SOIL MOISTURE RETRIEVAL USING IN SITU AND DATA SIMULATION REGULARIZED DEEP LEARNING MODELS

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ABSTRACT

Retrieval of Surface Soil Moisture (SSM) over large scales at high spatial resolution is crucial for numerous applications. Existing solutions rely on the analysis of remote sensing platforms or in situ measurements that are either too coarse in their resolution or too localized to address the aforementioned need. In this work, we propose a novel deep learning approach for reliably estimating SSM at a high spatial resolution of 1 km over broad regions. To achieve this objective, the proposed framework employs a Convolutional Neural Network that can capture both multi-modal and spatial correlations. Introducing a novel loss function, the proposed scheme can leverage limited in situ observations while also generating estimates consistent with physical models. This is achieved through the utilization of coarse-resolution data assimilation estimates. For training and assessing the performance of the proposed framework, a novel dataset is generated by combining information from remote sensing, in situ measurements, and data assimilation estimates. Experimental analysis demonstrates that the proposed approach can provide accurate retrieval of SSM, significantly outperforming existing products.

***Index Terms*—** deep learning, soil moisture, data assimilation

1. INTRODUCTION

Residing at the land-atmospheric boundary, surface soil moisture (SSM), i.e., volumetric water content at the top 5 cm of soil, has a profound effect on Earth's water and energy cycles, playing a critical role in weather prediction and climate modeling [1]. Therefore, estimation of SSM at a high spatial and temporal resolution on a global scale is fundamental for understanding hydrometeorological water and energy flux processes [2]. To achieve a reliable estimation of SSM, three main sources of data are available, namely, observations from *remote sensing* platforms, measurements from *in situ* sensor networks, and estimates generated by physics-driven *data assimilation* processes [3, 4].

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In the case of remote sensing, several platforms, including the ASCAT, AMSR-E, SMOS, and SMAP, have been considered for SSM retrieval [3]. In such instances, observations undergo processing through various algorithms to extract the desired physical variables from raw observations. This process often relies on specific models, such as the tau-omega radiative transfer model, particularly in the context of microwave brightness temperature observations [5]. Unlike remote sensing methods, in situ sensor networks such as ISMN [6] can deliver precise retrievals with exceptionally high temporal resolution. Nevertheless, these in situ observations are highly localized. Finally, measurements are integrated with physical laws, such as the governing equations for soil water flow, to estimate SSM on a global scale through data assimilation processes [7, 8]. Despite the potential of data assimilation models, the accuracy of estimations is constrained by the quality of the forcing data and the parameterization of physical rules, which may be incorrect, while also suffering from coarse resolution estimations [9].

Although application-dependent, a spatial resolution of 10 km and a temporal resolution of 2 to 3 days has been considered adequate for tasks like resolving hydro-meteorological water and energy flux processes at global scales. While the retrieval of SSM at a broader scale is valuable, regional and local studies, particularly those addressing agricultural crop yield prediction and intelligent irrigation management, necessitate SSM estimation at a resolution of at least 1 km or finer. This accommodates the specific spatial characteristics of each region [10, 11].

In this paper, we present a novel SSM retrieval approach, capable of producing high spatial resolution retrievals, by integrating all three sources of data, namely in situ, remote sensing, and data assimilation. The proposed approach is based on the introduction of Deep Learning and more specifically, Convolutional Neural Networks (CNNs) which can seamlessly encode both spatial and inter-modality correlations. A significant innovation in this study is the introduction of a composite loss function, which effectively accounts for the disparity between localized in situ measurements and coarse-resolution data assimilation estimates. To train and validate the proposed approach, we produced a new analysis-ready dataset that integrates observation from remote sensing platforms, specifically from the SMAP radiometer, and Sentinel 1 radar, in situ observations from ISMN, data assimilation estimates, and ancillary data, co-registered and re-mapped to 1 km EASE-Grid 2 resolution for June of 2017, 2018, and 2019.

2. STATE-OF-THE-ART

Recently, a new paradigm in remote sensing observation analysis considers data-driven approaches based on machine learning models for the retrieval of various geophysical characteristics, ranging from land cover and surface temperature to water quality, among others [12]. Successful paradigms extensively applied for remote sensing-based SSM retrieval encompass methodologies like random forests (RF), support vector regression (SVM), and artificial neural networks [13, 14].

In recent years, the field of machine learning has been taken by storm by a class of methods based on recent advancements in neural networks collectively known as Deep Learning. Deep Learning methods were explored for retrieving SSM from SMAP observations [15] to quantify the ability to extend the availability of estimations beyond the platform's operational lifetime. To capture the information encoded in time series, Long Short-Term Memory networks were explored for SSM estimation using SMAP and MODIS observations [16].

