Assessment of the SMOS inversion scheme for salinity and wind speed retrieval purposes

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Abstract
A simplified parallel version of the Soil Moisture and Ocean Salinity (SMOS) Level 2 Ocean Salinity (L2OS) processor is used to assess the optimal configuration of both the SMOS cost function and the corresponding minimization scheme for sea surface salinity (SSS) and wind speed (U10) retrievals. For such a purpose, both realistically simulated brightness temperatures (TBs) and a post-launch derived semi-empirical forward model are used. This study confirms the effectiveness of the L2OS configuration for SSS retrieval and provides the optimal configuration for U10 retrieval. A revised cost function formulation, where the observational term has more weight than the background one, is further assessed, which leads to smaller retrieval errors.

Keywords: SMOS, Bayesian-based inversion, Levenberg-Marquardt minimization scheme, Sea surface salinity, Sea surface wind speed.

Introduction
The Soil Moisture and Ocean Salinity (SMOS) mission is one of the European Space Agency (ESA) Earth Explorer Opportunity Missions, which was proposed in 1998 within the ESA Living Planet Program [Kerr et al., 2001]. It was launched in November 2009 with the purpose to provide global maps of both soil moisture (SM) and sea surface salinity (SSS) with both spatial and temporal resolutions adequate for climate and ocean general circulation studies. The payload embarked on SMOS includes the Microwave Imaging Radiometer using Aperture Synthesis (MIRAS), which is an L-band fully polarized 2-Dimensional (2-D) interferometric radiometer able to use the aperture synthesis to obtain high spatial resolution over a large swath [Martin-Neira and Goutoule, 1997]. It provides 2-D images of the ocean-surface brightness temperature (TB) for each overpass with a multi-angular imaging capability thus observing the same point on the Earth’s surface from a wide range of incidence angles, which is crucial for a successful retrieval of SSS. It must be pointed out that TB measurements acquired at L-band
over the ocean are mainly modulated by three geophysical variables, i.e. the SSS, the sea surface temperature (SST), and the sea surface roughness (SSR). As a matter of fact, the operational SMOS MIRAS TB measurements can be used in a multi-parametric inversion scheme to retrieve not only the SSS, but at the same time SST and sea surface roughness related parameters ($P_{\text{rough}}$), such as the sea surface wind speed ($U_{10}$) [Zine et al., 2008]. The sensitivity of SMOS TB measurements to $U_{10}$ substantially increases at high-wind conditions for which fair quality winds may be retrieved, as previously demonstrated for higher frequency radiometers such as the Advanced Microwave Scanning Radiometer-Earth Observing System (AMSR-E) and the WindSAT one [Quilfen et al., 2007]. However, the interesting advantage of the L-band SMOS instrument with respect to AMSR-E or WindSAT radiometer is its substantially lower sensitivity to cloud liquid water and rain, which enables wind retrievals in high wind conditions and the unique capability of providing such high wind information even under heavy rain conditions.

The retrieval of both SSS and other interesting geophysical parameters (e.g. SST, $U_{10}$, friction velocity or other roughness descriptors, etc.) is accomplished in the Data Product Generation System (DPGS) by means of the SMOS Level 2 Ocean Salinity processor (L2OS), which provides consistent retrievals of the above-mentioned parameters by efficiently processing geo-located TBs provided at the SMOS Level 1C (L1C) after the image reconstruction step, as described in [Zine et al., 2008]. The retrieval is conventionally accomplished by using a multi-parametric minimization algorithm based on the Levenberg-Marquardt (LM) procedure [Marquardt, 1963]. The latter aims at retrieving the geophysical parameters values (e.g. SSS, SST, $U_{10}$ and more generally $P_{\text{rough}}$), which minimize a maximum-likelihood Bayesian-based cost function. A suitable definition of this cost function, as well as the minimization strategy, is very important to obtain good performances for the retrieval of SSS, SST and $U_{10}$ from SMOS data. Although several pre-launch studies have been carried out to optimize the SMOS SSS inversion, little work has been done to revisit such studies after launch, once the first realistic post-launch forward models were derived. Moreover, no comprehensive studies have been carried out to assess the optimal SMOS cost function configuration for $U_{10}$ retrieval purposes.

The goal of this study is to develop a simplified parallel version of the L2OS inversion scheme for optimizing the retrieval of both SSS and $U_{10}$. For such a purpose, an assessment study of the optimal configuration of both the SMOS maximum-likelihood Bayesian-based cost function and the corresponding LM-based multi-parametric inversion scheme is accomplished over realistically simulated TBs by using a post-launch empirically-derived sea surface roughness forward model. Within such a framework, a sensitivity analysis of the SMOS cost function is carried out for different cost-function configurations. A review of the cost function weights as well as the minimization strategy is carried out to fully exploit both the SSS and the $U_{10}$ content of the SMOS data. The assessment is accomplished by only taking into the account the sea surface contribution of the SMOS forward model (hereinafter FM), which relates the L-band SMOS TB measurements and the ocean surface geophysical parameters to retrieve.

