

A machine learning-based geostatistical downscaling method for coarse-resolution soil moisture products

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Abstract

The land Surface Soil Moisture (SSM) products derived from microwave remote sensing have a coarse spatial resolution, therefore downscaling is required to obtain accurate SSM at high spatial resolution. An effective way to handle the stratified heterogeneity is to model for various stratifications, however the number of samples is often limited under each stratification, influencing the downscaling accuracy. In this study, a machine learning-based geostatistical model, which combines various ancillary information at fine spatial scale, is developed for spatial downscaling. The proposed support vector area-to-area regression kriging (SVATARK) model incorporates support vector regression and area-to-area kriging by considering the nonlinear relationships among variables for various stratifications. SVATARK also considers the change of support problem in the downscaling interpolation process as well as for solving the small sample size in trend prediction. The SVATARK method is evaluated in the Naqu region on the Tibetan Plateau, China to downscale the European Space Agency's (ESA) 25-km-resolution SSM product. The 1-km-resolution SSM predictions have been produced every 8 days over a six-year period (2010-2015). Compared with other two methods, the downscaled predictions from the SVATARK method performs the best with in-situ observations, resulting in a 23.6 percent reduction in root mean square error and a 10.7 percent increase in correlation coefficient, on average. Additionally, anomalously low SSM values, an indicator of drought, had a record low anomaly in mid-July for 2015, as noted by previous studies, indicating that SVATARK could be utilized for drought monitoring.

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Abstract: The land Surface Soil Moisture (SSM) products derived from microwave remote sensing have a coarse spatial resolution, therefore downscaling is required to obtain accurate SSM at high spatial resolution. An effective way to handle the stratified heterogeneity is to model for various stratifications, however the number of samples is often limited under each stratification, influencing the downscaling accuracy. In this study, a machine learning-based geostatistical model, which combines various ancillary information at fine spatial scale, is developed for spatial downscaling. The proposed support vector area-to-area regression kriging (SVATARK) model incorporates support vector regression and area-to-area kriging by considering the nonlinear relationships among variables for various stratifications. SVATARK also considers the change of support problem in the downscaling interpolation process as well as for solving the small sample size in trend prediction. The SVATARK method is evaluated in the Naqu region on the Tibetan Plateau, China to downscale the European Space Agency’s (ESA) 25-km-resolution SSM product. The 1-km-resolution SSM predictions have been produced every 8 days over a six-year period (2010-2015). Compared with other two methods, the downscaled predictions from the SVATARK method performs the best with in-situ observations, resulting in a 23.6 percent reduction in root mean square error and a 10.7 percent increase in correlation coefficient, on average. Additionally, anomalously low SSM values, an indicator of drought, had a record low anomaly in mid-July for 2015, as noted by previous studies, indicating that SVATARK could be utilized for drought monitoring.

Key Words: Downscaling, Support vector regression, Area-to-area kriging, Soil moisture

1 Introduction

Land surface soil moisture (SSM) is an essential hydro-ecological parameter for monitoring energy, water, and carbon cycles (Seneviratne et al., 2010; Bateni and Entekhabi, 2012). Continuous SSM at fine spatial resolutions provides crucial information for hydrological models, precipitation forecasting models, land-atmosphere models, drought and flood forecasting, and vegetation growth monitoring (Krishnan et al., 2006; Wang et al., 2016; Dorigo et al., 2017). In general, soil moisture is acquired by using in-situ measurements (Dobriyal et al., 2012), including wireless sensor networks (Kerkez et al., 2012) and Cosmic-ray Soil Moisture Observing System (Zreda et al., 2012), which have helped overcome the sparse sampling and poor dynamic limitations of traditional in-situ methods. These ground-based measurements methods require continuous financial support and suitable ground conditions and are limited to small monitoring areas. With the development of active and passive microwave remote sensing techniques (Petropoulos et al., 2015), it becomes possible and more convenient to acquire SSM information dynamically at different spatiotemporal resolutions over large areas. A series of SSM products derived from various satellite-based microwave sensors has been released (Njoku et al., 2003; Parinussa et al., 2014; Meissner et al., 2018). However, with spatial resolutions of tens of kilometers, the current microwave-based SSM products are limited to large-scale monitoring applications.

