

Synthesizing high-resolution satellite salinity data based on multi-fractal fusion

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Abstract

The spaceborne platform has unprecedentedly provided the global eddy-permitting (typically about 0.25°) products of sea surface salinity (SSS), however the existing SSS products can hardly resolve mesoscale motions due to the heavy noises therein and the over-smoothing in denoising processes. By means of the multi-fractal fusion (MFF), the high-resolution SSS product is synthesized with the template of sea surface temperature (SST). Two low-resolution SSS products and four SST products are considered as the source data and the templates respectively to determine the best combination. The fused products are validated by the *in situ* observations and intercompared via SSS maps, Singularity Exponent maps and wavenumber spectra. The results demonstrate that the MFF can perform a good work in mitigating the noises and improving the resolution. The combination of the climate change initiative SSS and the remote sensing system SST can produce the 0.1° denoised product whose global mean standard derivation of salinity against Argo is 0.21 and the feature resolution can reach 30–40 km.

Key words: sea surface salinity, multi-fractal fusion, high resolution

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1 Introduction

As an essential climate variable (ECV), the ocean salinity plays an important role in the global water cycle, climate change and ocean circulation (Vinogradova et al., 2019). However, to date the salinity observations have been sparse and sporadic before the realization of the remote sensing of salinity in the last decade. Based on the L-band (about 1.4 GHz) sensor, three missions can measure sea surface salinity (SSS) from space, including the soil moisture and ocean salinity (SMOS) (Font et al., 2010) (2009 to present), the Aquarius (Le Vine et al., 2010) (2009–2015) and the soil moisture active passive (SMAP) (Entekhabi et al., 2010) (2015 to present). These missions can typically provide the quasi-weekly SSS products on an eddy-permitting grid (1° for Aquarius). Even so, the reliance of the resolution on the size of the antenna and the low sensitivity of salinity to the brightness temperature have limited the resolution and accuracy of SSS products (Reul et al., 2020). Besides, the quality of remotely sensed salinity data is vulnerable to radio frequency interference (RFI), land-sea contamination and spatial-temporal drifts (Martín-Neira et al., 2016). As a result, the quality of the first versions of the SSS products is quite poor. Taking the first SMOS SSS product as an example, the global standard deviation (STD) of the level 2 (L2) data with respect to Argo can reach over 1 (Boutin et al., 2012; Reul et al., 2012).

Due to the ongoing efforts of researchers to advance the capabilities of retrieval and correction algorithms, the new versions of SSS products are more reliable, of which the typical STD of the quasi-weekly level 3 (L3) SSS products with respect to the *in situ* near surface salinity can be about 0.2 in the open ocean (Bao et al., 2019; Boutin et al., 2018; Meissner et al., 2018; Olmedo et al., 2017; Tang et al., 2017). These remotely sensed data products

have thus promoted studies on large-scale salinity-related ocean phenomena, such as El Niño and the Southern Oscillation (ENSO) (Hasson et al., 2018; Qu and Yu, 2014). However, the SSS maps are still too noisy to highlight mesoscale motions. Besides, the SSS maps are intrinsically deficient in mesoscale research due to the limited footprint of the SSS sensors. Most of the former works employed the monthly SSS data or relaxed the SSS to a coarser resolution, thus only the about 100 km eddies or fronts may be extracted (Kao and Lagerloef, 2015; Maes et al., 2014; Melnichenko et al., 2017). Consequently, the key to improving the resolution of SSS data lies in the mitigation of noises without blurring the mesoscale features.

In general, the mitigation of noise is often accompanied by the decrease of resolution. Most of the existing L3 products are denoised by means of a two dimensional (2D) filter (e.g., the Gaussian filter) or objective analysis (OA) (Reul et al., 2020). Although effective in eliminating noise, the utilization of the 2D filter inevitably results in artificial cross-isohaline mixing, lowering the capability to resolve mesoscale eddies and fronts (Buongiorno Nardelli et al., 2016). Besides, the 2D filter is only applicable to white noises and fails to eliminate spatially-varying noise (Turiel et al., 2014). Therefore, efforts to synthesize satellite-derived SSS data in combination with other sources of data are necessary (Vinogradova et al., 2019).

One solution to synthesize high-quality SSS is based on the fusion of *in situ* near surface salinity (NSS) data. The NSS can be taken as the reference in the neural network to correct the satellite salinity (Mu et al., 2019; Vernieres et al., 2014) or can be directly blended with the satellite salinity via OA (Droghei et al., 2016). This approach is generally considered to be reasonable because the uncertainty of the *in situ* NSS is usually lower than the

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satellite salinity. However, there can be large differences between the quasi-pointwise *in situ* NSS and the footprint-averaged SSS as measured by the satellite due to the near surface stratification and the sub-footprint variability (Boutin et al., 2016). Moreover, the *in situ* NSS is too sparse to improve the resolution of the SSS map.

Another solution is to take other satellite data as the template under the hypothesis of the similarity between the SSS and the template. Typical algorithms include the SST-based-covariance optimal interpolation (OI; Buongiorno Nardelli, 2012) and the multi-fractal fusion (MFF) algorithm (Umbert et al., 2014), which are claimed to improve the resolution of SSS maps taking SST as the template. Given that the parameters of OI are difficult and rely on the covariance of the SST, the fusion of OI is not sufficiently flexible to be transplanted to multiple SST templates. Consequently, this method will not be discussed further in this paper. As for the MFF, the essence of the (scalar) multifractal fusion is to carry out a local regression between the gridded SSS and the gridded SST (Olmedo et al., 2016; Umbert et al., 2014). This non-parametric method has proved to be effective in boosting the capability of the SSS map in resolving mesoscale eddies (Isern-Fontanet et al., 2016; Umbert et al., 2015). This technique has been applied to the SMOS SSS, producing the nominal 0.05° SMOS Barcelona Expert Center (BEC) L4 SSS products (Olmedo et al., 2017) based on the SST of the operational sea surface temperature and sea ice analysis (OSTIA; Donlon et al., 2012). However, this product cannot effectively resolve the features that are finer than 100 km (Buongiorno Nardelli et al., 2016). This issue results partly from the over-smoothing of the OSTIA. As revealed by Reynolds and Chelton (2010) and Chin et al. (2017), the feature resolution of OSTIA is about 100 km despite its nominal resolution of 0.05°.

Consequently, the existing L4 salinity product cannot actually attain mesoscale resolution. The quality of the fused SSS product synergized by MFF is determined by the input SSS data and the SST template (which will be discussed in Section 2.1). For one thing, several centers are processing the SSS data and disseminating the products, of which the best one for MFF input has not been discussed. Furthermore, the oversmoothed OSTIA has been demonstrated to be an inappropriate template. Please note that multiple sensors including the about 1 km infrared sensors can measure the SST from space (Ciani et al., 2020), thus SST products can theoretically reach mesoscale or even finer resolution. Nevertheless, the selection of the SST template has not been fully considered by researchers.

In this paper, both the input data of the SSS and the template data of the SST are evaluated and selected for MFF. The fused products are validated by *in situ* observations and the use of various methods to determine the most appropriate combination of the SST and the SSS.

This paper is organized as follows. In Section 2, the MFF method and the evaluation methods are described. In Section 3, the data and experiments employed are highlighted. In Section 4, the templates for fusion are selected and the synthesized products are evaluated. The discussion and summary are presented in Sections 5 and 6, respectively.

2 Methods

2.1 Multi-fractal fusion method

It is challenging to derive the quantitative relationship between the SSS and the SST because of the complexity of the governing equations. The multi-fractal theory provides a new approach for quantifying the relationship between the SSS, the SST

and other ocean scalars from a geometric perspective (Turiel et al., 2005; Isern-Fontanet et al., 2007; Nieves et al., 2007; Olmedo et al., 2016; Turiel et al., 2008; Umbert et al., 2014). Justification of this theory has been provided by Umbert et al. (2014) and Olmedo et al. (2016). A concise overview of the theoretical basis of multi-fractal fusion now follows.

The association between the geometric structure of the SSS and the SST at any point $\vec{x}$ can be expressed as [see Olmedo et al., (2016) for more details]

$$\begin{cases} T_\psi |\nabla S|(\vec{x}, r) = \alpha_S(\vec{x}) r^{h(\vec{x})} + o(r^{h(\vec{x})}), \\ T_\psi |\nabla \theta|(\vec{x}, r) = \alpha_\theta(\vec{x}) r^{h(\vec{x})} + o(r^{h(\vec{x})}), \end{cases} \quad (1)$$

where $T_\psi |\nabla S|(\vec{x}, r)$ ($T_\psi |\nabla \theta|(\vec{x}, r)$) represents the modulus of the gradient of the SSS (SST) projected on a given wavelet function ψ ; $\alpha_S(\vec{x})$ ($\alpha_\theta(\vec{x})$) denotes the amplitude factor of the SSS (SST); r is the non-dimensional scale parameter. The singularity exponent h is a dimensionless quantity depicting the fractal structure. Note that h is the same for the SSS and the SST and represents the correspondence of their fractal structures.