The paper is organized as follows: in section 2 the theoretical background relevant to the SMOS cost function multi-parametric inversion scheme used in this study is provided. In section 3, a detailed analysis of the SMOS cost function is carried out. In section 4, a thorough simulation experiment is carried out to determine the optimal cost function configurations for both SSS and $U_{10}$ retrieval purposes. In section 5, the experiments carried out in sections 3 and 4 are revisited using the revised cost function formulation used in the SMOS operational processor. In section 6, the conclusions are drawn.
Theoretical background
In this section, the theoretical background of the SMOS FM, the Bayesian-based cost function and the LM inversion scheme, which are used in the paperwork, is described.

Forward Model
The forward model (FM) that relates the sea-surface contribution of the L-band SMOS TB measurements to the geophysical parameters of the ocean surface (i.e. SSS, SST and $U_{10}$) can be expressed as follows [Guimbard et al., 2012]:

$$TB_{model}(\theta, SSS, SST, U_{10}) = TB_{flat\_sea,p}(\theta, SSS, SST) + TB_{rough\_sea,p}(\theta, U_{10}) \quad [1]$$

where $TB_{flat\_sea,p}$ is the TB measurement of a flat sea surface, $TB_{rough\_sea,p}$ is the contribution of sea surface roughness, $p$ is the polarization and $\theta$ is the incidence angle. The term $TB_{flat\_sea,p}$ is modeled according to the following Equation:

$$TB_{flat\_sea,p}(\theta, SSS, SST) = \left[1 - R_{flat\_sea,p}(\theta, \varepsilon)\right] \cdot SST \quad [2]$$

where $R_{flat\_sea,p}$ is the Fresnel reflection coefficient and $\varepsilon$ is the dielectric constant of seawater. The latter is typically described by means of the Klein and Swift dielectric model [Klein and Swift, 1977], i.e. a reasonably accurate model for the L-band emissivity of a flat sea surface. Regarding the term $TB_{rough\_sea,p}$, three different roughness models are currently used in the L2OS processor for SSS retrieval purposes. The first two are based upon a similar theoretical electromagnetic scattering approach [Yueh et al., 1988; Yueh et al., 1994]. The first one is referred as the two-scale model [Dinnat et al., 2002] and the second one as the small slope approximation/small perturbation method (SSA/SPM) model [Irisov, 1997; Johnson and Zhang, 1999]. The latter has been defined in the L2OS processor as the weighted sum by foam fraction of the SSA/SPM emission and foam emission [Camps et al., 2004]. The foam model is based on [Reul and Chapron, 2003], and its implementation is fully described in [Font et al., 2009]. In this paper, the third L2OS roughness model, i.e. an empirically derived model [Guimbard et al., 2012], is used. This model, which is based on a neural network (NN) approach, relates the TB rough-sea contribution to $\theta$ and $U_{10}$ in the following way:

$$TB_{rough\_sea,p} = \sum_{j=1}^{m} W_j \tanh \left(b_j + \sum_{i=1}^{n} w_{ij} x_i \right) + B \quad [3]$$

where $x$ is the normalized input two-row vector $[\theta, U_{10}]$; $(w_{ij}, b_j)$ are the weights and the biases of the single hidden layer defined in the NN approach, respectively; $(W_j, B)$ are the weights and the biases of the output layer defined for the NN approach, respectively; and $(j,i)$ are the number of neurons and input variables defined in the NN approach, respectively [Guimbard et al., 2012].
**SMOS Bayesian-based cost function**

Based on the FM described in section 2.1, the retrieval of both SSS and other geophysical parameters (e.g. SST and $U_{10}$) is performed by the L2OS processor through a multi-parametric inversion scheme based on a maximum-likelihood Bayesian approach [Gabarró et al., 2009]:

$$X^2 = \frac{1}{N_{\text{obs}}} \sum_{n=1}^{N_{\text{obs}}} \left( \frac{TB_{\text{meas}}_n - TB_{\text{model}}_n(\theta_n, SSS, SST, U_{10})}{\sigma_{TB_n}} \right)^2 + \sum_{j=1}^{M} \left( \frac{P_j - P_{j0}}{\sigma_{P_{j0}}} \right)^2$$  \[4\]

where $N_{\text{obs}}$ is the number of L-band SMOS TB observations, which depends on the SMOS acquisition mode (in this study, the inversion is performed in dual-polarimetric mode, i.e., accounting for both vertically- and horizontally-polarized TB measurements). The first term of Equation [4] is referred to as the observational term, since it represents the contribution of both measured and modeled (using the previously defined FM) MIRAS TB observables ($TB_{\text{meas}}_n$ and $TB_{\text{model}}_n$, respectively), properly weighted by the radiometric noise ($\sigma_{TB_n}$). The second term of Eq. [4] is referred to as the background term since it represents the contribution of the background or auxiliary *a priori* information ($P_{j0}$) which is provided as a constraint for each geophysical parameter to retrieve ($P_j = SSS$, SST, $U_{10}$), weighted by its corresponding uncertainty value $\sigma_{P_{j0}}$. Eq. [4] takes into account that errors on both TB measurements and auxiliary geophysical parameters are assumed to be Gaussian and un-correlated. Previous studies [Gabarró et al., 2009] showed that the definition of the optimal cost function is not straightforward and a suitable definition of the Bayesian-based cost function is very important to obtain good performances for the retrieval of SSS, SST and $U_{10}$ parameters from SMOS TB measurements.

