Soil moisture retrieval using neural networks: application to SMOS

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Abstract—A methodology to retrieve soil moisture (SM) from SMOS data is presented. The method uses a Neural Network (NN) to find the statistical relationship linking the input data to a reference SM dataset. The input data is composed of passive microwaves (L-band SMOS brightness temperatures, $T_b$’s) complemented with active microwaves (C-band ASCAT backscattering coefficients), and MODIS NDVI. The reference SM data used to train the NN are ECMWF model predictions.

The best configuration of SMOS data to retrieve SM using a NN is using $T_b$’s measured with both H and V polarizations for incidence angles from 25° to 60°. The inversion of soil moisture can be improved by $\sim 10\%$ by adding MODIS NDVI and ASCAT backscattering data and by an additional $\sim 5\%$ by using local information on the maximum and minimum record of SMOS $T_b$’s (or ASCAT backscattering coefficients) and the associated SM values. The NN inverted SM is able to capture the temporal and spatial variability of the SM reference dataset. The temporal variability is better captured when either adding active microwaves or using a local normalization of SMOS $T_b$’s. The NN SM products have been evaluated against in situ measurements, giving results of comparable or better (for some NN configurations) quality to other SM products.

The NN used in this study allows to retrieve SM globally on a daily basis. These results open interesting perspectives such as a near real time processor and data assimilation in weather prediction models.

Index Terms—Soil Moisture and Ocean Salinity (SMOS), MODIS, ASCAT, Soil Moisture, Artificial Neural Networks, ECMWF.

I. INTRODUCTION

SOIL MOISTURE represents less than 1/10000 of the total water of our planet but it plays an important role as it affects the water and energy exchanges at the land surface/atmosphere interface and it is the reservoir of water for agriculture and vegetation in general. Surface soil moisture (hereafter SM) is also a key parameter for hydrological models as it controls important processes such as runoff and it is an important parameter to monitor for flood risk evaluation.

The thermal emission of the Earth at low microwave frequencies (L band i.e., 1.4 GHz) depends essentially on the soil temperature and the amount of soil moisture. The brightness temperature decreases as the amount of soil moisture increases. Therefore, the soil moisture content can be derived from microwave observations at these frequencies. A passive L-band radiometer presents the advantage with respect to active systems at higher frequencies that the measurement is less sensitive to soil roughness and vegetation. This is the concept of the Soil Moisture and Ocean Salinity (SMOS) satellite [1], which is the first mission specifically designed to perform remote sensing measurements of soil moisture and ocean salinity [2].

The SMOS soil moisture operational algorithm [3] is based on a direct or forward model and an optimal estimation approach: a model of the soil physics and the radiation transfer thought the vegetation is used to simulate L-Band brightness temperatures (hereafter $T_b$’s) for a set of physical parameters, soil composition, and moisture content and vegetation opacity. The modeled $T_b$’s are compared to those measured by SMOS. The SM content and the vegetation opacity can be estimated using an iterative process to minimize difference of the model output with respect to the observations. This type of iterative solution using a direct model is said to be local because an independent minimization process needs to be performed for each new observation.

The second approach is finding an inverse model that provides SM values directly from a given set of measured $T_b$’s. Neural networks (NNs) are an efficient mathematical method to obtain such an inverse model. In contrast to the direct model approach discussed above, an inverse model using NNs is a global method that aims at building an inverse model at once using a relatively large number of observations, instead of applying a direct model for each new observation.

NNs have been successfully applied to many inverse problems in the remote sensing field such as the retrieval of atmospheric [4], [5], ocean [6], [7] and continental surface parameters such as surface heat fluxes [8], [9]. NNs have also been applied to retrieve soil moisture at small scale from Synthetic Aperture Radar [10]–[13] or radiometric [14]–[16] observations. These studies are devoted to agricultural fields or to the watershed scale and the NNs were trained with simulated $T_b$’s or backscattering coefficients using radiative
transfer and backscattering models. NNs have been compared to other methods as the Bayesian approach or the Nelder-Mead simplex algorithm. It has been found that all of those methods give similar results but the NNs are faster [12]. The potential of this approach has also been studied to retrieve SM from Sentinel-1 SAR observations [17]. Recently, radiative transfer models have been discussed as a possible approach to train NNs to retrieve SM from SMAP observations [18].

A different approach is to use in situ measurements of SM as reference to train the NNs. This approach has been used to link a total of 3000 \( T_{b} \)’s measurements obtained with the AMSR-E radiometer with in situ measurements of SM in Mongolia and Australia [19]. The trained NN has been applied to one AMSR-E pointing in the north of Italy and compared to and Australia [19]. The trained NN has been applied to one AMSR-E radiometer with in situ measurements of SM in Mongolia and Australia [19]. The trained NN has been applied to one AMSR-E pointing in the north of Italy and compared to and Australia [19]. The trained NN has been applied to one AMSR-E radiometer with in situ measurements of SM in Mongolia and Australia [19]. The trained NN has been applied to one AMSR-E pointing in the north of Italy and compared to and Australia [19]. The trained NN has been applied to one AMSR-E radiometer with in situ measurements of SM in Mongolia and Australia [19].

Two preliminary studies using simulated SMOS data before the launch of the satellite were done by [26] and [27]. The first one was devoted to the use of NNs to measure the sea surface salinity and the second one to the retrieval of SM. To our knowledge, the current work is the first attempt to use NNs to retrieve SM from actual SMOS data.

The rest of the paper is organized as follows: Sect. II presents the different datasets used in this study. Works that used NNs to retrieve SM globally before the launch of SMOS [22]–[24], have used NNs to do a non-linear mapping from a input space of low dimension (typically 1-5) to the one-dimensional output space (SM). SMOS works in full polarization mode and for a wide ranges of incidence angles from 0° to ~ 60°. Therefore, even working with angle-binned data, only using SMOS, the dimension of the input space can be as high as 24 (12 angle bins of 5° width per polarization), many more than any other NN scheme to retrieve SM discussed in the literature. Thus, it is important to start with a sensitivity analysis of the different datasets to SM and to adopt a good strategy of dimensionality reduction. This is presented in Sect. III. A discussion of the neural network approach can be found in Sect. IV while the results are presented in Sect. V. The evaluation of the NN SM retrieval is discussed in Sect. VI in comparison with ECMWF SM, in situ measurements and previous NN retrievals. Finally, Sect. VII summarizes the conclusions.

II. DATA

This section describes the different datasets used in this study. The goal is to construct a data base to train the neural networks (hereafter NN) by collocating a dataset of geophysical variables including a reliable SM estimate with real SMOS observations and other complementary data.

A. SMOS data

As already mentioned, SMOS [1], [2] measures the thermal emission from the Earth at a frequency of 1.4 GHz in full-polarization and for incidence angles from 0° to ~ 60°. SMOS has 69 antennas with a diameter of 16.5 cm distributed in a Y-shaped structure with 4.5 m long arms to perform interferometry and synthesize an aperture of ~ 7.5 m [28], [29]. The satellite is tilted by 32.5°. The projection of the synthesized beam on the Earth surface is in general an ellipse whose axis-ratio and orientation depends on the observed point position. The field of view, defined as the projection of the full width at half maximum of the synthesized beam over land, changes from ~ 30 to ~ 50 km and it is 43 km on average over the field of view [2]. The satellite follows a sun-synchronous polar orbit with 6:00 am/pm equator overpass time (being 6:00 am the local solar time at ascending node).
To retrieve SM from SMOS $T_b$’s using NNs, one would like to use brightness temperatures with the more straightforward physical interpretation, i.e., in the Earth polarization reference frame. In addition, as a NN should have as input a vector of constant length, it is needed to work with fixed angle bins. Therefore, we have used the Level 3 Brightness Temperature (L3TB) from the CATDS (Centre Aval de Traitement des Données SMOS). The L3TB product [30] is a daily global brightness temperature dataset in a 0.25° EASE grid [31] obtained from the L1B product [32]. It includes all the $T_b$’s acquired on a given day, transformed to the ground polarization reference frame (horizontal, H, and vertical, V, polarization), and averaged within 5°-width incidence angle bins. The center of the first angle bin is 2.5°. Ascending and descending orbits are processed separately.

