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Estimating soil moisture in gullies from adjacent upland measurements through different observation operators

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SUMMARY

Soil moisture datasets in large gullies are rare due to the difficulty of direct sampling in such landform. This study attempted to estimate spatial soil moisture averages in gullies from measurements of adjacent uplands by using observation operators, based on three-year soil moisture datasets in a gully catchment of the Loess Plateau. Soil moisture datasets in 2010 and 2011 were used for developing observation operators and those in 2012 were used for validation. Several nonlinear and linear methods including cumulative distribution function (CDF) matching method, linear regression (LRG) method, mean relative difference (MRD) method and linear rescaling (LRS) method were used to define observation operators. The results showed observation operators significantly improved the predictions compared to when using spatial averages of uplands as the direct surrogates for gullies. Among different methods, the CDF matching method performed best in estimating soil moisture in gullies followed by the LRG, LRS and MRD methods. Validation analysis showed that the linear observation operators such as LRS, MRD and LRG had better temporal transferability than the nonlinear operators. The MRD observation operators for various layers could successfully transfer in time whereas temporal transferability only succeeds to a limited extent for other observation operators. Furthermore, the MRD, LRG and LRS methods exhibited better vertical transferability than the CDF matching method. However, the transferability of observation operators across the whole root zone layers was not successful.

1. Introduction

Gullies represent a serious land degradation form, which occur globally in areas with crusting soils, such as loess (European belt, Chinese Loess Plateau, North America), sandy soils (Sahelian zone, north-east Thailand) and dispersive soils prone to piping and tunneling (Valentin et al., 2005). Although gullies are not directly involved in agricultural activities, they are closely associated with many hydrological processes since they geographically connect hillslopes and channels. Thus the hydrologic characteristics of gullies may greatly affect watershed discharge and sediments deposition. Several studies have shown that erosion from gullies were responsible for most deposition of sediments in downstream pools (Li et al., 2003; Valentin et al., 2005). Surface runoff and severe disturbance of vegetation organization (then degrades soil structure) are usually two necessary conditions for water erosion happening which is responsible for the occurrence and evolution of gullies (Tang, 2004). In semiarid areas, soil moisture is a key eco-hydrological variable (Ludwig et al., 2005). It switches the generation of surface runoff (Brocca et al., 2008) and affects the vegetation growth and distribution (Rodriguez-Iturbe et al., 1999). Therefore, the knowledge of soil moisture is critical for understanding gully evolution and the eco-hydrological processes in gullies (Gao et al., 2011).

Several efforts have been made to collect soil moisture in gullies (van den Elsen et al., 2003; Melliger and Niemann, 2010; Gao et al., 2011). These studies reported different values and behaviors of soil moisture between gullies and hillslope uplands. However, soil moisture datasets in large gullies are still scarce, and widespread in situ sampling in large gullies is difficult and costly due to steep slopes and complex topography. Remote sensing sensors/techniques are promising methods for soil moisture retrieving for ungauged areas (Brocca et al., 2011; Khan et al., 2011). However, ground validation and calibration were rarely conducted in places where gullies are prevalent. Gao et al. (2013) found that soil moisture time series in gullies could be reliably estimated from

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observations of adjacent uplands where soil moisture sampling are much easier. In their study, the primary method for soil moisture estimation in gullies was time stability analysis which was induced by Vachaud et al. (1985) to characterize the time-invariant associations between spatial locations and classical statistical parametric values. They found more than one upland location was temporally stable with respect to spatial averages in gullies. Nevertheless, time stability features of soil moisture fields are largely affected by many geographical and meteorological factors including topography, soil properties, vegetation and precipitation (Grayson and Western, 1998; Mohanty and Skaggs, 2001; Jacobs et al., 2004, 2010; Hu et al., 2010; Joshi et al., 2011). However, only a few studies have conducted validation to test the temporal robustness of time-stable locations (e.g., Martínez-Fernández and Ceballos, 2005; Jacobs et al., 2010). Therefore, it is uncertain as to whether a time-stable location maintains its rank with time or if the rank of surface soil moisture is consistent with time-stable observations at deeper depths (Han et al., 2012; Heathman et al., 2012).

In recent years, observation operators termed by Drusch et al. (2005) were used to transform point soil moisture observations to spatial averages for a field. De Lannoy et al. (2007) and Han et al. (2012) derived observation operators mainly by cumulative distribution function (CDF) matching method. They found that field soil moisture averages were accurately estimated from point observations by CDF matching method. Other methods including linear regression method and mean relative difference method were also used to define observation operators, and similar results were reported (Han et al., 2012). Moreover, Han et al. (2012) tested the spatial–temporal transferability of observation operators. They found observation operators successfully transferred in space (two different fields and two different layers), whereas failed to transfer between two years. Observation operators have also been used to transform remote sensing soil moisture to model predictions or in situ soil moisture measurements (Drusch et al., 2005; Brocca et al., 2011; Matgen et al., 2012).

On the Loess Plateau of China, large gullies (with depth from several meters to tens of meters, even deeper than 100 m) are important compositions of landscapes. Especially in the hilly region of the Loess Plateau, gullies occupy 50–60% of the total area with densities of 3–8 km km^{-2} (Huang and Ren, 2006). In this study, we attempt to propose different nonlinear and linear methods including cumulative distribution function (CDF) matching, linear regression (LRG), mean relative difference (MRD) and linear rescaling (LRS) to define observation operators for transforming soil moisture of hillslopes (uplands) to spatial averages of gullies. Most of these methods have been widely used for validating satellite soil moisture products and assimilating remote sensing data into land surface models with the purpose of bias reduction. However, the feasibility for these methods in rescaling hillslope soil moisture into gullies has never been documented. Moreover, the estimation errors for various observation operators were evaluated. The temporal robustness of these observation operators and their transferability across root-zone layers were also tested. Note that this study only focuses on spatial averages of soil moisture in gullies and uplands.

2. Methods

2.1. Methods for defining observation operators

The nonlinear cumulative distribution function (CDF) matching method and linear methods including linear regression (LRG), mean relative difference (MRD), and linear rescaling (LRS) methods were used to define observation operators. A summary of the characteristics of these methods was indicated in Table 1.

