Sea Surface Salinity Products Validation Based on Triple Match Method

Jin Wang [ORCID], Weifu Sun, and Jie Zhang

Abstract—Since satellites have observed the sea surface temperature (SSS) from space for years, the scientific community has devoted many efforts to the validation of satellite SSS products. Typically, this validation procedure is based on the "double match" method between the *in situ* and remote-sensed measurements. However, this direct comparison has its limitations because it does not take into account sampling error of different SSS sources. Actually, the *in situ* method presents the pointwise measurements and the satellite data are the spatial average within its footprint, so the *in situ* data contain the true small-scale SSS signal which cannot be resolved by satellite data. Researchers introduce the representativeness error to describe the small-scale signal. However, the estimation of representativeness error remains challenging. In this study, based on the constancy of salinity variance, we develop a new method to estimate the representativeness error and apply it to the triple collocation dataset of Argo data and L3 SSS product of soil moisture active/passive (SMAP) and soil moisture and ocean salinity (SMOS). The representativeness error is estimated to be 0.093 psu^2 in global oceans. The random error of Argo data is better than 0.21 psu which is superior to SMAP and SMOS. Considering the different sampling resolution of SMAP and SMOS, the quality of SMAP SSS product (0.33 psu) is slightly better than SMOS (0.41 psu).

Index Terms—Representativeness error, sea surface salinity, soil moisture active/passive (SMAP), SMOS, triple match.

I. INTRODUCTION

SEA surface salinity (SSS), as well as the sea surface temperature (SST), is a key parameter to describe the ocean's role in the global water cycle [1]. Before the launch of the first L-band radiometer, SMOS, in 2009, the *in situ* measurements (drifters, mooring buoys, profiling floats, ships, stations) are the main sources of ocean salinity information for decades [2]. However, the *in situ* measurement has its limitations because of its sparse spatial coverage relative to space-borne observations. The space-borne L-band radiometer SMOS, Aquarius, and soil moisture active/passive (SMAP) can map the global oceans in

several days and provide unprecedented satellite-derived SSS datasets [3], [4]. Since the quality of SSS data product is crucial for the application of the remote-sensed SSS datasets based on the direct comparison between remote sensing and *in situ* observations, the scientific community has devoted enormous efforts to the validation of the satellite SSS data in global oceans [5]–[7].

However, there are two limitations in this double match method. First, it assumes the *in situ* observations have no error and explains the difference between satellite data and *in situ* data to be the error of the former [8]. Researchers have proved that the statistical characteristics of both *in situ* measurement and the true signal variation can affect the difference between satellite and *in situ* data [9]. Consequently, the direct comparison procedure cannot give an accurate description of the satellite-derived observations error without the prior knowledge of characteristics of *in situ* measurement and true SSS variation. To address this problem, researchers developed the triple match method to estimate the random errors of three independent and collocated datasets (for example, *in situ*, remote sensing, and model data). The triple match method is first used to assess the measurement error of sea surface wind products [9]. Then it is applied to the soil moisture [10], wave [11], and SSS [12] products.

The second limitation of direct comparison is about the sampling error which is caused by the different sampling resolution of *in situ* (buoys) measurements and remote sensing [13]. Apparently, the *in situ* data represent the "point" measurements and can reflect all small-scale SSS variations. By contrast, the antenna footprint of a spaceborne L-band radiometer is about 40–100 km, which means the satellite-derived SSS data cannot resolve an SSS signal whose spatial scale is smaller than a few tens of kilometer. To resolve this problem, researchers introduce the "representativeness error" to describe this small-scale signal which is observed by a high-resolution system but not by the low-resolution system [9]. However, the accuracy estimate of representativeness error still remains challenging.

In this article, using Argo observations and L3 SSS product of SMAP and SMOS, we develop a new method to estimate the representativeness error and apply it to the triple match dataset (Argo, SMOS, and SMAP). The sampling scales of different SSS products are studied and the random errors of all three SSS datasets are obtained and discussed. Section II introduces the datasets involved in this study and the triple match method. The main results of representativeness error estimation, random errors of all SSS datasets, and a further discussion about the double match and triple match are discussed in Section III and the conclusion is summarized in Section IV.