As the satellite progresses, any given location on the Earth’s surface is “seen” a number of times at different incidence angles depending on the location with respect to the satellite subtrack: the further away, the fewer the angular acquisitions [2]. Fig. 1 show the number of $T_b$’s measurements (in H polarization) as a function of the incidence angle and the distance to the satellite subtrack (parameter $X_{\text{swath}}$) for a subset of L3TB data. Along track, a wide range of angles is obtained (0 to 60°). On the opposite, the only angle range that it is accessible all across the swath is from 40° to 45°.

The data base constructed for this project also contains information from the CATDS L3 UDP (User Data Product) [30], such as the SM obtained by the SMOS operational algorithm (hereafter SMOS L3SM), and the probability of having a Radio Frequency Interference (RFI) at a given position (parameter $\text{RFI}_{\text{Prob}}$).

B. ASCAT data

The Advanced Scatterometer (ASCAT) is a real aperture radar operating at 5.255 GHz (C-band) onboard EUMETSAT’s Meteorological Operational (MetOp) satellite [33]. MetOp is in a sun-synchronous orbit, with equator crossing times of approximately 21:30 local time for the ascending overpass and 09:30 for the descending overpass. ASCAT uses fan-beam antennas that covers two 550-km swaths which are separated from the satellite ground track by about ~ 336 km. ASCAT measures the backscattered radiation at incidence angles from 25° to 65°.

Passive and active microwaves have different sensitivity to SM, vegetation and roughness. In the case of SMOS and ASCAT, the observing frequency is also different. Thus, ASCAT data is a potentially useful data set to complement SMOS in the framework of NN inversions. However, in order to use ASCAT as input to the NNs, a pre-processing step is necessary to interpolate the backscatter coefficients to the single constant incidence angle. The adopted pre-processing scheme is inspired from the processing chain of the ERS and ASCAT SM products [34], [35]. The reference incidence angle has been chosen to be 40° as it is in the middle of the observed incidence angle range [34]. The relationship between backscatter and incidence angle is linear over a large range of angles, therefore the angle interpolation has been done using a linear regression. The time window used to compute the regression has to be large enough to ensure the robustness of the regression, while ensuring that the surface conditions other than SM (in particular the vegetation, which affects the slope) remain nearly constant. As a good compromise, the time window has been chosen to be seven days ending the day one wants to estimate the backscattering coefficient for an incidence angle ($\theta$) of 40° (hereafter $\sigma_{40}$). The slope of the line fitted to the points is determined in the data of this window. In general, the fitted line does not goes through the backscattering coefficient measured for the time $t$ of interest (which has been acquired at a variable angle from 25° to 65°). Therefore, a line with the same slope but containing the measurement at time $t$ is computed. This is the line used to estimate $\sigma_{40}$. In summary, the seven-day window is used to compute the slope of the $\sigma(\theta)$ function but the actual line used to compute $\sigma_{40}$ is shifted to take into account the backscattering at time $t$, which depends mainly on the SM content. For many grid points the backscatter coefficient can been measured several times per day at different incidence angles, both in ascending and descending overpasses. A $\sigma_{40}$ is computed from each $\sigma$ value. Finally, the different values are averaged to obtain a daily estimation of $\sigma_{40}$.

The more elaborated processing discussed by [34] computes not only the slope but also the curvature of the $\sigma(\theta)$ function. In addition, data from several years are used to reduce the uncertainties in the $\sigma_{40}$ estimates by computing averaged values for a particular period of the year. However, Sects. V and VI show that the simpler ASCAT data processing discussed in the current study is enough to show the complementarity of passive and active microwaves to retrieve SM.

C. ECMWF models

The ECMWF products used in this work are operational Integrated Forecasting System (IFS) models with the “Hydrology-improved Tiled ECMWF Scheme for Surface Exchanges over Land” (H-TESSEL) [36]. A significant improvement of H-TESSEL took place in November 9th, 2010.
with the addition of: (i) a simplified Extended Kalman Filter for the global operational soil moisture analysis [37], (ii) a new snow analysis based on NESDIS snow cover data at 4 km resolution [38] and, (iii) a monthly varying climatology of leaf area index (LAI) based on MODIS data [39]. Therefore, in this study only data from November 9th, 2010 have been used.

The original ECMWF IFS products used in this study have a native resolution of ~25 km [40] similar to that of the CATDS grid. They have been re-sampled to the CATDS EASE grid and temporally interpolated to the time of the SMOS acquisitions for ascending and descending orbits (the IFS products have a temporal sampling of 3 hours). We will use the volumetric moisture content in the first layer (0-7 cm depth, hereafter ECMWF SM$_{L1}$) of these models as reference or target SM to train the neural networks. In addition, we have used the snow depth and the soil temperature in the first layer to filter out regions with snow or frozen soils.

D. MODIS NDVI

The SMOS signal is affected by the vegetation water content. In addition, the presence and amount of vegetation is correlated with SM in many ecosystems. Therefore, a vegetation index could improve the SM retrieval, as it has been found in previous works using other satellite observations and a similar methodology [22], [41].

Here, the MODIS Normalized Difference Vegetation Index (NDVI) product MYD13C1 has been used. The MODIS NDVI product contains atmospherically corrected bi-directional surface reflectances masked for water, clouds, and cloud shadows. Global MYD13C1 data are cloud-free spatial composites of the gridded 16-day 1-kilometer MYD13A2, and are provided as a level-3 product projected on a 0.05° geographic Climate Modeling Grid (CMG). Cloud-free global coverage is achieved by replacing clouds with the historical MODIS time series climatology record.

A zero-order spatial interpolation of the 0.05° MODIS grid to the 0.25° CATDS grid has been done. In addition, the 16 days MODIS NDVI value for a given grid point is assigned to that point for the previous 8 days and the following 7 days, without any temporal interpolation. This approach presents the advantage of giving a rough estimate of the vegetation characteristics without imposing strong constrains for instance in an operational context. It will be seen in the following that the introduction of such information actually improves significantly the SM retrieval (Sect. V).

E. Wetlands

The emissivity of water being typically half of that of dry soil, the brightness temperatures measured by SMOS over water bodies are significantly lower to those measured over soil, even with a high SM content. Big water bodies are filtered using land-water masks. The problem is dealing with inundated areas. If the SMOS pixel is completely covered by free water, the point is easily filtered out using $T_b$ thresholds (see Sect. III-A). For the pixels partially inundated, the situation is more complex. Therefore, in order to have a clean dataset to train the NNs, it is pertinent to introduce an information on wetlands extension on the data base.

There are several wetland extension datasets such as the NASA JPL Wetland Extent database [42], the Global Lakes and Wetlands Database (GLWD) [43] and the Global Inundation Extent from Multi-Satellites (GIEMS) dataset [44]. The last two ones have been extensively validated at global scale [45], [46] but the GLWD is a static dataset without temporal variation estimations. Therefore, we have used the GIEMS monthly averages of wetland extensions.

F. Texture

Soil texture is a fundamental information when dealing with SM as, for instance, the emissivity of a sand or clay soil with the same volumetric SM will be very different (e.g. [47]). This is a consequence of the soil micro-physics as even if the total volumetric soil moisture is the same, there would be many more free water molecules in a sandy soil that will absorb the Earth thermal radiation, reducing the emissivity and the observed $T_b$’s. Therefore, giving a texture information to the NN can be important in particular to achieve good retrievals for intermediate values of SM, as those values can be easily measured in soils with a variety of textures. Therefore, the sand and clay fractions from the ECOCLIMAP [48] soil texture maps has been added to the database. This is the same texture information that is used by the SMOS L2 and L3 algorithms [3], [30].