In this paper, two different maximum-likelihood Bayesian-based cost functions have been considered starting from the general formulation given in Eq. [4]. The first formulation of the SMOS Bayesian-based cost function consists of an observational term only, (i.e. the unconstrained configuration) where no geophysical parameters are constrained in the minimization procedure:

$$X^2 = \frac{1}{N_{\text{obs}}} \sum_{n=1}^{N_{\text{obs}}} \left( \frac{TB_{\text{meas}}_n - TB_{\text{model}}_n(\theta_n, SSS, SST, U_{10})}{\sigma_{TB_n}} \right)^2$$  \[5\]

The second formulation of the Bayesian-based cost function consists of both an observational and a background term (i.e. the fully constrained configuration), where the geophysical parameters are constrained in the minimization procedure and thus *a priori* information is used:

$$X^2 = \frac{1}{N_{\text{obs}}} \sum_{n=1}^{N_{\text{obs}}} \left( \frac{TB_{\text{meas}}_n - TB_{\text{model}}_n(\theta_n, SSS, SST, U_{10})}{\sigma_{TB_n}} \right)^2 + \left( \frac{SSS - SSS_{\text{prior}}}{\sigma_{SSS_{\text{prior}}}} \right)^2 + \left( \frac{SST - SST_{\text{prior}}}{\sigma_{SST_{\text{prior}}}} \right)^2 + \left( \frac{U_{10} - U_{10_{\text{prior}}}}{\sigma_{U_{10_{\text{prior}}}}} \right)^2$$  \[6\]
The background terms, i.e., the 2nd, the 3rd and the 4th terms in [6], represent the SSS, SST, and U10 constraints, respectively, which include auxiliary or a priori information (i.e. SSS_{prior}, SST_{prior}, and U10_{prior}, respectively) and its corresponding uncertainty (σ_{SSS_{prior}}, σ_{SST_{prior}} and σ_{U10_{prior}}, respectively). The lower the uncertainty (σ) of an auxiliary parameter is, the higher the impact of that auxiliary value in the retrieval is (i.e., higher constraint).

Based on the second formulation of the Bayesian-based cost function, other hybrid configurations (with one or two parameter constraints) can be considered to analyze the capabilities of the corresponding cost function for SSS, SST and U10 retrieval purposes.

**LM multi-parametric inversion scheme**

The retrieval of SSS, SST, and U10 parameters from the SMOS Bayesian-based cost function is conventionally accomplished by L2OS processor through a multi-parametric minimization algorithm based on the Levenberg-Marquardt (LM) procedure [Marquardt, 1963]. The latter is considered a very computationally effective iterative scheme, thus providing accurate values of the cost function minima in relatively small number of iterations. The LM scheme involves an iterative algorithm aimed at retrieving the geophysical parameters values (i.e. SSS, SST, U10) that minimize the SMOS Bayesian-based cost function. The goal of each iteration is to find a perturbation to the geophysical parameters that reduces the value of the cost function until its minimum value is reached [Marquardt, 1963]. Therefore, in the presence of multiple minima (which may result from the inversion of non-linear FMs such as the SMOS one), LM will converge in one of the minima, thus providing a single solution. Besides the fact that the convergence may happen in a secondary minimum (i.e., not the most representative or likely in terms of the probability of being the true solution), providing a single solution in case of multiple minima generally leads to poor quality retrievals since the full information content of the inversion is not taken into account [Portabella and Stoffelen, 2004]. A minimization scheme, which allows detecting and characterizing such multiple minima together with a comprehensive ambiguity removal scheme [e.g., Vogelzang et al., 2009], is required in such cases.

In this paper, the LM multi-parametric inversion scheme is adopted by considering the convergence criteria defined in the L2OS processor [SMOS Team, 2011], which state that the convergence is achieved when both the cost function value (inversion residual) does only marginally change (below a certain threshold) from one iteration to the next and the increments in geophysical parameters are small with respect to a fixed threshold.

**Sensitivity Analysis of SMOS Bayesian-based cost function**

In this section some meaningful synthetic results are discussed, which are relevant to the sensitivity analysis of the SMOS Bayesian-based cost function configurations described in section 2. The analysis aims at assessing: a) the SMOS TB sensitivity with respect to SSS, SST, U10; b) the possible presence of multiple-minima solutions for the SMOS cost function; c) the effect of constraints on the SMOS cost function retrieval solutions.

