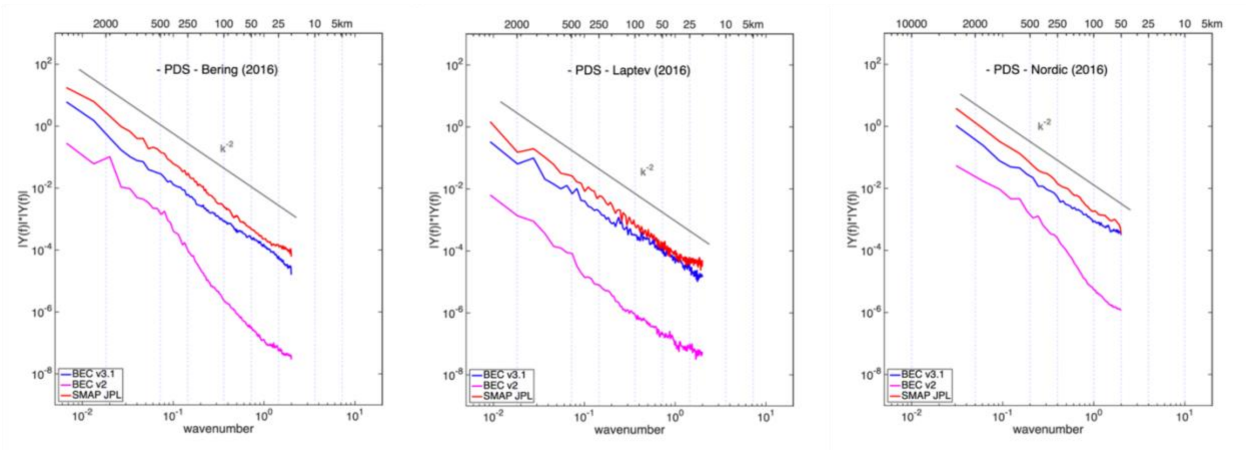


Figure 22: PDS mean over year 2016 for SMOS BEC v3.1 (blue), SMOS BEC v2 (magenta) and SMAP JPL (red). Slope of k-2 is used as a reference (grey line).

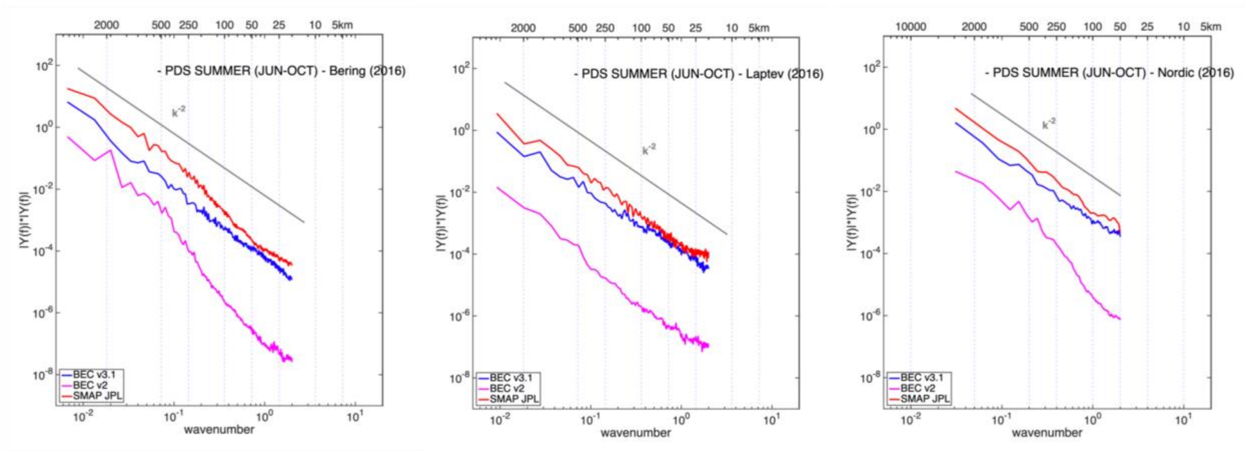


Figure 23: PDS mean for months from June to October 2016 for SMOS BEC v3.1 (blue), SMOS BEC v2 (magenta) and SMAP JPL (red). Slope of k-2 is used as a reference (grey line).