III. DATA ANALYSIS

A. Time period and data filtering

The data sets presented in Sect. II have been compiled from Nov 9th, 2010 (ECMWF models with improved surface physics, see above) to December 31st, 2012. From this data set we have extracted a subset to perform a sensitivity analysis and the training of the neural networks. The subset samples one full year from two from April 1st, 2011 to March 31st, 2012 to capture the year cycle. During this period, one day over four is kept for the analysis. For each selected day, the subset only contains one grid point every two in latitude and longitude, reducing the total number of points by a factor of 4. Grid cells with a latitude higher than 75° or lower than -60° or corresponding to water bodies are excluded. Points with frozen soil (soil temperature in the first layer of ECMWF models lower than a threshold of 274 K) or covered by snow (as predicted by ECMWF models) at a given time are also filtered out. The data subset does not include points for which the monthly average wetland fraction is higher than 10%. Regarding the SMOS data, grid cells with a cumulative probability of the presence of RFI higher than 20% or with $T_b$’s lower than 50 K or higher than 400 K are filtered out. Finally grid cells corresponding to sites of the USDA-NRCS SCAN network (USA) are also removed from this subset as these sites will be used to perform independent a posteriori tests of the NN retrieval performance (Sect. VI-D).

The distribution of SM in the filtered subset is relatively uniform from 0 to ~0.5 m$^3$/m$^3$ except for the values close to zero. In contrast there is a small number of points with very
high SM values from 0.53 to 0.8 m³/m³ that correspond to peat soils in the arctic regions during northern summer. Those organic soils with SM values of 0.53-0.8 m³/m³ can de facto be considered as inundated wetlands and the number of these points is less than 1% of the total number of points. Therefore they have been filtered out.

The total number of points in the training subset having simultaneously well defined SMOS \( T_b \)'s for incidence angles from 0 to 60\(^\circ\), ASCAT \( \sigma_{40} \), MODIS NDVI and ECMWF SM\(_1\) is \( \sim 10^5 \). This number increases by a factor of 3.4 if only SMOS incidence angles from 25\(^\circ\) to 60\(^\circ\) are requested as the swath that can be used is wider (Fig. 1).

**B. Sensitivity to soil moisture**

In order to better understand the sensitivity of SMOS \( T_b \)'s and other observables to SM, the filtered data subset has been used to compute Pearson correlations coefficients \( |R| \) of those observables with respect to ECMWF SM\(_1\). Fig. 2 and Table I show the results.

1) **SMOS brightness temperatures:** The correlation of SMOS \( T_b \)'s and ECMWF SM\(_1\) is globally low both for H and V polarization (blue and red circles, respectively). The correlation increases (in absolute value) for V polarization for increasing incidence angles up to \(|R|=0.61\). Fig. 2 also shows the correlations of other quantities derived from SMOS \( T_b \)'s such as the \( T_b \)'s divided by the soil temperature of the first layer of ECMWF model predictions (blue and red crosses for H and V polarizations, respectively), which are an approximation to the soil emissivity. Nevertheless, the correlation with SM is very close to that of the \( T_b \)'s. The correlation of the normalized polarization difference \(((T_b^H - T_b^V) / (T_b^H + T_b^V)), \) black diamonds) shows a positive correlation with SM but the absolute values are not higher than those obtained for the \( T_b \)'s alone. The relatively low correlation coefficients discussed above imply that a careful selection of the best set of SMOS \( T_b \)'s is needed to ensure a good retrieval using neural networks.

2) **Other physical magnitudes:** In addition to SMOS \( T_b \)'s, the correlation of other physical magnitudes with respect to ECMWF SM\(_1\) are shown in Table I. The correlation of the soil temperature and the soil sand and clay fractions with ECMWF SM\(_1\) is lower than 0.5. The clay fraction is positively correlated with SM because water molecules are captured within the clay. The sand fraction is negatively correlated with the SM content in the first few centimeters of soil (where the thermal emission from the Earth detected by SMOS comes from) because sand favors infiltration. In contrast, the correlation of the daily estimate of ASCAT \( \sigma_{40} \) and SM is 0.62 and that of MODIS NDVI with SM is 0.80. This high value is partly due to the high seasonal patterns present both in NDVI and SM in some regions of the globe, as shown for instance by [41].

3) **Local normalization of SMOS \( T_b \)'s:** It is possible to pre-process SMOS \( T_b \)'s to compute a local index (hereafter index \( I_1 \)) by normalizing from 0 to 1 the brightness temperature for each polarization and incidence angle. First, the maximum \( (T_b^{max}) \) and minimum \( (T_b^{min}) \) of the \( T_b \)'s in the time series for a given grid point \((i, j)\) are computed. Then, at a time \( t \), the index \( I_1 \) is computed as follows:

\[
I_1(t, i, j) = \frac{T_b(i, j) - T_b^{min}(i, j)}{T_b^{max}(i, j) - T_b^{min}(i, j)}
\]

(1)

This computation is not a trivial normalization of the brightness temperatures globally because it is done independently for each grid point. Fig. 2 shows the correlation of the index \( I_1 \) with respect to ECMWF SM\(_1\) for each incidence angle (blue and red triangles for H and V polarization, respectively). In contrast to the original \( T_b \)'s, the correlation of \( I_1 \) index with SM is almost independent of the incidence angle with a value of \( \sim -0.4 \).

The index \( I_1 \) can be used to define a new index \( I_2 \) using the SM values at each grid point \((i, j)\) at the time when \( T_b \) reaches its minimum \( SM^{T_b^{min}}(i, j) \) and maximum \( SM^{T_b^{max}}(i, j) \) as follows:

\[
I_2(t, i, j) = SM^{T_b^{min}}(i, j) + [SM^{T_b^{max}}(i, j) - SM^{T_b^{min}}(i, j)] \times I_1(t, i, j)
\]

As \( I_1 \), the index \( I_2 \) is computed for each incidence angle bin and polarization at the time \( t \) of the SMOS acquisition.

The information content of index \( I_2 \) is very strong as it contains a local information on the dynamic ranges of both the measured \( T_b \)'s and the model SM. Fig. 2 shows the

![Fig. 2. Correlation R of H and V brightness temperatures (circles), brightness temperatures divided by the soil temperature (crosses), normalized indexes \( I_1 \) (triangles) and \( I_2 \) (squares) with respect to ECMWF SM\(_1\). Blue symbols correspond to H polarization and red to V polarization. Black diamonds give the correlation for the normalized polarization ratio (see Sect. III).](image-url)
correlation \( R \) of the index \( J_2 \) with respect to ECMWF SM\(_1\) for each incidence angle (blue and red squares for H and V polarization, respectively). Like index \( I_1 \), the correlation of index \( I_2 \) with SM is almost independent of the incidence angle. In contrast, correlation increases up to values of 0.90-0.92. Table I also shows the correlation with ECMWF SM\(_2\) of the locally normalized index \( I_2 \) computed with ASCAT \( \sigma_{40} \) \( (I_2^{\sigma_{40}}) \), which is also very high (0.87).

The definition of indexes \( I_1 \) and \( I_2 \) is inspired by the so-called “change detection” approach used for SM retrieval with ERS and ASCAT scatterometer data [49]. However, one should bear in mind that in the current study the indexes \( I_1 \) and \( I_2 \) are just local normalizations. In contrast, the ASCAT SM retrieval is not a mere scaling between dry and wet soil conditions as done by index \( I_1 \), but also corrects for vegetation effects. In addition, the ASCAT SM retrieval does not use modeled SM data as reference as used for calculating index \( I_2 \). Instead, dry and wet reference values are estimated by analyzing several years of data [35]. Nevertheless, as discussed above, these simple normalization indexes can be used to improve the performances of the NN retrieval (see also Sect. V).

IV. METHOD: NEURAL NETWORKS

Multilayer feedforward neural networks are universal approximators [50] and a very efficient method to find a function linking a set of input data to SM. In particular, the NN approach can exploit the synergy of different instruments due to its truly multivariate nature and its non-linear capacities [51]. It has been shown that the NN is able to exploit complex interactions among the satellite data so that combining a priori the satellite information into the retrieval scheme gives better results than a posteriori combination of individually retrieved products [21].