Many approaches have been developed for downscaling these coarse scale SSM products. Some of these benefit from ancillary information that captures the variations of SSM at fine resolution, combined with correlated variables (Ge et al., 2019). There are two main sources of ancillary variables: active microwave data and visible/infrared data. Change detection based downscaling algorithms (Piles et al., 2009; van der Velde et al., 2015) and Bayesian merging methods (Zhan et al., 2006; Wu et al., 2017) have been proposed to downscale the coarse SSM by using active microwave data. The active microwave technique is highly sensitive to SSM and can even penetrate clouds, however it is greatly affected by soil roughness and vegetation. An

alternative downscaling approach is to use fine resolution optical/thermal data. A number of downscaling algorithms have been developed to generate fine-resolution SSM, such as Disaggregation based on Physical And Theoretical scale Change (Merlin et al., 2015; Malbêteau et al., 2016), trapezoid-based methods (Yang et al., 2015; Babaeian et al., 2018), regression-based approaches (Duan et al., 2016; Liu et al., 2018) and geostatistical methods (Mukherjee, 2015; Jin et al., 2018). For downscaling with optical/thermal data, the statistical correlation between SSM and ancillary variables or physically based models have been explored (Peng et al., 2017).

Chauhan et al. (2003) proposed an empirical polynomial fitting downscaling approach using a polynomial regression at coarse spatial resolution to obtain the fine-spatial-resolution SSM. Since then, further polynomial fitting downscaling methods have been presented by employing multiple data sources or different ancillary parameters (Piles et al., 2014; Knipper et al., 2017), such as land surface temperature (LST), vegetation information, brightness temperature, albedo, evapotranspiration and terrain indices. Meanwhile, geographically weighted regression, which takes into consideration local characteristics (Song et al., 2019), and machine learning algorithms have been introduced into downscaling. Machine learning algorithms such as random forest and support vector regression (SVR) perform better in capturing the nonlinear relationships among variables and have been widely applied to downscaling SSM (Zhao et al., 2018; Abbaszadeh et al., 2019). Some studies directly combined the fine-resolution trend and coarse-resolution residual to predict the fine-resolution SSM (Im et al., 2016; Wei et al., 2019). Interpolation techniques such as bilinear interpolation and kriging interpolation have been generally used in residual analysis for approximating the actual fluctuations (Song and Jia, 2016; Chen et al., 2019). Geostatistical methods with a focus on the spatial correlation between variables have been increasingly applied in downscaling (Kaheil et al., 2008; Djamai et al., 2016). However, these downscaling approaches ignore the change in supports before and after downscaling. Due to the stratified heterogeneity in geographical variables, downscaling models for various stratifications established in the scaling process (Ge et al., 2019) are limited to the smaller samples captured by the model. The SVR approach, benefiting from its high generalization ability, could provide a solution to the small sample size problem (Srivastava et al., 2013).

Considering all the previous machine learning algorithms, this paper proposes a new machine learning-based geostatistical model that integrates SVR and area-to-area kriging (ATAK) to achieve spatial downscaling by fusing various ancillary variables. The proposed support vector area-to-area regression kriging (SVATARK) can tackle the modifiable areal unit problem, as well as model the complex nonlinear relationship among variables in the downscaling process. The downscaling approach was employed to predict 1-km-resolution SSM data by downscaling ESA's 25-km-resolution SSM product, Climate Change Initiative (CCI), with consideration of land cover types. Downscaled SSM predictions were produced every eight days over the Naqu region in the central Tibetan Plateau (TP), and were evaluated using in-situ SSM measurements. A comparison of the SSM residuals obtained from the ATAK method versus the residuals from bilinear interpolation and kriging interpolation indicated advantages of the SVATARK downscaling approach.

