



1	Blending SMAP, Noah and In Situ Soil Moisture Using Multiple Methods
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#### 7 Abstract

8 Soil moisture can be obtained from in-situ measurements, satellite observations, and model 9 simulations. This study evaluates different methods of combining model, satellite, and in-situ soil 10 moisture data to provide an accurate and spatially-continuous soil moisture product. Three 11 independent soil moisture datasets are used, including an in situ-based product that uses regression 12 kriging (RK) with precipitation, SMAP L4 soil moisture, and model-simulated soil moisture from 13 the Noah model as part of the North American Land Data Assimilation System. Triple collocation 14 (TC), relative error variance (REV), and RK were used to estimate the error variance of each parent 15 dataset, based on which the least squares weighting (LSW) was applied to blend the parent datasets. 16 These results were also compared with that using simple average (AVE). The results indicated no 17 significant differences between blended soil moisture datasets using errors estimated from TC, REV or RK. Moreover, the LSW did not outperform AVE. The SMAP L4 data have a significant 18 19 negative bias (-18%) comparing with *in-situ* measurements, and *in-situ* measurements are valuable 20 for improving the accuracy of hybrid results. In addition, datasets using anomalies and percentiles 21 have smaller errors than using volumetric water content, mainly due to the reduced bias. Finally, 22 the in situ-based soil moisture and the simple-averaged product from in situ-based and Noah soil 23 moisture are the two optimal datasets for soil moisture mapping. The in situ-based product 24 performs better when the sample density is high, while the simple-averaged product performs 25 better when the station density is low, or measurement sites are less representative. 26 **Keywords:** soil moisture; in situ network; remote sensing, regression kriging; triple collocation;

27 relative error variance;

28





#### 29 **1. Introduction**

30 Soil moisture is a critical component of the climate system. It modulates the exchange of 31 water and energy between land and atmosphere through evapotranspiration (Seneviratne et al., 32 2010). Soil moisture has great value for understanding and predicting soil erosion and water quality (Keesstra et al., 2016; Abbaspour et al., 2015), agricultural and water resource management 33 34 (Pittelkow et al., 2015; Dobriyal et al., 2012), runoff and flooding (Brocca et al., 2010; Wanders et 35 al., 2014), drought monitoring (Dai, 2013; Wang et al., 2011) and weather and climate forecasting (Hirschi et al., 2011;Seneviratne et al., 2010). Despite the importance of soil moisture, accurate, 36 37 spatially-continuous soil moisture datasets with high temporal and spatial resolution are elusive.

38 There are three primary sources of soil moisture information: remote sensing (RS) 39 observations, Land Surface Models (LSMs), and in-situ measurements. Microwave remote sensing 40 is responsive to surface (~5-cm) soil moisture in regions with sparse to moderate vegetation density. 41 The passive microwave satellites that are currently in orbit include the Soil Moisture and Ocean 42 Salinity (SMOS) satellite (launched 2009, 35 km resolution, Kerr et al. (2001)), the Advanced 43 Microwave Scanning Radiometer 2 (AMSR2) (25 km resolution, Imaoka et al. (2010)) onboard the GCOM-W1 satellite, and the Soil Moisture Active Passive (SMAP) satellite (launched 2015, 44 45 9 km resolution, Entekhabi et al. (2010)). The Advanced Scatterometer-A/B (ASCAT-A/B) 46 (Wagner et al., 2013) on board of the Meteorological Operational (METOP) satellite series 47 (launched 2006 and 2012 respectively, 25 km resolution) is an active microwave satellite in orbit. 48 The coarser spatial resolution of these sensors is compensated by their greater spatial coverage and 49 more frequent revisit times. In contrast, the active synthetic aperture radar (SAR) systems, such as 50 the one onboard the RADARSAT-2 satellite (launched 2007, 3 m resolution) (Lievens and 51 Verhoest, 2012) and the ones onboard the Sentinel-1 (A/B) satellite constellation (launched in





2014 and 2016, respectively, 5 m resolution) (Paloscia et al., 2013), provide soil moisture
information at finer spatial resolution, but with limited spatial coverage and less frequent revisit
times.

55 A limitation of all microwave RS soil moisture datasets is that they can only measure soil 56 moisture in the top 5 cm (or less) of the soil due to the limited penetration depth of microwave 57 signals. In addition, they cannot detect soil moisture under snow or ice, or in frozen soils. There 58 are also challenges with retrievals in areas with complex topography, dense vegetation, near water bodies, or cities (Wagner et al., 1999; Parinussa et al., 2011). Ford and Quiring (2019) compared 59 the RS soil moisture datasets from SMAP (SMAP L3 and SMAP L4), SMOS and ESA-CCI with 60 61 in-situ measurements and found the SMAP L3 product consistently performed best among the four. 62 Model-simulated soil moisture is another source of spatially-continuous soil moisture. The 63 NOAA Climate Prediction Center (CPC) (Huang et al., 1996), Global Land Data Assimilation System (GLDAS) (Rodell et al., 2004) and North American Land Data Assimilation System 64 65 (NLDAS) (Mitchell et al., 2004) all provide simulated soil moisture operationally at various depths and time scales. Compared with in-situ measurements, Chen et al. (2013) found all four GLDAS 66 67 LSMs systematically underestimate the surface soil moisture in the Tibetan Plateau. Bi et al. (2016) 68 also found that all the GLDAS LSMs are strongly correlated with observations, but the Mosaic 69 model consistently has larger biases than other LSMs (the largest bias reaches  $0.192 \text{ m}^3\text{m}^{-3}$ ) in the 70 Tibetan Plateau. By comparing GLDAS Noah model with the Standardized Precipitation Index 71 and a multi-satellite surface soil moisture product, Spennemann et al. (2015) found that GLDAS Noah accurately captured the variability of soil moisture anomalies over southern South America, 72 73 but the accuracy varied both regionally and seasonally. Soil moisture simulations from NLDAS 74 phase 2 (NLDAS-2) are also found to have large biases when compared to in-situ observations





(Xia et al., 2014). Specifically, the Noah and VIC models tend to overestimate soil moisture, while
Mosaic and SAC models underestimate soil moisture when compared with in-situ observations
(Xia et al., 2015). Ford and Quiring (2019) compared the modeled soil moisture from NLDAS-2
and CPC with in-situ measurements and that the found NLDAS-2 models consistently performed
better than the CPC model.

80 Similar to RS soil moisture, model-simulated soil moisture is difficult to validate because of the scale mismatch and the in-situ networks are not dense enough to adequately resolve soil 81 82 moisture variability within each LSM pixel. In addition, the reliability of model-simulated soil 83 moisture varies significantly from model to model, and over time and space (Ford and Quiring, 84 2019; Spennemann et al., 2015). Models generally perform well in representing the variations in 85 soil moisture and soil moisture anomalies (Downer and Ogden, 2003; Meng and Quiring, 86 2008; Albergel et al., 2012), but they tend to have large biases in simulating the absolute volumetric 87 water content of the soil (Xia et al., 2015;Bi et al., 2016).

88 In-situ soil moisture measurements from individual field campaigns and regional and national soil moisture monitoring networks are invaluable for calibrating and validating LSMs and 89 90 RS-based soil moisture datasets and other hydrological and climatological studies. Great efforts 91 have been made to assemble, homogenize, and standardize in-situ soil moisture measurements 92 from different networks, time frames, sensors, depths and format (Cosh et al., 2016;Dorigo et al., 93 2013; Zhang et al., 2017a; Ford and Quiring, 2014). Currently, the coordinated in-situ soil moisture 94 networks include the International Soil Moisture Network (ISMN) (Dorigo et al., 2011) and the North American Soil Moisture Database (NASMD) (Quiring et al., 2016). Despite the coordinated 95 96 and standardized in-situ measurements, the number of stations and networks measuring soil 97 moisture continuously is still very limited at either regional or global scale. In addition, the small





98 spatial representativeness of in-situ data (a point measurement) also limits its application at larger

99 spatial scales.