According to Umbert et al. (2014), a proportional relationship can be derived based on Eq. (1) via a smooth, slow-varying function $\Phi(\vec{x})$.

$$\nabla S(\vec{x}) = \Phi(\vec{x}) \nabla \theta(\vec{x}), \quad (2)$$

where $\Phi(\vec{x})$ is considered to be a matrix, however the integration of the gradient of the SSS would introduce large systematic errors (Olmedo et al., 2016). As a result, the $\Phi(\vec{x})$ has to be simplified as a scalar $a(\vec{x})$ quantity and Eq. (2) can thus be integrated directly giving Eq. (3).

$$S(\vec{x}) = a(\vec{x})\theta(\vec{x}) + b(\vec{x}), \quad (3)$$

where the intercept b is calculated by $b(\vec{x}) = \langle S(\vec{x}) \rangle - a(\vec{x}) \langle \theta(\vec{x}) \rangle$, where $\langle \cdot \rangle$ is the local average operator, namely, a local 2D filter. Then Eq. (3) can be transformed into Eq. (4).

$$S(\vec{x}) = a(\vec{x})(\theta(\vec{x}) - \langle \theta(\vec{x}) \rangle) + \langle S(\vec{x}) \rangle. \quad (4)$$

The right part of Eq. (4) consists of two terms. The first term is characterized by the difference between the SST map and the filtered SST map. It is this term that transmits the frontal or singular structures of the SST map to the SSS map. Determined by the feature resolution of the template, this singular term is the guarantee that MFF will improve the resolution of the SSS map. The second term is the background SSS, where both the small-scale signals and the noises are removed.

2.2 Evaluation methods

2.2.1 Denoising performance

In situ (Argo or mooring buoys) near the surface are used to validate the denoising performance of the fused SSS. Considering the innate differences resulting from the sub-footprint variability and the near surface stratification (Boutin et al., 2016), differences of >1 between the *in situ* NSS and the SSS products are excluded. The standard deviation (STD) and mean of the difference between the *in situ* NSS and the satellite-derived SSS are calculated to quantify the level of noise and the bias of the product, respectively.

2.2.2 Wavenumber spectra

The feature resolution of the SSS map may be quantified by the wavenumber spectra. A reasonable slope for the SSH spectra in the mesoscale band should be between $-11/3$ [predicted by the surface quasi-geostrophic (SQG) turbulence] and -5 [predicted by the quasi-geostrophic (QG) turbulence] (Xu and Fu, 2011, 2012), while the spectrum of a passive tracer should be about -2 along the isopycnals (Callies and Ferrari, 2013). Given that the temperature and the salinity are not always density-compensated (as well as other reasons that are beyond the scope of this paper), the spectral slopes of the SST and the SSS products do not totally follow the -2 law but usually range from -3 to -2 (Chin et al., 2017; Ciani et al., 2020; Droghei et al., 2018; Reynolds and Chelton, 2010).

The calculation of the wavenumber spectrum is based on the method of Buongiorno Nardelli et al. (2016). Considering that the frontal variations in the ocean are mainly meridional, only the meridional spectrum is discussed in this paper. At each longitude, the SSS values are linearly detrended and then transformed by the fast Fourier transformer (FFT). The Blackman-Harris window is applied to reduce the leakage of the spectral power. The plot of the wavenumber spectra is the logarithmic plot with x -axis as the wavenumber and y -axis as the power spectral density (PSD, computed by the amplitude of FFT).

Note that “feature resolution” in this study refers to the capability of one product to resolve the features of oceanic motions. This capability is characterized by the sharp decline of the wavenumber spectrum. Please note that no standard or quantitative definition of feature resolution has been defined authoritatively. Hereafter, we define the “feature resolution” as the reflection point between the reasonable cascade of PSD and the sharp drop of PSD that results from the over-smoothing. In contrast, there is usually a reflection point where the spectrum becomes flat, which is defined as the “effective resolution” hereinafter, corresponding to a signal-to-noise ratio of about 1. Generally speaking, the “true resolution” of a specific product should be between two reflection points.

3 Data

3.1 SSS data

Although multiple SSS products are available, only the SMOS-based products can provide the long record of data from 2010 to the present. Two SMOS-based SSS products are thus considered in this paper.

The SMOS BEC L3 binned SSS product is retrieved from the non-Bayesian algorithm (Olmedo et al., 2017). This product blends the SSS data measured by SMOS and binned onto a $0.25^\circ \times 0.25^\circ$ grid. The temporal resolution of 9-d running. A series of reprocessing has been employed, including a geophysically-consistent filtering criterion, an empirical correction to reduce the biases, an interpolation scheme to improve the near-coast values and an estimate of the uncertainty (Olmedo et al., 2021). Consequently, the systematic errors have been effectively removed and the effect of noises has been mitigated. There are two versions of BEC L3 SSS products, namely the “high-resolution version” (hr) and the “low-resolution” (lr) version. The hr version retains the potential mesoscale features from SMOS retrievals, while the lr version has removed part of mesoscale features through the 50 km Gaussian filter. The hr version is selected as the source data considering the fusion of a truly high-resolution SSS product.

The climate change initiative (CCI) SSS dataset is produced

by the European Space Agency (ESA) CCI project. This product blends the data from three existing SSS missions including SMOS, Aquarius and SMAP. It has been sampled spatially on a 25 km equal area scalable earth (EASE) grid with a sampling time of 1 d. The blending is based on the optimal interpolation and a series corrections and calibrations, e.g., the correction of latitudinal biases and the correction of individual SSS. The comparisons with *in situ* data indicate much better performances than the ones obtained with a single satellite data product (Boutin et al., 2020).

3.2 SST data

Two types of sensors can measure the SST from space, i.e., the microwave sensor and the infrared sensor. The microwave sensor is unaffected by cloud cover but the resolution is lower (about 25 km), while the infrared sensor can measure the near-coastal values and the resolution is higher (about 9 km or 1 km). Although multiple SST products blend the data from multi-sensors, the differences in the specific data used and the fusion scheme can result in a divergence in data quality. Four SST products are considered in this paper and are now introduced.

The optimum interpolation SST (OISST) is a $(1/4)^\circ$ daily product that can provide a long-term record of the SST. This dataset incorporates multi-source observations including those via satellites, ships, buoys, and Argo floats. The advanced very high resolution radiometer (AVHRR)-only product is employed here.

The OSTIA SST is a daily product and has a nominal spatial resolution of $0.05^\circ \times 0.05^\circ$ (Donlon et al., 2012). The OSTIA program is run by the Met Office and the dataset is provided by the Copernicus Marine Environment Monitoring Service (CMEMS). This product fuses *in situ* and satellite data from both infrared and microwave radiometers by means of objective analysis.

The office of satellite and product operations (OSPO) SST analysis is a daily product on a global 0.054° grid. This analysis blends the data from AVHRR, the visible infrared imager radiometer suite (VIIRS), the geostationary operational environmental satellite (GOES) imager, the Japanese advanced meteorological imager (JAMI) and *in situ* data.

The remote sensing systems (REMSS) MW_IR OI SST product is also employed. The product blends microwave data and infrared data (MW_IR) at 9 km resolution. The spatial resolution is 0.1° and the temporal resolution is daily.

3.3 *In situ* data

The near surface salinity for the Argo floats of the global argo observational data set from the China Argo Real-time Data Center (Li et al., 2019) was used for validation. This data set is the quality re-controlled product of all of the profiles in the Global Data Assembly Center (GDAC). Only the data with quality control (QC) flag = 1 (“the highest quality”) are considered. To match the daily SSS map, the shallowest Argo salinity above 10 m in a 9-d temporal window was selected. The SSS field was then interpolated onto the positions of these Argo floats by means of the bilinear interpolation. In this way, a pair of SSS measurements together with their co-located Argo near surface salinity (NSS) observations were obtained for comparison purposes.

The tropical atmosphere ocean (TAO) mooring array can provide time series for salinity. This data set undergoes a series of QC measures and only those data whose QC flag = 1 (“good”) are used. The daily observations of 1-m salinity are employed as the NSS.

3.4 Data source

The Argo profiles of global argo data set (V3.0) can be available by the official website: <http://www.argo.org.cn/index.php?m=content&c=index&a=lists&catid=26>. The buoys data of TAO are available at <http://www.pmel.noaa.gov/gtmba/>. The BEC SSS is available at <http://bec.icm.csic.es/ocean-global-sss/>. The CCI SSS can be obtained from <https://catalogue.ceda.ac.uk/uuid/aea368301bff448bbbea7e90e66819e5>. The OISST is available at <https://psl.noaa.gov/data/gridded/data.noaa.oisst.v2.highres.html>. The OSTIA data set (SST_GLO_SST_L4_NRT_OBSERVATIONS_010_001) is disseminated by Copernicus Marine Service: <https://resources.marine.copernicus.eu/>. The OSPO data set can be retrieved from https://www.ncei.noaa.gov/access/metadata/landing-page/bin/iso?id=gov.noaa.nodc:GHRST-Geo_Polar_Blended-OSPO-L4-GLOB. The REMSS data set is available at <https://www.remss.com/measurements/sea-surface-temperature/oisst-description/>.