2.1.1. CDF matching method

Cumulative distribution function (CDF) matching method has been used in many hydrological applications with the purpose of bias correction, data assimilation, and rescaling of different sets of observations. Reichle and Koster (2004) used this technique to define observation operators for bias reduction in satellite-retrieved surface soil moisture. Drusch et al. (2005) derived observation operators by using this method for direct assimilation of remote sensing data into model results. Liu et al. (2011) employed this approach to merge soil moisture retrieves of passive and active satellite sensors. The CDF matching method has also been used for spatial soil moisture averages estimation. De Lannoy et al. (2007) and Han et al. (2012) used the CDF matching method to derive observation operators for field soil moisture averages estimation from point observations. In their studies, observation operators were presented in the form of polynomial equations. The CDF matching method, in this study, was used as the primary method to define observation operators through polynomial fit. A pre-analysis was conducted to determine the optimal order of polynomial equations, although the third-order polynomial equation was often employed (Drusch et al., 2005; De Lannoy et al., 2007; Han et al., 2012). The results of pre-analysis showed that the fifth order was best (Fig. 1) and thus was selected for analysis in this study. The detailed procedures of the CDF matching method used are summarized as follows:

(1) Rank the spatial averages of soil moisture content for uplands (μ) and gullies (η).
(2) Compute the differences in soil moisture between the corresponding elements of each ranked dataset.

$$\delta'_k = \eta'_k - \mu'_k \tag{1}$$

where η'_k and μ'_k denote the ranked spatial averages for gullies and uplands, respectively, for k = 1, 2, ..., T, where T denotes the number of the datasets.

(3) Apply the fifth-order polynomial fit to the ranked soil moisture values and the corresponding differences.

$$\tilde{\delta}'_k = k_0 + k_1\mu'_k + k_2\mu'^2_k + k_3\mu'^3_k + k_4\mu'^4_k + k_5\mu'^5_k \tag{2}$$

(4) Compute the estimated spatial averages in gullies from the estimated difference.

$$\tilde{\eta}'_k = \mu_k + \tilde{\delta}'_k \tag{3}$$

Eq. (2) serves as the observation operator for each dataset to remove the systematic differences of spatial averages between gullies and uplands.

2.1.2. Linear methods

2.1.2.1. LRG method. Linear regression analysis has been shown an effective method to upscale point measurements to field averages (De Lannoy et al., 2007; Han et al., 2012; Teuling et al., 2006). In this study, a simple linear relationship was used as the third method to estimate spatial averages in gullies. This method was as follows:

$$\tilde{\eta}_j = b + a\mu_j \tag{4}$$

where b and a are the intercept and the slope coefficient, respectively. In this method and the following linear methods, only time series datasets were used for analyses. Here j = 1,2,...,N, where N is the total number of sampling events.

2.1.2.2. MRD method. This method is based on the concept of mean relative difference (MRD) between spatial averages for uplands and gullies. For a given depth, the relative difference between spatial soil moisture averages for uplands (μ_j) and gullies (η_j) is defined as:

$$\beta_j = \frac{\mu_j - \eta_j}{\eta_j} \tag{5}$$

Table 1
Overall description of different methods for defining observation operators.

Full name	Abbreviations	Type	No. of parameters	The highest order
Cumulative distribution function matching	CDF matching	Nonlinear	6	5
Linear regression	LRG	Linear	2	1
Mean relative difference	MRD	Linear	1	1
Linear rescaling	LRS	Linear	4	1

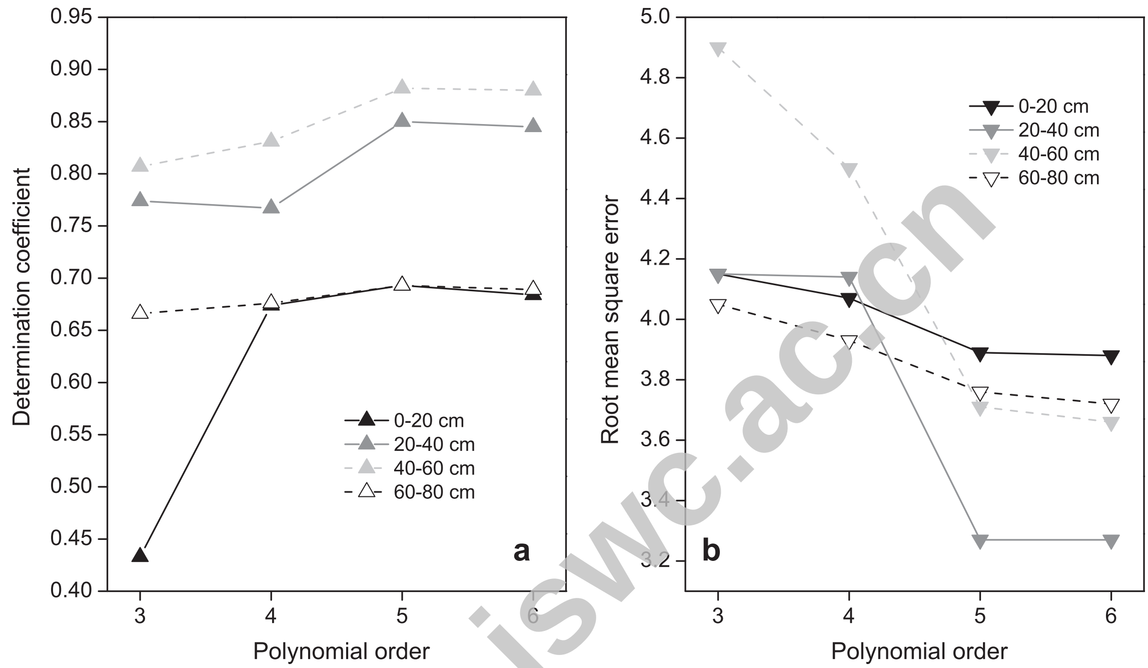

Fig. 1. Pre-analysis statistics of determining the optimal order of polynomial fitting equations by using cumulative distribution function (CDF) matching method, (a) determination coefficient and (b) root mean square error.

Rearrange Eq. (6), η_j can be expressed as:

$$\eta_j = \frac{\mu_j}{1+\beta_j} \tag{6}$$

Since similar soil moisture time series existed for uplands and gullies (Fig. 2), we assumed a constant offset β, i.e., the temporal mean of β_j over the study period, to represent β_j. Then spatial averages for gullies could be estimated as:

$$\tilde{\eta}_j = \frac{\mu_j}{1+\beta} \tag{7}$$

where T is the total number of sampling events when soil moisture was sampled simultaneously for gullies and uplands.In fact, the MRD method is a special LRG method as assuming $a = \frac{1}{1+\beta}$ and $b = 0$. However, the MRD method differs from the general LRG method because a special parameter β is needed to be calibrated.