**TB sensitivity versus SSS, SST and U10**

A single study case is fully presented and detailed, where the noise-free SMOS Bayesian-based cost function is tested over different configurations, according to the Equations [5] and [6]. A reference marine scenario is considered, where SSS_{true} = 35psu, SST_{true} = 20°C
and $U_{10,\text{true}} = 5\text{m/s}$. With respect to the observational term Eq. [5] and first term in Eq. [6], noise-free TBs are simulated in a dual-polarimetric mode for $\theta$ values ranging between 0° and 55°. A constant radiometric noise $\sigma_{TB} = 2\text{K}$ is considered to weight every simulated horizontally-polarized (H-pol) and vertically-polarized (V-pol) SMOS TBs. With respect to the background term in Eq. [6], no errors are assumed in the simulated measurements and the reference a priori values, i.e. $\text{SSS}_{\text{true}} = \text{SSS}_{\text{prior}}$, $\text{SST}_{\text{true}} = \text{SST}_{\text{prior}}$ and $U_{10,\text{true}} = U_{10,\text{prior}}$. Each auxiliary a priori parameter is provided with a reference uncertainty of $\sigma_{\text{SSS}_\text{prior}} = 0.3\text{psu}$, $\sigma_{\text{SST}_\text{prior}} = 1\text{°C}$ and $\sigma_{U_{10,\text{prior}}} = 1.5\text{m/s}$, respectively. Note that the true geophysical parameter values defined in Gabarró et al. [2009] are used here for intercomparison purposes. They correspond to a typical marine scenario that accounts for the relationship among SSS, SST and $U_{10}$. However, the priors’ uncertainties differ somewhat from those used by Gabarró et al. [2009]. The former, as defined above and in Table 1, are more realistic and similar to those used by the L2OS processor. Moreover, these uncertainty values are in line with previous assessment studies of SSS [Delacroix et al., 2006; Philipps et al., 2007], SST [Reinolds et al., 2007] and $U_{10}$ [Vogelzang et al., 2011] uncertainties.

| Marine scenario (true values) | SSS (psu) | SST (°C) | $U_{10}$ (m/s) |
|------------------------------|-----------|----------|----------------|
| Warm water / Low wind        | 36        | 30       | 5              |
| Warm water / High wind       | 36        | 30       | 14             |
| Cold water / Low wind        | 33        | 0        | 5              |
| Cold water / High wind       | 33        | 0        | 14             |

| Simulated a priori values    | SSS$_{\text{true}} + \mathcal{N}(0, \sigma_{\text{SSS}}=0.3\text{psu})$ | SST$_{\text{true}} + \mathcal{N}(0, \sigma_{\text{SST}}=1\text{°C})$ | $U_{10,\text{true}} + \mathcal{N}(0, \sigma_{U_{10}}=1.5\text{m/s})$ |

In Figure 1, the 2-D contour plots of the SMOS Bayesian-based cost function are shown in different configurations, when varying SSS and $U_{10}$ (SSS and SST) over the whole range of possible solutions, while holding the SST ($U_{10}$) to the original true value. This sensitivity analysis is similar to the one carried out by Gabarró et al. [2009]. In contrast with the latter, where a pre-launch derived FM (based on platform campaign data) was used, the current analysis uses the post-launch derived FM described in section 2, where the rough sea contribution to TB is empirically derived [Guimbard et al., 2012].

In general, the simulated results presented here are in line with the ones obtained by [Gabarró et al., 2009]. In detail, when considering the observational term only and hence the unconstrained cost function configuration [Eq. 5], the ideal (noise-free and un-biased) simulated TB measurements are characterized by very low sensitivities with respect to SSS, SST and $U_{10}$ variations (see the broad minimum in Fig. 1a and the vertical contours in Fig. 1b). In detail, these sensitivities are quite of the same magnitude order for both SSS and $U_{10}$ parameter values (the cost-function exhibits similar value for a wide range of SSS and $U_{10}$ values), whereas a smaller sensitivity for SST is provided (the cost-function exhibits similar value for a wide/small range of SST/SSS values, see the vertical contours in Fig. 1b). Therefore, assuming that the SMOS TB sensitivities are realistic, it is clear that the cost function configuration [Eq. 5] will lead to large retrieval errors when real (noisy and biased) TB observables are used.
Figure 1 - 2-D Contour plots of the SMOS Bayesian-based cost function in the $U_{10}$-SSS and SST-SSS planes, when (a)-(b) considering the un-constrained configuration [Eq. 5], (c)-(d) the $U_{10}$ and SST constrained configurations, respectively, (e)-(f) the fully constrained configuration [Eq. 6]. Note that the $U_{10}$-SSS (SST-SSS) plane plots correspond to cuts of the 3-dimensional cost function at the true SST=20°C ($U_{10}$=5 m/s).
When only one parameter is restricted (see Figs. 1c and 1d) and therefore a partially-constrained hybrid cost function configuration is taken into account, the cost function minimum and the corresponding SSS, SST and U_{10} solution values are better defined over the whole range of possible solutions. Conversely, when all the constraints are used (see Figs. 1e and 1f) and therefore Eq. [6] is taken into account, both the cost function minimum and the corresponding SSS, SST and U_{10} solution values are the best defined. Note that the x and y ranges of Figures 1e and 1f have been reduced to better discern the contour lines, indicating that indeed the cost function minima are substantially better defined in these figures than in Figures 1c and 1d, notably when compared to Figures 1a and 1b (unconstrained cost function). As such, assuming un-biased TBs and reference a priori values, the fully-constrained cost function provides more accurate geophysical parameter retrievals than either the un-constrained or the partially constrained cost function configurations. All the results gathered by using simulated ideal TB measurements have been confirmed when realistically simulated noisy TB measurements are used (not shown).