CNNs represent a distinct departure from traditional machine learning approaches for SSM. Unlike methods that solely consider independent spatial locations for retrieval, CNNs retain and leverage information encoded in spatial correlations. CNNs were utilized for SSM retrieval from the AMSR-E brightness temperature measurements which were trained to predict the SSM estimated from the European Centre for Medium-range Weather Forecasts (ECMWF) model in [17]. CNNs were recently considered in [18] for SMAP downscaling, which was found to perform better compared to SVMs and RFs. A successful CNN architecture called ResNet was considered in [19] where it was found to achieve higher retrieval accuracy compared to random forests.

A CNN was employed for downscaling SMAP radiometer brightness temperature measurements, focusing only on the period when both SMAP radar and radiometer were operational [20]. In [21], a CNN model was proposed for SSM estimation from SMAP, however, this model did not assume the availability of in situ observations or observations from multiple satellite platforms. This work was extended in [22] to include both SMAP and Sentinel 1 observations. In [23], a Generative adversarial network was introduced in conjunction with a physics-based tau-omega model for retrieval.

3. PROPOSED APPROACH

Our modeling framework considers three data sources, namely in situ, remote sensing, and data assimilation generated data. The primary objective of the proposed SSM retrieval scheme is to establish a mapping from remote sensing observations to surface-level soil moisture values. This mapping aims to ensure that the estimated values align with both in situ observations and data assimilation estimates. Fig. 1 provides a high level block diagram of the proposed framework.

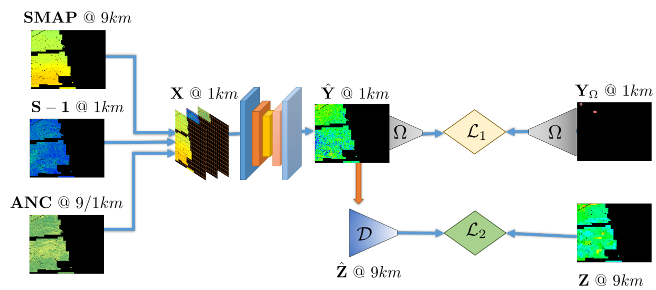

Fig. 1. Block diagram of the proposed framework: Remote sensing observations from SMAP at 9 km, Sentinel 1 at 1 km, and ancillary measurements are incorporated into the CNN model. The model initially produces high spatial resolution SSM estimations and subsequently generates a lower-resolution version.

To formulate the problem within a learning framework, it is essential to establish the concepts of training/validation examples that will be presented to the machine learning system. Given the input $\mathcal{X} \in \mathbf{R}^{m \times m \times k}$, the objective of the proposed approach is to predict $\mathbf{Y} \in \mathbf{R}^{m \times m}$ where m corresponds to spatial indexing and k to the dimensionality of the input signal. Effectively, for a given target resolution, each spatial location i, j, corresponds to a grid cell of fixed spatial resolution. Nevertheless, $\mathbf{Y}$, the actual SSM for every location on a 1 km grid within a specific region is not accessible, neither during the training nor the validation phases.

To address the lack of proper ground-truth target values, we consider two different sources of data as reliable proxies to these values, namely the measurements from the in situ sensors at 1 km, denoted by S_Ω, and estimations derived from the data assimilation platform denoted by $\mathbf{Z} \in \mathbf{R}^{n \times n}$, where n is the index at the coarse resolution. Given that the spatial resolution of data assimilation models is significantly lower than the target resolution, for the sample region, $n \leq m$.

In the ideal case, the objective is to use training data to produce a function $f(\mathbf{w}) : \mathcal{X} \xrightarrow{\mathbf{Y}}$, where $\mathbf{w}$ are the weights of the CNN. To obtain a reliable mechanism for translating remote sensing observations to geophysical values, the parameters $\mathbf{w}$ of the CNN model f must be estimated. This is achieved by minimizing the error between estimated and measured (in situ) SSM values and is encoded in the function

$$\mathcal{L}_1 = \|P_\Omega(\hat{Y}) - P_\Omega(S)\|_2^2 \quad (1)$$

where $P_\Omega(\cdot)$ is the sampling operator which only retains the values at locations where in situ measurements are available.

In addition to minimizing $\mathcal{L}_1$ which focuses on high quality estimation using point-like ground-truth, we also introduce $\mathcal{L}_2$ to match the predicted SSM at image-level, but at a courser-resolution of 9 km, to the estimated SSM in the L2 product:

$$\mathcal{L}_2 = \|\mathbf{Z} - \mathcal{D}(f(\mathbf{X}; \mathbf{w}))\|_2^2, \quad (2)$$

where $\mathcal{D}$ is a downsampling operator responsible for generating a coarse resolution estimation of $\mathbf{Y}$. More specifically, the spatial subsampling operator $\mathcal{D}$ corresponds to filtering the high resolution estimated SM with a low-pass filter to remove high frequency components before applying spatial subsampling through an average pooling operation.