The remainder of the paper is organized as follows. Section 2 describes the downscaling methodology, including the downscaling strategy during the experiment. Both the study area and the data sets are introduced in Section 3. Section 4 validates the downscaled predictions and discusses the comparison results. Finally, some conclusions are summarized in Section 5.

2 Methodology

The proposed SVATARK downscaling method mainly consists of both trend and residual models. In this section, we briefly describe the downscaling model components SVR and ATAK and the experimental downscaling scheme.

2.1 Support vector regression method

Support vector machines (SVMs) have been widely applied to classification and regression, which minimize both empirical risk and structural risk to seek the best compromise between the complexity and learning capability of a model (Srivastava et al., 2013; Sujay and Deka, 2014). For regression, SVR was first introduced by Vapnik et al. (1997). Let $\chi = \{x_i, y_i; i = 1, \dots, n\}$ be the training dataset with ancillary vectors x_i and corresponding targets y_i . The input space χ can be mapped into some feature space Φ using the nonlinear function $\varphi = \chi \rightarrow \Phi$. In the feature space Φ , the training data may exhibit linearity, which can be approximated by linear regression. The general form of the nonlinear SVR function can be expressed as:

$$\overline{f(\omega, b) = \omega \bullet \varphi(x) + b}, \quad (1)$$

where ω and b are the parameter vectors. The kernel function $K(x_i, x_j) = \langle \varphi(x_i) \bullet \varphi(x_j) \rangle$ can be used to calculate the inner products in the feature space Φ . By introducing α_i and α_i in the dual form to solve the optimization problem in SVR, the regression function of the nonlinear SVR allowing the kernel function is expressed as:

$$\overline{f(x_i) = \sum_{k=1}^n (\alpha_k - \alpha_k) K(x_i, x_k) + b}. \quad (2)$$

More details about the nonlinear SVR can be found in Smola and Schölkopf (2004). It is well known that the kernel function and its hyper-parameters have a great impact on the performance of nonlinear SVR model. In our study, ε -SVR is used with the Gaussian radial basis function as its kernel function. The relevant penalty coefficient and gamma can be optimized by minimizing the model error. The SVR was implemented in R “e1071” package (Meyer et al., 2015). Owing to the stratified heterogeneity, the SVR models are established for different land cover types, considering that different underlying surfaces might influence the relationship among SSM and ancillary variables.

2.2 Area-to-area kriging method

The area-to-area kriging is a case of areal interpolation, which changes the supports before and after the interpolation (Kyriakidis, 2004). A linear combination of areal data is used to predict other areal values. The target areal value z over a given unit u_α is estimated with the K neighboring observations at units u_i :

$$\overline{z(u_\alpha) = \sum_{i=1}^K \lambda_i(u_\alpha) \bullet z(u_i)}, \quad (3)$$

where $\lambda_i(u_\alpha)$ is the weight assigned to $z(u_i)$, which can be calculated by minimizing the prediction error variance. The corresponding kriging system is written as:

$$\overline{\begin{cases} \sum_{j=1}^K \lambda_j(u_\alpha) \bullet \overline{C}(u_i, u_j) + \mu(u_\alpha) = \overline{C}(u_i, u_\alpha), & i = 1, \dots, K \\ \sum_{j=1}^K \lambda_j(u_\alpha) = 1 \end{cases}}, \quad (4)$$

where $\mu(u_\alpha)$ is the Lagrange multiplier, $\overline{C}(u_i, u_j)$ and $\overline{C}(u_i, u_\alpha)$ are block-to-block covariance terms. The most important step for the implementation of ATAK is to obtain the point support covariance for deriving the covariance terms. A deconvolution procedure can be used to achieve the point support covariance Goovaerts (2008). In our study, 25 neighboring pixels were employed to predict the target area of ATAK.