4 Results

4.1 Selection of SST templates

As shown in Eq. (4), the feature resolution of the fused SSS product relies mainly on the template of the SST. Consequently, the selection of the SST template is an essential step in the fusion

of the high-resolution SSS product. The wavenumber spectra for the four candidate SST templates were computed to decide the best template. The selection criterion is the best agreement between the feature resolution and the nominal resolution. Four regions were considered, i.e., the Southern Indian Ocean (SIO; 10°–50°S, 70°–100°E), the Gulf Stream (GS; 30°–50°N, 30°–80°W), the Kuroshio Current (KC; 25°–50°N, 140°–180°E) and the Tropical Pacific (TP; 30°S–30°N, 120°–180°W). Among these four regions, the GS and the KC are two of the most energetic regions that are characterized by strong currents and abundant eddies, while the SIO and TP are characterized by salinity fronts. As shown in Fig. 1, the spectrum for each product cuts off at the Nyquist frequency according to the grid resolution. It can also be seen that in the four selected regions, the PSD of the OISST is almost the highest of the four products at large scale, but it decays rapidly at 100–150 km and the slope drops to -5 . This demonstrates that the feature resolution of the OISST is far coarser than the nominal resolution of about 50 km. Only those motions whose scales are larger than 150 km can be effectively reflected. The spectrum of the OSTIA at 50–150 km is very close to that of the OISST and is also characterized by the sharp drop of the PSD. It turns out that the OSTIA is such an over smoothed product that its feature resolution is at the same level as that of the OISST, despite the far higher nominal resolution (0.05°) of the former.

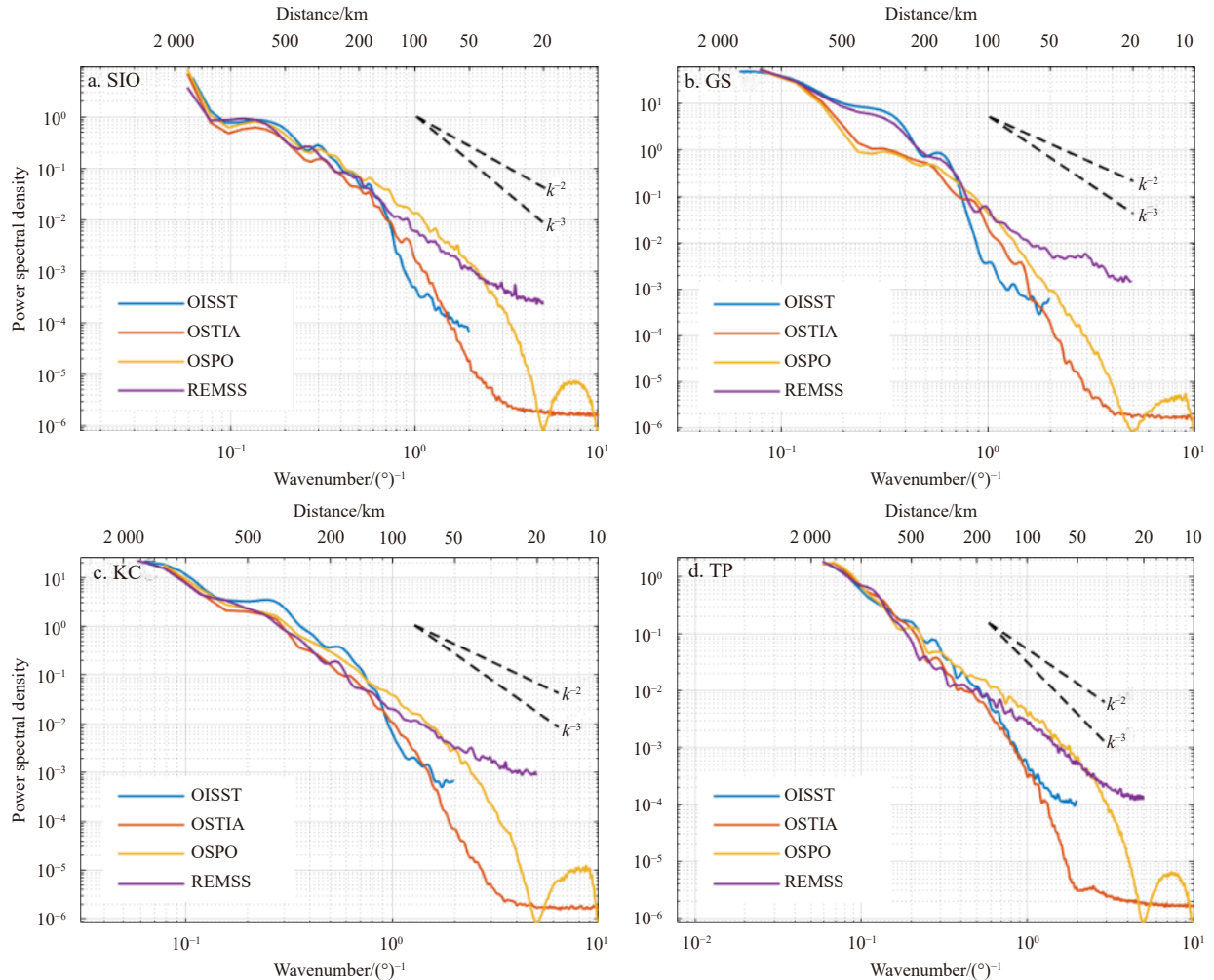


Fig. 1. The meridional wavenumber spectra for the four SST products. a–d. Southern Indian Ocean (SIO), Gulf Stream (GS), Kuroshio Current (KC), and Tropical Pacific (TP). k denotes the wavenumber.

The spectrum of the OSTIA flattens out at about 75 km in the TP (Fig. 1d) and at about 35 km in the SIO, GS, and KC (Figs 1a–c). In this case, the scale that is finer than 35 km is totally dominated by white noises. The PSD of the OSPO is clearly higher than that of the OSTIA at the mesoscale band. The slopes of the OSPO in the SIO (Fig. 1a), KC (Fig. 1c) and TP (Fig. 1d) remain at about -3 at the scale of 50–200 km. This indicates that the mesoscale motions can be resolved by the OSPO in these three regions. In the GS (Fig. 1b) area, the spectrum of the OSPO decreases rapidly at 100 km, corresponding to the relatively low capability of the OSPO in resolving mesoscale eddies in the GS. Note that a mountain-like pattern occurs from 35 km to the finer scale, which results from the ineffective interpolation of low-resolution data onto the high-resolution grid. This reflects the fact that the grid resolution of the OSPO (0.05°) is “wasted”. The PSD of the REMSS can decay naturally from the large scale to the mesoscale in all four regions except for the GS. A reasonable spectrum for the slope of between -2 and -3 occurs in the SIO (Fig. 1a), the KC (Fig. 1c) and the TP (Fig. 1d), except for the narrow flattening trend near the Nyquist frequency. This demonstrates that the effective resolution of the REMSS is around 30–40 km, which is very close to the grid resolution (0.1° , about 20 km). The spectral behavior is supportive of the high quality of the REMSS for research on mesoscale motions. It must be noted that the product is not perfect, considering the anomalous spectrum in the GS (Fig. 1b) at about 50 km. Nevertheless, the REMSS is the only product that can effectively resolve motions with a scale of 50 km among the four

SST products.

Based on the above analysis, the OISST and the OSTIA cannot effectively resolve the mesoscale features within 100 km, while the grid resolution of the OISST is roughly comparable with the effective resolution. Considering that the potential application of ocean salinity to climatological analysis, the OISST is considered to be suitable to play the role of a low-resolution template. For the two 0.05° SST products, i.e., the OSPO and the OSTIA, there is a significant mismatch between the nominal resolution and the feature resolution. Taking the OSPO or the OSTIA as the template would not only fail to synthesize high-resolution SSS products, but also increase the burden of computation and storage. Conversely, the REMSS is verified to be a truly eddy-resolving product and its grid resolution is comparable to its feature resolution. Consequently, the REMSS is selected as the high-resolution template in the SSS fusion.