2.1.2.3. LRS method. LRS method has been widely used to validate satellite soil moisture products (e.g., Brocca et al., 2010a; Draper et al., 2009). One distinctive characteristic for this method is that the rescaled values have the same temporal mean and variance with the original datasets. Here, we will test whether this method was viable to define observation operators for estimating spatial averages of gullies. This method was described as follows:

$$\hat{\eta}_j = (\mu_j - \bar{\mu})\frac{s(\eta)}{s(\mu)} + \bar{\eta} \tag{8}$$

where $\hat{\eta}_j$ is the rescaled spatial average of gullies; $\bar{\mu}$ and $\bar{\eta}$ are the temporal means of μ_j and η_j , respectively; $s(\eta)$ and $s(\mu)$ are the standard deviation of μ_j and η_j in time, respectively.

2.2. Validation method

Previous studies have shown that short-term sampling may lead a failure of temporal transferability of observation operators (Han et al., 2012). Therefore, we used the soil moisture datasets in 2010 and 2011 to derive observation operators for each depth while the datasets in 2012 would be used for validation. The statistical metrics in Section 2.3 were used to evaluate the performances of these methods.

2.3. Statistical metrics

Determination coefficient (R^2), root mean square error (RMSE), and mean bias error (MBE) were calculated as measures of the goodness-of-fit between observed (E_j) and estimated (O_j) spatial averages of gullies. They are defined bellows:

$$R^2 = \frac{\left(\sum_{j=1}^{T}(E_j - \overline{E}_j)(O_j - \overline{O}_j)\right)^2}{\sum_{j=1}^{T}(E_j - \overline{E}_j)^2 \sum_{j=1}^{T}(O_j - \overline{O}_j)^2} \tag{9}$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{T}\sum_{j=1}^{T}(E_j - O_j)^2} \tag{10}$$

$$\mathrm{MBE} = \frac{1}{T}\sum_{j-1}^{T}(E_j - O_j) \tag{11}$$

where T is the total number of sampling days, while $\bar{E}_j$ and $\bar{O}_j$ are the temporal means of E_j and O_j, respectively.

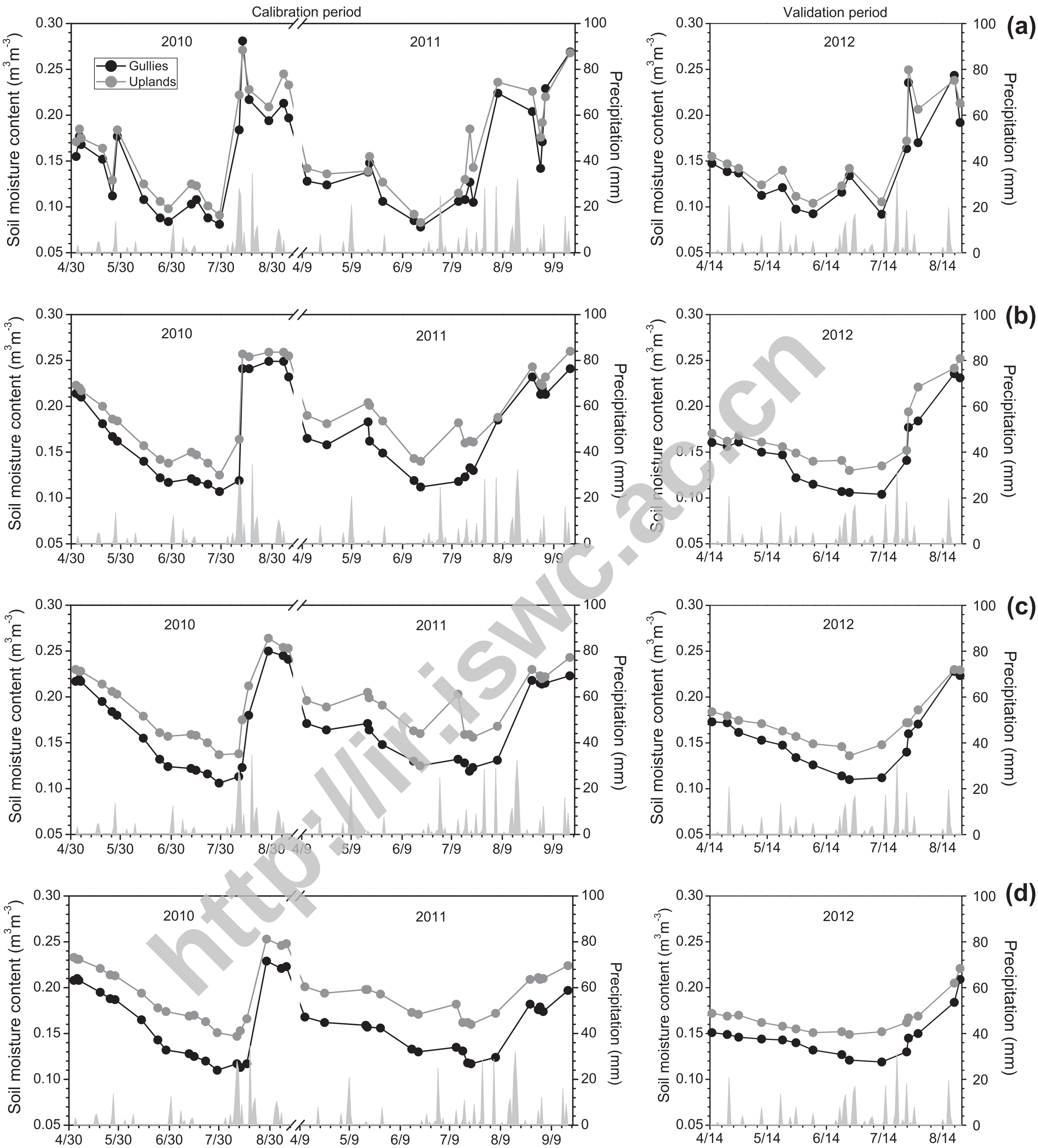

Fig. 2. Time series of soil moisture for gullies and uplands during calibration and validation periods, (a) 0–20 cm; (b) 20–40 cm; (c) 40–60 cm; and (d) 60–80 cm.