Combining the loss functions in Equations 1 and 2, a novel composite loss function can be created. In this case, the objective is expressed as

$$\min_{\theta} \mathcal{L}(\mathbf{w}) = \min_{\mathbf{w}} \big(\mathcal{L}_1(\mathbf{w}) + \alpha \mathcal{L}_2(\mathbf{w})\big), \quad (3)$$

where α is a regularization parameter controlling the impact of data assimilation versus in situ measurements. In our experiments α was set to 10^{-3}.

To achieve the sought-out objective, we designed a deep neural network for the specific task. The proposed network is 31-layer CNNs with 53.000 parameters. The architecture is similar to a U-Net architecture, featuring an encoding and a decoding part. The architecture is segmented into blocks of 3D convolutions, each followed by pooling for downsampling, and subsequent upsampling layers. Input corresponds to 3D image patches of size $256 \times 256 \times 13$ at high resolution (1 km) while two outputs are produced both of size 256×256, the first one corresponding to high spatial resolution output (1 km) and the second to the coarse resolution (9 km).

4. EXPERIMENTAL ANALYSIS

4.1. Data sources

To train and validate the proposed approach, we generated a first-of-its-kind analysis-ready dataset for remote-sensing soil moisture estimation. The data sources used in our analysis include active and passive microwave remote sensing observations, ancillary data, and in situ measurements. Specifically,

- Coarse-resolution (9 km) brightness temperature T_B observations at horizontal and vertical polarization from the NASA SMAP L-band radiometer (1 km or better)
- Fine-resolution (1 km) SAR backscatter (sigma-0) imagery at horizontal and vertical polarization from the ESA C-band Sentinel-1A/B satellites.
- In situ observations from the U.S. Climate Reference Network (USCRN) and the SNOTEL network that are part of the ISMN network, comprising a set of 114 and 415 sensors, respectively, distributed across the Continental United States (CONUS).
- Data assimilation products, specifically, the SMAP L4 Surface and Root Zone Soil Moisture Geophysical Data product (SMAP_L4_SM) [1]. The algorithm employs an ensemble Kalman filter to integrate SMAP 9 km downscaled brightness temperature observations with SM estimates from a customized version of the NASA Goddard Earth Observing System (V5) Land Data Assimilation System (LDAS).
- Ancillary observations, and more specifically: land surface temperature from the NASA GEOS-5; vegetation water content from MODIS; clay fraction and bulk density from SoilGrid; land cover type from the MODIS IGBP product; elevation from the SRTM product; and precipitation from the GPM mission.

4.2. Satellite derived SSM product

The baseline model for SSM retrieval is the 9 km SMAP L2 product produced by the Backus-Gilbert optimal interpolation scheme. In addition to the baseline model, we also consider the high resolution enhanced L2 product which combines the SMAP L-band radiometer data with Sentinel-1 C-band radar data [24]. This product contains calibrated, geolocated, time-ordered brightness temperature during 6:00 a.m. descending (and 6:00 p.m. ascending) half-orbit passes and Sentinel 1 C-band backscatter coefficients, transformed to sigma-naught (σ_0) values, at a spatial resolution of 1 km.

4.3. Experimental results

We consider observations from CONUS and focus on June 2017, 2018, and 2019. All datasets are georeferenced at the same 1 km EASE-2 grid. We consider locations where a valid measurement is available, either from a single sensor or the average value from multiple sensors, and use this value as the expected value for this location (1km grid cell).

To quantify the performance, the entire dataset was split into training and validation sets. To produce the training set, 70% of the sensors were used as training examples, while the remaining 30% were employed for validation. To quantify the performance, we employ the unbiased Root-Mean-Squared Error (ubRMSE) metric.

Fig. 2 presents the evolution of SSM retrieval error as a function of the training epoch of the proposed CNN, while

[1]Reichle, R., G. De Lannoy, R. D. Koster, W. T. Crow, J. S. Kimball, and Q. Liu. 2021. SMAP L4 Global 3-hourly 9 km EASE-Grid Surface and Root Zone Soil Moisture Analysis Update, Version 6. Global. Boulder, Colorado USA. NASA National Snow and Ice Data Center Distributed Active Archive Center. doi: https://doi.org/10.5067/6P2EV47VMYPC. 11/2021.

also including the retrieval error for the enhanced SMAP L2 product which incorporates Sentinel 1 observations at 1 km. Note that this error is measured with respect to the values acquired by the specific set of in-situ sensors (and not cal/val sites that are employed in SMAP). The figure demonstrates that the proposed approach outperforms the existing SMAP product by a large margin both for the case of training and validation datasets, although effects of overfitting are present in the model. Furthermore, the results also indicate that the proposed approach does not suffer from bias, unlike the case of the SMAP product.