The feedforward network used in this work has two layers. Many tests were done to determine the optimal architecture, the transfer functions and the minimization algorithms. Above 5-7 neurons in the hidden layer (depending on the dimension of the input vector) the results do not improve anymore and remain constant up to 20 neurons. Using a NN with three layers (two hidden layers) does not improve the results. This is in agreement with Cybenko [52], who showed that a network with a single layer of sigmoid functions can approximate any continuous function. Using a logarithmic-sigmoid function or an hyperbolic tangent sigmoid function (tansig) gives results in perfect agreement. Several minimization algorithms were tested, finding no differences except in computing time, therefore the Levenberg-Marquard algorithm was preferred. The low sensitivity of the results to those parameters is due to the large statistics in the training database, which contains more than 3 \( 10^8 \) vectors. Therefore, the results shown in the following have been obtained with 10 nodes or neurons in the hidden layer and with tansig transfer functions. The second layer is composed of a single node with a linear function. For each neuron in the first layer, the input vector (including a unity element, the bias) is multiplied by a vector of weights using a scalar product. The activation functions associated to each neuron are applied to those scalars. The operation is repeated for the second layer. The vector containing the outputs of the first layer of neurons plus a unity element is again multiplied by a vector of weights and the linear combination is used as the input of the neuron of the second layer constituted of a linear function. Therefore, for an input vector of 8 elements, for instance, a neural network with the former structure will have a total of \( (8+1) \times 10 + (10+1) \times 1 = 101 \) free parameters corresponding to 10 weight vectors of 9 elements and 1 weight vector of 11 elements.

For each input vector containing a combination of SMOS \( T_b \)’s, ASCAT \( \sigma_{40} \), MODIS NDVI and other data, there is an associated target containing a ECMWF SM\(_1\) value. The output of the NN is compared to the target and the weights are adjusted by minimizing a cost function (Mean Squared Error). The minimization has been done by gradient backpropagation with the Levenberg-Marquard algorithm (using the Matlab Neural Network library). The input and the targets have been normalized to fall in the range [-1, 1], as this optimizes the training of the NN.

Data in the period from January 1st, 2012 to December 31st, 2012 have been selected for the training (\( \sim 3 \times 10^6 \) vectors). This data subset has been decomposed randomly in 60 % actually used for the training, 20 % for validation and 20 % for test purposes such as to compute the global correlation of NN outputs with the reference SM (Tables II and III). The validation dataset is used to detect signs of overlearning during the minimization (learning). This occurs when the correlation of retrieved SM and target SM improves for the training dataset but the performances start to degrade on the validation dataset. Actually, no signs of overlearning have been detected as the training data base is composed of a large number of statistically significant data. The minimization has been stopped after 30-50 iterations once the cost function has approached asymptotically a minimum. The effect of the weight initialization on the minimization results has been tested, finding that the effect is negligible.

Once the training is done, more independent tests have been performed using data from a period that has not been used for the NN training (November 2010 to December 2011), or for locations of in situ stations, from November 2010 to December 2012, since as mentioned in Sect. III-A data from these locations have been removed from the training dataset.

V. RESULTS

A. Using SMOS \( T_b \)’s as input

1) Selection of SMOS \( T_b \)’s: As discussed in Sect. III, an appropriate selection of the incidence angles of the SMOS observations is necessary to ensure the best SM retrieval in a fraction of the swath as large as possible. Table II shows a comparison of the SM produced by several NNs applied to ascending orbits data of the test subset (Jan 2012 - Dec 2012) with respect to ECMWF SM\(_1\) using three different metrics: the correlation coefficient (R), the root mean squared difference or “error” (RMSE), and the mean absolute difference or “error” (MAE). The retrieval is better using only H polarization than using only V polarization (see for instance results for NN inversions with 7 \( T_b \)’s in H polarization in the
angle range from 25 to 60° “7Tb H 25-60” and the results for the equivalent model with \( T_h \)'s in V polarization “7Tb V 25-60”). Using a combination of H and V \( T_h \)'s gives better results than using just H or V \( T_h \)'s alone (see for instance the results for NN inversions with 7 \( T_h \)'s in H polarization and 7 \( T_h \)'s in V polarization in the angle range from 25 to 60° “14Tb HV 25-60” and the results for the equivalent model with \( T_h \)'s in V polarization “7Tb H 25-60”), which is logical as the input vector dimension increases by a factor of two. Adding the normalized polarization difference as input (NN 14Tb, 7(V-H)/(H+V)) does not improve the results.

Regarding the incidence angle range, Table II shows the results for SM inversions obtained with different sets of input data. The retrieval performance actually improves from using H and V \( T_h \)'s in the angle range from 25 to 45° (“8Tb HV 25-45”) to 20°-50° (“12Tb HV 20-50”) and 25°-60° (“14Tb HV 25-60”). In contrast, using \( T_h \)'s in the 20°-60° range (16Tbs 20-60) does not improve the quality of the NN SM anymore, while it decreases the width of the swath in which the SM can be obtained (Fig. 1). Therefore, the best set of SMOS \( T_h \)'s to retrieve SM using NNs is composed of 7 \( T_h \)'s for angle bins from 25° to 60° for both H and V polarizations (a total of 14 \( T_h \)'s).

### Table II

<table>
<thead>
<tr>
<th>Input data</th>
<th>R</th>
<th>RMSE</th>
<th>MAE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Using only SMOS brightness temperatures</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>7Tb V 25-60</td>
<td>0.68</td>
<td>0.117</td>
<td>0.093</td>
</tr>
<tr>
<td>7Tb H 25-60</td>
<td>0.71</td>
<td>0.113</td>
<td>0.091</td>
</tr>
<tr>
<td>8Tb HV 25-45</td>
<td>0.74</td>
<td>0.104</td>
<td>0.082</td>
</tr>
<tr>
<td>12Tb HV 20-50</td>
<td>0.76</td>
<td>0.105</td>
<td>0.081</td>
</tr>
<tr>
<td>14Tb HV 25-60</td>
<td>0.80</td>
<td>0.093</td>
<td>0.072</td>
</tr>
<tr>
<td>14Tb HV 25-60, 7(V-H)/(H+V)</td>
<td>0.80</td>
<td>0.093</td>
<td>0.072</td>
</tr>
<tr>
<td>16Tb HV 20-60</td>
<td>0.79</td>
<td>0.097</td>
<td>0.075</td>
</tr>
<tr>
<td>Using soil temperature and texture</td>
<td></td>
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<tr>
<td>14Tb, T</td>
<td>0.83</td>
<td>0.086</td>
<td>0.066</td>
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<tr>
<td>14Tb, tex</td>
<td>0.84</td>
<td>0.084</td>
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<td>0.078</td>
<td>0.059</td>
</tr>
<tr>
<td>14Tb,NDVI, tex</td>
<td>0.89</td>
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<td>0.054</td>
</tr>
<tr>
<td>14Tb,NDVI, T</td>
<td>0.90</td>
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<td>0.052</td>
</tr>
<tr>
<td>Using ASCAT</td>
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<tr>
<td>14Tb,( \sigma_{40} )</td>
<td>0.84</td>
<td>0.085</td>
<td>0.071</td>
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<tr>
<td>14Tb,( \sigma_{40} ),NDVI</td>
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<tr>
<td>14Tb,( \sigma_{40} ), NDVI, tex</td>
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<td>0.066</td>
<td>0.050</td>
</tr>
<tr>
<td>Using local information on extreme Tb's</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>14Tb,14T1</td>
<td>0.83</td>
<td>0.088</td>
<td>0.067</td>
</tr>
<tr>
<td>14Tb,14T1,NDVI</td>
<td>0.88</td>
<td>0.075</td>
<td>0.057</td>
</tr>
<tr>
<td>14Tb,14T1,NDVI, tex</td>
<td>0.90</td>
<td>0.067</td>
<td>0.050</td>
</tr>
</tbody>
</table>