4.2 Validation against in situ data

After selection of the SST templates, four combinations of MFF fusion were considered for this study, namely, the OISST and REMSS as the templates along with the BEC and CCI as the source data. To highlight the merits of MFF, the original product and the 50-km Gaussian-filtered products were also validated. By subtracting the salinity of the satellite data from the NSS of Argo, the differences between the salinity products for each satellite and Argo were compared, as shown in Fig. 2. There are many large differences in the original data of the BEC (Fig. 2a), which

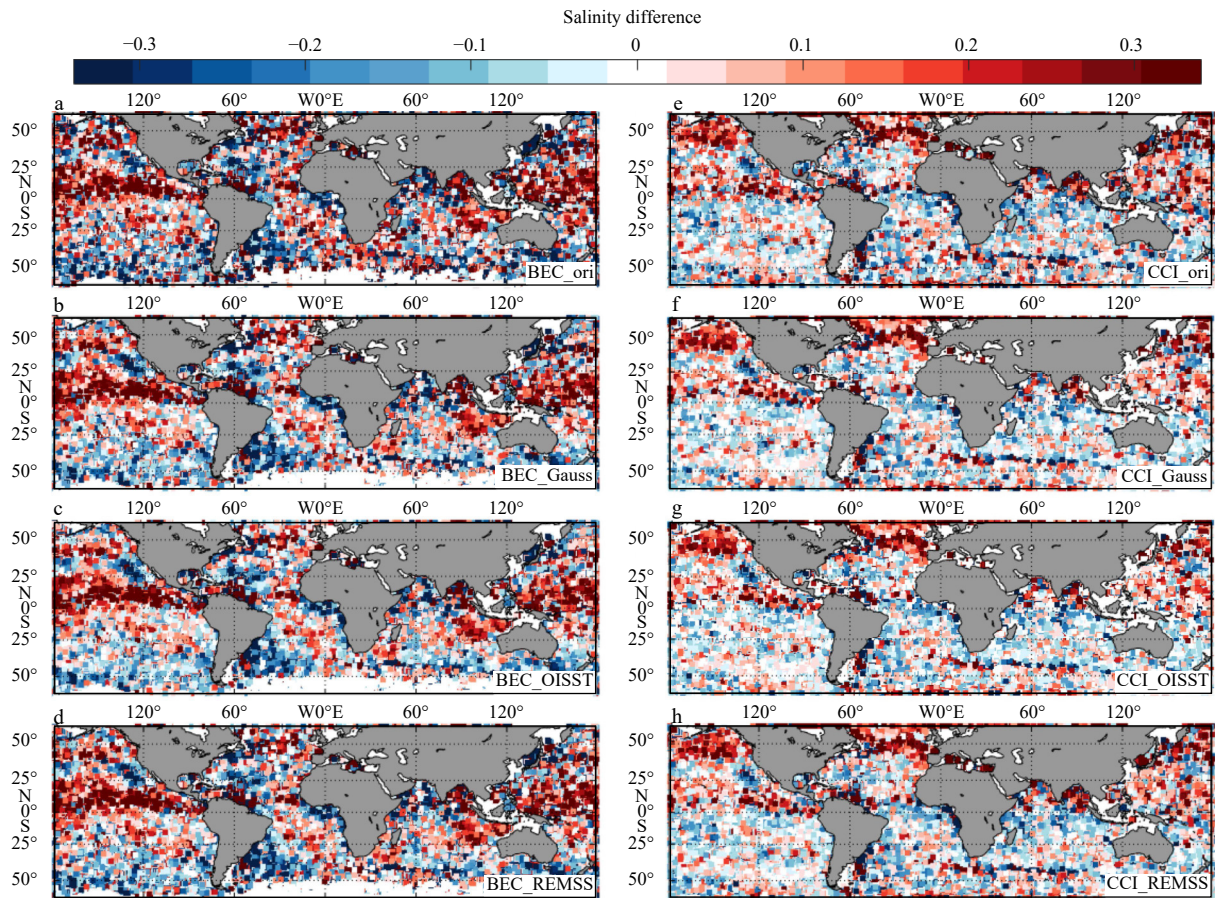


Fig. 2. The differences between the different salinity products and Argo (located at the pixels). BEC: BEC-based products; CCI: CCI-based products; ori: original product; Gauss: Gaussian-filtered product; OISST: multi-fractal fusion product with OISST template; REMSS: multi-fractal fusion product with REMSS template.

are mainly located in the low-latitude sea area of the Pacific Ocean (corresponding to a heavy precipitation area in the inter-tropical convergence zone), the strong current area in the western boundary, the diluted water areas (Bay of Bengal, Amazon River Estuary, etc.) and the sea areas with large evaporation (Arabian Sea, Mediterranean Sea, etc.), etc. The largest difference of salinity was more than 0.5. The CCI data (Fig. 2e) effectively eliminated the salinity errors in these corresponding regions, and in the Southern Hemisphere, a large area with a reduction in the difference was evident. This indicates that the CCI data can effectively reduce both the random errors and the systematic bias of the SSS. There are still clear differences between the CCI data in those strong flow areas and those diluted water areas, but this does not necessarily demonstrate the errors of the CCI data. These large values are in good agreement with the inconsistent observations revealed in the study by Yan et al. (2021), indicating that most of these differences are likely be attributed to the inherent differences between the *in situ* observations and the remotely sensed observations.

Through comparison of the different panels in the same column, it can be noted that the differences between the fused products and the original products are not visually significant. Although a seemingly small reduction of salinity error (e.g., 0.05–0.10) cannot be highlighted easily in the figure, the improvement of data quality is quite significant considering the magnitude of the error (about 0.2–0.3) of the SSS products.

However, a large number of extreme value pixels in the BEC products are effectively removed in the CCI products, e.g., in the tropical Pacific and the Amazon plume. This suggests that the calibration and correction processes of the CCI can effectively mitigate the errors, while the fusion algorithm provides a complementary means for improving the quality of the SSS products only.

To further quantify the differences between satellite-based salinity and Argo salinity, the bias, the STD and the correlation coefficients (Corr) were computed and the values are shown in Fig. 3. In addition to the regions in Fig. 1, four additional regions were considered, including the global ocean (Glo; 60°S–60°N, 180°W–180°E), the Agulhas Current (AC; 20°–40°S, 20°–60°E), the Bay of Bengal (BoB; 10°–30°N, 80°–100°E) and the Amazon plume (Amazon; 10°S–10°N, 30°–60°W). It can be seen in Fig. 3a that both the BEC and the CCI are unbiased globally. Meanwhile, the Corrs for all products were >0.9. The STD for the original data of the BEC was 0.39, which was much larger than that of the CCI (0.22). Both the Gaussian filter and the MFF can effectively reduce the STD for the BEC, especially for the MFF fusion product with the template of the OISST (STD about 0.28). The denoising performance was not significant in terms of the CCI product, indicating that most of errors were eliminated in the original data. For the SIO (Fig. 3b) and the TP (Fig. 3e), the STDs for the CCI-related products were 0.15 or lower, and the Corrs were around 0.98. These statistics demonstrate the high quality of the CCI in

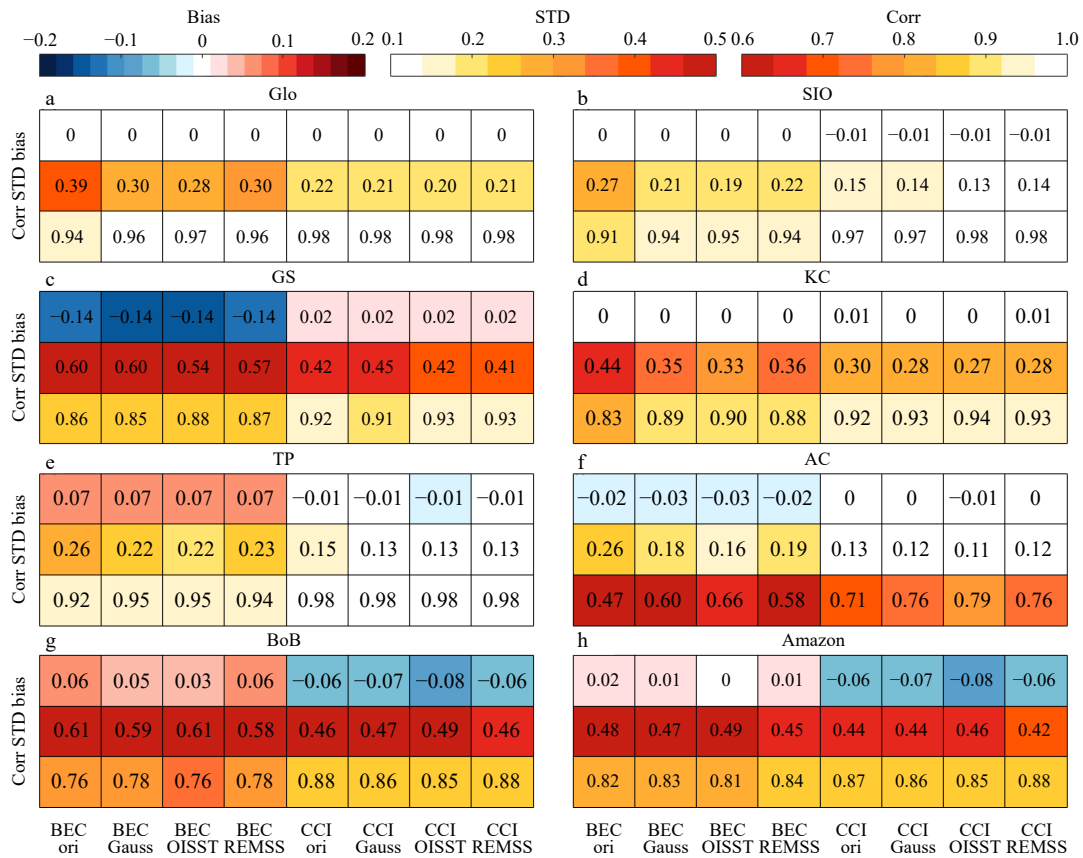


Fig. 3. The statistics for the different SSS products with respect to Argo. Eight regions were examined. For each panel, the bias, the STD, and the correlation coefficient are plotted from top to bottom, respectively. a–h. Global ocean between 60°S and 60°N (Glo); South Indian Ocean (SIO); Gulf Stream (GS); Kuroshio Current (KC); Tropical Pacific (TP); Agulhas Current (AC); Bay of Bengal (BoB); Amazon plume (Amazon). BEC: BEC-based products; CCI: CCI-based products; ori: original product; Gauss: Gaussian-filtered product; OISST: multi-fractal fusion product with OISST template; REMSS: multi-fractal fusion product with REMSS template.

the open ocean. The STDs for the BEC-based products in these two regions were still significantly inferior to that of the CCI_ori product, even though the Gaussian filter and MFF can lower the STD.