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II. Datasets and Method

As is described in the previous section, we cannot accurately estimate the random error of SSS data based on the direct comparison between *in situ* and satellite data. In this section, we apply the triple match method to investigate the random error of different SSS products. In fact, as long as the datasets are independent and error distributions are close to Gaussian, the triple match method can obtain the random error of all datasets [14]. So triple match procedure is applied widely in the error characterization analysis of remote sensed datasets. With regard to the SSS, we should choose three independent SSS sources for the triple match method. As is well known, there are three satellite missions which focus on SSS remote sensing, i.e., SMOS, Aquarius, and SMAP. Aquarius has stopped operating since June 2015, and the scientific data product of SMAP is processed by remote sensing system (RSS) since April 2015, so there is barely any temporal coverage between Aquarius and SMAP data. For *in situ* data sources, mooring buoys (TAO, RAMA, PIRATA) provide valuable SSS information in the tropical oceans. But these mooring buoys cannot cover the global oceans, especially some strong transient dynamics regions which have much larger sampling errors than open oceans [13]. As a result, we use the Argo *in situ* dataset to achieve a global estimation of representativeness error. Besides the satellite and *in situ* measurements, there are also climatology field or model results of SSS such as world ocean atlas (WOA) and hybrid coordinate ocean model (HYCOM). WOA climatology is a set of objectively analyzed climatological fields of various oceanic parameters, including the ocean salinity. However, as [16] has pointed out, the WOA climatology assimilates multiple *in situ* data sources such as station data, conductance temperature depth (CTD) probes, gliders, and especially, the Argo buoys. So, the independence between the WOA field and Argo *in situ* data is doubted and we exclude WOA product in this study. Meanwhile, HYCOM product also assimilates various *in situ* data sources including Argo buoy, and we do not use the HYCOM field in our research too. Finally, Argo buoy, SMAP, and SMOS data are involved in this study.

A. Argo

The Argo project is a global ocean array of more than 3800 profiling floats which measure the temperature, salinity, currents, and bio-optical parameters profiles from the sea surface to 2000 m every ten days [17]. The Argo project is the first global system to achieve continuous monitoring for the upper ocean parameters and all Argo data are made publicly available within hours after collection. We use the Argo data processed by the French Research Institute for Exploitation of the Sea (IFRE-MER) from the year of 2015 to 2017 and extract the salinity, location, and time of observation and the quality flag of salinity from the raw data blocks. Some quality control procedures are applied to Argo data. Only the data of the best quality (the quality flag equals one) are involved in this study. For the Argo buoy whose profiler type is SOLO or PROVOR, we use the shallowest salinity data between 5 and 10 m, because of the problem of water pumping at a depth less than 5 m [18]. For the other Argo profiles, we use the shallowest salinity measurements between 0.5 and

10 m. Finally, the amount of effective Argo measurements is more than 3 54 000.

B. SMAP

SMAP was launched by NASA on, 31 January 2015 [19]. Equipped with the L-band radiometer and radar which share a 6 m reflector antenna, SMAP can map the global oceans in two to three days at a 40-km resolution. Although the primary objective of SMAP mission is monitoring the land surface soil moisture and freeze–thaw state, SMAP also has the capability of SSS remote sensing, based on its L-band radiometer observations. Particularly after Aquarius ended its mission on June 7, 2015, because of a power supply failure, SMAP has become the only in-orbit space-borne L-band radiometer of NASA. Thus, the scientific community carries out extensive research on SSS retrieval based on SMAP observations [20]. RSS provides the SMAP L2 swath data product and L3 eight-days running average product of 0.25° spatial resolution [21]. We downloaded the SMAP L3 data (V4.0) from the year of 2015 to 2017 from the RSS FTP site (ftp://ftp.remss.com/smap).