3. Soil moisture datasets

3.1. Study site

The study site is in the Yuanzegou watershed (37°15′N, 118°18′E) (Fig. 3), located in the north central area of the Loess Plateau, China. This watershed has an area of 0.58 km^2 with a gully area of 0.31 km^2 (53.4% of the total). This region has a semiarid continental climate (Gao et al., 2011) with mean annual precipitation of 505 mm. Detailed meteorological information for this area refers to Gao et al. (2011). The elevation of the Yuanzegou catchment ranges from 865 to 1105 m. The main gully extends from south to north, where steep slopes (35–90°) prevail. Much of the gully bottom comprises exposed bedrock with only a thin soil layer (<20 cm). The loess soil of this watershed is a silt loam (belonging to the Inceptisols, USDA). The uplands are composed of various hillslopes with the length of tens to hundreds of meters and relatively gentle gradients (<35°). The gullies are covered by sparse perennial grassland; there are four land uses in the uplands, namely cropland, grassland, fallow land and jujube orchards. The

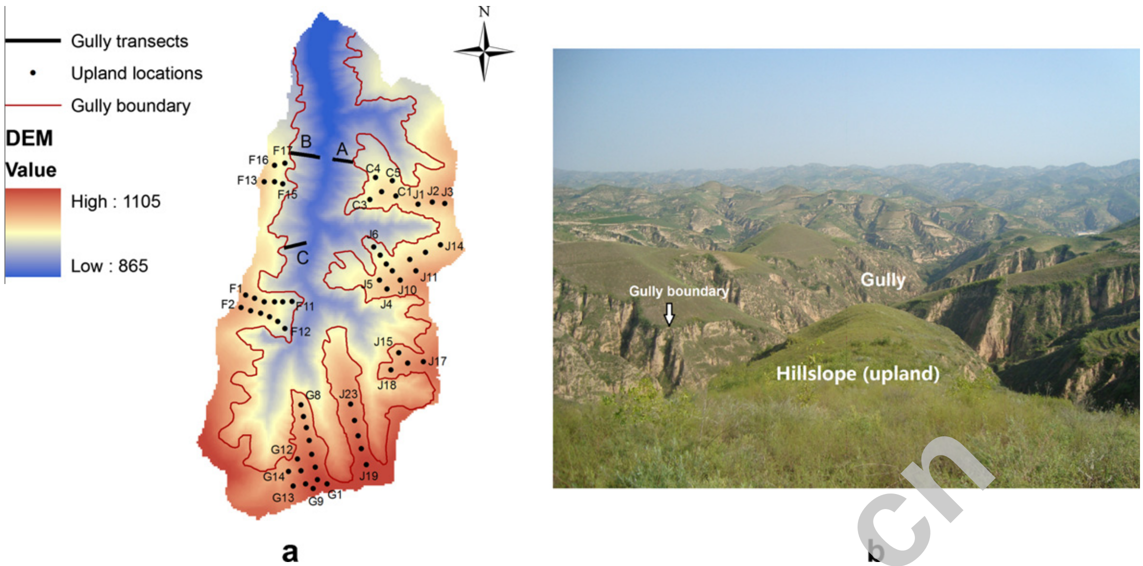

Fig. 3. Topography of the study site and sampling locations distribution, (a) DEM; (b) slope; and (c) photos of gullies.

topographic maps (DEM with a 5-m resolution) with the location of sampling points for soil moisture and a picture of the study catchment are shown in Fig. 3a and b, respectively.

3.2. Soil moisture datasets

A total of 19 sampling locations along three transects (A, B, and C) with length from 50 to 80 m along gully sidewalls were established for soil moisture collection (Fig. 1). These locations cover different topographic types (ridges, pipes and plain surfaces) in gullies according to Gao et al. (2011). Soil moisture was not sampled in gully bottom because most of them are exposed to bedrock. For the uplands, a total of 59 sampling locations were established to collect soil moisture of hillslopes. The sampling points were distributed along transects to include different topographic features, i.e., upper, middle and lower positions on slopes. These sampling points were also located in areas with different land uses (cropland, grassland, fallow and jujube orchards), and at least nine points were sampled for each land use (Fig. 3). Soil moisture in the 0–80 cm with an interval of 20 cm was collected by using a portable Time Domain Reflectometry (TDR) system termed as TRIME-IPH (IMKO, Ettlingen, Germany). This TDR system was local calibrated through gravimetric method. The details of calibration procedure were described in Gao et al. (2011). From 3 May 2010 to 19 September 2011, a total of 52 sampling events were recorded. We selected 36 out of the 52 sampling events for developing observation operators in this study because there was a large number of missing values for the rest. From 15 April to 23 August 2012, a total of 15 sampling events were conducted and these data would be used for validating observation operators. On each sampling event, the all samples were collected within one day to minimize soil water temporal variations as much as possible.

4. Results

4.1. Soil moisture temporal patterns

Fig. 2a–d shows the soil moisture time series at different depths for uplands and gullies during both calibration and validation periods. Overall, similar temporal patterns were observed for gullies and uplands; soil moisture increased after rain events and decreased thereafter, whereas noticeable lags of response to rainfall existed in deeper depths. Soil moisture for uplands always exhibited higher values than gullies except for a very few sampling days (e.g., 12 August 2010) in the 0–20 cm. The difference between soil moisture for gullies and uplands increased with depths. This could be ascribed to the much steeper slope in gullies which is not favorable for soil moisture infiltration towards deeper depths. It is worth noting that for each depth, the soil moisture difference between uplands and gullies decreased following rainstorms and increased during inter-rainstorm periods.

4.2. Performances of observation operators and validation

In this section, we first showed how the original CDFs of spatial soil moisture averages in uplands were transformed to the ones in gullies based on soil moisture datasets in 2010 and 2011. Then we compared the results of different transforming methods in estimating spatial averages in gullies. Finally, validation analysis based on soil moisture data in 2012 was conducted to test the temporal robustness of these observation operators.