**Multiple-minima assessment**

In this section, some relevant results are presented, which aim at demonstrating the lack of secondary minima and therefore the validity of the LM minimization scheme, even when realistically simulated noisy TB measurements and noisy auxiliary a priori information are used. The reference marine scenario described in section 3.1 is considered, together with the same configuration parameters previously defined for the un-constrained [Eq. 5] and the fully constrained [Eq. 6] cost functions. In contrast with section 3.1, a Gaussian noise with zero mean and standard deviation $\sigma_{TB} = 2K$, $\sigma_{SSS} = 0.3\text{psu}$, $\sigma_{SST} = 1^\circ\text{C}$, and $\sigma_{U_{10}} = 1.5\text{m/s}$ (see Tab. 1) is added to simulated H/V-pol TB observables, $SSS_{true}$, $SST_{true}$ and $U_{10\_true}$, respectively, to provide noisy TB measurements and noisy background terms, with corresponding uncertainties. In Figure 2 it is shown the behavior of the un-constrained cost function [Eq. 5], whose values are plotted against the whole range of SSS, SST and U_{10} solution values, respectively, for the simulated marine scenario. This result consistently demonstrates the lack of secondary minima for the SMOS cost function both when only the observational term [Eq. 5] is taken into account and when realistically simulated noisy TB observables are in place. All the results are further confirmed by considering the sample 2-D contour plots shown in Figure 3, where a cut of the 3-dimensional (3-D) SMOS Bayesian-based cost function [Eq. 6] at the original true SST value (i.e. the $U_{10\_SSS}$ plane) is shown. It is clearly demonstrated that a unique absolute minimum numerical value is retrieved for the cost function observational term (un-constrained configuration) (Fig. 3a), the background term (Fig. 3b), and the subsequent SSS-U_{10} constrained cost function configuration (Fig. 3c). Moreover, Figure 3 shows a case where a large inconsistency between the observational and the background terms is present (see large discrepancy between the minimum values in Figs. 3a and 3b). For such case, the presence of secondary minima is more likely. However, this is not the case mainly because the background term associated with both SSS_{prior} and U_{10\_prior} dominates the cost function solution with respect to the observational term (the minimum in Fig. 3c is much closer to that in Fig. 3b than to that in Fig. 3a). As a result, the presence of multiple minima in the SMOS minimization procedure can be discarded when considering the SMOS general cost function formulation [Eq. 4], thus validating the LM scheme used in the L2OS processor.
Effects of constraints

In this section, some relevant results are presented, which aim at demonstrating the impact of the cost function background terms (i.e., SST, SSS, and $U_{10}$ constraints) in the retrieval of geophysical parameters from (noisy) realistically simulated SMOS data. The analysis is presented by taking into account the un-constrained [Eq. 5], the SST constrained and the fully (i.e. SST-SSS-$U_{10}$) constrained [Eq. 6] configurations of the SMOS Bayesian-based cost function by considering a sample test case relevant to the marine scenario defined in section 3.2.

As mentioned in section 3.1, the SMOS TBs have a significantly lower sensitivity to SST changes than to SSS and $U_{10}$ changes. As such, the need for an SST-constrained cost function configuration to optimize SSS and $U_{10}$ retrievals is first investigated. Synthetic results are
shown in Figure 4, where the probability density function (pdf) or normalized histogram of the difference between the retrieved and the true SST values are shown for both the unconstrained [Eq. 5] and the SST-constrained cost function configurations (see the solid and the dotted lines in Fig. 4, respectively).

![Image](image_url)

**Figure 3** - Synthetic results relevant to a sample simulation, where the noisy realistically simulated SMOS Bayesian-based cost function is tested with respect to the reference marine scenario described in section 3.2. 2-D Contour plots of (a) the observational term (i.e. the un-constrained configuration), (b) the $U_{10}$-SSS background term and (c) the $U_{10}$-SSS constrained cost function configuration in [Eq. 6] over the $U_{10}$-SSS plane, when fixing SST to its true reference value.

The results agree with the sensitivity analysis described in section 3.1, showing that the very low TB sensitivity to SST changes leads to large SST retrieval errors, with SST retrieval values close to the extremes of the FM look-up table. Since this large SST retrieval error does negatively impact the quality of SSS and $U_{10}$ retrievals (not shown), fixing or constraining the SST in the SMOS cost function is required to optimize SSS and $U_{10}$ retrievals.
Other meaningful results are shown in Figure 5, where the normalized histograms of the difference between the retrieved and the true values (solid lines) and between the retrieved and a priori values (dotted lines) are provided for both SSS (Fig. 5a) and U_{10} (Fig. 5b) parameters, when considering the fully constrained cost function configuration [Eq. 6]. Figure 5 shows that a (strong) background term associated to one of three geophysical parameters dominates the SMOS cost function solution with respect to the observational term. In detail, the SSS-SST-U_{10} triplet solution converges to the auxiliary a priori information of each retrieved geophysical parameters. This is due to the relatively low sensitivity of SMOS TBs to SSS, SST and U_{10} (see section 1). Hence, to optimize the information content of SMOS TB measurements, no SSS (U_{10}) constraints can be used to derive SSS (U_{10}).
Optimal SMOS cost function configuration for SSS and $U_{10}$ retrieval