In contrast, the BEC SSS v2 PDS (magenta) consistently describes the geophysical structures up to 250km wavelength (PDS slope similar to -2). For smaller scales there was a decrease of the

PDS slope, indicating a loss of signal, especially in Nordic Seas and Bering Strait due to an over smoothing in the optimal interpolation algorithm.

7 Summary and Conclusions

The present document reflects the results of the validation exercise done for the Arctic+ SSS v3.1 product developed within the project.

The inter-comparison with respect to BEC v2.0 product has been carried out to assess the impact of the algorithm changes into the quality of the product respect to the data version available before the project.

The following aspects have been verified as valid during the validation exercise, both native to Arctic v3.1 product as well as coming from the inter-comparison exercise:

1. Arctic+ SSS v3.1 product introduces an improvement in the number of SSS retrievals obtained from SMOS TBs for the Arctic region. This improved number manifests as a significant reduction of presence of gaps within the product with respect to the initial version BEC v2.0.
2. The new product also benefits of a polar grid in EASE v2.0 format, which is a standard for the research and operations in the region, improving its useability.
3. Arctic SSS+ v3.1 product has been built with minimal external information, being mainly developed using SMOS data exclusively. Whereas this is an advantage in some respects, it raised specific issues impacting data quality that could be addressed in the future.
4. In this sense, additional work could be done to improve the TB climatology used in the retrieval, as it seems the main factor behind the increase of bias in certain regions of the Arctic+v3.1 vs the BEC v2.0 product. Note that BEC v2.0 product uses in-situ based climatology and a bias correction against ARGO, which explains also why metrics are better against certain in-situ databases (i.e., ARGO floats).
5. Comparisons with ARGO inform that BEC v2.0 and Arctic v3.1 products are of similar quality for the regions where ARGO are present (mainly the Greenland and Norwegian seas). The time series analysis, however, reveals some specific limitations within the Arctic+ v3.1 product, including unexplained seasonality (probably instrument-driven patterns) and larger errors in 2011, which is likely to relate to RFI. Results are also slightly noisier in Arctic v.3.1 than in BEC v2.0, with an overall increase of the noise of 0.1 p.s.u. Nevertheless, in terms of overall biases, both products score similarly. Still, the detected limitations give room for improvement and correction, and a better understanding of how the retrieval method is impacted by these peculiarities is required.
6. Matchups with TARA, however, are inclined in favour of the Arctic+ v3.1 product vs BEC v2.0. It is here where the innate smoothing and effective scales of BEC v2.0 are highlighted, which manifests as a worse skill to map spatial variability. Nevertheless, metrics with TARA are not simple to interpret due to the lack of synopticity of the dataset (acquired over a relatively long period of time, i.e., representing different observational conditions) and the lack of spatial homogeneity of the sampling.

7. Because of the above, it is possible to conclude that Arctic+ v3.1 has generally a better skill to describe horizontal SSS gradients than BEC v2.0 and maps better processes at better effective spatial resolution. This comes, however, at the price of an increase of bias in some case, and a larger noise level in general. Those two, however, could be largely compensated by a completer and more advanced L3 mapping technique, as current L3 maps have very little processing, they are not denoised nor data quality has been homogenized.
8. Also related to TARA datasets, Arctic+ v3.1 improves SSS estimates based in SMOS data for some key areas, like the Beaufort Sea, which is good news as some of those areas are now in the focus of the Arctic scientific community.
9. The introduction of the triple collocation also helped to assess properly the differences existing between the derived satellite products. The metrics presented including SMAP data show that Arctic+ v3.1 dataset is the best of the three products used in the collocation exercise (BEC v2.0, Arctic+ v3.1 and SMAP). In particular, the triple collocation also shows that of the three, SMAP data yields the largest errors.
10. The outcome of the triple collocation is interesting because this technique mainly addresses random error levels, rather than systematic errors. As the method extracts the expected natural variability from the common information between the compared products, it means that the fraction of information relevant for studies contained in Arctic+ v3.1 product is the largest of the three products. Mind that triple collocation using these products is relative, as the lack of an in-situ source within the set of datasets used in this metric implies that ground truth information is obtained by pure triangulation of the three observables.
11. The analysis of the spatial wave spectrum is also an important metric to assess the results and helped to confirm what was also observed in some of the other datasets: that Arctic+ v3.1 data is the one containing the most information at smaller spatial scales, what results in a better effective spatial resolution and, thus, more accurate description of Arctic SSS processes.