Five-order polynomial curves and the corresponding coefficient values for different depths were shown in Fig. 4 and Table 2, respectively. Significantly different fitting curve was observed for the 0–20 cm compared to other depths. However, very similar fit-

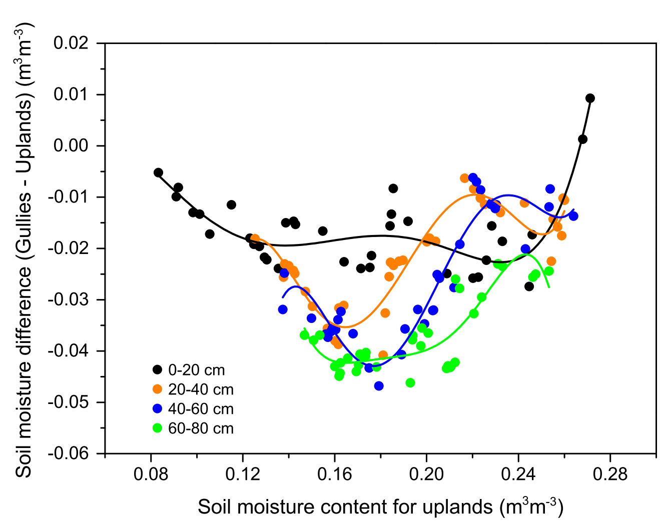

Fig. 4. Five-order polynomial fitting through cumulative distribution function (CDF) matching method for different depths.

ting curves existed between 20–40 and 40–60 cm. This suggests that observation operators defined by CDF matching method may be not successful to transfer across the whole root-zone layers. In-depth analysis on the vertical transferability of observation operators was shown in Section 4.3. Fig. 5 shows how CDFs of soil moisture for gullies were rescaled to the ones for gullies at various layers. In general, the transformed and original CDFs of soil moisture in gullies were very similar, suggesting the CDFs of spatial averages in uplands were successfully rescaled to spatial averages in gullies. It is worth noting that as calculating the errors between estimated and observed soil moisture values, time series datasets rather than ranked datasets should be used.

The other methods including LRG, MRD and LRS were also used to estimate spatial averages in gullies. The coefficients of the corresponding transforming equations were listed in Table 2. The statistical metrics defined in Section 2.3 were used to evaluate the performance of the different transforming methods and were presented in Table 3. Overall, estimations through observation operators were significantly better than when directly using upland measurements as the surrogates of spatial averages in gullies. Among different transforming methods, the CDF matching method showed the best results for each depth with the highest R^2 values and the lowest RMSE for each depth. The LRG method was considered as the second best method because it had the lower estimation errors than MRD method in terms of RMSE and MBE, while LRG and LRS showed very similar values for various statistical measures. To compare the details of estimation results, the time series of the estimated soil moisture through these methods were graphically shown in Fig. 6. It also indicated that CDF matching, LRG and LRS methods performed better than MRD method. Moreover, it is noteworthy that the estimated values for MRD method significantly underestimated the observed values over wet period.

Validation analysis based on soil moisture datasets in 2012 was used to check the temporal robustness of different observation operators with the results indicated in the latter section of Table 3. In general, the CDF matching method performed more poorly over the validation period than the linear methods except for the surface layer (0–20 cm). For the subsurface layers, RMSE during the validation period increased by 89.3–122.2% as compare to the values over the calibration period. Among the linear methods, relatively poor performances were observed for LRG and LRS methods; for the LRG method, the RMSE values in the 40–60 and 60–80 cm during the validation period were 37.6% and 113.1% higher than those in the calibration period, respectively; for the

Table 2
Coefficients of transforming equations for estimating spatial averages in gullies from soil moisture of uplands.

Methods	LRG		MRD	CDF					
Coefficients	a	b	β	k_0	k_1	k_2	k_3	k_4	k_5
0–20 cm	0.979	−1.297	0.126	−0.158	7.508	−127.390	958.018	−3329.155	4362.336
20–40 cm	1.128	−4.633	0.150	−9.428	271.039	−3047.535	16715.110	−44776.631	46958.005
40–60 cm	1.237	−7.284	0.188	−18.505	488.734	−5074.749	25850.253	−64641.518	63566.171
60–80 cm	1.148	−6.591	0.255	18.603	−488.654	5097.289	−26444.264	68191.188	−69861.989

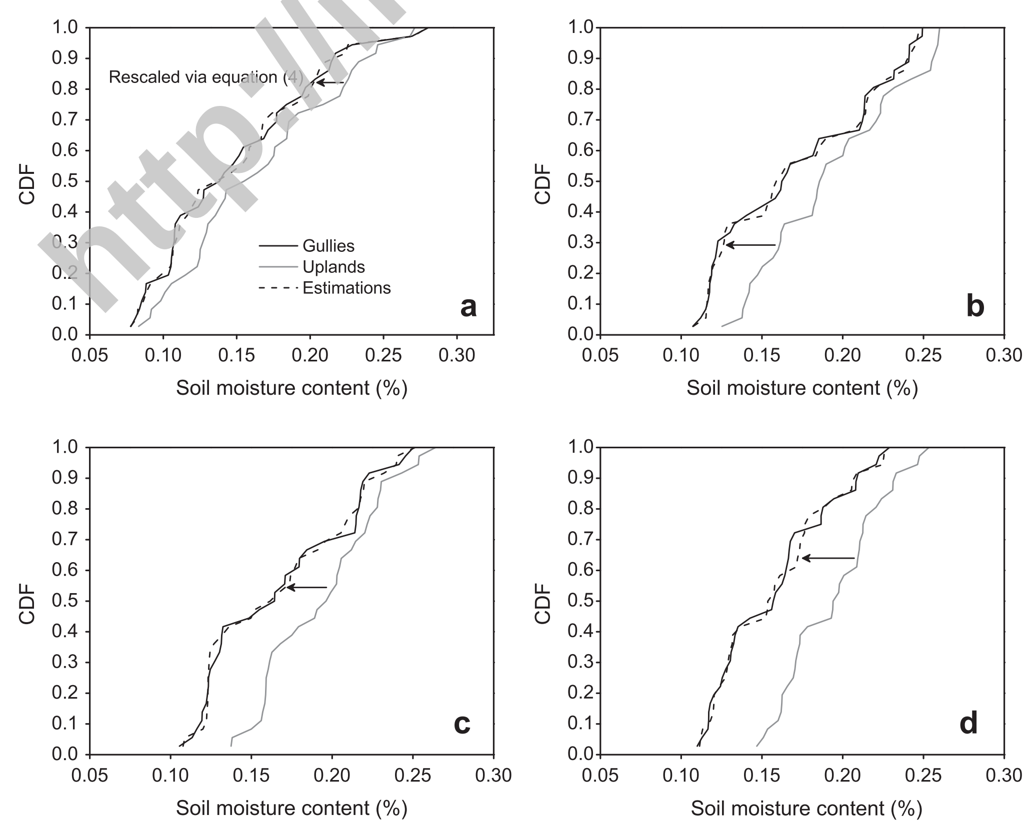

Fig. 5. CDFs of observed and predicted soil moisture in gullies for different depths (a) 0–20 cm; (b) 20–40 cm; (c) 40–60 cm; and (d) 60–80 cm.

Table 3
Performance comparison of different transforming methods and the results of cross validation. All of R^2 values are significant at the level of $p < 0.01$.