2) Adding additional data as input:

a) Soil temperature and texture: In a first approximation the \( T_h \) is the product of the soil temperature multiplied by the emissivity. Therefore it is interesting to test the effect of adding the soil temperature as one of the input vector elements for the NN. In addition, the emissivity depends on the dielectric constant of the soil, which depends itself on soil texture (and moisture content, of course). Thus, some information on the soil texture, namely the clay and sand fractions, can potentially improve the SM retrieval. Table II shows the performance of the NN retrieval when adding soil temperature and texture information in addition to 7 SMOS \( T_h \)'s for H and V polarization in the angle range from 25° to 60°. The addition of temperature or clay and sand fractions improves the correlation of SM retrieved by NN and ECMWF SM by 4% (\( R \)). Everything together improve \( R \) by 8%. Fig. 3 shows scatter plots of SM retrieved by NN versus ECMWF SM. Interestingly, adding the sand and clay fractions breaks a bi-modality that is present for intermediate SM values in the scatter plot of SM retrieved by a NN with only SMOS \( T_h \)'s as input versus ECMWF SM.

b) Using a vegetation index: In the presence of vegetation, the \( T_h \)'s measured by SMOS will also depend on the vegetation opacity which attenuates soil radiation and depolarizes the soil signal. Therefore, some information on the vegetation estate is a potential valuable input for the NN. On the other hand, as discussed in Sect. III, the correlation of MODIS NDVI (with only two reference dates per month) and SM is actually very high (\( R \sim 0.8 \)), in good agreement with previous studies using other datasets at a monthly scale [22], [24], [41]. This correlation comes from the global close relationship of SM and vegetation at a seasonal scale length, but of course one cannot retrieve accurately the highly changing dynamics of surface SM (at a time scale of a few hours) using just NDVI. In contrast, NDVI helps significantly the retrieval of SM by NN, providing a good “seasonal first guess” while SMOS \( T_h \)'s are instantaneous estimations of the SM content. Table II shows that NDVI actually improves the NN retrieval by 8% (model “14Tb’s, NDVI”). While the retrieval improves by 11% when adding also soil texture and temperature information (model “14Tb, NDVI, tex, T”), reaching a significantly high correlation of \( R = 0.9 \).

c) Effect of adding active microwaves: NN retrievals combining active and passive microwave observations have been tested using ASCAT and SMOS data. Using jointly SMOS and ASCAT for SM retrieval at a daily scale is non-trivial since SMOS and ASCAT do not observe the same point at the same time (Sect. II) and SM can change rapidly at the scale of hours. In the current study, the ASCAT active microwave information has been introduced as a daily averaged value, which could damp the sensitivity to SM variations. In addition this value will be compared to ECMWF SM1, bi-modality that is present for intermediate SM values in the scatter plot of SM retrieved by a NN with only SMOS \( T_h \)'s as input versus ECMWF SM1.

Developing an optimized multi-sensor retrieval is out of the scope of this study, which is mainly devoted to SMOS. However, this relatively simple ASCAT data processing is enough to show that adding active microwaves to the retrieval can improve significantly the results (see Sect. VI-B).
Fig. 3. SM computed by applying the trained NN to ascending orbits data of the test subset (Jan 2012 - Dec 2012) versus ECMWF SM. From top to bottom and from left to right, the scatter plots correspond to NN’s with the following input data: “14Tbs”, “14Tbs, T, tex”, “14Tbs, σ,40, tex, NDVI”, and “14I2, I2,σ,40” (see Sect. V for a detailed description of those NN retrievals). The black dashed line is the 1:1 line and the black solid line is the regression line. The linear regression equation is given in the bottom of each panel.

II shows the results of SM retrievals using SMOS + ASCAT data. Adding ASCAT improves the SM retrieval by 5% ($R$). Adding NDVI and soil clay and sand fractions increase $R$ up to 0.91. In this case, adding the soil temperature to the input vector does not improve the performance of the retrieval [53].

4) Using local information on the $T_b$’s dynamic range:

Table II shows the results of NN retrievals using index $I_1$. Adding this index to the input vector increases the correlation of NN SM and ECMWF SM$_1$ from $R = 0.80$ (model “14Tb’s”) to $R = 0.83$ (model “14Tb’s, $I_1$”). Adding the vegetation index the correlation increases to $R = 0.88$. Adding the soil texture information the correlation increases to $R = 0.90$, which equals the highest value obtained without $I_1$. In this case, adding the soil temperature to the input vector does not add any information. The advantages of a retrieval “14Tb’s,$I_1$, NDVI, tex” with respect to “14Tb’s, NDVI, tex, T” is that it only needs two remote sensing data sets (daily SMOS data and a NDVI estimation every 15 days) and a static texture information. Therefore, once the NN is trained, using model “14Tb, $I_1$, NDVI, tex”, the SM can be retrieved without ECMWF data.

B. Using local information on the $T_b$’s and SM dynamic range

As discussed in Sect. III, local information on the $T_b$’s and SM dynamic range can be used to define the index $I_2$, which becomes the physical magnitude that shows the highest correlation with ECMWF SM$_1$ (Fig. 2). Of course, this is logical as in this case the NN gets as input some information on the SM magnitude that should be retrieved. Since the linear correlations of $I_2$ and SM are very high, it is likely that using $I_2$ the NN does not need as many input elements as the NN using $T_b$’s as input. Actually, even using only one angle bin for the two polarizations (“2$I_2$ HV40-45”), the

<table>
<thead>
<tr>
<th>Input data</th>
<th>$R$</th>
<th>RMSE</th>
<th>MAE</th>
</tr>
</thead>
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<tr>
<td>2$I_2$, HV40-45</td>
<td>0.91</td>
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</tr>
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<tr>
<td>6$I_2$, HV30-45</td>
<td>0.92</td>
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<td>8$I_2$, HV25-45</td>
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</tr>
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<td>10$I_2$, HV25-50</td>
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<td>0.93</td>
<td>0.058</td>
<td>0.042</td>
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Using additional information:

<table>
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<tr>
<th>Input data</th>
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<th>MAE</th>
</tr>
</thead>
<tbody>
<tr>
<td>14$I_2$, $I_2$,σ,40</td>
<td>0.94</td>
<td>0.055</td>
<td>0.040</td>
</tr>
<tr>
<td>14$I_2$, $I_2$,σ,40, NDVI</td>
<td>0.94</td>
<td>0.053</td>
<td>0.038</td>
</tr>
<tr>
<td>8$I_2$, $I_2$,σ,40</td>
<td>0.94</td>
<td>0.055</td>
<td>0.040</td>
</tr>
<tr>
<td>8$I_2$, NDVI</td>
<td>0.94</td>
<td>0.055</td>
<td>0.039</td>
</tr>
<tr>
<td>8$I_2$, NDVI, $I_2$,σ,40</td>
<td>0.94</td>
<td>0.053</td>
<td>0.038</td>
</tr>
</tbody>
</table>
correlation coefficient $R$ obtained applying the trained NN to ascending orbits data of the test subset (Jan 2012 - Dec 2012) is already higher than 0.9 (Table III). In addition, such retrieval methodology would allow to retrieve SM for the whole SMOS swath. Correlation increases when adding more $I_2$ indexes for other angle bins up to four angle bins in the range 25-45° and two polarizations (“$B I_2$ HV25-45°” input). Using more angle bins reduces the RMSE without an increase of $R$. Table III shows the result for two polarizations and 7 angle bins $-14 I_2-$, which is the equivalent configuration to that giving the best results when using $T_b$’s). Using $8 I_2$ and NDVI the retrieval still improves by $\sim 1\%$. The same score ($R=0.94$) is also obtained with “$14 I_2, I_2^{25-45}$”. When using index $I_2$, adding the soil temperature and even the soil texture to the input vector does not add any information with respect to the previous models. This is because, the $I_2$ index contains implicitly this information from the local SM values for the extreme $T_b$’s.