100 To fully apply in-situ soil moisture on a continuous basis, a variety of approaches have 101 been adopted to generate spatial continuous soil moisture datasets based on in-situ measurements. 102 For example, Takagi and Lin (2012) used regression kriging (RK) along with five topographic 103 variables (elevation, curvature, slope, upslope contributing area, and topographic wetness index) 104 to generate soil moisture maps of the Shale Hills. The RMSE of RK predictions ranged from 0.03 to 0.08 m<sup>3</sup>m<sup>-3</sup> in the surface layer (0-10 cm). Yao et al. (2013) compared ordinary kriging (OK), 105 106 inverse distance weighting (IDW), linear regression and regression kriging (RK) to estimate soil 107 moisture at small catchment (2 km<sup>2</sup>) with complex terrains. The auxiliary variables used in RK 108 and linear regressions were land use types, slope, and annual average solar radiation. They found 109 both OK and IDW did not perform well in complex terrains, while RK performed best with mean 110 Nash-Sutcliffe Efficiency (NSE) of 0.69 followed by linear regression. Yuan and Ouiring (2017) 111 compared the reduced optimal interpolation (ROI) based on in-situ and simulated soil moisture from VIC model with co-kriging and IDW methods for surface soil moisture mapping in 112 113 Oklahoma, and found that ROI performs better than the other two methods with a mean NSE around 0.58 and a mean absolute error 0.03 m<sup>3</sup> m<sup>-3</sup>. 114

In general, the RK method performs better than other geostatistical and non-geostatistical methods (Keskin and Grunwald, 2018), but it requires a relatively high density of soil moisture measurements, strong correlations between soil moisture and auxiliary variables and the accurate measurement of auxiliary variables (Li and Heap, 2011;Keskin and Grunwald, 2018). In addition, none of the RK-gridded soil moisture datasets have been compared with the model-simulated and satellite-derived soil moisture.





121 In summary, each source of soil moisture data has its strengths and weaknesses. However, 122 none of them, at least by themselves, are adequate for providing accurate soil moisture data at high 123 temporal and spatial resolutions. Therefore, it is useful to combine these three independent data 124 sources to capitalize on the strengths of each and to generate an optimal soil moisture product to 125 facilitate real-world applications. There are a number of methods that are commonly used for 126 blending together different soil moisture datasets, including triple collocation (TC) (Stoffelen, 127 1998) with least square weighting (LSW) and simple averaging (averaging parent datasets using 128 equal weighting). For example, Yilmaz et al. (2012) generated a hybrid soil moisture anomaly 129 product at 0.25° grid by merging model-derived soil moisture, thermal infrared RS-soil moisture, 130 and microwave RS-based soil moisture using TC and LSW. The TC-merged product had less 131 uncertainty, but it did not outperform the simple averaging method. Zeng et al. (2016) also used 132 TC with LSW to blend the soil moisture from two satellite (AMSRE and ASCAT) and one 133 reanalysis soil moisture product (ERA-Interim). Their merged product performed better than 134 simple averaging in the sub-humid and semi-arid regions, but the performances of TC with LSW and simple averaging were similar in arid regions. 135

136 There are a number of knowledge gaps that still exist, including (1) of the lack of in-situ 137 soil moisture inclusion in product blending. Current studies mainly focus on combining modeled 138 and RS soil moisture, rather than combining all three sources (modeled, RS and in-situ). In-situ 139 measurements can be useful for improving the accuracy of hybrid soil moisture datasets. (2) There 140 is no comprehensive evaluation of different data blending methods. In addition to TC, there are a 141 variety of other methods that are available for combining different datasets such as Kriging and 142 Relative Error Variance (REV) (Vinnikov et al., 1996;Ford and Quiring, 2019). Therefore, it would be helpful to compare the accuracy of different blending methods to identify the optimal 143





144 approach for soil moisture. (3) The impact of measurement units (e.g., volumetric water content, 145 soil moisture anomalies, and percentiles) is unknown. For example, is it better to convert all of the 146 soil moisture measurements to anomalies or percentiles before blending? (4) A simple and 147 operational methodology is still needed for accurate daily soil moisture mapping with high spatial 148 resolution. Current methods to generate gridded soil moisture data products cannot produce data 149 with sufficient spatial resolution for many agricultural and hydrological applications.

This paper addresses all four of these knowledge gaps by assessing different blending methods to merge model-simulated, RS-based and in-situ soil moisture data into a 4-km soil moisture product. The impact of different measurement units (absolute, anomalies and percentiles) on the accuracy of the blended product are also investigated. Finally, two optimal datasets are identified and the utility of these datasets are demonstrated.

#### 155 **2. Study area and data**

156 This study is conducted in the south-central region of the United States, covering four states, 157 including Texas, Oklahoma, Arkansas, and Louisiana with a total area ~1,150,400 km<sup>2</sup>. The south-158 central U.S. an important agricultural region in the U.S., but also one that is drought-prone (Tian 159 and Quiring, 2019). For example, the four states account for about 10% of national winter wheat 160 production in 2017 (National Agricultural Statistics Service). According to the Köppen climate 161 classification, the climate of this region varies from warm temperate (about three-fourths of the 162 region) in the east to the arid (about one-fourth of the region) in the west (Kottek et al., 2006). The 163 annual average temperature gradually decreases from south (27 °C) to north (13 °C), and the mean 164 annual precipitation gradually increases from west (<25 cm) to east (>190 cm).

165 This study uses in-situ measurements of soil moisture, satellite-observed soil moisture, 166 model-simulated soil moisture, precipitation and air temperature data. Detailed information on the





- 167 spatial and temporal resolution, period of record and measurement depths are listed in Table 1. To
- 168 facilitate comparison, the common period of record from 2015/03/31 to 2018/12/31 (SMAP
- 169 product) were extracted for all datasets.
- 170
- 171 Table 1. Summary of datasets used in this study

<b>D</b> ( <b>d</b>							
Data Sources		Temporal	Temporal	Spatial	Measurement		
		Domain	resolution	resolution*	depths (cm)		
	OKM	1998-present	Daily	115 out of 129	5, 25, 60, 75		
				sites			
	WTM	2002-present	Daily	64 out of 70	5, 20, 60, 75		
Ten aiten		_	-	sites			
m-situ	SCAN	1994-present	Daily	21 out of 219	5, 10, 20, 50, 100		
				sites			
	CRN	2009-present	Daily	15 out of 147	5, 10, 20, 50, 100		
		_	-	sites			
SMAP L4		2015/03/31 -	3 hours;	9-km	5, 0-100		
		present	latency: 2 days				
NLDAS_V2 Noah		1979-present	Hourly	1/8°	0-10, 10-40, 40-100		
Model		_	-				
DDIGM	ppt,	1981-present	Daily	4-km			
FRISM	tmp						

172 \*: The in-situ measurements are point-based, thus the spatial resolution for in-situ data refers to

the number of stations used in this study out of a total number of stations of the sparse network.

## 175 2.1 In-Situ Soil Moisture Measurements

176 The in-situ soil moisture data are collected from four sparse networks: Oklahoma Mesonet (OKM), West Texas Mesonet (WTM), Soil Climate Analysis Network (SCAN) and Climate 177 178 Reference Network (CRN). Daily soil moisture measurements were obtained from North 179 American Soil Moisture Database (NASMD) in the units of volumetric water content (m<sup>3</sup> m<sup>-3</sup>) 180 (Quiring et al., 2016). Since different networks collect data at different time intervals ranging from 181 every 5 minutes to once per day, for consistency a single morning measurement (7 am LST) is 182 extracted to represent the daily value. This is not ideal, but it is reasonable for applications in which 183 diurnal variations in soil water content are inconsequential, such as drought monitoring. The raw





- 184 measurements have passed through the Quality Assurance and Quality Control (QAQC) process
- 185 (Ford and Quiring, 2014), with dubious or questionable values been removed and filled. The near-
- 186 surface measurements (5 cm) from a total of 215 stations (Fig. 1) were obtained for this study.



187

Fig. 1 Study area and stations for in-situ soil moisture measurements. Background map (USA
 Topographic Basemap) Copyright:© 2013 National Geographic Society, i-cubed

190 2.2 SMAP-L4 Soil Moisture

191 The SMAP Level-4 Surface and Root-Zone Soil Moisture are adopted in this study because 192 it provides a temporally complete set of global soil moisture data. The SMAP L4 product is a 193 merged soil moisture product from SMAP L-band brightness temperature observations and 194 estimates from the NASA Catchment land surface model using a data assimilation system (Reichle 195 et al., 2018). The L4 Geophysical Data are used, which are available from 31 March, 2015 to 196 present (with 2-3 days latency). They include both surface (0-5 cm) and root-zone (0-100 cm) soil 197 moisture every 3 hours at a spatial resolution of 9-km. The unbiased RMSE for SMAP L4 SM surface and root zone soil moisture are reported to be 0.038 m<sup>3</sup> m<sup>-3</sup> and 0.030 m<sup>3</sup> m<sup>-3</sup> respectively 198





199	(Reichle et al., 2017). Finally, to be consistent with the in-situ measurements, the SMAP L4
200	product with time slot covering 7 am are extracted each day to represent the daily soil moisture
201	from 2015/03/31 to 2018/12/31. The nearest neighbor assignment is used to resample SMAP L4
202	surface soil moisture from 9-km to 4-km to match the spatial resolution of other datasets (e.g.,
203	PRISM).