C. SMOS

SMOS is the first satellite mission with the main objective focused on the SSS remote sensing from space which was launched on 2 November 2009 from the Plesetsk Cosmodrome in northern Russia. With the L-band Microwave Imaging Radiometer with Aperture Synthesis (MIRAS), SMOS can provide the global ocean's salinity in 2–3 days with a 30–100 km solution [1]. The Centre Aval de Traitement des Données SMOS - Production & Dissemination Center (CATDS-PDC) develops various high-level SMOS SSS products with different resolutions. We use the L3 ten-days average debiased salinity field (V3.16) at 25 km spatial resolutions which mixes both ascending and descending orbits and this product covers the oceans between 50 °N–50 °S.

D. SSS Data Collocation

The three SSS data sets used in this study are provided with different spatial and temporal resolutions. Therefore, a data collocation procedure is taken to construct the spatial and temporal match dataset. Obviously, Argo data present the pointwise observations at ten-days intervals. SMAP dataset is the eight-days running average at daily scales and SMOS data is provided as ten-days average. For SMAP data, we take the central day as the observation date to temporally collocate with Argo data. And the 40 km grid of SMAP product which is the closest to Argo location is regarded as spatially match data. For the SMOS dataset, the central two days (i.e., day 5 and day 6) is taken as the observation dates and collocated with Argo-SMAP match-up dataset. We also use the SMOS product grid closest to Argo-SMAP observations to achieve the spatial collocation. Finally, we get more than 40 000 collocated data in the triple match dataset. It is worth noting that Argo data are beneficial to achieve a collocated dataset which covers the global oceans, especially the regions with high SSS variability. The spatial distribution of triple match data is shown in Fig. 1.
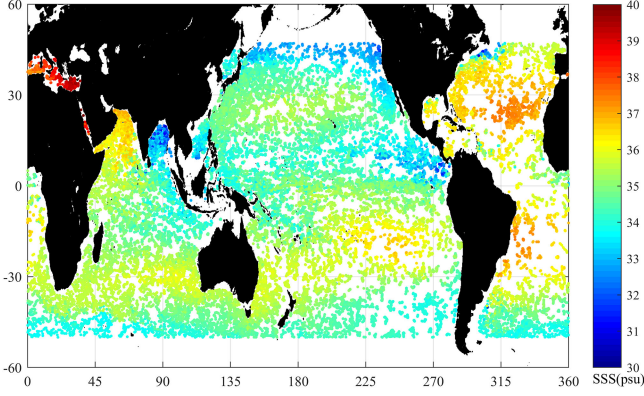
Fig. 1. Distribution of collocated data.

E. Triple Match Method

As is described in prior sections, different SSS data sources have different sampling resolutions. Suppose there are three SSS datasets S_i (such as buoy, satellite, and model data) which is arranged in the descending order of spatial and temporal scales

$$S_i = a_i S + b_i + \delta_i \qquad (i = 1, 2, 3) \tag{1}$$

where a_i and b_i are the scaling and bias calibration coefficients of SSS systems, and δ_i is the random error. S is true SSS variation that can be resolved by all three systems. Generally, the three SSS systems have different sampling scales. For example, the buoy measurements which present the pointwise observations has the smallest sampling scale, whereas the sampling scale of satellite and model data is much bigger because of the spatial average or smoothing. So, S represents the SSS signal resolved by the largest scale (lowest resolution) system, i.e., the scale of S_3. Because the system 1 and 2 have a higher resolution, there are small scale SSS signals which are observed by S_1 and S_2 but not by S_3. This small scale SSS variation is defined as the representativeness error, r^2, which can be estimated by the correlated part of the random error of system 1 and 2 [22]

$$\langle \delta_1 \cdot \delta_2 \rangle = r^2 \tag{2}$$

where the symbol $< >$ means averaging. Meanwhile, since the system 3 cannot observe this small SSS signal, the random error of system 3 is uncorrelated to system 1 and 2

$$\langle \delta_1 \cdot \delta_3 \rangle = \langle \delta_2 \cdot \delta_3 \rangle = 0 \tag{3}$$