2.3 Support vector area-to-area regression kriging

The proposed SVATARK is based on SVR for trend prediction and ATAK for residual prediction. Let $Z(S_i)$ and $X_k(S_i)$ be the target and k ancillary random variables at coarse pixel S_i . The nonlinear regression model between $Z(S_i)$ and $X_k(S_i)$ can be obtained using Equation (2), denoted by $f_{\text{SVR}}(\bullet)$. Assuming that the statistical relationship among variables is scale-invariant, the trend component of the fine spatial resolution can be estimated by using the coarse regression function:

$$\overline{m(s_j) = f_{\text{SVR}}(x_k(s_j))}, \quad (5)$$

where $x_k(s_j)$ represent k ancillary variables of fine pixels s_j .

The residual component of the fine spatial resolution is estimated using Equation (3), interpolating the coarse residual with I neighboring coarse pixels $e(S_i)$:

$$\begin{aligned} e(s_j) &= \sum_{i=1}^I \lambda_i(s_j) \bullet e(S_i) \\ &= \sum_{i=1}^I \lambda_i(s_j) \bullet [Z(S_i) - f_{\text{SVR}}(X_k(S_i))], \end{aligned} \quad (6)$$

where $\lambda_i(s_j)$ are the weights assigned to I neighboring coarse pixels for the prediction at fine resolution.

Combining Equations (5) and (6), the SVATARK downscaling model prediction $z(s_j)$ can be expressed as:

$$\begin{aligned} z(s_j) &= m(s_j) + e(s_j) \\ &= f_{\text{SVR}}(x_k(s_j)) + \\ &\quad \sum_{i=1}^I \lambda_i(s_j) \bullet [Z(S_i) - f_{\text{SVR}}(X_k(S_i))]. \end{aligned} \quad (7)$$

2.4 Downscaling strategy

LST, Normalized Difference Vegetation Index (NDVI), land cover (LC), Blue Sky Albedo (BSA), Digital Elevation Model (DEM), aspect and slope were used as ancillary variables to downscale the CCI SSM product over thirty-six months (during May to October, 2010-2015). Considering the relatively low coverage of daily remotely-sensed observations, the 8-day composites of all variables were employed by using average aggregation to maintain stability and representativeness of each variable. A spatial-temporal prediction method (Gerber et al., 2018) was adopted to replace the missing values for LST and BSA due to cloud cover. Prior to performing the downscaling algorithm, a bias correction step (Djamai et al., 2016) was used for remotely-sensed SSM data to reduce the influence of the original SSM product. The downscaling procedure is shown in Figure 1, including the downscaling and validation processes.

After all data processing steps, including resampling aggregation, gap filling and bias correction, the 25-km and 1-km variables with full spatial coverage for each 8-day period was achieved, as well as the 8-day in-situ measurements within $1 \text{ km} \times 1 \text{ km}$ grids. Three downscaling methods were implemented, involving the proposed SVATARK method and two benchmark methods. The two benchmark methods interpolate coarse regression residuals by applying kriging and bilinear interpolation, denoted by SVRK and SVRB respectively. In the trend prediction process, the SVR models were established for each land cover type. In the experiments, SSM values for water bodies and permanent snow and ice were not included. The downscaled SSM were validated by ground-measured SSM with four classical statistical metrics, including correlation coefficient (R), mean absolute error (MAE) ($\text{m}^3 \cdot \text{m}^{-3}$), root mean square error ($RMSE$) ($\text{m}^3 \cdot \text{m}^{-3}$) and slope ($SLOP$).

Please Insert Figure 1 here.

3 Study area and data description

3.1 Study area

The study area is $3 \times 3^\circ$ ranging from 30.0° to 33.0°N and 90.5° to 93.5°E in the Naqu region located in the center of the Tibetan Plateau (TP), China. Due to the influence of the South Asian summer monsoon, the annual precipitation is approximately 500 mm in most of the central TP, with 75% of precipitation events occurring between June and August (Yang et al., 2013). Soil thawing and freezing take place around each May and November, respectively. As seen in Figure 2, most of the study area has a main vegetation type of high elevation alpine grasslands. The period of interest is during the growing season (May 1 to October 31) during 2010 to 2015. In the following dynamic analysis, five ground stations were employed, and three of them were identified as Station A, Station B and Station C. The network area covers all of the ground sites.