Ideally, computing local extreme $T_b$’s and the associated SM values should be done in a period as long as possible to have robust results. In the present study the extreme values have been computed using 2.5 years of data. The effect of using a shorter period has also been tested. When computing the extreme values using only 1 year of data, the global correlation obtained for a given NN configuration decreases by $\sim 2\%$.

The advantage of using $I_2$ is that it allows to perform good retrievals even with a small number of observables given as input to the NN and that it gives the best results in terms of quality metrics with respect to the reference SM dataset. The disadvantage is that potential errors in the local SM time series extreme values used to compute index $I_2$ will be easily replicated in the NN retrieval. In contrast, when not using any SM information as input to the NN, the non-linear regression done during the NN training makes the NN less sensible to outliers in the reference SM dataset [23].

VI. DISCUSSION

A. Reference NN retrievals: maps

Five of the best NN models have been selected to perform further evaluation of different SM retrievals using NNs. Those retrievals are shown in Table IV. The retrieval NNSM$_1$ uses as input similar information to that used by the SMOS L3 operational algorithm: SMOS $T_b$’s, soil texture and temperature and a vegetation index (NDVI for NNSM$_1$ and LAI for SMOS L3). Retrieval NNSM$_2$ also uses the local normalized $T_b$’s ($I_1$) in addition to SMOS $T_b$’s and NDVI. Retrieval NNSM$_3$ also uses ASCAT data as input. Finally, retrievals NNSM$_4$ and NNSM$_5$ use the change detection approach with SMOS $I_2$ indexes and NDVI (NNSM$_4$) or $I_2^{25-40}$ (NNSM$_5$). In addition, the best retrieval using only SMOS data as input (NNSM$_6$) has also been selected in order to compare its performances with those using the multi-sensor approach.

The Level 3 CATDS SMOS products are divided in ascending (equator overpass at 6 am) and descending (6 pm) half-orbits. The reason is that sources of radio-frequency interference (RFI) are often directional and they affect differently morning and evening overpasses. In addition, the evaluation of SMOS products against in situ measurements has shown different results for morning and evening overpasses (see also Sect. VI-D and references therein). Therefore, in the current study, data from ascending and descending orbits are also processed independently.

The reference NN retrievals have been applied to SMOS data from descending orbits instead of data from ascending orbits as those presented in Tables II and III. The results are shown in Table IV. The NN retrieval quality is comparable (within 1%) to that using ascending orbits.

Fig. 4 shows an example of the retrieval NNSM$_2$ for ascending and descending orbits on August 22, 2011 and the corresponding ECMWF SM$_1$. In addition, the lower panels of Fig. 4 show the monthly average of SM obtained with the retrieval NNSM$_5$ for July 2010 and the corresponding average of ECMWF SM$_1$. The NN retrievals reproduce the main spatial structures of the ECMWF SM$_1$ dataset. The most significant differences in this example are the drier soil predicted by the NN retrieval in western USA, central Asia and Australia. In addition, the NN retrieval predict somewhat wetter soil in the Sahara desert borders.

From the input-data/SM relationship learned globally and over a long time period during the training phase, the NN gives the most likely SM value for a given set of input data [54]. Even if the NN has been trained with ECMWF SM$_1$, the NN output over a given region at a given time does not necessarily equals the ECMWF SM$_1$ value because the retrieval is driven by the remotely sensed data. In the case shown in Fig. 4, taking into account the global input-data/SM relationship learned by the NN, the ECMWF SM$_1$ values in the western USA, central Asia, Australia and the Sahara-border are not the most likely SM values. At least in the USA, the values predicted by the NNSM retrieval can actually be a statistical correction of ECMWF estimates, as other studies have already shown that ECMWF models are on average too wet in the west of the USA [40], [55].

B. Temporal correlation

In order to get further insight on the ability of the neural network with different input data to capture the temporal and spacial variability of the reference ECMWF SM product, it is pertinent to compute temporal ($R_{\text{temp}}$) and spatial correlations ($R_{\text{spa}}$) of the NN products with respect to the SM used as reference. This approach has already been used in previous studies [24].
The temporal correlation is defined as the Pearson correlation of the NN SM and ECMWF SM$_1$ time series of each grid point. $R_{\text{temp}}$ has only been computed if the time series for the whole period of this study contains more than 30 points. Fig. 5 shows maps of $R_{\text{temp}}$ for the different retrievals. First, there exist regions with negative correlation such as the Sahara region. Fig. 6 shows the variance of the ECMWF SM$_1$ time series for each grid point. There are clear similarities between the variance and the $R_{\text{temp}}$ maps, showing that regions with negative $R_{\text{temp}}$ are those where the variance of the local time series is very low. In addition, in this arid region the SM content is also very low. Therefore, the relative uncertainties of the different SM estimations are very high. This makes that when comparing two different SM products over these areas, the correlation is low in absolute value and can even be negative.

It is interesting to note that there are significant differences for the different NNSM retrievals that were not obvious in the global correlations shown in Tables II and III. Table V shows the average $R_{\text{temp}}$ computed for each of the maps in Fig. 5. Both for retrievals using SMOS $T_b$’s or the change detection approach, those with a better ability to capture the temporal dynamics of the ECMWF SM$_1$ data are those that include active microwaves data as input (NNSM$_3$ and NNSM$_5$, respectively). This is in agreement with previous studies that already pointed out the good performance of active microwave data to capture the soil moisture temporal variability [24], [56]. However, it is worth-noting that the passive microwaves ability to capture the temporal variability can be similar to those of active microwaves when using the local normalization of SMOS $T_b$’s (index $I_1$) in addition to the $T_b$’s themselves as input to the NN (retrieval NNSM$_2$, Table. V). Even retrieval NNSM$_6$, using only SMOS $T_b$’s and $I_1$ shows a better ability to capture the temporal variability of SM than retrieval NNSM$_4$. Both NNSM$_2$ and NNSM$_3$ give an average $R_{\text{temp}}$ higher than retrieval NNSM$_4$, which uses the SM change detection approach. Nevertheless, the best $R_{\text{temp}}$ is obtained when using this approach both with active and passive microwaves as input to the NN (SMNN$_5$). With the exception of retrieval NNSM$_1$, the multi-sensor retrievals perform better than the best SMOS-only retrieval by 8-17%.

C. Spatial correlation

In addition to the maps of local temporal correlation, it is interesting to compute time series of global daily correlations, which are sometimes called “spatial” correlations, by computing the Pearson 1-D correlation coefficient comparing the values of two daily SM maps (NN SM and ECMWF SM$_1$) for all grid points. One should bear in mind that these values are not the 2D cross-correlation of the two SM maps but in the following, the “spatial” correlation, $R_{\text{spa}}$, terminology will be used for simplicity.

Fig. 7 shows the time series of spatial or daily correlation of retrievals NNSM$_1$ and NNSM$_5$ with respect to ECMWF
SM₁. Time series of $R_{spa}$ for retrievals NNSM₂ and NNSM₃ are very similar to that of NNSM₁ (and NNSM₄ very similar to NNSM₅) and they are not shown in this figure. Table VI gives the mean $R_{spa}$ for each retrieval as computed from the corresponding time series. The time series of $R_{spa}$ show a seasonal oscillation, with slightly lower values for the months of northern summer. This is because the frozen soil and

snow pack filter keeps more points in this months coming from northern high latitude regions. This imply that NN SM predictions are less consistent with ECMWF SM₁ in these regions (the maps of $R_{temp}$ also show lower values in the northern regions). The typical amplitude of the seasonal oscillation in the $R_{spa}$ time series is $\sim 10\%$ for retrievals NNSM₁₋₃ and $\sim 5\%$ for retrievals NNSM₄₋₅. The mean values of $R_{spa}$ are 0.90-0.91 for retrievals NNSM₁₋₃ and 0.94 for retrievals NNSM₄₋₅. The retrieval NNSM₆, which uses only SMOS data as input, shows an ability to capture the SM spatial variability that is 6-10% lower than that of the multisensor retrievals. All these values are in perfect agreement with the global correlation computed with the test dataset during the training period discussed in Sect. V.