### 204 2.3 NLDAS-2 Noah Soil Moisture

205 This study uses the simulated soil moisture from the NLDAS-2 Noah model. The Noah 206 model provides hourly soil moisture fields at 1/8° grid from 1979 to present. The Noah model has 207 four soil layers: 0-10 cm, 10-40 cm, 40-100 cm, and 100-200 cm, but only the top layer is used 208 in this study. Details about the NLDAS-2 configuration of the Noah LSM can be found in Xia et 209 al. (2012). To be consistent with the in-situ measurements, the Noah output at 7 am are extracted 210 each day to represent the daily soil moisture, and the data from 2015 to 2018 are adopted to match 211 the record length of the SMAP data. Finally, the nearest neighbor method is used to resample the 212 simulated soil moisture from 12.5-km to 4-km to match with other datasets.

#### 213 2.4 PRISM Climate Data

The PRISM (Parameter-elevation Relationships on Independent Slopes Model) datasets are developed by Oregon State University's PRISM Climate Group (Daly et al., 2008). They are official climatological data sets of the USDA. PRISM use surface stations and a weighted regression scheme to generate daily updated spatial mapping of climate variables (e.g., precipitation, temperature, dew point, vapor pressure deficit) over the contiguous United States. There are more than 13,000 quality controlled surface stations used for precipitation interpolation and more than 10,000 stations used for temperature interpolation (Daly et al., 2008). The





- climatological normals (average monthly and annual conditions over 1981-2010) and monthly and
- daily data are available at 4-km and 800-m resolution from 1981 to present.

The 4-km daily precipitation from PRISM are used in this study. Since there is strong coupling between soil moisture and precipitation (Koster et al., 2004), precipitation has been widely used as an important input for soil moisture estimation in various LSMs (Liu et al., 2018;Xia et al., 2012;Liang et al., 1996). Here, the Antecedent Precipitation Index (API) is calculated based on precipitation and adopted for soil moisture interpolation using in-situ measurements and regression kriging. The API index is introduced in Section 2.5.2 and regression kriging is introduced in Section 3.

230 2.5 Data Preparation

## 231 2.5.1 Anomalies and Percentiles

232 The volumetric water content of the soil varies as a function of weather conditions, soil 233 characteristics, vegetation, topography, among other factors, and so it cannot be directly compared 234 between different locations. In contrast, relative measures of soil wetness, such as anomalies and 235 percentiles can used to standardize soil moisture from different sensors and locations and make 236 them comparable (Ford et al., 2015; Zhang et al., 2017a). In this study, anomalies and percentiles 237 are calculated for all 3 datasets (In-situ, SMAP, NLDAS and PRISM). Anomalies are calculated 238 by removing the seasonal climatology from the absolute soil moisture at each day (Crow and Van 239 den Berg, 2010). The climatological mean is calculated using a moving-window approach (Chen 240 et al., 2017), which averages all available soil moisture estimates across all years within a 31-day 241 window (Dong et al., 2018) centered on the target day.

242 Percentiles are calculated using an empirical probability distribution function and moving
243 window approach as well. At each day of the year, all the data fall within a 31-day window centered





244 on that day was used to construct the empirical probability distribution function. Ford et al. (2016) 245 found sample sizes of 93 to 186 daily soil moisture observations were required to generate robust 246 percentiles. In our case, SMAP has the shortest data record (3 years), thus has 93 data points (31 days in window  $\times$  3 years) from which to build the distribution and compute the quartiles and 247 248 percentiles. This has met the sampling size to generate robust percentiles. For other datasets, the 249 total length of records is used to generate the percentiles (e.g., 20 years for in-situ, 40 years for 250 NLDAS). Percentiles range from 0 or (0%) to 1 (or 100%), which corresponds to the driest (0%)251 and wettest (100%) soil conditions at a specific site over the entire study period.

## 252 2.5.2 Antecedent Precipitation Index (API)

The API is precipitation-based moisture index. It is used to indicate the wetness of a location and has been widely applied in drought monitoring (Crow et al., 2012a), runoff forecasting (Anctil et al., 2004), soil moisture estimation (Ochsner et al., 2019) and crop yield prediction (Zhang et al., 2017b). API takes preceding precipitation into account to estimate the current moisture status, and is formulated as (Kohler and Linsley, 1951):

258 API(i) = API(i-1) \* k + PPT(i)(1)

Where API(i) is the API at day i, PPT(i) is the precipitation occurring on day i; k is an empirical decay factor between 0.80 and 0.98 (Heggen, 2001). In this study, a set of k values (from 0.80 to 0.99) is tested to determine the optimal k value that results in the highest correlation between API and soil moisture based on 215 stations. Fig. S1 shows the variation in correlation as a function of different k values. The highest correlation (r = 0.4) is achieved at k = 0.92. Therefore, k = 0.92 is used in this study for API calculation.





#### 265 2.5.3 Site Selection

In this study, 40% of the stations with soil moisture measurements (88 sites) are used for modeling (black circles in Fig. 1), while the remaining 60% of stations (127 sites) are used for outof-sample validation. The 88 modeling sites are selected based on the Index of Temporal Stability (ITS) (Jacobs et al., 2010;Zhao et al., 2010). ITS is an indicator of the temporal representative locations. The location with the lowest ITS value is the location with the highest temporal stability. The ITS at location i ( $ITS_i$ ) is calculated as:

272 
$$ITS_i = \sqrt{MRD_i^2 + SDRD_i^2}$$
(2)

273 
$$MRD_i = \frac{1}{T} \sum_{j=1}^{T} RD_{i,j}$$
(3)

274 
$$SDRD_{i} = \sqrt{\frac{1}{T-1}\sum_{j=1}^{T} (RD_{ij} - MRD_{i})^{2}}$$
(4)

275 
$$RD_{ij} = \frac{\theta_{ij} - \overline{\theta_j}}{\overline{\theta_j}}$$
(5)

276 Where  $\theta_{ij}$  is individual daily measurement of soil moisture at location  $i \subset [1, ..., N]$  and 277 time j  $\subset$  [1, ..., T], and  $\overline{\theta}_i$  is the spatial average of soil moisture at all locations at time j.  $RD_{i,i}$  is 278 the relative difference of location i at time j, which is introduced by Vachaud et al. (1985).  $MRD_i$ 279 is the mean relative difference of location i. It averages the RD at location i across an entire period 280 (T days), and represents the location's temporal bias or whether the location is wetter or drier than 281 the average of the area during T days.  $SDRD_i$  is the standard deviation of the RD at location i. It 282 describes the degree of the temporal stability of a location, or whether a location is temporally 283 stable. Therefore, a temporally representative site is one with a small mean bias and can be characterized by low values of both MSD and SDRD, and a low value of ITS (Cho and Choi, 284 285 2014;Penna et al., 2013;Brocca et al., 2012).





Since anomalies can be negative, the absolute value of the difference between  $A_{i,j}$  and  $\overline{A_j}$ 

(Eq. 6) is adopted to represent the relative difference of anomalies at location i and time j  $(RD_A_{ij})$ 

288 (Wang et al., 2017;Mittelbach and Seneviratne, 2012):

$$RD_{-}A_{ij} = |A_{i,j} - \overline{A_{j}}| \tag{6}$$

290 where  $\overline{A}_{j} = \frac{1}{N} \sum_{i=1}^{N} A_{ij}$ , indicates the spatial average of anomalies of all stations at time j.

291 In this study, the 88 modeling sites are selected by three steps: (1) Calculate and rank the 292 ITS of 215 stations in ascending order; (2) Evenly divide the ranked ITS into four groups; (3) 293 Within each group, select the 22 sites with the smallest ITS values. The 88 sites are selected in this 294 way to ensure an evenly sampled sites across the ITS range, which best mimic the reality that in-295 situ stations have different temporal representativeness. Although ITS ranking using absolute soil 296 moisture, anomalies and percentiles are not exactly the same, the differences are minor. To be 297 consistent across datasets and facilitate comparison, the same 88 (127) sites selected using the 298 absolute soil moisture were used for calibration (validation) using soil moisture anomalies and 299 percentiles, because the selected sites are also evenly distributed within the ITS range calculated 300 by anomalies and percentiles (Fig. S2).

# 301 3. Blending Methods

The soil moisture blending schemes used in this study are summarized in Fig. 2. Two categories of parent datasets are adopted in this study (Fig. 2). The first category is consist of SMAP observations, NLDAS simulations, and RK-gridded soil moisture using in-situ soil moisture and API. The datasets from the first category are implemented with three data formats: absolute values (PP1), anomalies (PP2), and percentiles (PP3). The second category consists of



309



- 307 the RK-gridded soil moisture (PP4) using in-situ soil moisture with the absolute values of API,
- 308 SMAP, and NLDAS soil moisture respectively.