Please Insert Figure 2 here.

3.2 In-situ measurements

The Naqu network was established in July of 2010 for monitoring SSM and soil temperature, and comprises of 57 ground stations. The ground stations provide SSM and soil temperature at four different depths of 0-5, 10, 20 and 40 cm, with 30-min and daily sampling intervals. The data are published by the National Tibetan Plateau Data Center from August 1, 2010 to October 31, 2014 (<http://data.tpsc.ac.cn/en/data>). The available daily SSM data at depths of 0-5 cm was collected during the period of interest to evaluate the downscaling performances. Not all in-situ measurements were available during the study period at the 57 ground stations because some stations have been out of operation. The mean and standard deviation (SD) values of in-situ SSM are shown in Figure 3 during the available study period for both daily and eight-day cases.

Please Insert Figure 3 here.

3.3 Coarse-resolution surface soil moisture product

In 2012, the ESA CCI project for SSM was established to fulfill global long-term SSM monitoring by merging multiple available active and passive microwave-based SSM products (Wagner et al., 2012). That same year, the first SSM product from the ESA CCI (v0.1) was publicly released. By involving new sensors and improving the merging scheme, the subsequent SSM dataset has been updated over an extended spatiotemporal coverage. The daily SSM product provides a consistent SSM record from 1978 to the present. The latest version (v04.4) of the ESA CCI SSM product at depths of 0.5-5 cm was used in this study, with a spatial resolution of 0.25 degree (<https://www.esa-soilmoisture-cci.org>). The SSM data were interpolated and resampled to $25 \text{ km} \times 25 \text{ km}$ regular grids (Figure 2).

3.4 MODIS products

The Moderate Resolution Imaging Spectroradiometer (MODIS) is a key instrument onboard the Terra and Aqua satellites. Fine-resolution ancillary variables LST, NDVI, BSA and LC information were collected from the Version 6 products of Aqua MODIS (<https://lpdaac.usgs.gov/>). The daily LST and 16-day NDVI were provided by MYD11A1 and MYD13A2 at 1-km resolution, while the 16-day albedo and annual LC were provided by MCD43A3 and MCD12Q1 at 500-m resolution. The BSA data were calculated from shortwave radiation of MCD43A3, which uses a linear combination of the black-sky and white-sky albedo data, with weights of 0.34 for the former and of 0.66 for the latter. All MODIS products were reprojected consistently with the ESA CCI product. Missing values were filled using the aforementioned spatiotemporal prediction method to ensure complete coverage. The LST and NDVI data were resampled and aggregated into 1 km \times 1 km and 25 km \times 25 km regular grids. The average aggregations of BSA and modal aggregations of LC were achieved at both fine and coarse grids.

3.5 DEM products

The DEM at 90-m resolution provided by the NASA Shuttle Radar Topographic Mission (SRTM) within the study area was employed. The Void Filled DEM product was downloaded from <https://www.usgs.gov/centers/eros>. The DEM data were resampled into 1 km \times 1 km and 25 km \times 25 km regular grids by using average aggregations. The basic terrain factors at 1 km and 25 km, including aspect and slope, were calculated from the DEM information.