Statistics	0–20 cm			20–40 cm			40–60 cm			60–80 cm		
	R^2	RMSE	MBE	R^2	RMSE	MBE	R^2	RMSE	MBE	R^2	RMSE	MBE
CDF	0.951	1.19E−02	−1.78E−04	0.961	9.51E−03	−4.05E−04	0.955	9.48E−03	1.93E−04	0.939	8.73E−03	−2.62E−04
LRG	0.937	1.35E−02	6.84E−06	0.948	1.09E−02	2.14E−06	0.939	1.09E−02	5.73E−06	0.928	9.43E−03	−5.33E−06
MRD	0.937	1.45E−02	−2.10E−03	0.948	1.57E−02	−3.53E−03	0.939	1.80E−02	−3.96E−03	0.928	1.42E−02	−2.56E−03
LRS	0.937	1.36E−02	2.64E−17	0.948	1.10E−02	1.11E−16	0.939	1.10E−02	4.64E−17	0.928	9.52E−03	−1.68E−17
Upland	0.937	2.13E−02	1.65E−02	0.948	2.48E−02	2.17E−02	0.939	3.01E−02	2.68E−02	0.928	3.84E−02	3.70E−02
Validation												
CDF	0.963	1.05E−02	4.61E−03	0.844	1.80E−02	7.07E−03	0.857	2.05E−02	1.57E−02	0.935	1.94E−02	1.85E−02
LRG	0.966	9.39E−03	2.96E−03	0.934	1.24E−02	6.04E−03	0.970	1.50E−02	1.36E−02	0.947	2.01E−02	1.94E−02
MRD	0.966	1.12E−02	4.24E−03	0.934	1.27E−02	3.98E−03	0.970	1.63E−02	9.22E−03	0.947	1.50E−02	1.24E−02
LRS	0.966	9.63E−03	3.77E−03	0.934	1.27E−02	5.97E−03	0.970	1.49E−02	1.36E−02	0.947	2.14E−02	2.07E−02

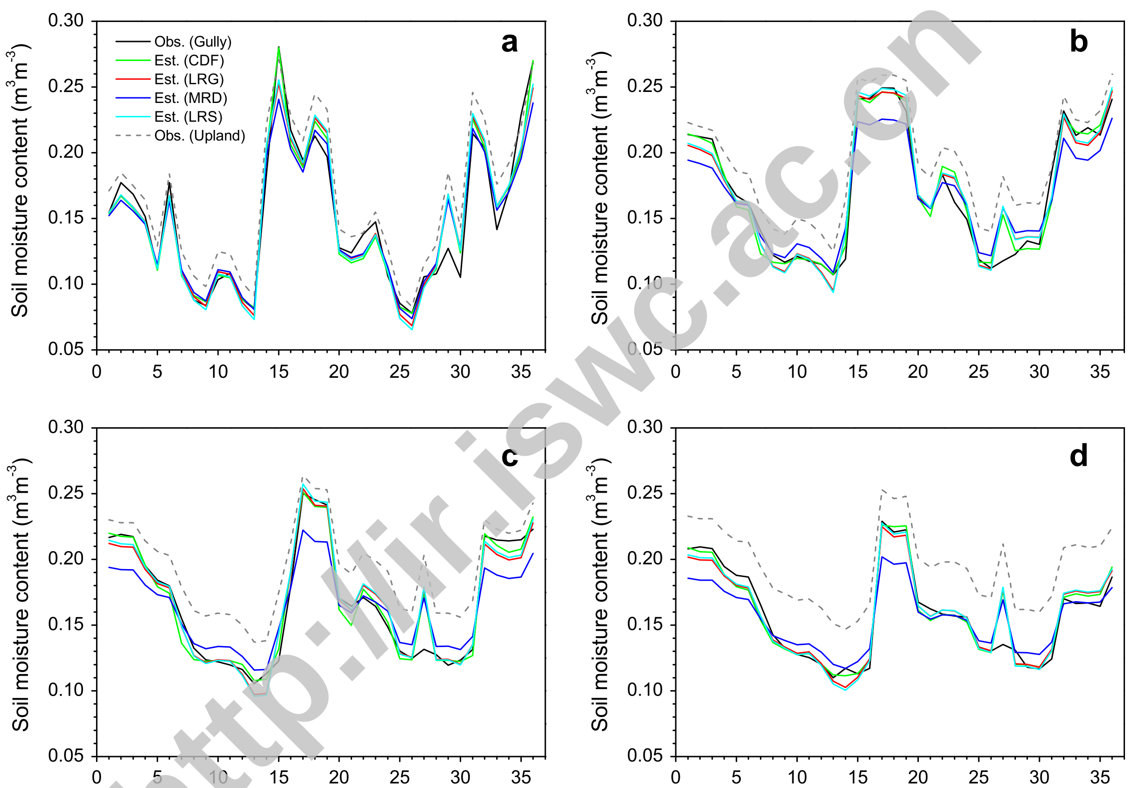

Fig. 6. Time series of soil moisture for gully averages, upland averages, and predictions through different transforming methods (a) 0–20 cm; (b) 20–40 cm; (c) 40–60 cm; and (d) 60–80 cm. The *x* coordinate shows the temporal order of sampling over the study period.

LRS method, the RMSE values over the validation period increased by 35.5% and 124.8% in the two corresponding depths, respectively. This means that the temporal transferability of observation operators defined by the CDF matching, LRG and LRS methods depends on depths and performed better for shallow depths. However, for the MRD method, higher R^2 and lower RMSE values were observed at various depths during validation period, indicating the successful transferability of these observation operators in time. We also showed the time series of observed and estimated soil moisture for different methods graphically in Fig. 7. It indicated that the MRD method performed best especially for subsurface layers and the differences of soil moisture contents for different methods increased with depths.

4.3. Transferability of observation operators for different layers

In this section, we tested if the observation operators for one given depth were applicable in other depths. Table 4 shows the relative bias errors for different statistical measures (R^2, RMSE and MBE) as applying observation operator for a given depth into other depths compared to the original observation operator for these corresponding depths. The relative bias errors were calculated as follows:

$$\varepsilon = \frac{\lambda' - \lambda}{\lambda} \tag{12}$$

where ε is the relative bias error; λ is the value of a given statistical measure as the original observation operator is used; λ' is the value of a given statistical measure as the observation operator for other depths is used. Here we set a threshold for the critical measures R^2 and RMSE in terms of the relative bias error λ to judge the success/failure of the vertical transferability of observation operators. For the specific case in this study, we define that the vertical transferability fails if the absolute value of the relative bias error (λ) exceeds 50%.