Fig. 2 Framework of soil moisture blending, and their associated parent datasets, data format,
blending methods and output products.

## 312 **3.1 Regression Kriging (RK)**

Regression Kriging (RK) is one of the most popular and robust hybrid spatial interpolation techniques in the digital mapping of soil properties (Keskin and Grunwald, 2018). RK combines a regression between the target variable and auxiliary variables with simple kriging of the regression residuals (Hengl et al., 2007;Odeha et al., 1994). Previous studies revealed RK often outperforms non-geostatistical methods (Mishra et al., 2010;Yang et al., 2019;Li and Heap, 2011), ordinary kriging (Hengl et al., 2004), and co-kriging (Eldeiry and Garcia, 2010). The RK models can be expressed as two parts (Hengl et al., 2004):

320 
$$\hat{z}(s_0) = \hat{m}(s_0) + \hat{e}(s_0)$$
 (7)

Where  $\hat{m}(s_0)$  is the fitted trend,  $\hat{e}(s_0)$  is the interpolated residual. In this study, the trend term  $\hat{m}(s_0)$  is fitted by a linear model between the auxiliary variable and soil moisture.

323 
$$\widehat{m}(s_0) = \widehat{\beta} \cdot q(s_0) \tag{8}$$





Where,  $\hat{\beta}$  is the estimated model coefficients using generalized least squares,  $q(s_0)$  is the auxiliary variable (e.g., API) at the target location  $s_0$ . The residual from the linear model is then interpolated

326 by simple kriging with an assumed 0 mean.

327 
$$\hat{e}(s_0) = \sum_{i=1}^n \lambda_i \cdot e(s_i) \tag{9}$$

Where,  $\lambda_i$  are kriging weights determined by the spatial dependence structure of the residual, and *e*(*s<sub>i</sub>*) is the residual at location *s<sub>i</sub>*. By adding the kriging residuals to the predicted trend, the final RK prediction are obtained. RK also provide the error estimation of predicted values as (Hengl et al., 2007):

332 
$$\sigma_{RK}^{2}(s_{0}) = (C_{0} + C_{0}) - c_{0}^{T} \cdot C^{-1} \cdot c_{0} + (q_{0} - q^{T} \cdot C^{-1} \cdot c_{0})^{T} \cdot (q^{T} \cdot C^{-1} \cdot q)^{-1} \cdot (q_{0} - q^{T} \cdot Q)^{-1} \cdot (q_{0} - q)^{-1} \cdot (q)^{-1} \cdot (q)^{-1} \cdot (q)^{-1} \cdot (q)^{-1} \cdot (q)^{-1} \cdot (q)$$

Where C is the covariance matrix of the residuals,  $C_0 + C_0$  is the sill variation,  $c_0$  is the vector of covariance of residuals at the unvisited locations, q is a matrix of predictors at the sampling locations, and  $q_0$  is the vector of p+1 predictors (p=1 in our case).

In this study, two sets of auxiliary variables are tested for RK. The first set of auxiliary variables are API in the format of absolute values, anomalies, and percentiles respectively. Given that precipitation is the chief driver of soil moisture, and a strong positive relationship was observed between the soil moisture and API over the contiguous United States (Fig. S3), thus API can be used as an important predictor of soil moisture variations. The second set of auxiliary variables are respectively the SMAP L4 and the NLDAS surface soil moisture in the format of volumetric water content (Fig. 2).

## 344 **3.2 Triple collocation (TC)**

Triple collocation (TC) is a technique for estimating the error variance (errVar, m<sup>3</sup> m<sup>-3</sup>) of three independent datasets with respect to the unknown truth (Stoffelen, 1998). It assumes a linear





347 error model (Eq. 11- Eq.13) between each product and the unknown truth (t). The errors from the 348 independent sources are assumed to have zero mean  $(E(e_i) = 0)$  and are uncorrelated with each 349 other  $(Cov(e_i, e_i) = 0, i \neq j)$  and with the truth  $(Cov(e_i, t) = 0)$ . TC analysis has been widely 350 used to estimate the errors of various measurement systems, such as the ocean waves (Caires and 351 Sterl, 2003), wind fields (McColl et al., 2014; Stoffelen, 1998), leaf area index (Fang et al., 2012), 352 precipitation (Roebeling et al., 2012), and soil moisture (Su et al., 2014; Yilmaz et al., 2012; Dorigo 353 et al., 2010; Gruber et al., 2013). Gruber et al. (2016) reviewed the previous TC analysis on soil 354 moisture, and found there are two different notations of TC formula, the difference notation 355 (Stoffelen, 1998;Scipal et al., 2008;Yilmaz et al., 2012) and the covariance notation (Stoffelen, 356 1998;McColl et al., 2014). They demonstrated that two different notations are mathematically 357 identical in the ideal case that each product is bias-free ( $\alpha_i = 0$  in Eq. 11 to Eq. 13). However, in 358 reality, there is always bias in each product, which results in a slightly different value of errVar 359 estimated using the two notations. The difference notation format of TC accounts for the total 360 errVar (including variance from both bias  $\alpha_i$  and error term  $e_i$ ), while the covariance notation of 361 TC only focuses on the errVar from the error term  $(e_i)$ . In this study, the difference notation of TC 362 is adopted to account for the total error variance of parent datasets.

363  $\theta_K = \alpha_K + \beta_K \theta_t + e_K \tag{11}$ 

364	$\theta_S = \alpha_S + \beta_S \theta_t + e_S$	(12)
		· · ·

365  $\theta_N = \alpha_N + \beta_N \theta_t + e_N \tag{13}$ 

Where,  $\theta_i$  (i  $\in$  (S, N, K)) are three collocated soil moisture datasets for SMAP, NLDAS and RK-gridded soil moisture, respectively;  $\theta_t$  is the unknown true soil moisture;  $\alpha_i$  (i  $\in$  (K, S, N)) and  $\beta_i$  (i  $\in$  (K, S, N)) are systematic additive and multiplicative biases of product i with respect to the truth, and  $e_i$  (i  $\in$  (K, S, N)) are the additive zero-mean random errors for each system. When





anomalies or percentiles are used, the additive bias  $\alpha_i$  can be deemed as zero, because these two

- 371 methods either removed the climatology mean from each product or standardized each product.
- 372 A reference dataset must be selected from the three input datasets and rescaling is required
- 373 to transfer the other two datasets into the same observation space of the reference dataset. Our
- 374 preliminary results showed that the choice of reference dataset did not impact the final results, thus
- 375 the RK-gridded soil moisture is selected as the reference dataset in this study ( $\theta_R = \theta_K$ ). The
- 376 rescaling method (Eq. 14) from Dorigo et al. (2010) is used.

377 
$$\theta_i^* = \overline{\theta_R} + \sqrt{\frac{VAR(\theta_R)}{VAR(\theta_i)}} \cdot (\theta_i - \overline{\theta_i})$$
(14)

378 Where,  $\overline{\theta_R}$  and  $VAR(\theta_R)$  are respectively the mean and variance of the reference soil moisture.

379 After the rescaling of the parent datasets, Eq. (11) to (13) can be rewritten as:

- $\theta_K^* = \beta_K \theta_t + e_K^* \tag{15}$
- $\theta_S^* = \beta_K \theta_t + e_S^* \tag{16}$
- $\theta_N^* = \beta_K \theta_t + e_N^* \tag{17}$

383 where,  $\theta_i^*$  (i  $\in$  (K, S, N)) are the rescaled soil moisture datasets. Finally, the error variances can be

384 estimated by averaging the cross-multiplied differences between the three datasets:

385 
$$\sigma_K^{*2} = \overline{(\theta_K^* - \theta_S^*)(\theta_K^* - \theta_N^*)}$$
(18)

386 
$$\sigma_S^{*2} = \overline{(\theta_S^* - \theta_K^*)(\theta_S^* - \theta_N^*)}$$
(19)

387 
$$\sigma_N^{*\,2} = \overline{(\theta_N^* - \theta_S^*)(\theta_N^* - \theta_K^*)}$$
(20)

Different combinations of triplets are also tested in this study to examine the impact of triplets on TC estimates. The triplet candidates include the in-situ measurements (denoted by "I" in the following figure and text), the SMAP L-4 surface soil moisture (denoted by "S"), simulated soil moisture from NLDAS-2 Noah model (denoted by "N"), and the RK-gridded soil moisture





using regression kriging (denoted by "K"). Four combinations of the candidates are tested,
including (I, S, N), (I, K, S), (I, K, N), and (K, S, N). The triplet candidates are extracted from the
127 out-of-sample stations. Scipal et al. (2008) found at least 100 collocated triplet samples are
required for a reliable estimation of the variance. In our case, the time series from 2015/03/31 to
2018/12/31 is used for TC analysis, which results in 1372 collocated triplet samples at every station
with a serially complete record. The stations with less than 100 observations are removed from the
TC error estimation.