In the GS region (Fig. 3c), the original BEC product showed a significant negative bias of -0.14 and a high STD of 0.6 , while the original CCI product was slightly biased (0.02) and had a much lower STD (0.42). Instead of improving the quality of the SSS product, the Gaussian filter actually increased the STD of the CCI and decreased the Corrs of both the BEC and the CCI. Nevertheless, the MFF can still take effects in the GS, especially for the BEC-fused product with the template of the OISST. The statistics for the KC (Fig. 3d) were dissimilar to those for the GS, but more similar to those for the SIO. Both the MFF and the Gaussian filter can effectively reduce the STD and improve the Corr, especially for the BEC products. A similar pattern of statistics can also be seen for the AC (Fig. 3f), except for the extremely low correlation value, i.e., lower than 0.8 . Especially, the Corrs of the BEC-based product can be as low as 0.66 , albeit the correlation has been significantly improved by the MFF. This demonstrates that the remotely sensed SSS product cannot perform satisfactorily in depicting the structure within the AC.

In the Bay of Bengal (BoB) (Fig. 3g) and the Amazon plume (Fig. 3h), neither the Gaussian filter nor the MFF can effectively improve the statistics of the SSS products. Note that the Gaussian filter is an effective tool for mitigating the random errors, while the performance of the MFF depends on the template of the SST. The poor performance of the Gaussian filter and the MFF high-

lights the special distribution of errors in these two regions. The variation of the salinity in the BoB and the Amazon is dominated by the motion of freshwater. The variation of the freshwater is independent of the variation in the temperature. Meanwhile, the low sensitivity of the remote sensor to freshwater can import large systematic errors into the SSS products. Consequently, the MFF and the Gaussian filter are not applicable. In this case, the quality of the SSS products is determined by a series of algorithms concerned with data retrieval, calibration, and correction, resulting in divergent statistics for the two products. In the BoB, the STDs/Corrs of the CCI-based products were significantly lower/higher than those of the BEC-based products, while the positive biases of the BEC-based products turned negative for the CCI-based products. For the Amazon, the STDs/Corrs for the BEC-based products were comparable to that of the CCI-based products. Meanwhile, the biases were amplified in terms of the CCI-based products.

The SSS products were further validated by the 1-m salinity of the TAO buoys. Only the data whose quality flag was 1 were considered. As revealed in Tang et al. (2017), several buoys on the date line were erroneous and thus were excluded. The results are shown in Fig. 4, where the color bar is consistent with Fig. 3, i.e., the lighter color corresponds to a better agreement with TAO. The statistics for the different products at each mooring buoy are plotted in terms of 8 pixels, the distribution of which is shown in the bottom diagram in Fig. 4.

As can be seen from Fig. 4a, the BEC-based SSS products (i.e., the upper four pixels at each mooring buoy) were biased by

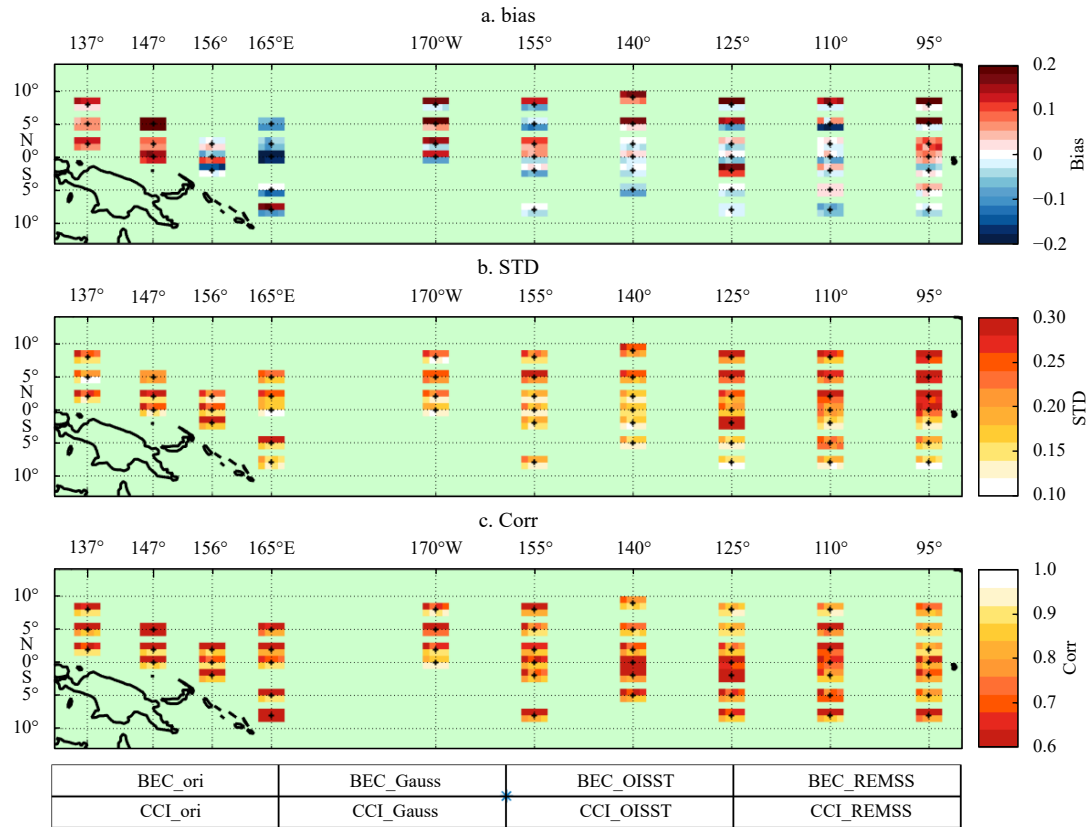


Fig. 4. The bias (a), the STD (b) and correlation coefficient (c) for the different SSS products with respect to the series of TAO. Each star point labels the position of the mooring buoy, encompassed by the distribution of $2 \text{ pixel} \times 4 \text{ pixel}$. As shown in the diagram at the bottom, the upper four pixels represent the BEC-based products while the lower four pixel represent the CCI-based products. BEC: BEC-based products; CCI: CCI-based products; ori: original product; Gauss: Gaussian-filtered product; OISST: multi-fractal fusion product with OISST template; REMSS: multi-fractal fusion product with REMSS template.

>0.1 at multiple sites, and the biases cannot be removed by the Gaussian filter or the MFF, e.g., the data for the four buoys at 170°W . The CCI-based products (i.e., the lower four pixels at each mooring buoy) effectively calibrated the bias at most buoys, whereas there were still some buoys with heavy bias, such as the three buoys at 147°E . In Fig. 4b, the STDs for all products at all buoys were within 0.3, which is consistent with the results in Fig. 3e. It is easy to check that the STDs for the CCI-based products was lower than that for the BEC-based products at most buoys. Meanwhile, the contribution of the Gaussian filter and the MFF to reducing the STD (i.e., the color of pixel gradually becoming lighter from left to right) can be seen, e.g., at several buoys at 137°E . Focusing on Table 1, the STD of salinity can be reduced from 0.25 to about 0.2 for BEC and from 0.14 to 0.11 for CCI. There was no significant difference between the STDs of the

Gaussian-filter products and those of the MFF products, indicating that the comparable denoising capability of the two algorithms. Similar characteristics can also be found in Fig. 4c, namely, the better performance of the CCI-based products versus the BEC-based products and the comparable performance between the Gaussian filter and the MFF, which can be highlighted from the correlation coefficients in Table 1. On the one hand, the Gaussian filter and MFF were carried out only from the spatial dimension perspective, while the time series of the mooring buoys were not effectively denoised. On the other hand, the eddy motions in the tropical ocean are not quite active. Consequently, the performance of the MFF was not significant compared with the Gaussian filter for the validation with respect to the mooring buoys. Nevertheless, the evidences are supportive of a denoising capability for the MFF at least at large scales.