In this section, results on the assessment of the SMOS Bayesian-based cost function multi-parametric inversion scheme in terms of the optimal retrieval of SSS and $U_{10}$ are presented. The inversion is accomplished through the LM procedure [Marquardt, 1963; SMOS Team, 2011] described in section 2.3. Note that the LM parameters and convergence criteria used in this analysis correspond to the ones defined in the SMOS L2OS processor [SMOS Team, 2011]. Although somewhat different than the default ones [Marquardt, 1963], they provide very similar inversion results (inter-comparison not shown). Based on this rationale, synthetic results are obtained by considering realistically simulated noisy TB measurements and noisy auxiliary *a priori* information on SSS, SST and $U_{10}$, with reference to the four simulated marine scenarios described in Table 1. These marine scenarios are based on both geophysical grounds and forward model sensitivities. As derived from Klein & Swift, 1977 [Guimbard et al. 2012], the flat sea (roughness) model sensitivity to SSS (sea surface wind) changes is the highest at warm waters (high winds) and the lowest at very cold waters (low winds). Moreover, the different scenarios well represent the characteristic geophysical conditions found in vast regions of the ocean, notably the tropics and the high latitudes.

The general cost function formulation [Eq. 4] and its most relevant configurations [Eq. 5], [Eq. 6] (note that other hybrid cost function configurations have been tested but only the most relevant are shown) are assessed in terms of optimal SSS and $U_{10}$ retrievals, accounting for the four marine scenarios defined in Table 1. In detail, special attention is paid to the SST, SST-SSS, SST_{fixed}-SSS-$U_{10}$ and the fully constrained (SST-SSS-$U_{10}$) cost function configurations. The analysis is provided in terms of mean error ($\mu$), root mean square error (RMSE) and standard deviation (STD) error values. Simulated results are shown in Figures 6 and 7, where the SSS and $U_{10}$ retrieval error results are plotted against the above mentioned cost function configurations, respectively, when considering the four simulated marine scenarios in Table 1.

The results are in line with the sensitivity analysis results provided in section 3. In fact, it is demonstrated that the SMOS Bayesian-based cost function inversion scheme can be both simplified and improved either by fixing the SST parameter to an auxiliary value or, equivalently, by using a (strong) SST background term in the cost function formulation. This is due to the low SST sensitivity of SMOS TB measurements. As a consequence, no useful SST information can be derived though from SMOS data (see Figs. 6 and 7).

With respect to the optimal SSS retrieval problem, simulated results demonstrate that the SST-$U_{10}$ constrained cost function configuration (or the fully constrained cost function configuration with a very high $\sigma_{SSS\_prior}$ value of 100psu, as used in the L2OS processor) is the optimal one. This is especially true for a marine scenario with warm water and low wind conditions, where low statistical errors are obtained due to the high sensitivity of TB measurements to SSS changes (see Fig. 6).

With respect to the optimal $U_{10}$ retrieval problem, simulated results demonstrate that the SST-SSS constrained cost function configuration is optimal for the retrieval of $U_{10}$. This is especially true for a marine scenario with cold water and high wind conditions where low statistical errors are obtained due to the high sensitivity of SMOS TB measurements to $U_{10}$ changes (see Fig. 7).
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Figure 6 - SSS retrieval results of the SMOS LM inversion procedure for the SST, SST-SSS, SST_{fixed} - SSS-U_{10} and the SST-SSS-U_{10} constrained cost function configurations, with σ_{SSS-prior} = 100psu. Marine scenario with (a) warm water and low winds, (b) warm water and high winds, (c) cold water and low winds, (d) cold water and high winds.

Other results are summarized in Tables 2 and 3, where the retrieval error analysis is carried out in terms of μ, RMSE and STD values by considering the optimal SSS and U_{10} retrieval cost function configurations, respectively, with reference to a more realistic case study in which the simulation accounts for the different range of θ, N_{obs}, and σ_{TB} values according to several SMOS swath configurations. In particular, simulations are carried out at nadir and 300km cross-track location, as well as at the Alias-Free (AF) and the Extended Alias Free (EAF) Field of View (FOV) [Zine et al., 2008]. The results in Tables 2 and 3 refer to nadir simulations. At 300km cross-track location, the results (not shown) are similar to those in Tables 2 and 3, although with slightly higher errors. The results, obtained for the marine scenarios of Table 1 and the optimal SSS and U_{10} retrieval cost function configurations, are in line with previous ones.