## 399 **3.3 Relative Error Variance (REV)**

Relative Error Variance (REV) is the ratio of measurement error variance to real soil
moisture variance. It measures the displacement of autocorrelation in a measured quantity.
Delworth and Manabe (1988) recognized that a soil moisture time series behaves like a first-order
Markov process. Later Vinnikov and Yeserkepova (1991) validated and confirmed this and noted
the autocorrelation function of soil moisture can be expressed as an exponential form of lag length:

405  $\gamma(\tau) = \exp(-\tau/T)$ (21)

where  $\gamma(\tau)$  is the autocorrelation function,  $\tau$  is the lag, and T is the decay time scale. Robock et al. (1995) also found a linear best fit of  $\ln(\gamma)$  verse  $\tau$  does not cross zero at a value of  $\gamma(\tau = 0) =$ 1. The displacement of the autocorrelation  $\gamma(\tau)$  at  $\tau = 0$  is related to the measurement error (*a*) as:

409 
$$\gamma(\tau = 0) = 1 - a$$
 (22)

410 Successively, Vinnikov et al. (1996) partitioned the soil moisture variation into red noise 411 ( $\sigma^2$ , actual variance of the soil moisture measurement) and white noise ( $\delta^2$ , random error of 412 measurements), and noted that the ratio  $\delta^2/\sigma^2$  can be used as a measure of the random error in the 413 measurement. Dirmeyer et al. (2016) related the ratio  $\delta^2/\sigma^2$  to the measurement error (*a*), and 414 used it to estimate the random measurement error of different sparse soil moisture networks. Ford





and Quiring (2019) applied relative error variance (REV) to quantify the proportion of
measurement error within real soil moisture variance, as:

417 
$$REV = \frac{\delta^2}{\sigma^2} = \frac{a}{(1+a)}$$
(23)

Thus, a higher REV value represents a larger proportion of random measurement error. REV is a powerful measurement of random measurement error or uncertainties, and it does not require independent data, unlike the TC method.

### 421 **3.4 Least square weighting (LSW)**

422 Yilmaz et al. (2012) adopted the least square framework to achieve an objective blending 423 of satellite and modeled soil moisture. The same methodology was adopted by Zeng et al. (2016) 424 to merge the satellite and reanalysis soil moisture data. In this study, the least square weighting 425 (LSW) is used to blend soil moisture data from satellite, model and in-situ measurements based on 426 error variances estimated from the TC, REV and RK methods, respectively (Fig. 2). The desired 427 estimate of soil moisture ( $S_m$ ) via blending different sources of data using least squares framework, 428 can be expressed as:

429 
$$S_m = w_x S_x + w_y S_y + w_z S_z$$
 (24)

430 Where,  $w_x$ ,  $w_y$  and  $w_z$  are the relative weights of three parent datasets  $S_x$ ,  $S_y$  and  $S_z$  respectively. 431 Then a cost function (J) is constructed using the weights and the error variance of the parent 432 datasets, such that:

433 
$$J = \sigma_m^2 = w_x^2 \sigma_x^2 + w_y^2 \sigma_y^2 + w_z^2 \sigma_z^2$$
(25)

434 Where,  $\sigma_x^2$ ,  $\sigma_y^2$ , and  $\sigma_z^2$  are the estimated error variance for the three parent datasets. To have an 435 unbiased estimation of  $S_m$ , the sum of weights should be 1 ( $w_x + w_y + w_z = 1$ ), thus:

436 
$$J = w_x^2 \sigma_x^2 + w_y^2 \sigma_y^2 + (1 - w_x - w_y)^2 \sigma_z^2 \qquad (26)$$





437 Finally, by minimizing the cost function and the partial derivative of function J with respect 438 to  $w_x$  and  $w_y \left(\frac{\partial J}{\partial w_x} = 0, \frac{\partial J}{\partial w_y} = 0\right)$ , the optimal estimation of the weights are obtained as

439 
$$w_{\chi} = \frac{\sigma_y^2 \sigma_z^2}{\sigma_x^2 \sigma_y^2 + \sigma_x^2 \sigma_z^2 + \sigma_y^2 \sigma_z^2}$$
(27)

440 
$$w_{y} = \frac{\sigma_{x}^{2} \sigma_{z}^{2}}{\sigma_{x}^{2} \sigma_{y}^{2} + \sigma_{x}^{2} \sigma_{z}^{2} + \sigma_{y}^{2} \sigma_{z}^{2}}$$
(28)

441 
$$w_z = \frac{\sigma_x^2 \sigma_y^2}{\sigma_x^2 \sigma_y^2 + \sigma_x^2 \sigma_z^2 + \sigma_y^2 \sigma_z^2}$$
(29)

It can be seen that the weights are functions of the error variance of the parent datasets, and the product with larger error variance will be given smaller weights and vice versa. If only blending two soil moisture datasets, the least square method can be applied similar, with weights:

445 
$$w_x = \frac{\sigma_y^2}{\sigma_x^2 + \sigma_y^2}$$
(30)

446 
$$w_y = \frac{\sigma_x^2}{\sigma_x^2 + \sigma_y^2}$$
(31)

In this study, all three parent datasets (K, S, N) and combinations of two from them (KS,
KN, SN) are tested to generate hybrid datasets. By comparing the hybrid results using all three and
two out of three datasets, the optimal blending product can be identified using the least datasets
while maintaining the accuracy.

#### 451 **3.5 Goodness of fit**

In this study, 88 sites (40%) out of the total 215 stations were used for RK modeling, while the remaining 127 sites (60%) were used for out-of-sample validation. The Mean Absolute Error (MAE), Root Mean Square Error (RMSE), the Nash-Sutcliffe Efficiency (NSE) score, and the decomposition of Mean Square Error (MSE) by its mean difference (MSE\_MD<sup>2</sup>) and its pattern variation (MSE\_VAR) were used for the validation and comparison of hybrid datasets. The





- 457 decomposition MSE is helpful to diagnose whether the error is mainly due to the bias or variation.
- 458 A detailed description of above mentioned indicators (including equations) are provided in
- 459 Supplementary Text S1.
- 460 **4. Results and Discussions**

### 461 **4.1 Patterns of parent datasets**

462 Fig. 3 compares three statistic features, such as mean, standard deviation (STD) and 463 coefficient of variation (CV) of the absolute values of four soil moisture datasets over 127 out-of-464 sample sites. The four datasets include the in-situ soil moisture measurements, the RK-gridded soil 465 moisture from API (K-API) and the SMAP and NLDAS soil moisture. Compared with in-situ 466 measurements, the three soil moisture datasets (K-API, SMAP and NLDAS) show an underestimation of soil moisture (Fig. 3a) with bias ratios of -9%, -18% and -8%, respectively. 467 468 The large negative bias of SMAP L4 data indicates that the produce may overestimate dryness if 469 used alone without animalization or standardization. The largest values of STD are observed for 470 in-situ soil moisture, followed by SMAP and K-API, while NLDAS has the smallest STD values 471 (Fig. 3b). This is reasonable since field measurements are point scale and contain more information 472 on spatial heterogeneity and thus exhibit a higher degree of variability. As spatial resolution 473 increases, a smoother pattern and less variability are expected. Another reason that NLDAS has 474 the smallest STD is because the model-simulated soil moisture are solved at each grid cell using a 475 land surface model. SMAP presents the highest (and significantly larger than others) CV among 476 all datasets (Fig. 3c), which indicates that there is a large degree of variability in the SMAP soil 477 moisture. The large CV of SMAP is jointly attributed to its small mean value and large STD. In 478 contrast, the NLDAS has the smallest CV among all datasets (Fig. 3c), which is mainly due to its 479 smallest STD among all datasets. K-API has the most comparable CV values and smaller range





- 480 than that of in-situ measurements. This indicates that K-API is the product that is most similar to
- 481 the in-situ measurements.





Fig. 3 Comparison of the (a) means, (b) standard deviation and (c) coefficient of variation of four datasets over 127 out-of-sample sites. The four data sets include the in-situ soil moisture measurements, the kriged soil moisture from API (K-API) and the SMAP and NLDAS soil moisture. All datasets are in the format of absolute values.