Table 1. Bias, STD, and correlation coefficients (Corr) of different salinity products w.r.t TAO 137e5n corresponding to Fig. 4

Metrics	BEC- or CCI-based	Ori	Gauss	MFF_OISST	MFF_REMSS
Bias	BEC	0.05	0.06	0.05	0.06
	CCI	0.05	0.07	0.06	0.06
STD	BEC	0.25	0.19	0.21	0.20
	CCI	0.14	0.11	0.12	0.11
Corr	BEC	0.43	0.54	0.50	0.52
	CCI	0.79	0.85	0.84	0.85

4.3 Assessment of the resolution

The resolution of the different SSS products can be assessed qualitatively from inspection of the images shown in Fig. 5. The images of the two original SSS products were noisy, where hardly any organized motions such as front and eddies can be seen. The contours of the BEC (Fig. 5) were much more congested than those of the CCI (Fig. 5), however, it cannot be determined whether mesoscale signals have been totally masked by the noise. Although the Gaussian filter can improve the quality of the BEC (Fig. 5), the map for the SSS was still dominated by noise,

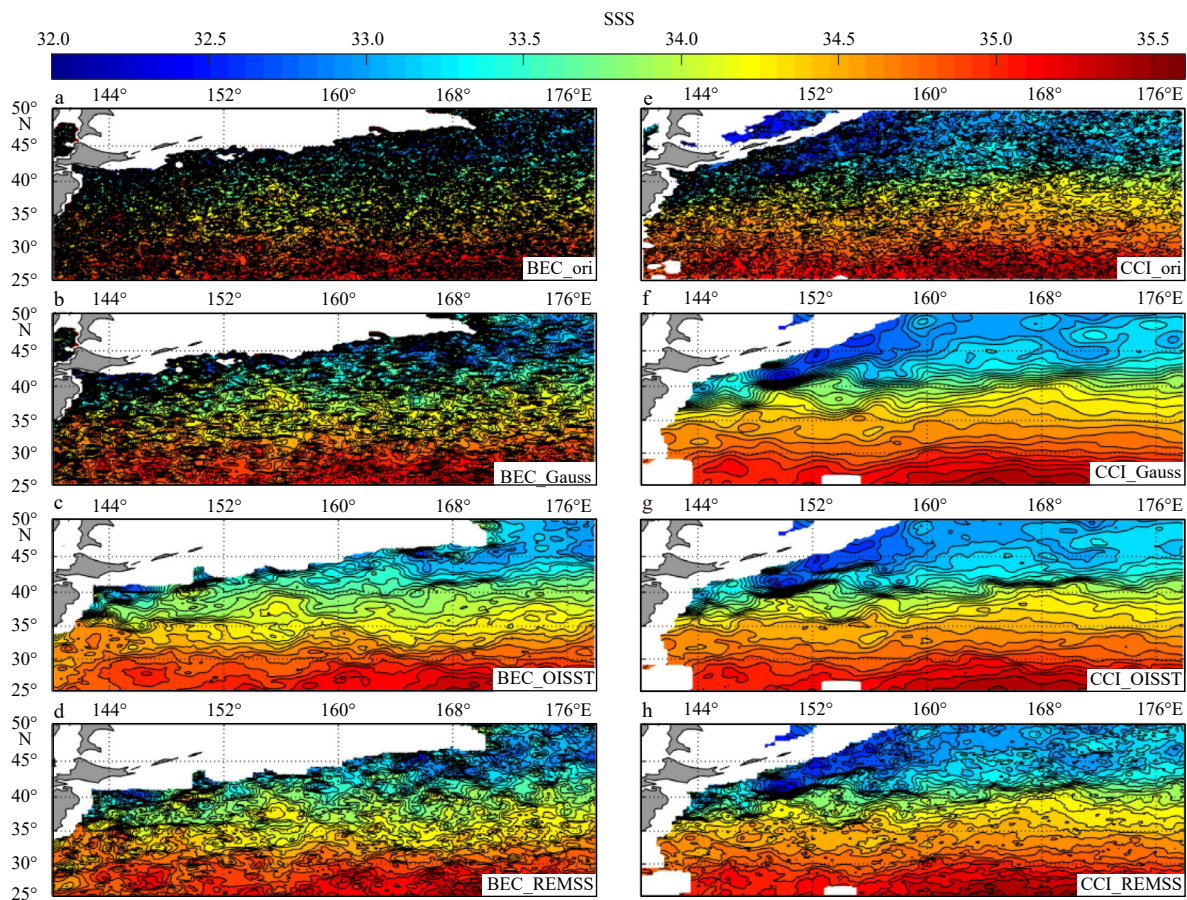


Fig. 5. Maps of the different SSS products in the region of the Kuroshio Current on March 15, 2016. The same contours are plotted in each panel ranging from 32.0 to 35.5 at the interval of 0.1. BEC: BEC-based products; CCI: CCI-based products; ori: original product; Gauss: Gaussian-filtered product; OISST: multi-fractal fusion product with OISST template; REMSS: multi-fractal fusion product with REMSS template.

which corresponded to the spatially dependent noise that cannot be mitigated by the Gaussian filter. Nevertheless, the noise has been effectively eliminated in terms of the CCI's Gaussian filter product (Fig. 5), where the frontal structure and large eddies can be clearly observed. The better application of the Gaussian filter demonstrates that the calibration and correction processes of the CCI can take effect in removing the systematic errors. Taking the OISST as the template, the MFF products can eliminate the noises of the BEC product (Figs 5c and g), even when these noises cannot be effectively denoised by the Gaussian filter. This indicates that the MFF can not only remove the white noise, but also mitigate the spatially-dependent noises. In the case of the CCI data, compared with the Gaussian filter product, the MFF product presented a stronger and narrower salinity front. The rationale for the frontal structure will be further validated by the wavenumber spectra. The MFF products (Figs 5d and h) with the high-resolution REMSS template presented detailed structures, such as the small eddies. The BEC_REMSS contained more small-scale structures than the CCI_REMSS, however, it cannot be demonstrated whether these structures corresponded to signals or noises given the lack of mesoscale observations.

The singularity exponent (SE) is an exponent representing the fractal structure, i.e., the geometric structure (Hoareau et al., 2018). The isoline of the SE extracted from the ocean scalars (e.g., SST, SSS, chlorophyll) should be consistent with the streamline (Nieves et al., 2007; Turiel et al., 2008; Pont et al., 2009). The more

detailed and clearer SE isolines correspond to higher resolution, while the negative values correspond to strong currents. The computation of the SE relies on the horizontal gradient and can be obtained via the graphical user interface (GUI) provided by the BEC singularity analysis service (<https://bec.icm.csic.es/data/singularity-analysis-service/>). The SE maps corresponding to Fig. 5 are shown in Fig. 6. Hardly any stream-like SE structures can be seen from the products of BEC_ori, BEC_Gauss and CCI_ori (Figs 6c, b, and c), e.g., the main axis of the Kuroshio extension was masked by noise. The Gaussian filter product of CCI (Fig. 6f) showed a smoothed SE structure in the region. However, the SE map was extremely fuzzy, indicating that the detailed fractal structure was removed by the Gaussian filter. As for the two products fused by the template of the OISST (Figs 6c and g), the SE maps showed clear frontal structures. Comparing panel Figs 6f and g, the maps demonstrate that the fractal structure was blurred as a result of applying the Gaussian filter but the structure can be restored by the MFF. However, the fractal structure of the BEC_OISST product was notably different from that of the CCI_OISST product, which suggests that the horizontal gradient of at least one product was distorted. In Figs 6d and h, fine streamlines were shown and a number of mesoscale eddies were effectively depicted. Nevertheless, the Kuroshio extension was obscure in the BEC_REMSS product. It would appear that the gradient of the BEC product is problematic, and this needs to be confirmed in future work.