Table 2 - SSS retrieval results for the optimal SST-U_{10} constrained cost function configuration, when using the general formulation [Eq. 4] for the simulated AF and EAF-FOV at nadir location.

| SSS (psu)       | μ     | RMSE     | STD     |
|-----------------|-------|----------|---------|
|                  | AF    | EAF      | AF      | EAF  | AF    | EAF  |
| Warm water / Low wind | 0.02  | 0.48     | 0.48    | 0.43 | 0.48  | 0.43 |
| Warm water / High wind | -0.01 | 0.07     | 0.77    | 0.81 | 0.77  | 0.81 |
| Cold water / Low wind | -0.07 | -0.05   | 1.47    | 1.44 | 1.47  | 1.44 |
| Cold water / High wind | 0.19  | 0.19     | 2.56    | 2.57 | 2.55  | 2.57 |
Figure 7 - \( U_{10} \) retrieval results of the SMOS LM inversion procedure for the SST, SST-SSS (\( \sigma_{\text{SSS-prior}} = 100 \text{psu} \)), SST-SSS (\( \sigma_{\text{SSS-prior}} = 0.3 \text{psu} \)) and SST-SSS-\( U_{10} \) (\( \sigma_{\text{SSS-prior}} = 0.3 \text{psu} \)) constrained cost function configurations. Marine scenario with (a) warm water and low winds, (b) warm water and high winds, (c) cold water and low winds, (d) cold water and high winds.

Table 3 - \( U_{10} \) retrieval results for the optimal SST-SSS constrained cost function configuration, when using the general formulation [Eq. 4] for the simulated AF and EAF-FOV at nadir location.

| \( U_{10} \) (m/s) | \( \mu \) | RMSE | STD |
|-------------------|----------|------|-----|
| Warm water / Low wind | 0.01     | -0.01 | 1.19 | 1.14 | 1.19 | 1.14 |
| Warm water / High wind | 0.03     | -0.06 | 0.77 | 0.7  | 0.7  | 0.7  |
| Cold water / Low wind | 0.01     | -0.02 | 0.98 | 0.83 | 0.98 | 0.83 |
| Cold water / High wind | -0.03   | 0.0   | 0.55 | 0.49 | 0.55 | 0.49 |

Assessment of the Operational SMOS cost function formulation

In this section, the experiments of sections 3 and 4 are repeated but for a revised Bayesian-based cost function formulation used by the SMOS operational processor (L2OS). As detailed in (SMOS Team, 2011), the default L2OS inversion procedure is performed with a revised cost function formulation, which excludes the factor “\( 1/N_{\text{obs}} \)” in the observational term of Eq. [4]:

\[
X^2 = \sum_{n=1}^{N_{\text{obs}}} \left( \frac{TB_{\text{meas}} - TB_{\text{mod}}(\theta_n, SSS, SST, U_{10})}{\sigma_{TB_h}} \right)^2 + \sum_{j=1}^{M} \left( \frac{P_j - P_{j0}}{\sigma_{P_j0}} \right)^2 \tag{7}
\]
As shown in section 3.3, the cost function constraints have a strong weight in the inversion procedure due to the generally low sensitivity of SMOS TBs to SSS, U_{10}, and SST changes. As such, the optimal cost function configurations obtained in section 4.1 are very much influenced by this effect. In other words, no SSS (U_{10}) constraint can be used to derive SSS (U_{10}), since the a priori value of SSS (U_{10}) clearly dominates the retrieval. The revised formulation [Eq. 7] enhances the weight of the observational term with respect to the a priori information (background term) and thus the impact of the former term in the SSS and U_{10} retrievals.

Figure 8 - Normalized histograms of the difference between the retrieved and the true values (solid lines) and between the retrieved and a priori values (dotted lines) for U_{10}. The retrieval is performed with the fully constrained cost function configuration (SST-SSS-U_{10}) of the revised formulation [Eq. 7]. (a) Marine scenario described in section 3.2. (b) Marine scenario with cold water (SST = 0°C) and high winds (U_{10} = 14m/s) for SSS = 33psu.

First, the sensitivity analysis (section 3.1), the LM minimization scheme assessment (section 3.2), and the analysis of the effects of constraints in the SMOS cost function (section 3.3) are repeated with the revised formulation [Eq. 7]. Simulated results (not shown) generally agree with those of the general formulation [Eq. 4], when considering the un-constrained, the fully constrained and other hybrid partially constrained cost function configurations. However, slightly different results are obtained when analyzing the effects of constraints in the fully constrained revised cost function formulation [Eq. 7]. In fact, the use of a U_{10} constraint can be valuable for optimizing U_{10} retrievals from SMOS TB measurements (see Fig. 8), especially when considering a marine scenario with cold water and high wind conditions (see Fig. 8b). On one hand, the retrieved U_{10} does not converge towards the a priori U_{10} (the dotted line histograms in Fig. 8 are clearly broad); on the other hand, the retrieved U_{10} is closer to the true U_{10} than to the a priori U_{10} (the solid line histograms are narrower than the dotted line ones, notably in Fig 8b). In contrast, the effect of a SSS constraint in the revised formulation [Eq. 7] is generally strong although not as strong as with the general formulation [Eq. 4] (not shown), notably for warm waters where the TB sensitivity to SSS changes is maximum. Regarding the optimal cost function configuration for SSS retrievals (section 4), the results of the revised formulation [Eq. 7] agree with those of the general formulation [Eq. 4], showing that the SST-U_{10} constrained configuration is the optimal one, although lower retrieval errors are obtained with the revised formulation
Regarding the optimal cost function configuration for $U_{10}$ retrievals (section 4), the results of the revised formulation [Eq. 7] show that the SST-SSS-$U_{10}$ (i.e. fully) constrained configuration is the optimal one, whereas those of the general formulation [Eq. 4] show that the SST-SSS constrained configuration is the optimal one (see section 4). Moreover, the retrieval errors obtained with the revised formulation [Eq. 7] are lower than those obtained with the general formulation [Eq. 4] (compare Tab. 5 with Tab. 3).