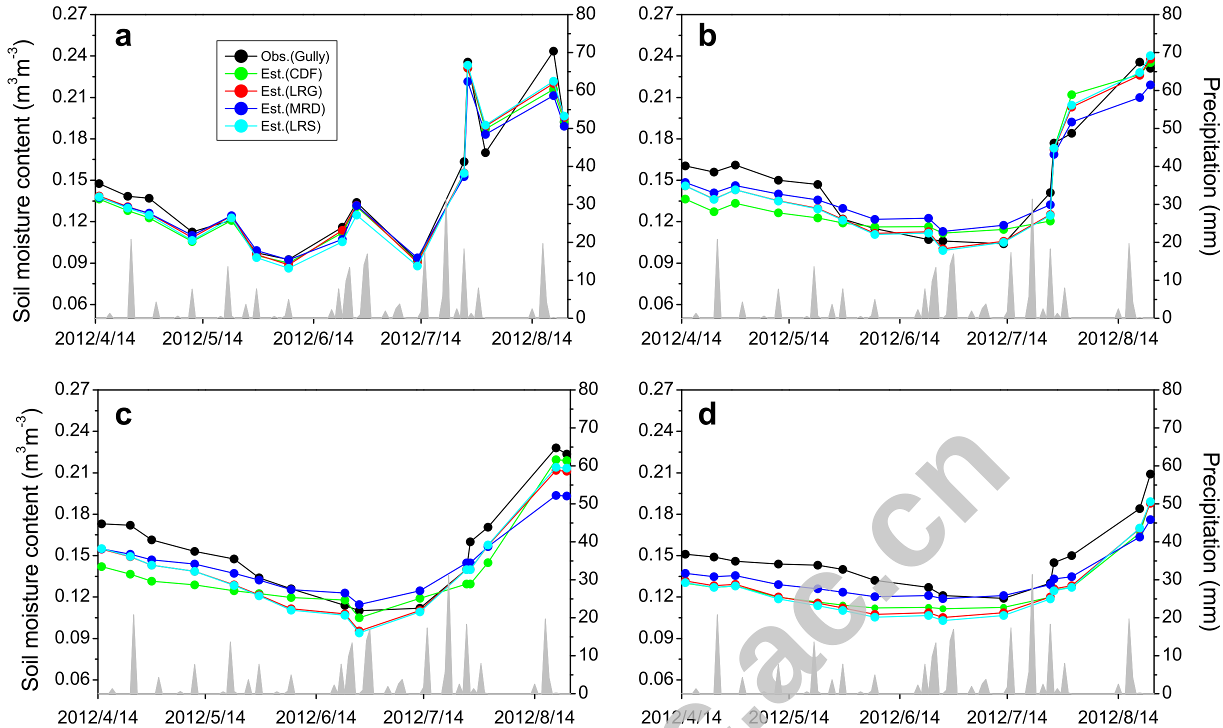

Fig. 7. Time series of observed and estimated soil moisture contents through various methods during the validation period, (a) 0–20 cm; (b) 20–40 cm; (c) 40–60 cm; and (d) 60–80 cm.

Table 4
Vertical transferability of various observation operators. Row A represents the relative bias errors for various measures (R^2, RMSE and MBE) as using observation operators at 0–20 cm into other depths compared to the original observation operators for these corresponding depths. Similarly, Row B represents the relative bias errors as using observation operators at 20–40 cm into other depths. And Row C and D represent the relative bias errors as using observation operators at 40–60 cm and 60–80 cm into other depths, respectively. Positive values mean increases of statistical measures and negative values mean decreases of statistical measures.

	20–40 cm			40–60 cm			60–80 cm		
	R^2	RMSE	MBE	R^2	RMSE	MBE	R^2	RMSE	MBE
A									
CDF	−2.5%	37.7%	803.7%	−3.4%	74.1%	−4239.9%	−1.6%	140.5%	6732.1%
LRG	0.0%	22.0%	>10,000%	0.0%	56.9%	>10,000%	0.0%	139.7%	<−10,000%
MRD	0.0%	−6.4%	−99.7%	0.0%	−5.0%	25.3%	0.0%	36.6%	−689.8%
LRS	0.0%	17.3%	>10,000%	0.0%	52.7%	>10,000%	0.0%	139.5%	>10,000%
	0–20 cm			40–60 cm			60–80 cm		
B									
CDF	−27.1%	474.8%	<−10,000%	−2.2%	32.9%	−2929.0%	−4.2%	121.1%	5587.0%
LRG	0.0%	32.6%	<−10,000%	0.0%	16.5%	>10,000%	0.0%	93.0%	<−10,000%
MRD	0.0%	7.6%	143.3%	0.0%	−6.1%	−63.9%	0.0%	19.7%	−553.1%
LRS	0.0%	37.5%	<−10,000%	0.0%	16.4%	>10,000%	0.0%	97.5%	>10,000%
	0–20 cm			20–40 cm			60–80 cm		
C									
CDF	−50.6%	1816.0%	<−10,000%	−1.5%	40.9%	−1586.4%	−2.2%	63.8%	3083.2%
LRG	0.0%	90.4%	<−10,000%	0.0%	19.3%	<−10,000%	0.0%	50.6%	<−10,000%
MRD	0.0%	24.8%	362.4%	0.0%	17.2%	151.8%	0.0%	1.4%	−341.4%
LRS	0.0%	98.5%	<−10,000%	0.0%	20.9%	<−10,000%	0.0%	58.6%	>10,000%
	0–20 cm			20–40 cm			40–60 cm		
D									
CDF	−81.4%	2017.6%	>10,000%	−6.0%	106.1%	−2964.2%	−1.9%	64.6%	4760.1%
LRG	0.0%	120.0%	<−10,000%	0.0%	74.3%	<−10,000%	0.0%	41.3%	<−10,000%
MRD	0.0%	64.1%	714.3%	0.0%	58.0%	395.8%	0.0%	26.1%	220.7%
LRS	0.0%	132.4%	<−10,000%	0.0%	75.5%	<−10,000%	0.0%	38.2%	<−10,000%

In general, the MBE indicated the greatest changes as observation operators for other depths were applied while R^2 had the lowest changes. The vertical transferability of observation operators differed with methods. Among different methods, the CDF matching method showed the poorest vertical transferability; as observation operators for subsurface layers were applied to the surface layer, the R^2 decreased by 27.1–81.4%; as to RMSE, the increases of 9 out of 12 values exceeded 50%, with the highest increase of 2017.6%. However, the MRD method showed the best vertical transferability with slight changes of R^2 and the lowest increases of RMSE (10 out of 12 values less than 50%). Overall, the vertical transferability of observation operators across root zone layers was only successful to a limited extent and failed to transfer across the whole root zone layers.