In any case, the $R_{spa}$ time series imply that the NN retrieval is robust as its performances when applied to data not included in the training dataset are comparable to the performances obtained over the training period.

### D. Comparison with in situ measurements

A full validation of SMOS L3 SM, ECMWF SM₁ and NN SM with respect to in situ measurements for a variety of ecosystems, physical conditions, or regions is beyond the scope of this paper. However, it is interesting to compare the different NN retrievals discussed above to in situ measurements. Therefore, the reference NNSM retrievals, SMOS L3 SM and ECMWF SM₁ have been compared to in situ measurements made by the SCAN network of the US Department of Agriculture [57]. This network has already been used to evaluate modeled SM products as well as SM retrievals from remote

![Fig. 5. Maps of temporal correlations for models NNSM 1 to 6 (from top to bottom) applied to SMOS ascending orbits.](image1)

![Fig. 6. Variance of the reference ECMWF SM₁ time series in logarithmic scale.](image2)

<table>
<thead>
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<th>Retrieval</th>
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<th>mean $R_{temp}$ D orbits</th>
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</tr>
<tr>
<td>NNSM₂</td>
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<tr>
<td>NNSM₃</td>
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<td>NNSM₄</td>
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</tr>
<tr>
<td>NNSM₅</td>
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</tr>
<tr>
<td>NNSM₆</td>
<td>0.48</td>
<td>0.53</td>
</tr>
</tbody>
</table>

![Table V](table1)
sensing data (ASCAT, SMOS...), including monthly estimates using NNs [24],[40],[55]. The SCAN data have been obtained from the International Soil Moisture Network [58]. Since L-band radiation is emitted by the first few centimeters under the soil surface [59], the SM products have been compared to in situ SM measurements in the 0-5 cm depth range. A total of 188 time series of in situ measurements have been used to evaluate the SM products. The in situ measurements have been compared with the closest CATDS EASE grid point. The different SM products have been compared at the time of SMOS overpasses. The in situ SM is measured every 30 minutes. Thus, the closest measurement in time to the SMOS overpass has been selected.

Of course, one should keep in mind that in situ sensors make a local measurement that is not necessarily representative of the spatial resolution of the remote sensors or the numerical weather prediction models (tens of kilometers). Some reasons of possible discrepancies are the presence of irrigated areas, water bodies or local precipitations within the SMOS synthesized beam footprint. In addition, the topography or soil texture differences will affect the hydrological processes taking place at the scale of tenths of km, making a single point measurement not representative of the remotely sensed area. However, the large number of SCAN sites allows to do a statistical analysis of the results. In order to have as consistent statistics among the different products as possible, for each time series, it has been used only the times for which all in situ, ECMWF SM1, SMOS L3 SM and NN SM are available. In addition, a minimum number of 30 days per time series has been required to compute statistics. The computation has been done independently for ascending and descending SMOS orbits in the full period of this study (Nov 2010 - Dec 2012). It is important to remind that, as mentioned in Sect. III, the EASE grid points corresponding to SCAN sites have been voluntarily excluded from the training data base for them to be used as testing data.

For each site, the standard deviation of the difference (STDD) of ECMWF SM1, SMOS L3 SM and NNSM with respect to the in situ measurement has been computed. In addition, the Pearson correlation (R) of those products with respect to the in situ SM and the bias (defined as the mean of the difference time series) have also been computed. Finally, the minimum, maximum, mean and median values of all those metrics have been calculated. The results are summarized in Table VII.

The retrieval NNSM1, which uses as input similar information to that used by the SMOS L3 algorithm, shows a correlation with the in situ measurements similar to that of SMOS L3 SM. Both for ascending and descending SMOS orbits, NNSM1 and SMOS L3 SM give the lowest average correlation with the in situ data (0.52 and 0.45-0.48 for ascending and descending orbits, respectively). The correlation is higher for the SMOS-only retrieval NNSM6 that uses index $I_1$ (0.53-0.55) and it increases to 0.59-0.61 for NNSM retrievals that include active microwaves data and/or a SM change detection approach ($I_2$) such as NNSM 2, 4 and 5. Interestingly, the NNSM4 retrieval, which uses locally normalized brightness temperatures ($I_1$), also gives R values of the same order, confirming the interest of this approach that does not include any a priori information on SM to capture the temporal variability of the SM time series (see also Sect. VI-B). ECMWF SM4 also shows a correlation with the in situ measurements of 0.59-0.61 both for ascending and descending orbits.

Regarding the STDD, the highest values are given by the SMOS L3 SM time series (0.06-0.07) followed by ECMWF SM1 ($\sim 0.05$). NNSM 1-3 retrievals present a STDD of 0.04-0.05, and those using the change detection approach NNSM 4-5 present a fairly low STDD of ($\sim 0.03$). Regarding the bias, NNSM retrievals show a positive bias similar to the ECMWF SM1, which is logical as the NNs have been trained with ECMWF data. In contrast, SMOS L3 SM shows a negative bias. The bias values obtained for ECMWF SM1 and SMOS L3 SM are in agreement with previous SM products evaluation studies over the SCAN sites [40],[55] and other USA watersheds [60],[61].

The correlations obtained at the time of SMOS descending overpasses are clearly lower than those for ascending overpasses for all SMOS-based products (NNSM and SMOS L3SM). This is also in agreement with previous studies, which have interpreted this fact as the possible effect of convective rainfall, which occurs during the day affecting potentially differently the local in situ measurement and the $\sim 40$ km remote sensing measurement and decreasing the
correlation for descending overpasses, which take place in the afternoon/evening [62]. However, it is interesting to note that proportionally, the difference in correlation for ascending and descending orbits is lower for NNSM retrievals using the daily \( \sigma_{40} \) estimation from active microwaves (NNSM 2) and for the retrievals using the change detection approach.

In summary, the comparison of the NNSM retrievals to USDA/SCAN in situ measurements shows the good performances of these retrievals. Products NNSM 4 and 5 (using the local extremes of SMOS brightness temperatures and the associated ECMWF SM\(_1\) values) give the best statistics of all the SM products discussed in this study (ECMWF SM\(_1\), SMOS L3, NNSM).

E. Comparison with previous NN retrievals of SM at global scale

The use of NNs to perform a SM retrieval from multi-instrument observations has already been studied using active microwaves (ERS), passive microwaves (SSM/I), NDVI (AVHRR) and skin temperature (ISCCP) as input data [22]–[24]. The NNs were trained with different surface physics models forced with numerical weather prediction models. In all those studies the NN approach was evaluated with monthly averages while the current paper describes a daily retrieval. Nevertheless, it is interesting to compare some results of the current study to those of previous studies since they use the approach proposed by [22] but with different input datasets.

The monthly SM inversion using NNs by [23] and the JULES land surface model show a global correlation \( R \) of 0.92. The SM inversion discussed in the current paper is able to capture the variability of ECMWF model SM in daily basis as it shows a global correlation varying from 0.9 to 0.94 depending on the exact input datasets. On the other hand, the spatial and temporal correlations between the retrieved and the reference monthly SM average found in [24] are 0.81-0.90 and 0.54-0.67, respectively. In the current work, the spatial and temporal correlation in between the daily retrieved SM and the reference one has been found to be 0.90-0.95 and 0.47-0.58, respectively (Tables V and VI). Therefore, the values obtained in the current study for the temporal correlation at daily bases are close to those obtained by [24] using monthly averages.

Finally, the monthly SM estimation by [24] has also been compared to the in situ measurements from the SCAN network obtaining a temporal correlation of -0.07, much lower than that of other SM products like HTESSEL (0.72). In contrast, the daily NNSM retrievals discussed in the current study show a similar temporal correlation to that of ECMWF/HTESSEL (\( \sim 0.60 \), Table VII).