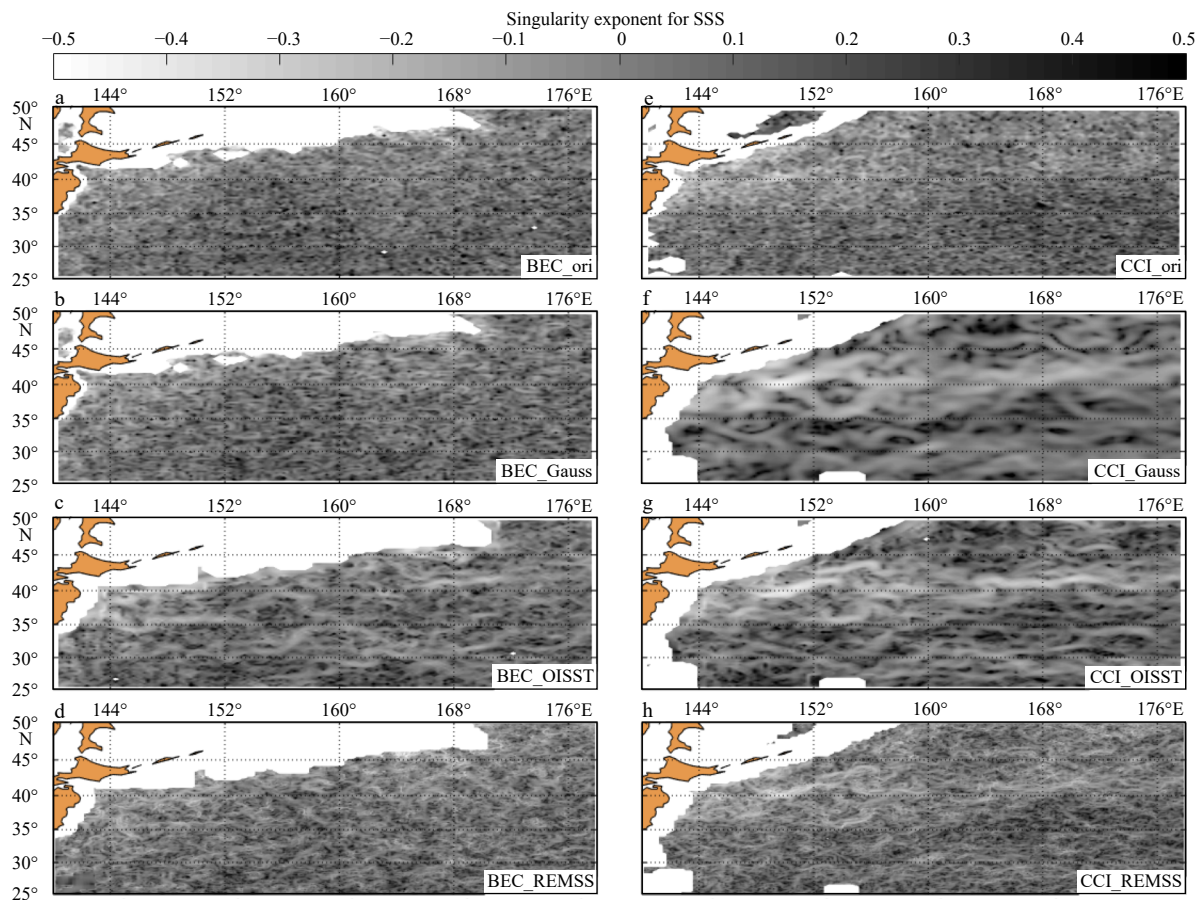


Fig. 6. Maps of the singularity exponents for the different SSS products in the region of the Kuroshio Current. The same contours are plotted in each panel ranging from -0.5 to 0.5 at the interval of 0.01 . BEC: BEC-based products; CCI: CCI-based products; ori: original product; Gauss: Gaussian-filtered product; OISST: multi-fractal fusion product with OISST template; REMSS: multi-fractal fusion product with REMSS template.

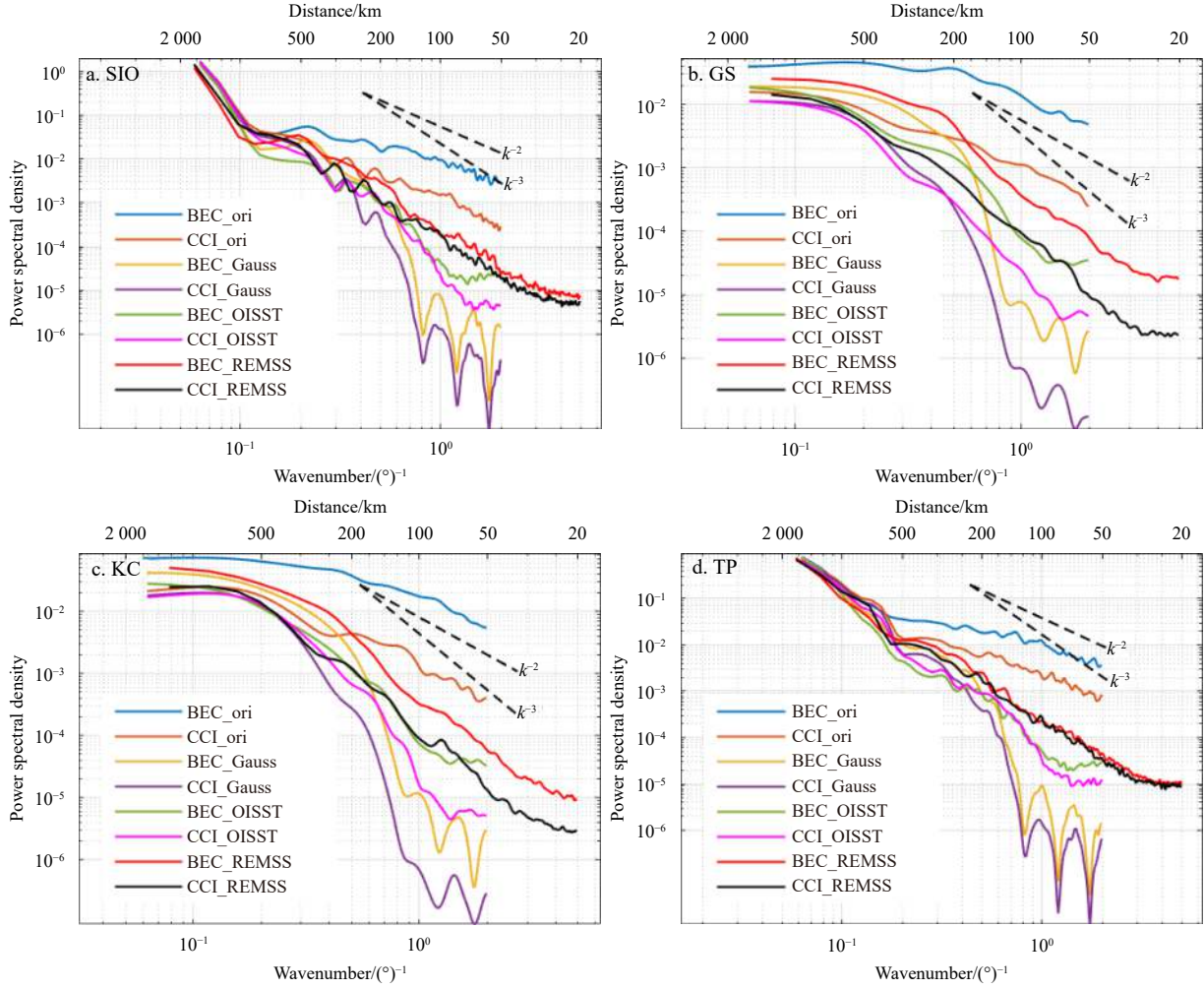


Fig. 7. The meridional wavenumber spectra for the SSS products. a–d. Southern Indian Ocean (SIO), Gulf Stream (GS), Kuroshio Current (KC) and Tropical Pacific (TP). BEC: BEC-based products; CCI: CCI-based products; ori: original product; Gauss: Gaussian-filtered product; OISST: multi-fractal fusion product with OISST template; REMSS: multi-fractal fusion product with REMSS template.

To analyze quantitatively the feature resolution of the different products, the wavenumber spectra of the four regions were examined. The spectra are presented in Fig. 7. In the SIO (Fig. 7a), the PSD of the original BEC data was the highest and the slope is quite flat, which demonstrated the dominance of white noises. The PSD of the original CCI data was relatively low and the slope was reasonable, indicating that the quality of the CCI data is higher than that of BEC. The PSD of the two Gaussian filter products dropped rapidly at 200 km, corresponding to a decrease in the capability to resolve the motions within 200 km. The spectra begin to oscillate around 120 km, which means that signals finer than this scale can no longer be resolved by the Gaussian filter products. The Gaussian filter is based on the average of the moving window, which results in the pseudo mixing across isohalines and consequently a degradation in the effective resolution. Two fusion products based on the OISST template showed lower PSD values. 150 km was the node where the slope drops sharply, i.e., features finer than 150 km were blurred in the two OISST-based products. The spectral behavior of the two fusion products was basically consistent with the SST template. Similar to the OISST, the spectra levelled off at about 75 km, corresponding to the dominance of white noise at a scale finer than 75 km.

In the SIO (Fig. 7a), the spectra of the two fusion products based on the REMSS template were similar. The PSD decayed

from the large scale to 30–40 km following a reasonable slope of between -2 and -3 . Then the spectra become flatter and the PSD was dominated by white noises. The situation of the TP in Fig. 7d was similar to that of Fig. 7a. It can be judged that in these two open oceanic regions, the effective resolution of the two salinity products based on the OISST template was approximately 75 km, and that based on the REMSS template was approximately 40 km.

For the two strong current regions in Figs 7b and c, the PSD for the BEC_ori was significantly higher than that for any other product. Besides, the flat slope of the BEC_ori indicated the high level of noise in this product, which has been revealed qualitatively in the salinity and fractal maps of Figs 2 and 3. The PSD of CCI_ori was consistent with that of other products at large scale, however, the slope was flatter than -2 and the PSD was significantly higher than the other products, corresponding to a relatively low signal-to-noise ratio at the mesoscale. As for the products synergized by the Gaussian filter, the common problem of over-smoothing was also reflected in the data, while the PSD of the CCI_Gauss product was extremely low, highlighting the loss of resolution as a result of denoising. The slope of the fusion products based on the OISST template was close to -3 , which was more reasonable than that in Fig. 7a, indicating that the slightly higher feature resolution of the fusion products in the strong currents. Judging from the inflection points of the spectra, the effect-

ive resolution of the MFF_OISST product in the two strong current regions was about 75 km. The spectral slope of the fusion products based on REMSS was about -3 , and the spectrum levelled off at a scale of about 40 km in the GS. In the KC, a similar behavior in the spectra can be observed except that the levelling-off point was at about 30 km. Therefore, the sharp drop of the spectra never appears for the REMSS-based products, demonstrating the considerably high feature resolution in the two strong current regions.

Comparing the fusion data based on the two different templates, it can be seen that the high-resolution template can indeed improve the feature resolution of the SSS products, and the shape of the spectra of the MFF fusion data were consistent with the SST template in Fig. 1. Besides, the MFF can counteract the differences between the CCI and the BEC in spectral behaviors. Taking Figs 1a and d as an example, the spectrum of the BEC_REMSS and that of the CCI_ori were almost coincident despite the significant differences between the spectra of BEC_ori and that of CCI_ori. Nonetheless, the spectra of BEC_REMSS and CCI_REMSS can be significantly divergent when their original products are widely different, e.g., in Figs 1b and c.