5. Discussion

On the Loess Plateau, soil moisture in gullies is important because of the large proportion of gullies and its significant role in ecohydrological processes of catchments (Gao et al., 2013). Because of the difficulty of direct measurements, soil moisture in gullies is needed to be derived through indirect methods. In this study, we found that spatial soil moisture averages in gullies were estimated accurately from hillslope measurements by using observation operators.

We used the same soil moisture datasets here for developing observation operators with our previous study (Gao et al., 2013) in order to compare the estimation results of different methods. In our previous paper, time stability analysis was the primary method for estimation soil moisture in gullies. Compared to the error statistics in this paper, we found that very similar R^2 and RMSE values existed between time stability analysis and observation operators, which agrees with De Lannoy et al. (2007) and Han et al. (2012). This suggests that observation operators also could be used to estimate spatial averages of soil moisture from measurements of adjacent sites. However, we still recommend the observation operators derived by CDF matching method (higher accuracy than MRD and LR method) when estimate soil moisture in gullies from upland measurements (if available). This is due to the shortcomings of time stability analysis: (1) the uncertainty of identifying time-stable locations based on land surface features (e.g., soil texture, topography or vegetation); (2) the uncertainty of finding one single time-stable location for different periods and different depths (Han et al., 2012). Nevertheless, the CDF matching method is not perfect and is limited through the polynomial fit (Drusch et al., 2005). Additionally, careful application of MRD method should be required because it would underestimate wet conditions (Fig. 6).

The test of spatial and temporal transferability of observation operators in fact focuses on the transferability of parameters. Observation operators defined by the linear methods (LRG, MRD and LRS) showed better spatial and temporal transferability than the nonlinear CDF matching method, although the latter had better estimation accuracy in the calibration period. It is probably due to that linear observation operators contained much less parameters and lower order than the nonlinear one. For the linear observation operators, the LRS method contained four parameters; the LRG and MRD observation operators have two and one parameters, respectively. Nevertheless, the nonlinear CDF matching operators have six parameters and the highest order of five. This also could explain why the MRD observation operators had better spatial–temporal transferability than the LRS and LRG methods. As a result, this phenomenon implies that a larger number of parameters and a higher order of observation operators would increase the estimation accuracy of spatial averages in gullies but decrease the probability of success of transferability in space and time. Our results partly agreed with the findings of Han et al. (2012) who reported a failure of temporal transferability, for both linear and nonlinear observation operators, between two years as upscaling point measurements of permanent sampling location to field averages in two agricultural sites of Indiana. They guessed that rainfall characteristic was the main factor affecting the temporal transferability of observation operators. For our study, however, larger estimation errors during validation period were mainly observed at the subsurface layers (40–60 and 60–80 cm) (Table 3). Therefore, soil infiltration properties rather than rainfall characteristics may be primarily responsible for the failure of temporal transferability. However, Matgen et al. (2012) observed similar shapes of CDF-matching observation operators between two years when validating satellite soil moisture products, suggesting a successful temporal transferability of observation operators. Nevertheless, it is worth noting the soil depth of interest in their study was less than 10 cm; therefore, their findings were consistent with ours since successful temporal transferability of CDF matching operators at surface layer was also observed here (Table 3). Moreover, Han et al. (2012) found observation operators for CDF matching method were vertically transferable at two layers (5 cm vs. 20 cm). This may be due to only two shallow layers were of investigation in their study. Han et al. (2012) also showed the successful transferability of observation operators between two nearby study sites. Nonetheless, whether the observation operators in our site could be applied at other gully catchments in the Loess Plateau region is still not clear and future studies should focus on this possibility. In addition, Drusch et al. (2005) found that the temporal transferability of observation operators in transforming remote sensing maps of soil moisture to model results depends on geographic regions in USA. This means that geographic positions may be a physical factor affecting the temporal transferability of observation operators.

Other factors in terms of sampling distance and frequency, scales and support may also affect the applicability of observation operators. Sampling distance and frequency and support may affect whether the sampled soil moisture can represent the true spatial and temporal soil moisture characteristics of one site (Western and Blöschl, 1999), and thus could change observation operators. A large number of literatures have demonstrated that spatial and temporal scales greatly affected soil moisture features in space and time in terms of soil moisture variability and temporal stability (e.g., Brocca et al., 2010b; Martínez-Fernández and Ceballos, 2005; Zhu and Lin, 2011). Since observation operators are developed based on soil moisture spatiotemporal features, the spatial–temporal scales of soil moisture sampling should affect observation operators. However, the mechanisms of how sampling distance and frequency, scales and support affect observation operators are still not understood and thus needs in-depth studies.

This study provided more general knowledge of soil moisture in gully catchments and viable methods for estimating soil moisture in gullies. The results of this study are important because few of previous studies in this region investigated soil moisture in large gullies (e.g., Qiu et al., 2001; Fu et al., 2003; Chen et al., 2007; Hu et al., 2010; Wang et al., 2012a,b). The results presented here are expected to provide insights for land surface modeling and to improve the understanding of the hydrological effects of large gullies in this region. In addition, with the increasing availability of remote sensing soil moisture products, this study also provided possibility for calibration and validation of remote sensing soil moisture products in the Loess Plateau.

6. Conclusions

This study investigated the applicability of transforming hillslope soil moisture averages to those of gullies at four depths (0–20, 20–40, 40–60, and 60–80 cm) by using observation operators. Soil moisture datasets in 2010 and 2011 were used for defining observation operators and soil moisture datasets in 2012 were used for validation. Four different nonlinear and linear methods including cumulative distribution function (CDF) matching method, linear regression (LRG) method, mean relative difference (MRD) method, and linear rescaling method (LRS) were used to define observation operators. The results showed that CDF matching method performed best in estimating soil moisture in gullies, followed by LRG, LRS and MRD methods. Validation analysis indicated that linear observation operators performed better temporal transferability than the nonlinear CDF-matching observation operators which failed to transfer in time for the subsurface layers. Moreover, the MRD, LRG and LRS methods exhibited better vertical transferability than the CDF matching method. However, the transferability of observation operators across the whole root zone layers was not successful. This study indicated that a larger number of parameters and a higher order of observation operators would increase the estimation accuracy whereas decrease the probability of success of spatial and temporal transferability.

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