In addition, the triple match method assumes the SSS signal, S, is independent of the random error of all systems

$$\langle \delta_i \cdot S \rangle = 0 \ (i = 1, 2, 3) \tag{4}$$

Without loss of generality, we take S_3 as the calibration reference source which means $a_3 = 1$ and $b_3 = 0$. We introduce the first-order moment $M_i (i = 1, 2, 3)$ of all three systems

$$M_1 = a_1 \langle S \rangle + b_1$$
$$M_2 = a_2 \langle S \rangle + b_2$$
$$M_3 = \langle S \rangle \tag{5}$$

where the $\langle S \rangle$ denotes the average of the true SSS signal under the scale of system 3.

The second-order moment of M_{ii} and the second-order mixed-second-order moment of $M_{ij} (i \neq j)$ are

$$M_{ii} = \langle S_i \cdot S_i \rangle = a_i^2 S^* + \langle \delta_i^2 \rangle \ (i = 1, 2, 3)$$
$$M_{12} = \langle S_1 \cdot S_2 \rangle = a_1 a_2 S^* + r^2$$
$$M_{23} = \langle S_2 \cdot S_3 \rangle = a_2 S^*$$
$$M_{31} = \langle S_3 \cdot S_1 \rangle = a_1 S^*$$
$$S^* = (S - S)^2 = \langle S^2 \rangle - \langle S \rangle^2 \tag{6}$$

where S^* is the variance of the common SSS single of all three systems.

Based on (6), the variance of random errors δ_i, scaling calibration coefficients a_i, and the common SSS variance S^* are obtained

$$\langle \delta_i^2 \rangle = M_{ii} - a_i^2 S^*$$
$$a_1 = \frac{M_{12} - r^2}{M_{23}}$$
$$a_2 = \frac{M_{12} - r^2}{M_{31}}$$
$$S^* = \frac{M_{23} \cdot M_{31}}{M_{12} - r^2} . \tag{7}$$

Equation (7) indicates that the estimation of representativeness error will affect the SSS variance and the random errors δ_i. If the representativeness error is taken as zeros, as [8] has done in their research, it will cause an underestimation of δ_1, δ_2, and an overestimation of δ_3. Consequently, an optimal method of determining representativeness error is critical for SSS product assessment.

III. RESULTS AND DISCUSSION

A. Representativeness Error Estimation

The discussion in the previous section emphasizes the importance of r^2 estimation to SSS product assessment. However, the estimation of r^2 is still challenging. It is widely accepted that an optimal estimation of r^2 will lead to a good calibration of all three SSS systems. Portabella and Stoffelen [14] estimated the representativeness error by an analysis of power density spectra (PDS) of wind fields measurements. However, according to [12], the slope of PDS is quite sensitive to the noise of data which is relatively high for SSS product. As a result, it restricts applying this method to SSS product validation. Lin also developed a method to address representativeness error by repeating the triple match analysis for different r^2 values until an optimal intercalibration was achieved [22]. Lin argued that the r^2 value which resulted in a close-to-zero bias for both the *in situ* and satellite-derived data was considered to be the optimal one. In [12], Hoareau chose the r^2 value which made the linear regression slope of the calibrated data and reference data close to 1 (i.e., close to the diagonal in scatterplots) as the optimal estimation and applied this method to six salinity

products including the TAO buoys data, the GLORYS2V3 ocean reanalysis, Aquarius and SMOS maps, WOA 13 (World Ocean Atlas 2013), and WOA 09 climatology fields. But our numerical experiment shows some different results. Even under the ideal conditions which means we know the precise value of r^2, a_i and b_i, the effect of random error δ_i will cause the slope of linear regression to deviate from the diagonal.