487 **4.2 Errors of parent datasets** 

488 Fig. 4 shows the error (uncertainties) estimated using TC, REV and RK using different 489 combinations of parent datasets. Fig. 4 (a)-(d) reveal that the error estimated from TC depends on 490 the parent triplets used. Changing the parent triplets changes the magnitude and ranking of the 491 parent datasets. For example, the errors estimated for in-situ data are higher when it is grouped 492 with SMAP and NLDAS (Fig. 4a), than when it is grouped with K-API and NLDAS (Fig. 4b) or 493 with K-API and SMAP (Fig. 4c). In addition, in-situ data have significantly higher errors than 494 SMAP in Fig. 4(a), while Fig. 4c shows in-situ data have significantly lower errors than that of 495 SMAP. Similar, contrasting results are also found between In-situ and NLDAS by comparing Fig. 496 4a and Fig. 4b. These results indicate that TC only provides a relative measure of accuracy. Yilmaz 497 et al. (2012) also noted that TC is not ideal for capturing absolute error and can only estimate the 498 relative error. They found that the absolute error depends on the reference dataset selected.









Fig. 4 (a)-(d) Estimated errors (uncertainties) using TC with different combination of four datasets 500 (In-situ, K-API, SMAP and NLDAS soil moisture). (e) Estimated errors using REV for four 501 502 datasets; and (f) Estimated errors using RK for three datasets (K-API, SMAP and NLDAS soil 503 moisture). The datasets used here are absolute soil moisture over 127 out-of-sample stations. The 504 same color indicates the same dataset used in TC and REV analysis. Note, both TC and REV 505 provide one error estimation through the entire period (1372 days) for each station, while RK 506 provides one error estimation at each day for each station. Therefore, there are 127 points within 507 the boxplots using TC and REV (Fig. 6a-e), while there are 174244 points (127 sites\*1372 days) 508 within the boxplots using RK (Fig. 6f).

509 Moreover, our study reveals that the relative errors of a single soil moisture dataset, 510 estimated from TC, are sensitive to the choice of input datasets (Fig. 4a-d). Thus, caution should 511 be used when selecting the input datasets for TC analysis. In this study, K-API, SMAP and NLDAS 512 are used for soil moisture blending with TC error estimation (Fig. 4d). The error ranking of the





513 three datasets from TC are K-API>API>NLDAS (Fig. 4d), and the differences among the three

514 datasets are statistically significant.

515 Our study also demonstrates that the measurement units (Fig. S4) do not impact the relative 516 relationship (error ranking) between the different datasets. It is also interesting to note that the in-517 situ data always have relatively larger error when compared with other datasets using TC (Fig. 4a 518 to 8c). This may due to its high spatial representativeness errors (Miralles et al., 2010;Crow et al., 519 2012b;Yilmaz et al., 2012). If this is true, then using in-situ data as the ground truth for validation 520 may not be the best choice.

521 The REV (Fig. 4e) and RK (Fig. 4f) can also be used to estimate error in different datasets. 522 REV (Fig. 4e) and RK (Fig. 4f) provide consistent results and both indicate that K-API has significantly smaller errors than SMAP and NLDAS, while SMAP and NLDAS are similar (i.e., 523 524 there is not a statistically significant difference between the two). Although REV is a relative ratio 525 between measurement error variance to real soil moisture variance, unlike TC, it does not depend 526 on another dataset during calculation. Therefore, REV provides a consistent estimate for each 527 product that does not change depending on the other datasets that are included. By comparing Fig. 528 4(b)-(c) with Fig. 4(e), in-situ data have larger errors than K-API based on both the TC and REV 529 methods.

Fig. 5A and 5B illustrate the spatial distribution of errors estimated using TC (Fig. 5A) and REV (Fig. 5B) for the three parent datasets (K-API, SMAP and NLDAS). When using TC estimates, the results agree well with Fig. 4d. NLDAS has the smallest error among the three, with low errors found in the central and southwestern portions of the study area. The K-API has larger errors near the Gulf of Mexico and in Oklahoma, while SMAP has larger errors scattered throughout the study region. On the contrary, when using REV, the K-API has the smallest errors





536 among the three datasets over the entire study area, while SMAP data has larger errors in the

537 western part of the study region and NLDAS has larger errors in the eastern part of the study region.



538

Fig. 5 Spatial maps of errors (A and B) and LSW weights (C and D) based on errors from TC and
REV for each parent product. All products are in the format of absolute soil moisture. The black
circles indicate the locations of 127 out-of-sample stations.

542 4.3 Weights of parent datasets

Fig. 5C and 5D reveal the spatial distribution of LSW weights calculated using the errors estimated from TC and REV. Fig. 6 compares the weights derived from TC, REV and RK based on 127 out-of-sample stations. Generally, larger weights are given to the product with smaller





546 errors (Fig. 5), and the weighting of each product are not impacted by the data format used (Fig. 547 S5). When using TC, larger weights are given to the NLDAS (median value of 0.42) and SMAP 548 (median value of 0.32), while K-API tends to be given lower weight, with a median value about 549 0.2 (Fig. 6a). In contrast, higher weights are given to K-API (median value of 0.6), especially in 550 the central part of study area, when REV is used, while smaller weights are given to SMAP and 551 NLDAS with a median value of 0.2 for both (Fig. 6b). SMAP has higher weights in the eastern 552 part of the study region than in the west. NLDAS is given higher weights in the western part of the 553 study region (Fig. 5D). In general, the weighting scheme derived from TC (Fig. 5C and Fig. 6a) 554 has patterns that are opposite to those based on REV (Fig. 5D and Fig. 6b). It is also interesting to 555 note that the weighting scheme derived from RK (Fig. 6c) is similar to the mean weighting (0.33 556 weighting line in green). This analysis has demonstrated that the choice of weighting scheme can 557 have a substantial influence on the relative weights that are assigned to each product.



558



563 Considering each dataset has errors and the inclusion of additional datasets may increase 564 the uncertainty, therefore it is important to evaluate whether it is necessary to use all three soil 565 moisture datasets to achieve the highest accuracy. Therefore, we iteratively selected pairs of the





- parent datasets and generated a hybrid soil moisture product. The results for each combination are provided in Fig. 7. Similar to the results from Fig. 6 and Fig. S5, the TC and REV provide opposite weighting results, and the weighting from RK is similar to the simple average (equal weight of two datasets). This analysis also demonstrates that the data format has little impact on the results,
- 570 especially for REV (right column in Fig. 7).



571

Fig. 7 Weights of soil moisture products in the format of anomalies (top row) and percentiles
(bottom row) based on least square weighting using errors estimated from TC (left column) and
REV (right column). The green line indicates the simple average weighting scheme with equal





575 weight (0.5 here) for each product. K-A is short for regression kriging using API, K-S is short for

576 regression kriging using SMAP, and K-N is short for regression kriging using NLDAS data.

577 **4.4 Evaluation of hybrid results** 

578 Fig. 8 evaluates the hybrid results of soil moisture anomalies from different methods 579 (simple average (AVE), REV and TC) based on MAE, RMSE, MSE\_MD<sup>2</sup>, MSE\_VAR and NSE. 580 The assessment of hybrid datasets in other formats (absolute values, percentiles and RK-gridded 581 soil moisture) are presented in Fig. S6, S7 and S8, respectively. In terms of MAE (Fig. 8a), K-API 582 has the smallest errors (MAE<sub>median</sub> = 0.037) among the three parent datasets, while SMAP has the 583 largest errors (MAE<sub>median</sub> = 0.050) and NLDAS falls in the middle (MAE<sub>median</sub> = 0.046). The 584 analysis demonstrates that after blending the three parent datasets, the merged datasets do not 585 outperform the parent products, especially in comparison to K-API. Although the MAEs of the 586 AVE3, REV3 and TC3 are significantly smaller than that of SMAP and NLDAS (boxes' notches 587 do not overlap in Fig. 8a), they are not statistically significantly different from K-API (overlapped 588 notches in Fig. 8a). Our findings contrast with those of Yilmaz et al. (2012), who found that a 589 merged soil moisture product generated from ALEXI, Noah and LPRM using TC is more accurate 590 than the individual parent products. However, our study evaluated different parent datasets, and 591 the TC-based weights did vary with the input datasets (Fig. 4a-d). Since the K-API was found the 592 most accurate among the three parent products, and Yilmaz et al. (2012) did not use this product, 593 our results are not directly comparable. But both our study and Yilmaz et al. (2012) utilized 594 NLDAS Noah, and both studies found that the hybrid datasets that use NLDAS have smaller errors 595 (MAEs and RMSEs).









Fig. 8 Comparison of parent and hybrid products of soil moisture anomalies using different
blending methods (simple average (AVE), REV- and TC-based) on (a) MAE, (b) RMSE, (c) NSE,
(d) MSE\_MD<sup>2</sup> and (e) MSE\_VAR. The green line indicates the median error of K-API among 127
out-of-sample stations. AVE3, REV3 and TC3 respectively indicate the hybrid results using all
three parent products based on simple average, REV and TC analysis.