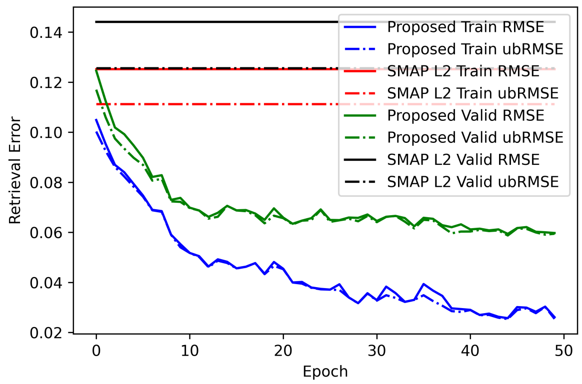

Fig. 2. Retrieval error (RMSE and ubRMSE) for the proposed model as a function of training epoch. The enhanced SMAP/Sentinel 1 L2 product at 1 km is also included for reference.

Fig. 3 provides an illustrative visualization of the derived SSM for a region in North Dakota, USA (46°46’01”N, 100°55’01”W). The figure presents the inputs (top left SMAP brightness temperature, top right Sentinel 1 backscatter), and retrieval at 1 km (middle left SMAP, middle right proposed) and at 9 km (bottom left SMAP, bottom right proposed). One can note the coarse band of higher SSM values in the coarse SMAP product in contrast to the smooth transition in the case of the proposed scheme.

Finally, in Fig. 4, a scatter plot comparing the retrieved and measured (from in situ) SSM values is depicted for both the training and validation sets. The outcomes suggest that the proposed scheme exhibits exceptional performance with the training data. However, for the validation data, some performance degradation is noticeable, although it is considerably less compared to the SMAP L2 product, which is characterized by substantial underestimation.

5. CONCLUSIONS

We demonstrated how utilizing coarse-resolution products generated by physics-driven data assimilation models and in-situ measurements from ground-based sensor networks can be efficiently integrated under a deep learning framework for soil moisture retrieval. Note that although the focus on soil moisture retrieval, the proposed framework can be readily applied for the retrieval of other climate variables like land surface temperature.

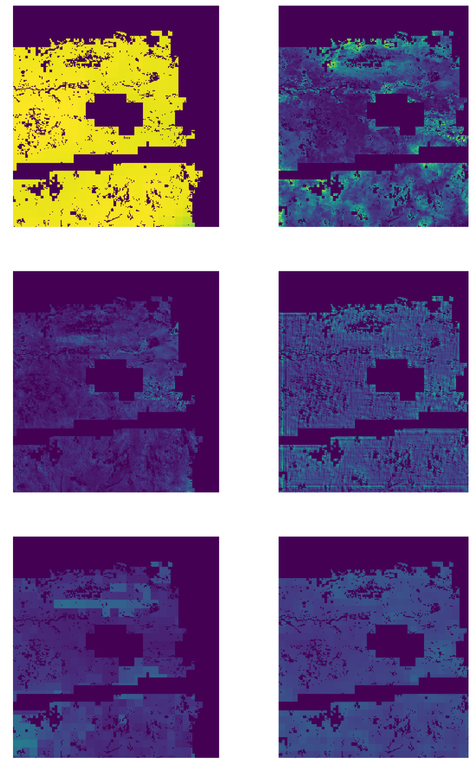

Fig. 3. Visualization of input data (top row), SSM estimates at fine resolution (middle row), and SSM estimates at coarse resolution (bottom row).

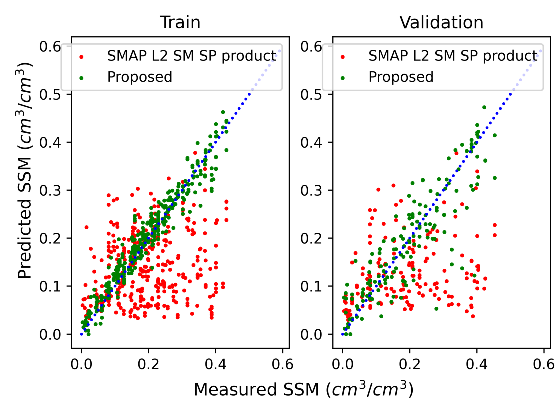

Fig. 4. Scatter plot of retrieval SSM against in situ measurements for the proposed and the SMAP L2 product.

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