Comparing Figs 1 and 7, the MFF could make the spectral behavior of the source data (SSS) approach that of the template (SST). The successful application of MFF relies on the similarity in the spectral behaviors of SST and SSS given that both of them exhibit the characteristics of the passive tracer to some degree. Consequently, not all ocean scalars are suitable to play the role of the template. For example, the spectrum for the SSH has been demonstrated to have a slope between $-5/3$ (predicted by the surface quasi-geostrophic turbulence) and -5 (predicted by the quasi-geostrophic turbulence) (Vergara et al., 2019), which means that the SSH cannot be an effective template to synthesize the SSS due to the much steeper slope.

5 Discussion

In this study, both the conventional Gaussian filter and the MFF method were applied to eliminate the noises in the SSS data. Through the verification of Argo and TAO, both the Gaussian filter and the MFF can effectively reduce the errors of the original SSS products, especially in the case of the BEC data, where the reduction of global mean STD can reach 0.09 (Fig. 3). However, as demonstrated in the BEC-based products in Figs 5 and 6, the Gaussian filter can mitigate the random errors but performed an unsatisfactory work in removing the spatially-varying errors. According to Eq. (4), the local average term $\langle S(\vec{x}) \rangle$ plays a similar role to that of a Gaussian filter in mitigating the random errors. Consequently, the transmission term $a(\vec{x})(\theta(\vec{x}) - \langle \theta(\vec{x}) \rangle)$ takes effects in mitigating the spatially-varying errors. Nevertheless, the denoising performance of MFF is only slightly better than the Gaussian filter, indicating that the transmission term contributes less than the local average term in reducing the magnitude of noises.

The coarse SE structure in Fig. 5f and the sharply dropped spectra in Fig. 7 indicate that the denoising performance of Gaussian filter comes at the expense of the degradation of feature resolution. As for the MFF, both the random errors and the spatially-varying errors can be removed (e.g., Figs 5c and d), while the feature resolution of the fused products can be improved instead corresponding to the SST templates. The results are supportive of the better performance of MFF compared to conventional Gaussian filter.

The quality of the fused SSS product is determined by the source data of SSS and the template of SST. In terms of two SSS

inputs, the original BEC product and the original CCI product present significant differences. In Figs 2–4, the BEC_ori was much noisier than the CCI_ori, e.g., the global mean STDs against Argo salinity were 0.39 and 0.22, respectively. Please note that the RMSD reduction of the Gaussian filter or the MFF is quite limited compared to that of changing the source data from BEC to CCI. In Fig 5a, the MFF and the Gaussian filter can lower the STD of BEC_ori from 0.39 to 0.30, which is also significant but is less effective than using the CCI product directly. On the other hand, the maps of the BEC-based products in Figs 5–6 suggest that unsolved problems are likely to exist in the BEC product. The isohalines of the BEC-based products were more chaotic (Figs 5a and 6a) than the CCI-based products (Figs 5e and 6e), corresponding to the dominance of noises in the original BEC product. In addition, the unorganized map of BEC_Gauss in Figs 5b and 6b demonstrates the heavy spatially-varying noises of BEC product. Even these noises can be removed by MFF in Figs 5c and d and Figs 6c and d, the structure of the Kuroshio Current extension and the corresponding SSS front cannot be highlighted by the BEC-based products. In contrast, the frontal structures were much clearer in terms of the CCI-based products in Figs 5g and h and Figs 6g and h. It turns out that the selection of a suitable SSS input is the fundamental step of fusion since part of the defects in the source data cannot be compensated by the MFF algorithm.

The most suitable templates were firstly selected from four SST products by means of the wavenumber spectra. The selection criterion was the best agreement between the feature resolution and the grid resolution. In Fig. 1, the wavenumber spectra demonstrate the sharp degradation of feature resolution of OISST, OSTIA and OSPO at the scales finer than 100 km. The nominal 0.05° OSTIA and OSPO products are oversmoothed and thus not recommended to play the role of the template. Consequently, the OISST was selected as the low-resolution template (0.25°) and the REMSS was selected as the high-resolution template (0.1°). In Fig. 3, the MFF can effectively denoise the original BEC product, while the denoising performance is not quite sensitive to the template, e.g., the global mean STD against Argo was 0.28 for BEC_OISST and 0.3 for BEC_REMSS (0.2 for CCI_OISST and 0.21 for CCI_REMSS) in Fig. 3a. From Figs 5–6, the clearer frontal structure can be seen from CCI_OISST product, while CCI_REMSS product can present finer features such as mesoscale eddies. From the spectral behaviors in Fig. 7, CCI_REMSS showed a reasonable slope (between -2 and -3) at the scales of 100 km to 40 km, while a sharp drop of PSD occurred at about 150 km and a flat spectrum was shown at scales finer than 100 km in terms of CCI_OISST. These evidences demonstrate the importance of template selection and its role in improving the feature resolution.

Comparing the above factors, namely the source data and the template, we can find that the source data mainly determine the magnitude of noises while the template dominates the feature resolution of the fused product. Please note that the fused products of BEC still presented even higher STD (0.28) than the original product of CCI (0.22) in Fig. 3a. In addition, the fused products of BEC showed different pattern with those of CCI in Figs 5 and 6, despite the similar spectral behavior in Fig. 7. Considering that the Kuroshio extension is not clearly shown by BEC-based products, we tend to believe that the BEC product is less suitable than the CCI product in synthesizing mesoscale SSS products. Although MFF has been demonstrated to be an effective tool in denoising and super-resolution, efforts are still worth taking in improving the retrieval, calibration and correction of re-

motely sensed SSS.

It must be noted that in those regions where the freshwater processes are active, such as BoB, neither the Gaussian filter nor the MFF can effectively eliminate the errors (Fig. 3). This result is not surprising since both random errors and systematic errors exist in these regions. Meanwhile, the poor resemblance between SSS and SST in these regions make the MFF algorithm less applicable. Consequently, the MFF could possibly increase the STD instead (e.g., the CCI_OISST product in Fig. 3g).

The time series of TAO cannot reflect effectively the merits of the MFF-fused products using the high-resolution REMSS template as in Fig. 4. This is due largely to the fact that the MFF is based on the geometric similarity but cannot take effects in the temporal dimension. It should be noted that the existing SSS products are quasi-weekly running products so that the remotely sensed salinity is under-sampled. As revealed in Yan et al. (2021), the temporal under-sampling can lead to a series bias between the SSS products and the *in situ* salinity. It is reasonable that the time series cannot be improved using two spatial filter algorithms. Future work will seek to address improvements in the denoising performance in the temporal dimension.

6 Conclusions

Based on the use of the MFF algorithm and the Gaussian filter together with the 0.25° OISST and 0.1° REMSS as templates, this study has synthesized multiple SSS products to optimize the fusion scheme. Through comparison with the *in situ* data and various indicators, the quality of the fused SSS products has been compared. The results show that the biases, the STDs and the Corrs for the BEC-based products are inferior to those of the CCI-based products for all regions. The Gaussian filter and the MFF can reduce significantly the STD and improve the correlation of the BEC except in the case of the BoB and the Amazon. However, the improvement of fusion algorithm on the CCI data is quite limited. In the global ocean out with the high latitude, the fused products of BEC have a bias of 0, a STD of 0.3 and a Corr of 0.97 with respect to Argo, while the fused products of CCI have a bias of 0, a STD of 0.2 and a Corr of 0.98. Meanwhile, for the strong currents of the KC, the GS, and the AC, the statistics for the BEC are significantly inferior to those of the CCI products. However, in the BoB and the Amazon, although the CCI yields better quality than the BEC, there are still large differences between the CCI and the *in situ* salinity. These differences probably reflect the intrinsic differences between the satellite observations and the *in situ* observations due to the sub-footprint variability and the near surface stratification (Boutin et al., 2016).

The BEC product is much noisier. Both the SSS map and the fractal structure demonstrate the higher signal-to-noise ratio of the CCI data. Nevertheless, the original products of the BEC and the CCI are still too noisy to depict mesoscale features. Although the Gaussian filter can effectively remove the random errors, the feature resolution of SSS could be degraded at the same time. This oversmoothed product can only be used in the climate research but cannot reflect mesoscale features. Through fusion of the MFF with the OISST template, the effective resolution of the BEC and the CCI products can reach about 75 km, whereas the mesoscale features are quite fuzzy, corresponding to the sharp drop in the wavenumber spectra. Nevertheless, the MFF-fused products with the REMSS template can reach a feature resolution of 30–40 km. The mesoscale features are effectively reflected by the maps of the SSS and the SE, especially for the CCI_REMSS product.

In conclusion, the MFF product of the CCI with the REMSS

template has lower error and higher resolution, and is potentially applicable to mesoscale research in the open ocean and in the strong current regions. However, in terms of the BEC products, only the large-scale features in the BEC_OISST product and the BEC_Gauss product are reliable. In those regions where freshwater motions are active, e.g., the BoB and the Amazon, the effects of both the Gaussian filter and the MFF are diminished, while the quality of the SSS products relies on the retrieval, correction, and calibration processes for the original data.

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