We present a new method to address the representativeness error. As is discussed by [22], besides the S_3, S_1, and S_2 can also be taken as the calibration reference. Without loss of generality, if the S_1 is chosen as the calibration reference, the SSS system S_i can be described as

$$S_1 = a_1 S + b_1 + \delta_1 = S' + \delta_1$$

$$S_2 = \frac{a_2}{a_1} S' + \left(b_2 - \frac{a_2}{a_1} b_1 \right) + \delta_2 = a'_2 S' + b'_2 + \delta_2$$

$$S_3 = \frac{1}{a_1} S' - \frac{b_1}{a_1} + \delta_3 = a'_3 S' + b'_3 + \delta_3. \qquad (8)$$

As is discussed in the Section II-E, the random error is obtained

$$\left\langle \delta_1^2 \right\rangle = M_{11} - a_1^2 S'^*$$

$$\left\langle \delta_2^2 \right\rangle = M_{22} - a_2^2 S'^*$$

$$\left\langle \delta_3^2 \right\rangle = M_{33} - S'^* \qquad (9)$$

where M_{ii} is the second-order moment of the system i. The SSS variance of system 1, S'^*, is

$$S'^* = \left\langle S'^2 \right\rangle - \left\langle S' \right\rangle^2 = a_1^2 S^* \qquad (10)$$

where S^* presents the variance of SSS signal of all three systems which is defined in the (6).

Similarly, when system 2 is taken as the calibration reference, SSS variance of system 2 is

$$S''^* = \left\langle S''^2 \right\rangle - \left\langle S'' \right\rangle^2 = a_2^2 S^* \qquad (11)$$

where S^* also presents the variance of SSS signal of all three systems.

It is obvious that, for given SSS systems, the spatial-temporal scales do not change which means the variance of SSS signal, S^*, should remain constant no matter which SSS system is chosen as the calibration reference. In other words, the S^* in (6), (10), and (11) should be the same. Consequently, the value of representativeness error which leads to a constant SSS variance S^* under different SSS calibration references is regarded as the optimal value. Based on this opinion, we present a new method to estimate the representativeness error. All three SSS Systems are chosen as the calibration reference respectively and based on each calibration reference, we calculate the S^* under different representativeness error values. Then the value of representativeness error, which makes the three S^* curves intersect is the optimal value.

The triple-match dataset of Argo, SMAP, and SMOS is used to estimate the representativeness error. As is described in Section II-E, to obtain a reasonable value of r^2, the three SSS systems should be sorted in the descending order of their resolving spatial-temporal scales. To determine the sampling scales of

TABLE I
FOUR TRIPLET SSS SOURCES COMBINATIONS

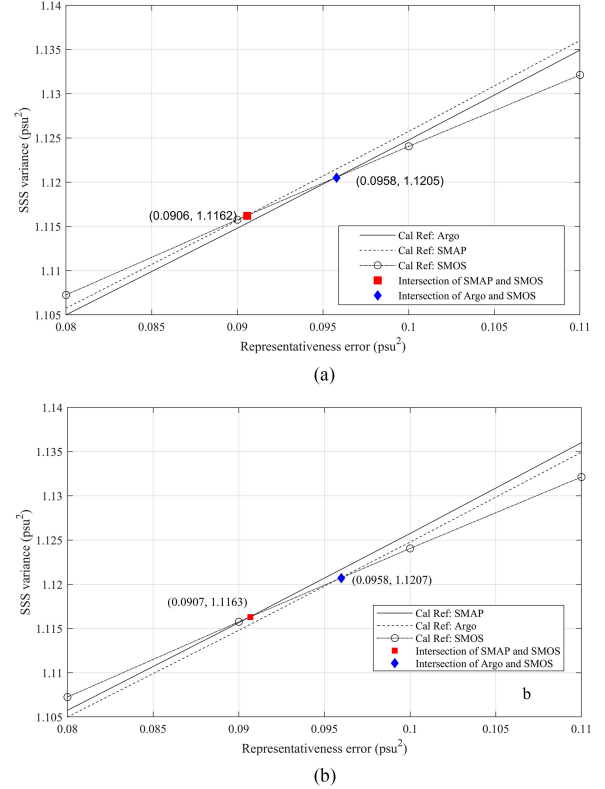| Data set	System1	System2	System3
D1	Argo	SMAP	SMOS
D2	SMAP	Argo	SMOS
D3	Argo	SMOS	SMAP
D4	SMAP	SMOS	Argo

Fig. 2. Relationship between S^* and r^2. (a) D1. (b) D2.