The current study using SMOS and previous studies of global SM retrieval using SSM/I [22]–[24] use the same approach (training a NN to link a multi-sensor input dataset to a reference SM from a land surface model). Therefore, the good temporal and spatial correlation between the NNSM retrievals obtained on a daily basis and ECMWF SM\(_1\) or in situ measurements confirm the strong sensitivity of SMOS to SM compared to the non-dedicated microwave observations used by those previous studies [22]–[24].

VII. SUMMARY AND CONCLUSIONS

A methodology to retrieve soil moisture from multi-instrument observations on daily basis has been presented. The approach is based on a feed-forward neural network using SMOS brightness temperatures (passive microwaves at 1.4 GHz), ASCAT backscattering coefficient (active microwaves at 5.3 GHz), MODIS NDVI and ECOCLIMAP soil texture maps. The neural networks have been trained using ECMWF Integrated Forecast System models, which include soil moisture estimations in the 0-7 cm depth range (ECMWF SM\(_1\)).

The best compromise to retrieve SM from SMOS \( T_b \)'s over a large fraction of the swath (\( \sim 670 \) km) is to use SMOS data in the incidence angle range from 25\(^\circ\) to 60\(^\circ\) (in 7 bins of 5\(^\circ\) width). The global correlation coefficient of the SM retrieved by NN and ECMWF SM\(_1\) is \( \sim 0.9 \) for NN retrievals that, in addition to SMOS \( T_b \)'s, use MODIS NDVI, soil texture and one of the following: (i) ASCAT \( \sigma_{40} \), (ii) ECMWF soil temperature or (iii) 14 normalized \( T_b \)'s computed using the minimum and maximum values of \( T_b \)'s for each incidence angle and polarization at each latitude and longitude grid point.

A change detection approach (defining a local normalization of brightness temperatures using the extreme values and the associated SM) has also been discussed. In this case, soil texture or temperature become irrelevant as the information is implicitly contained in the SM values for the extreme \( T_b \)'s. Using only this approach with SMOS \( T_b \)'s and ASCAT backscattering or NDVI, one can obtain a correlation \( R \) of 0.94 between the SM retrieved by NN and the reference ECMWF SM used as target for the NN learning phase. In addition, one advantage of the change detection approach is that good results can be obtained using SMOS data for a lower number of incidence angles, allowing a retrieval over a larger swath (and hence a better temporal coverage).

It has been shown that the NNs are able to capture the spatial and temporal variability of soil moisture. The temporal variability is better reproduced when using retrievals schemes that include active microwave information or, alternatively, using only passive microwave data that include a local normalization of SMOS brightness temperatures.

When compared to in situ measurements, the NNSM retrievals perform well. Actually, the NNSM retrievals that use a local normalization of the SMOS brightness temperatures and the associated extreme SM values give the best results of all the products evaluated in this study (ECMWF SML1, SMOS L3, NN SM).

We have discussed different strategies to retrieve SM from SMOS observations using NNs that perform very well. The best model would depend on the particular application of the NN retrieval. For instance, for an operational NN algorithm using ASCAT will require access to ASCAT data in real time and in addition this data has to be preprocessed to estimate the backscattering at 40\(^\circ\) incidence angle first, which can put strong constrains on an operational algorithm. In addition, requiring both SMOS and ASCAT observations of the same point reduces the coverage to the intersection of the swaths of the instruments of both satellites. In contrast, MODIS NDVI improves significantly the NN retrieval and it is a very soft
constraint to a real time pipeline as only one NDVI every 15 days is used for the NN retrieval. Adding soil texture improves the results by \(\sim 3\%\), but soil texture is a static information that does not make more complex a real time algorithm. Retrieval schemes using local normalization indexes need a few years of data for the indexes to be significant but they are less dependent on external datasets and they allow to retrieve SM over a larger swath because a lower number of incident angles are required.

Once trained, NNs are a very efficient method to retrieve SM. For instance, using the data filtering discussed in Sect. III, applying the NN to all SMOS ascending orbits in the data base discussed in this paper (with more than 2 years of data) takes \(\sim 150\) seconds on a standard desktop computer. This fact opens exciting perspectives for a near-real-time operational product.

Training NNs with a numerical weather prediction model ensures that the retrieved SM is consistent with the model. However, the NN SM can correct the model accordingly to the remote sensing observations. Therefore, this approach can be the basis for an efficient satellite data assimilation into numerical weather prediction models [22]. Meteorological offices need satellite data no more than 3 hours after sensing to be able to assimilate the observations in a forecasting system. A near-real-time algorithm using NNs such as those discussed in the current study will be able to retrieve SM fast enough to be assimilated into such a system.

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### References


### Table VII

**Comparison with in situ measurements.** The standard deviation of the difference (STDD), correlation coefficient (R) and bias has been computed for all SCAN sites with more than 30 coincident points in the four time series (NNSM, ECMWF, SMOS L3 and in situ). Using these metrics the minimum, mean, median and maximum values have been computed. The results are displayed for NNSM trained on SMOS ascending and descending orbits.

<table>
<thead>
<tr>
<th>SM product</th>
<th>STDD</th>
<th>R</th>
<th>Bias</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Min</td>
<td>Mean</td>
<td>Median</td>
</tr>
<tr>
<td>Ascending orbits</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NNSM1</td>
<td>0.018</td>
<td>0.046</td>
<td>0.043</td>
</tr>
<tr>
<td>NNSM2</td>
<td>0.017</td>
<td>0.049</td>
<td>0.046</td>
</tr>
<tr>
<td>NNSM3</td>
<td>0.013</td>
<td>0.044</td>
<td>0.041</td>
</tr>
<tr>
<td>NNSM4</td>
<td>0.006</td>
<td>0.029</td>
<td>0.026</td>
</tr>
<tr>
<td>NNSM5</td>
<td>0.005</td>
<td>0.027</td>
<td>0.023</td>
</tr>
<tr>
<td>NNSM6</td>
<td>0.025</td>
<td>0.055</td>
<td>0.056</td>
</tr>
<tr>
<td>ECMWF SM1</td>
<td>0.012</td>
<td>0.049</td>
<td>0.045</td>
</tr>
<tr>
<td>SMOS L3</td>
<td>0.027</td>
<td>0.060</td>
<td>0.059</td>
</tr>
</tbody>
</table>

| Descending orbits |      |      |      |     |      |      |      |     |
| NNSM1      | 0.019 | 0.045 | 0.041 | 0.097 | -0.12 | 0.45 | 0.47 | 0.92 | -0.096 | 0.070 | 0.061 | 0.30 |
| NNSM2      | 0.011 | 0.046 | 0.044 | 0.089 | -0.41 | 0.59 | 0.69 | 0.95 | -0.071 | 0.071 | 0.065 | 0.31 |
| NNSM3      | 0.014 | 0.043 | 0.038 | 0.084 | -0.17 | 0.56 | 0.63 | 0.93 | -0.074 | 0.063 | 0.059 | 0.30 |
| NNSM4      | 0.004 | 0.033 | 0.028 | 0.094 | -0.22 | 0.59 | 0.69 | 0.96 | -0.123 | 0.056 | 0.036 | 0.38 |
| NNSM5      | 0.003 | 0.032 | 0.026 | 0.100 | -0.18 | 0.59 | 0.66 | 0.95 | -0.138 | 0.057 | 0.041 | 0.39 |
| NNSM6      | 0.022 | 0.051 | 0.050 | 0.098 | -0.17 | 0.53 | 0.63 | 0.90 | -0.079 | 0.076 | 0.073 | 0.29 |
| ECMWF SM1  | 0.011 | 0.053 | 0.056 | 0.129 | 0.01 | 0.61 | 0.66 | 0.89 | -0.138 | 0.061 | 0.046 | 0.38 |
| SMOS L3    | 0.024 | 0.068 | 0.065 | 0.148 | -0.41 | 0.48 | 0.55 | 0.94 | -0.259 | -0.051 | -0.051 | 0.13 |


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Jana Kolassa, photograph and biography not available at the time of publication.

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