The lack of significant improvement of the merged datasets verses the parent products may be attributed to (1) sub-optimal weights because neither TC and REV consider temporal variations in errors. Both TC and REV give only one error estimation at each location for the entire period. In reality, the error in each parent product likely varies both spatially (from location to location) and temporally (from day to day). Thus, the temporally fixed error estimation that is provided by TC and REV is likely not optimal. (2) The in-situ measurements cannot be considered the "truth"





608 because they are point measurements that may not reflect the soil moisture value for each 4 km 609 grid cell. In addition, the use of in situ measurements as truth may also be biased towards the K-610 API. As we found in Fig. 4, the in-situ soil moisture have large spatial representativeness errors. 611 Even for the densest in-situ network used in this study, such as the Oklahoma Mesonet, there is 612 only one station within each 4-km grid cell. Considering K-API is generated using in-situ soil 613 moisture, the error patterns of K-API may follow closely with that of in-situ data, which is also 614 confirmed by Fig. 4. This bias may result in smaller errors of K-API when evaluated using in-situ 615 data. (3) The validation data are not spatially exhaustive. Although 60% (127) of total stations 616 have been used in the validation, they are still relatively sparse and not evenly distributed in the 617 study area. Fig. 1 shows most validation stations are clustered in Oklahoma and west Texas, while 618 few stations are located in south Texas, Arkansas and Louisianan. It is possible that the places 619 where hybrid results showed an improvement over the parent product (K-API) are not well 620 captured using only 127 stations.

When comparing the results from the various blending methods, there is no statistically significant difference between the merged datasets using AVE, REV or TC, even though the REVweighted datasets perform slightly better (slightly lower MAE/ RMSE, and slightly higher NSE) than other two methods. This indicates that the more complicated blending methods (LSW using TC and REV estimates) are not necessarily superior to the simple average. This result agrees with the findings from Yilmaz et al. (2012) that the merged soil moisture anomalies using LSW and TC estimates did not outperform the equally-weighted results.

628 Considering the different blending methods correspond to different weighting schemes 629 (Fig. 7 and Fig. S5), this result suggests two possible conclusions: (1) if the optimal weighting 630 (either TC- or REV-based) has been achieved, then the weighting scheme does not have a





631 significant impact on the merged results; (2) if the optimal weight has not been achieved, then 632 there is still an optimal weighting scheme to be identified that can significantly reduce the errors. 633 The evaluation of hybrid datasets using the two parent datasets (Fig. 8) suggests the first conclusion 634 (weighting scheme does not have a significant impact on the merged results) is most likely. 635 According to Fig. 6, the weights calculated using AVE, REV and TC-based methods have covered 636 all the possible weighting schemes of two datasets, including equal weighting (AVE) and two 637 cases of unbalanced weighing (the product given larger weights by TC will be given smaller weights by REV). Still, no significant differences are observed when different weighting schemes 638 639 are applied. In this case, the simple average (equal weighting) is recommended for soil moisture 640 blending, as the more complicated weighting schemes do not outperform this approach.

It is also found that the combination of SMAP and NLDAS (e.g., AVE(S,N), REV(S,N) 641 642 and TC(S,N)) result in a statistically significant increase in MAE values, while combining K-API 643 with either SMAP or NLDAS has similar accuracy as the merged datasets using all three datasets. 644 This indicates (1) incorporating three datasets may not be necessary to generate the most accurate 645 soil moisture product and, (2) in-situ measurement is valuable for improving the accuracy of 646 blended soil moisture datasets. K-API is the only dataset that incorporates the in-situ 647 measurements, and it has the lowest error among all parent datasets (Fig. 8). These results are 648 consistent when RMSE (Fig. 8b) or NSE (Fig. 8c) as considered instead of MAE.

The impact of data format on hybrid results is examined by comparing Fig. 8 with Fig. S6 to S8. It is found the MAE of hybrid datasets using anomalies (about  $0.035 \text{ m}^3\text{m}^{-3}$ ) is lower than that of the absolute datasets (about  $0.055 \text{ m}^3\text{m}^{-3}$ ). The hybrid datasets using anomalies and percentiles also have higher NSE (around 0.6) values than that of (around 0.3) absolute and RKgridded datasets. The improved performance of the anomaly and percentile datasets are mainly





due to the removal of bias error (MSE MD<sup>2</sup>). Using Eq.S2 to Eq. S4 from the Supplementary Text, 654 the MSE can be decomposed to differences in the mean or bias (MSE MD<sup>2</sup>) and differences in the 655 656 variance (MSE\_VAR). It is found that the bias for both the soil moisture anomalies (Fig. 8d) and 657 soil moisture percentiles (Fig. S6d) are close to zero. Therefore, most of their error is due to 658 differences in variance (Fig. 8e and Fig. S6e). This is reasonable since both anomalies and 659 percentiles are methods for standardizing the datasets and they are useful for removing the 660 systematic bias between different data sets (Ford et al., 2015; Zhang et al., 2017a). In contrast, the 661 errors of absolute soil moisture (Fig. S7d and S7e) and RK-gridded absolute soil moisture (Fig. S8d and S8e) have similar proportions of error that are due to bias  $(0.02 \text{ m}^3\text{m}^{-3})$  and variance  $(0.02 \text{ m}^{-3})$ 662 663 m<sup>3</sup>m<sup>-3</sup>). This indicates when using soil moisture data in absolute formats, the bias-related errors are present in the final datasets. 664

665 Fig. 9 shows maps of soil moisture anomalies on March 31, 2015 for each of the parent 666 datasets (a-c) and the merged datasets based on using three products (d-f) and two products (g-i). 667 There are distinct differences between the three parent datasets. The K-API (Fig. 9a) has a smoother pattern than the other two datasets. In addition, the in-situ anomalies (with blue dots 668 669 indicate positive anomalies and red dots indicate negative anomalies) seem to match better with 670 that of K-API. However, the differences between the maps become less distinguishable after blending the three datasets using AVE (Fig. 9d), REV- (Fig. 9e) and TC-based LSW (Fig. 9f). 671 672 There is also no dramatic change of spatial patterns when changing the number of input datasets from three (Fig. 9d) to two (Fig. 9g-i) using simple average, which agrees with the results from 673 674 Fig. 8.









**Fig. 9** Maps of parent and hybrid products of soil moisture anomalies on March 31, 2015. (a)-(c) present the three parent products (K-API, SMAP and NLDAS); (d)-(f) respectively represent the hybrid product from 3 parent products using simple average, least square weighting using REV estimated errors and TC estimated errors; (g)-(i) represent the hybrid products using simple average of two parent products. The red dots represent the in-situ stations with negative anomalies, the blue dots present the in-situ stations with positive anomalies, and the empty circles present the in-situ stations with no measurement on that day.







kriging performance declines as the data variation increases (Schläpfer and Schmid, 687 1999;Martínez-Cob, 1996;Li and Heap, 2011;Keskin and Grunwald, 2018). Gotway et al. (1996) 688 689 found that the performance of both inverse distance weighting and ordinary kriging declines as 690 CV increases when mapping soil properties. Based on a review of more than 50 spatial 691 interpolation studies, Li and Heap (2011) found that data variation has a significant impact on the 692 performance of spatial interpolation methods. Generally, accuracy decreases as CV increases. 693 Keskin and Grunwald (2018) also found an inverse relationship between the accuracy of RK 694 models and the variation of soil properties based on a review of more than 70 studies of RK model.



695

696 Fig. 10 The spatial distribution of MAE of AVE(K,N), K-API and ITS index using anomalies soil

<sup>697</sup> moisture.





- The correlation between temporal stability and error is further demonstrated in Fig. 11. The
- 699 results show that the MAE has a higher correlation with ITS than REV or CV. This finding is
- 700 consistent for all data formats (absolute, anomalies and percentiles). As the variability in the data
- 701 increases, the predictive accuracy of RK decreases.



702

Fig. 11 Relationship between MAE and three indices (ITS, REV and CV) using absolute soil
moisture (first row), anomalies (second row) and percentiles (third row).

Another interesting finding from Fig. 10 is that the MAEs of K-API (red circles) are generally smaller than that of AVE(K,N) (blue circles), especially in Oklahoma and northwest Texas. However, in places where in-situ measurements are sparse, such as the central to the south





708 of Texas and east Arkansas, the AVE(K,N) has similar and sometimes smaller MAE than K-API. 709 This indicates when in-situ measurements are sparse, using additional sources of soil moisture 710 information (such that from NLDAS) may help to increase the accuracy. To further confirm this 711 point, the assessment of K-API and AVE(K,N) with varying numbers of sampling points and 712 different sampling schemes are provided in Fig. 12 using (a) NSE and (b) MAE, respectively. 713 Three different sampling schemes are compared, including tail sampling (choosing sampling 714 points from the tail of ascending ITS), head sampling (choosing sampling points from the head of 715 ascending ITS) and even sampling (choosing sampling points evenly from the ascending ITS). 716 Since ITS is an indicator of the temporal stability, a more "representative" site is characterized 717 by a lower ITS. Therefore, the tail sampling scheme selects the least "representative" sites for RK, 718 head sampling selects the most "representative" sites for RK, while even sampling selects the sites 719 most close to the population distribution for RK.