### Conclusions

In this paper, an assessment of the SMOS Bayesian-based cost function has been carried out by means of a comprehensive simulation study. The main results are summarized as follows:

- Both ideal (noise-free) and realistically (noisy) simulated SMOS TB measurements exhibit very low sensitivities with respect to SSS, SST and $U_{10}$ variations. These sensitivities are of the same order of magnitude (although different) for both SSS and $U_{10}$ parameter values, whereas a substantially smaller sensitivity to SST changes is found;
- No useful SST information can be derived from SMOS TB measurements, due to their very low sensitivity to SST changes. As a result, the SMOS Bayesian-based cost function and the subsequent minimization scheme can be simplified and improved by either fixing or constraining SST to an auxiliary value;
- A unique absolute minimum numerical value for the SMOS Bayesian-based cost function is retrieved, which in turn corresponds to a single unique triplet solution of SSS-SST-$U_{10}$;
- A (strong) background term associated with any of three geophysical parameters dominates the retrieved solution with respect to the observational term. This is especially true when considering the general cost function formulation [Eq. 4]. However, the use of a $U_{10}$ constraint can be valuable for optimizing $U_{10}$ retrievals when excluding the factor “1/$N_{obs}$” in the cost function formulation, i.e., in the revised formulation [Eq. 7];
- The SST-$U_{10}$ constrained (i.e. L2OS) configuration is optimal for the SSS retrieval, both with [Eq. 4] and without [Eq. 7] the factor “1/$N_{obs}$” in the cost function formulation;

### Table 4 - SSS retrieval results for the optimal SST-$U_{10}$ constrained cost function configuration, when using the revised formulation [Eq. 7] for the simulated AF and EAF-FOV at nadir location.

| SSS (psu)          | AF       | EAF      | AF       | EAF      |
|--------------------|----------|----------|----------|----------|
| Warm water / Low wind | 0.01     | 0.01     | 0.37     | 0.34     |
| Warm water / High wind | 0.02     | 0.01     | 0.57     | 0.59     |
| Cold water / Low wind  | -0.07    | -0.04    | 1.24     | 1.11     |
| Cold water / High wind | 0.05     | 0.15     | 1.86     | 1.78     |

### Table 5 - $U_{10}$ retrieval results for the optimal SST-SSS-$U_{10}$ constrained cost function configuration, when using the revised formulation [Eq. 7] for the simulated AF and EAF-FOV at nadir location.

| $U_{10}$ (m/s) | AF       | EAF      | AF       | EAF      |
|----------------|----------|----------|----------|----------|
| Warm water / Low wind | 0.04     | -0.04    | 0.82     | 0.87     |
| Warm water / High wind | 0.03     | -0.03    | 0.67     | 0.63     |
| Cold water / Low wind  | -0.05    | -0.02    | 0.8      | 0.79     |
| Cold water / High wind | -0.06    | 0.01     | 0.54     | 0.5      |
The SSS-SST and the SST-SSS-U$_{10}$ (i.e. fully) constrained configurations are optimal for the U$_{10}$ retrieval, with [Eq. 4] and without [Eq. 7] the factor “$1/N_{obs}$” in the cost function formulation, respectively.

In conclusion, a parallel-simplified version of the L2OS Bayesian-based inversion scheme has been developed to optimize the retrieval of SSS and U$_{10}$. It shows that L2OS cost function configuration is optimal for the retrieval of SSS. However, a different cost function configuration is required to optimize U$_{10}$ retrievals. Such retrievals are most accurate under high wind conditions, where TB sensitivity to U$_{10}$ changes increases. As mentioned in section 1, the present study only takes into account the sea surface contribution to the TB measurements. Other contributions, e.g. the sky radiation, the sun glint, the atmospheric effects, the Faraday rotation, the vertical total electron content (TEC) and the Radio-Frequency interference (RFI), are not accounted. Some of these contributions, e.g., sky radiation, sun effects, and RFI, are nowadays still poorly modeled and/or detected/filtered. As such, they can introduce TB biases, which in turn can impact the SSS and U$_{10}$ retrieval quality. In particular, the optimal cost function configuration may also depend on the mentioned effects. As such, future work will focus on developing the L2OS parallel version with real data and provide feedback to the L2OS team.

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