Argo, SMAP, and SMOS, we analyze four triplet combinations in this section, as is shown in Table I. For spatial sampling, it is quite obvious that the Argo data which present the pointwise observation have the best spatial sampling resolution than SMAP and SMOS whose spatial resolutions are about 40 km. For temporal sampling, Argo buoys measure the SSS at ten-days intervals and the temporal resolution of the L3 SSS products used in this article is eight to ten days which is approximate to Argo data. As a result, in the dataset of D1, the Argo data are taken as the system 1. Then we assume the SMAP has a better resolution than SMOS, so the SMAP and SMOS are taken as the system 2 and 3. Certainly, this assumption will be tested later.

Based on D1, the relationship between S^* and r^2 under all three different calibration reference is shown in Fig. 2(a). It is found that the two intersection points of three curves are quite close. The curves of SMAP and SMOS intersect at 0.091 (r^2) and 1.116 (S^*). For Argo and SMOS, the curves intersect at 0.096 (r^2) and 1.121 (S^*). Then the same procedure is applied to the dataset of D2 and the results are shown in Fig. 2(b). It is obvious
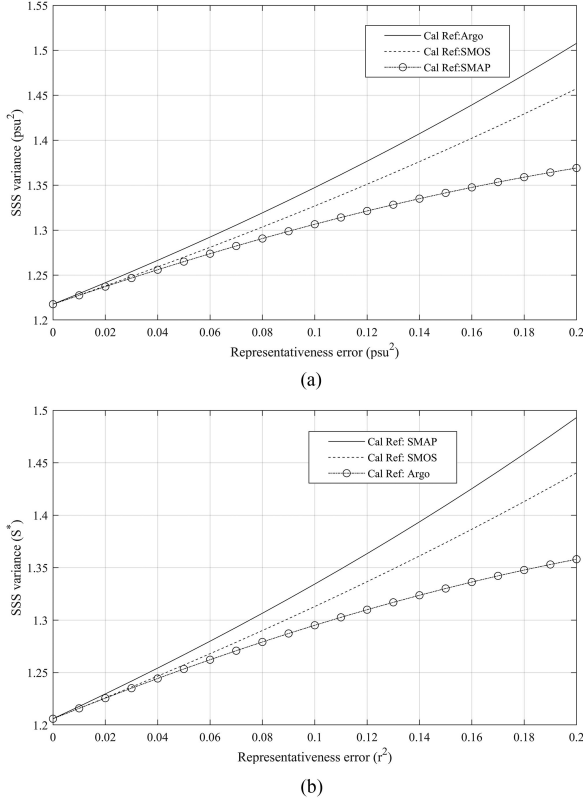
(a)

(b)

Fig. 3. Relationship between S^* and r^2. (a) D3. (b) D4.

that the results coincide with Fig. 2(a). These results confirm the assumption of SMAP having a smaller spatial-temporal scale than SMOS and the common small scale SSS signal which Argo and SMAP can observe (i.e., sampling error) is about 0.091–0.096 psu^2.

To validate the feasibility of the method, we also test the dataset of Argo_SMOS_SMAP (D3) which means we investigate the common SSS signal which can be observed by Argo and SMOS but not by SMAP. The results are shown in Fig. 3(a). Obviously, in Fig. 3(a), there is no intersection at the positive axis of r^2 for all three curves. It indicates there is no common SSS signal in Argo and SMOS observations on the scale of SMAP because the spatial-temporal scale of SMOS is bigger than Argo and SMAP. In Fig. 3(b), which is obtained by dataset D4, we can get a similar conclusion that SMAP and SMOS cannot catch a small scale SSS single on the sampling resolution of Argo data because Argo data has the smallest sampling scale.