Within the main difficulties found, limitations and lessons learned, we can enumerate the following ones:

1. The performance of validation in the Arctic region is rather complex due to the heterogeneity of the in-situ datasets, which either lack of temporal or spatial synopticity. Some of the sources only represent specific regions, at the risk of inducing bias by spatial selection when assessing the product entirely. Others are more representative spatially but lack of a proper temporal description of the variability. Thus, none of the datasets used can describe both aspects simultaneously, i.e., the validation requires certain quantities of interpretation of data to extract the actual quality of the product.
2. Metrics performed with TARA, as found in the literature for SSS products, are currently missing key elements in such validation. Whereas there is agreement is possibly the best tool to understand the capability of a satellite-based product in mapping horizontal

processes for SSS in the region, lot of care is required to select data and interpret the results. For instance, there is need to check on the representativity of TARA of a satellite footprint when the number of TARA measurements per cell drops significantly (as it is the case). Filtering in TARA impacts significantly to the results of the metrics. Thus, comparing metrics for products found in literature but with different treatment of TARA data is probably an error, as specific attention is required to what has been done to TARA and how the collocations are made.

3. It is also important to highlight that, when inter-comparing satellite-based SSS products, there is need to pay attention to the selected projections and grids. A fair set of metrics for inter-comparison only is possible over common points resolved at the same spatial scales. This means that QC for these products require to set the products into the same spatial grids and projections. By not doing so, significant errors may be introduced artificially in the metrics, and one or more products may be penalized because sampling strategies are different and thus, matchup database do not yield the same points and hence, information.
4. OMG experiment dataset is very interesting, but its data is probably not good for validation of satellite-based SSS products. The main reason is that EO SSS products face significant limitations to retrieve SSS very close to coast, where most of the OMG AXCTD were launched. In addition, the sparsity of the data in space also makes difficult to find common points when comparing various EO-based products.
5. Provision of the ice mask along the SSS product is relevant for the validation and understanding of the information. It helps to identify where there is actually missing data because of lack of performance in the retrieval vs where it is not possible to measure due to ice. It helps also to understand the behaviour of SSS close to ice patches in the region. Thus, adding this information to the product would be of help and should be addressed in the future. Some options would be to incorporate this from external sources, or derive the mask using SMOS information, as for example using the outputs of the cardioid model fitting over the dwell lines of SMOS.
6. Whilst the retrieval methodology helps significantly to mitigate impact of the RFI present in the region, Arctic+ v3.1 product is still impacted by them. It is understood that there are limits to what can be filtered in terms of RFI, but additional information could be delivered to the users to identify what grid points of the product are more affected by this problem.
7. Several issues have been identified associated to the TB climatology generated to support the retrieval. It could be convenient to revisit this aspect of the methodology to improve quality. A good example of this is the loss of quality in Arctic+ v3.1 within the Baffin Bay vs BEC v2.0.
8. Fundamental error associated to the Arctic+ SSS v3.1 retrieval are not coming only from the instrument, but also from the ancillary information. In particular, errors in wind speed and sea surface temperature (SST) could be of high relevance to understand the actual limit of quality in SSS from SMOS that could be achieved in the region. Whereas these aspects have not been explored explicitly within this project, they are known and may

have an impact. Thus, it could be necessary to revisit those datasets to enable improvement of the product. In particular SST is known to have specific limitations at high latitudes due to the persistence of clouds, which unable the use of IR information. Also, errors in SST are impacting specially SSS retrieval in cold waters, due to the loss of sensitivity of the dielectric constant model under such conditions.

9. Also connected with the above, further work could be done to improve the separability of regimes within the dielectric constant model. Being a key aspect of the retrieval, minimizing its limitations at extreme observational conditions (low SSS, low SST) is relevant for the future of EO-based SS products, not only for the Arctic region.

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