4 Results and discussion

4.1 Downscaled 1-km SSM

Figure 4 displays the 25-km SSM images in comparison with 1-km downscaled SSM predictions by three different models (i.e., SVATARK, SVRK and SVRB) for May 1 of 2011, July 20 of 2013 and September 22 of 2015. It can be inferred that the 1-km downscaled results provide more detailed information and variations of the SSM spatial distribution within each 25 km \times 25 km grid. The SSM data at fine spatial resolution can improve the characterization of the spatial variability of the SSM, which are useful for filling the gap between low-spatial-resolution SSM satellite observations and the needs of catchment-based or regional hydroecological studies. In the downscaled SSM images, the maximum and minimum values of SSM are shown in blue and red, respectively. The blue areas are near the water bodies and in areas with low elevation. Besides surface water, the negative correlation with elevation is another primary factor affecting the spatial distribution of SSM under a sub-frigid zone. The results from the proposed SVATARK method showed spatial patterns that were similar to those of the 25-km SSM, while SVRK and SVRB produced smoother downscaled results. The coherence of the ATAK predictions ensures that the average of the disaggregated predictions is equal to the original areal data, and confers the downscaled SSM of SVATARK a continuous pattern. Visual comparison of the downscaled SSM products confirmed that the failure of SVRK to predict extreme SSM and the failure of SVRB to properly capture high SSM were influenced by the kriging and bilinear interpolations. SVATARK exhibits better results in modeling extreme SSM (both maximum and minimum) than the other two downscaling methods.

Please Insert Figure 4 here.

The difference histograms of the downscaled results between SVATARK versus SVRB and SVRK are also shown in Figure 4. The three groups of histograms do not indicate large differences, perhaps because the same trend model was employed in all three downscaling methods. For the SVRB case, the minimum differences

range from $-0.068 \text{ m}^3 \cdot \text{m}^{-3}$ to $-0.033 \text{ m}^3 \cdot \text{m}^{-3}$ and the maximums range from $0.027 \text{ m}^3 \cdot \text{m}^{-3}$ to $0.036 \text{ m}^3 \cdot \text{m}^{-3}$, while the differences for SVRK span from $-0.063 \text{ m}^3 \cdot \text{m}^{-3}$ to $0.085 \text{ m}^3 \cdot \text{m}^{-3}$.

Although only three days of downscaled SSM predictions are presented in Figure 4, it is evident that the three downscaling approaches generate fine-resolution predictions with similar numerical distribution, which is reflected in the similar performance of the cumulative distribution functions (CDFs) derived from thirty-six-month data (Figure 5). Moreover, as found in the visual comparison, the CDFs and density plots of the three downscaled predictions match well with those of the 25-km SSM product (Figure 5). When comparing the differences of the density curves between 25-km SSM and the three downscaled SSM, SVATARK appears to have the closest match. Over the study area, the downscaled SSM by SVATARK is quite similar to the coarse SSM, both in spatial distribution and values. The following validations further demonstrate its improved performance.

Please Insert Figure 5 here.

4.2 Validation with the in-situ SSM measurements

The downscaled 1-km SSM of each algorithm were validated using the in-situ observations from 57 ground stations over the Naqu region within the available days from 2010 to 2014. Figure 6 shows the comparisons between ground observations and 1-km predictions of SVATARK, SVRK and SVRB. The SVRK model produces more accurate predictions than those of the SVRB-based SSM data with an *RMSE* value of $0.10 \text{ m}^3 \cdot \text{m}^{-3}$, a *MAE* value of $0.07 \text{ m}^3 \cdot \text{m}^{-3}$ and a *SLOP* value of 0.70, but with slightly smaller *R* value of 0.64. The comparison illustrates that the proposed SVATARK approach significantly outperforms the other two downscaling approaches with the smallest *RMSE* and *MAE* values of $0.08 \text{ m}^3 \cdot \text{m}^{-3}$ and $0.06 \text{ m}^3 \cdot \text{m}^{-3}$, the largest *R* and *SLOP* values of 0.72 and 0.71. The scatterplot from the SVATARK approach visually gathers along the 1:1 line and has the lowest dispersion. Because of the model prediction error, errors in input variables and the representativeness errors of different supports, there are some discrepancies between the 1-km downscaled results and in-situ measurements. Although the spatiotemporal prediction approach can help fill the missing values of remote-sensed data, the errors from this process can be propagated into the final results. In future research, more error analyses, especially before downscaling, should be performed to improve the downscaling accuracy. The improvements made by SVATARK are illustrated by an increase in *R* (0.06 or 10.7% on average) and a decrease in *RMSE* ($0.03 \text{ m}^3 \cdot \text{m}^{-3}$ or 23.6% on average) and slightly better *MAE* and *SLOP* values. A general improvement can be seen in Figure 7-9.