B. Random Error Assessment of SSS Products

In this section, based on the data set of Argo_SMAP_SMOS (D1), we take the representativeness error to be 0.093 (the mean value of 0.091 and 0.096) and calculate the random errors of all SSS systems. The results are shown in Table II. Obviously, regardless of which dataset is set to be the calibration reference, the random errors of all three SSS sources and the variance of SSS are quietly stable. The Argo in situ measurements have the best quality with a random error of 0.37 psu. The random

TABLE II
RANDOM ERROR AND SSS VARIANCE AT THE RESOLUTION OF SMOS

Calibration Reference	δ_{Argo}(psu)	δ_{SMAP} (psu)	δ_{SMOS} (psu)	S^*
Argo	0.37	0.44	0.41	1.118
SMAP	0.38	0.45	0.42	1.119
SMOS	0.37	0.45	0.41	1.118
Mean Value	0.37	0.45	0.41	1.118

error of SMOS SSS is 0.41 psu which is slightly superior to SMAP. However, it is worth noting that these results are obtained at the resolution of SMOS (system 3) which means there is a common SSS signal (r^2) observed by Argo and SMAP but not by SMOS. So, if we want to get the random error at the resolution of SMAP, the representativeness error is needed to subtract from the error variances of Argo (system 1) and SMAP (system 2) and add to the error of SMOS (system 3) [12]. As a result, at the resolution of SMAP, the random errors of Argo, SMAP, and SMOS are 0.21, 0.33, and 0.51 psu, respectively. We believe that a reasonable quality assessment procedure is to estimate the error of SSS data sources on their own sampling resolution. Therefore, the random errors of SMAP and SMOS are 0.33 and 0.41 psu, respectively and the data product quality of SMAP is slightly better than SMOS.

It is concluded that at both resolutions of SMAP and SMOS, the Argo buoys provide the best quality SSS measurements. It is remarkable that the Argo has the smallest sampling scale and as a result, there is still an SSS signal which Argo can resolve but SMAP cannot. Consequently, the random error of Argo is actually better than 0.21 psu.

C. Further Discussion About the Double Match Method

In this section, we will compare the results we got in Section III-B with double match procedure. Validation based the double match between satellite observation and in situ measurements is a wide-used method to estimate the quality of remotely sensed data [23], [24]. However, as is discussed in Section I, this method will lead to an overestimation to the remotely sensed data because it assumes the in situ data are perfect and does not separate the observation error and sampling error. To compare with the results of the triple match method, we also apply this double match procedure to the dataset of Argo, SMAP, and SMOS. And it is found that the random errors of SMAP and SMOS are 0.39 and 0.55 psu, respectively, which means that the double match method leads to an overestimation of 18% and 34% to the error of SMAP and SMOS data.

IV. CONCLUSION

The triple match method for SSS validation is an improved procedure compared with the double match method which assumes the in situ data are perfect and does not separate the observation error and sampling error. Sampling error, or representativeness error, which presents the small scale SSS signal

in the high-resolution system, is a key factor to be determined during the triple match procedure since it affects the validation results dramatically. However, the accurate estimation of representativeness error remains difficult. In this article, we present a new method to address the representativeness error based on the constancy of salinity signal variance for a given SSS triple match dataset. The results indicate that representativeness error in the SSS system of Argo, SMAP, and SMOS is about 0.093 psu^2 in global oceans. The Argo buoys provide the most accurate SSS observations with the random error better than 0.21 psu. At the resolution of SMOS, the random error of SMOS (0.41 psu) is better than SMAP (0.45 psu). However, at the resolution of SMAP, SMAP has a better random error (0.33 psu) than SMOS (0.51 psu). Generally, considering the different sampling resolution of SMAP and SMOS, the quality of the SMAP SSS product (0.33 psu) is slightly better than SMOS (0.41 psu). We also compare our results with the double match. The results show that the double match procedure will lead to an overestimation of 18% and 34% to SMAP and SMOS data.

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