**Fig. 12** Assessment of K-API and AVE(K,N) under different sampling scheme and sampling points in terms of (a) NSE and (b) MAE. Both the NSE and MAE are calculated using the out-ofsample stations over the entire study period. "Tail Sampling" indicate choosing sampling points from the tail of ascending ITS (denoted by line with square), "Head Sampling" indicates choosing sampling points from the head of ascending ITS (denoted by line with asterisk), while "Even





Sampling" indicates choosing sampling points evenly from the ascending ITS (denoted by linewith dot).

728 A positive NSE trend is observed as sample density increases (Fig. 12a). The most 729 significant improvement is observed for K-API using tail sampling (black line with squares). When 730 used alone, the K-API under tail sampling shows the lowest NSE values among all datasets using 731 all sampling schemes. However, when combined with the NLDAS, or the AVE(K,N) product (red 732 line with squares) using tail sampling shows comparable NSE values with other product and other 733 sampling schemes. Generally, the NSE variation of AVE(K,N) (red shaded area) under different 734 sampling schemes is much smaller than that of K-API product (grey shaded area). This indicates 735 that the hybrid product AVE(K,N) can reduce uncertainties and it is especially helpful for reducing 736 the errors caused by using too few stations or using unrepresentative stations, as compared with 737 the K-API product.

738 A decreasing trend in MAE is observed as sample density increases using both the tail and 739 even sampling schemes, which is consistent with the NSE results (Fig. 12b). Although the 740 AVE(K,N) has a larger MAE than K-API when using even sampling, the differences are not 741 statistically significant (p>0.05) based on ANOVA. However, when using tail sampling, the 742 AVE(K,N) shows a statistically significant (p<0.05) improvement over K-API, especially at lower 743 sample densities. The MAE of K-API is 0.055 m<sup>3</sup>m<sup>-3</sup> using 15 stations, but it drops to only 0.004 744  $m^{3}m^{-3}$  when AVE(K,N) is used. This indicates when sampling sites are less representative and 745 sparsely distributed, adding an extra source of soil moisture information (e.g., the product of 746 AVE(K,N)) significantly improves the accuracy. This finding has practical significance for real-747 world applications, where achieving dense and representative sampling is always challenging. The 748 Oklahoma Mesonet is a unique and uncommonly densely network, in most cases, soil moisture





stations are sparsely distributed. In these cases, the hybrid product, AVE(K,N), may perform better

than K-API.

751 It is also worth noting that the sampling scheme has a larger impact on RK results than the 752 sample density. Although increasing the station density generally improves the accuracy, the 753 improvement gradually decreases and it levels off when the number of stations is >50 (Fig. 12a 754 and b. This agrees well with previous findings (Yuan and Quiring, 2017). In contrast, the change 755 in the sampling scheme may yield a completely different trend of MAE. As shown in Fig. 12(b), 756 an increasing trend of MAE is observed for both K-API and AVE(K,N) when head sampling is 757 adopted. This increasing trend may due to the higher degree of heterogeneity in validation data of 758 head sampling. Considering the head sampling selects the most representative sites for RK 759 modeling, while the remaining sites are less representative and have larger temporal variability, 760 which may yield larger errors. Thus, the head sampling should be avoided for RK modeling, and 761 the even sampling scheme or the bootstrapping random sampling may be more reasonable. In 762 reality, the sampling sites are always a mix of more and less representative sites.

In summary, both increasing sample density and adding an extra source of soil moisture data can improve the accuracy, especially when the station representativeness and station density are low (Fig. 12). Increasing the station density helps to capture the spatial variation of the target variable, while using an additional source of soil moisture tends to lead to a more substantial improvement in accuracy.

#### 768 5. Conclusions

This work is the first study that compared multiple methods (REV-, TC- and RK-based LSW and simple average) and considered multiple data formats (absolute, anomalies and percentiles) for soil moisture blending from multiple sources, including satellite (SMAP L4-SM),





772 model (NLDAS-V2 Noah), and in-situ measurement. All soil moisture datasets are generated at 4-773 km spatial resolution and updated daily. The results indicate that the SMAP data have a large 774 negative bias (-18%) compared with in-situ measurements (Fig. 3), thus it should be used with 775 caution without standardization, especially for drought monitoring. Both the absolute and relative 776 errors from TC vary with the input datasets (Fig. 4). In contrast, REV provides an absolute measurement error, but in a relative (ratio) format. Generally, the TC-estimated error variance tend 777 778 to show the opposite pattern as REV. That is, the soil moisture products that have a low error 779 variance based on REV, tend to have a larger error variance using TC. The RK-estimated error 780 variances are similar for different datasets (Fig. 4 and Fig. 6).

The hybrid results are not sensitive to the weighting scheme that is used. There were no 781 statistically significant differences between the hybrid datasets when using different weighting 782 783 methods (TC, REV, RK). There is also no significant advantage to using more complicated 784 weighting (LSW) over the simple average (AVE). The merged products from two datasets (with 785 one fixed as K-API) are found to have comparable accuracy with merged products using three datasets. This indicates that in-situ measurements are valuable for improving the accuracy of 786 787 blended soil moisture datasets. In terms of different data formats (absolute, anomalies, percentiles 788 or RK-gridded soil moisture), the NSE for anomalies and percentiles (0.60) is higher than that of 789 absolute soil moisture (0.25) mainly due to reduced biases when using anomalies and percentiles 790 (Supplementary, Fig. 6-8). However, the relative errors (or error ranking) is independent of the 791 data format used. The errors from RK are highly correlated with ITS (Fig. 10 and Fig. 11). This 792 indicates that the predictive capability of RK decreases as the heterogeneity increases.

Both K-API and AVE(K,N) are recommended as optimal soil moisture datasets.
Considering the PRISM dates back to 1895 and NLDAS dates back to 1979, a long-term soil





795 moisture record can be generated by adopting the methods in this study. It is also found K-API can 796 be used alone if the station density is high (>50 stations in our case). However, when the station 797 density is low (<50 stations) and the stations are not representative, the hybrid product (AVE(K,N)) 798 has significantly better performance. Increasing station density helps to capture the spatial 799 variation of the target variable, while using an extra source of soil moisture information may help 800 to reduce the overall uncertainties (Fig. 12). This has significant practical implications for real-801 world applications because achieving a high density of stations that are spatially representative is 802 always challenging.

803 Finally, there are some limitations of this study, such as: (1) the soil moisture products used 804 in this study were extracted with time slot covering 7 am. However, a temporal mismatch between 805 different soil moisture products may still exist due to their different temporal resolutions. Future 806 work can adopt the daily average or other methods to ensure the temporal coherence of different 807 datasets. (2) this study only considered precipitation (API) in soil moisture kriging, while in future 808 studies other variables, such as soil properties, land cover and topography (DEM), may be helpful 809 for soil moisture estimation (Ochsner et al., 2019) and should be considered to improve the 810 accuracy using RK. (3) Geographically weighted regression kriging (GWRK) (Brunsdon et al., 811 1996; Fotheringham et al., 2003) considers the spatially non-stationarity relationships between 812 dependent variable and independent variables and weights the regression points by their distance 813 to the target point. Therefore, it may be more accurate than RK (Yang et al., 2019;Kumar et al., 814 2012), and should be explored in future studies for estimating soil moisture. (4) Further study is 815 required to test whether these conclusions are valid in other parts of the world.

816





### 817 Data Availability

- All datasets used in this study are publicly available. The SMAP data can be accessed through
- 819 National Snow and Ice Data Center (http://nsidc.org/data/smap). The NLDAS-V2 Noah soil
- 820 moisture products can be accessed through NASA's Earth Observing System Data and Information
- 821 System (EOSDIS) (https://disc.gsfc.nasa.gov/). The in-situ soil moisture measurements can be
- 822 accessed through the National Soil Moisture Network (http://www.nationalsoilmoisture.com/).

### 823 Author contribution

- 824 NZ designed and carried out the study under supervision of SQ. NZ prepared the original
- 825 manuscript and all the co-authors contributed scientifically by providing editing, comments and
- 826 suggestions.
- 827 **Competing interests.** The authors declare that they have no conflict of interest.

#### 828 Acknowledgement

- 829 This work was financially supported by the NOAA Modeling, Analysis, Predictions and
- 830 Projections (MAPP) "Developing National Soil Moisture Products to Improve Drought
- 831 Monitoring" project (Grant number: NA17OAR4310136).

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