Please Insert Figures 6-7 here.

Figure 7 presents the comparisons between ground observations and three downscaled results for each year. The CDFs of SSM measured by in-situ and downscaled results derived from three different algorithms are displayed in Figure 8. The performance shown by the four statistical metrics appears inconsistent from year to year when comparing the results of SVRK and SVRB methods. The SVRK results are frequently better than the SVRB's during the five-year period. In general, the SVATARK model produces the two highest statistical metrics (i.e., *R* and *SLOP*) and the two lowest statistical metrics (i.e., *RMSE* and *MAE*), followed the SVRK and SVRB models. The CDF comparison indicates that the downscaled results of SVATARK models show minimum deviations from the CDF calculated from the ground observations.

Please Insert Figure 8 here.

To explore the spatial distribution of the estimation errors, the *MAE* values from 2010 to 2014 of the 57 ground stations were calculated. Figure 9 visualizes the *MAE* of the downscaled results using SVATARK, SVRK and SVRB for each ground station with color bars. The *MAE* values tend to be higher in the upper left and middle part, likely due to higher topographic relief and the lack of the corresponding original remotely-sensed observations, which could introduce errors from filling gaps. The SVATARK model has the smallest *MAE* values at each station, suggesting a better performance than SVRK and SVRB. Further SSM analyses at each station are shown in section 4.3. Although the above validations were all taken at stations of grasslands, which is the main vegetation type in the Naqu region, the SVATARK method could theoretically result in accurate downscaling predictions from other areas given its ability to learn for small samples and the strong generalization of SVR, as well as the coherence of ATAK. The proposed method should be validated and applied to other land cover types in future work.

Please Insert Figure 9 here.

In addition to the representativeness errors, there is a bias between the coarse SSM product and the in-situ observations. To reduce the negative effect of the bias in the downscaled prediction accuracy, in this experiment the mean difference between the 25-km SSM values and the point supports was removed before downscaling. Considering that all the ground stations were installed on grasslands, this bias step was used without consideration of the differences resulting from topography and LC types. However, the remotely-sensed product might perform differently over various surfaces and therefore incorporation of the impact of LC types may be beneficial for improving the bias correction accuracy. In addition, how to determine whether bias needs to be applied to all coarse grids is still a problem, if the SSM can be effectively observed at some grids.

4.3 Dynamic analysis of downscaled SSM

The downscaled maps and validation analyses described in this study illustrate that the downscaled SSM results generally show a good performance compared with ground-based measurements and their spatial pattern follows those of the coarse SSM. In this section, we investigate whether the fine-resolution SSM predictions from the three downscaled methods also capture the temporal dynamics of ground-based SSM observations during the study period. Figure 10 shows the temporal variations of 1-km downscaled SSM derived from all three downscaling methods and in-situ observations at five ground stations (in Figure 2 and Figure 9) and at network scale (i.e., network area in Figure 2). There is a significant seasonal variation in the time series, generally reaching its highest value in August. By using average aggregation within the network domain, the aggregated values of ground measurements and 1-km SSM were obtained. Two statistical metrics, *MAE* and *RMSE*, were used to evaluate their performance.

Please Insert Figure 10 here.

In the proposed SVATARK downscaling method, the values of *MAE* and *RMSE* at all five stations range from $0.033 \text{ m}^3 \cdot \text{m}^{-3}$ to $0.065 \text{ m}^3 \cdot \text{m}^{-3}$ and from $0.041 \text{ m}^3 \cdot \text{m}^{-3}$ to $0.076 \text{ m}^3 \cdot \text{m}^{-3}$, respectively, where SVATARK is found to be more accurate than the other two approaches. From the time series comparisons at different ground stations (Figure 10(a-e)), the downscaled SSM predictions, especially of the SVATARK method, show temporal consistency with the in-situ observations, although there is a significant bias between them. This indicates that the downscaled SSM of SVATARK can describe the temporal changes of the in-situ SSM. The discrepancies are mainly because of the large scale differences between 1-km predictions and

point observations. The best performance was obtained at Station D, which has the lowest *MAE* of all stations. The variation in performance of various stations might be the result of the station’s location, which would affect the soil type and have different accuracy of the input variables. The range of values for the downscaled SSM are almost all less than the ground measurements’ range. This matches well with the fact that the range of SSM decreases dynamically from fine to coarse scales (Abbaszadeh et al., 2019). Areal-averaged downscaled SSM agrees well with the ground-based SSM in Figure 10(f). However, the discrepancies between three downscaled SSM and ground observations in the network area seem smaller than those of the stations, particularly for the SVRK and SVRB methods, perhaps due to the comparisons at the same scale. The errors associated with upscaling the SSM from 1-km and point scale to network scale require further research and exploration. Note that a better performance of the downscaled SSM is also obtained by using SVATARK.

Soil moisture is a direct indicator of agricultural drought. In-situ observations of SSM may not be able to assess drought conditions in a region, whereas the 1-km downscaled predictions could provide powerful data support. A simple relative drought analysis was attempted using the downscaled SSM of SVATARK. The pixels with anomalously low values in the downscaled images were counted by comparing the pixel values on the same date every year. The mean and standard deviation were calculated for each pixel. Pixels with a larger absolute value than the standard deviation were considered to be in a drought condition. The main idea behind this assumption is to find the pixel which has a low value and relatively large variation in SSM over the same period. Figure 11 shows the proportion of pixels with relatively smaller SSM in the downscaled images using SVATARK during study period. Several proportions are larger than 0.30, meaning that thirty percent of the 1×1 km pixels in the corresponding date have abnormally low values. The proportion values suddenly increase in mid-July 2015, indicating relative drought conditions. These results are consistent with Zhu et al. (2016). Although the SSM at 0-5 cm depth might have a limited ability to reflect soil drought without deep soil moisture, this preliminary attempt demonstrates that the proposed downscaling method could be used in drought remote sensing monitoring applications for a large area. The downscaled SSM could also help understand how often and where these droughts occur. In this study only four types of ancillary variables were employed, but rainfall (including its infiltration and runoff) also affects SSM variations, and should be explored as an ancillary variable in the downscaling process in future work.

Please Insert Figure 11 here.

5 Conclusions

In this study, we proposed a machine learning-based geostatistical downscaling method. The proposed SVATARK relies on SVR that expresses the nonlinear relationship between target (i.e., SSM) and ancillary variables (i.e., LC, LST, NDVI, BSA and terrain factors), and utilizes ATAK to achieve the predictions on changed supports. SVATARK was compared to the benchmark methods SVRK and SVRB to obtain 1-km predictions from a 25-km SSM product over the Naqu region during a thirty-six month period from 2010-2015. The downscaled predictions were validated using ground stations. In general, the comparison results indicate that the SVATARK downscaling approach obtained the greatest accuracy, and the dynamic analysis of 1-km SSM reached the same conclusion. The downscaled predictions were used to capture the abnormally low SSM by using a simple count analysis, which reveals the capability of monitoring the relative drought and could be further generalized for large areas with systematic analysis methods. The proposed SVATARK method is entirely general, and it can be employed to downscale or even upscale other continuous variables owing to the changes in the supports in ATAK. Other machine learning or deep learning methods such as random forest or neural network algorithms could be applied in trend predictions and could be integrated with ATAK for spatial scaling. The comparisons among different artificial intelligence algorithm-based

ATAK models will be explored in the future work.

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Conflicts of Interest

The authors declare no conflict of interest.

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