Dear Editor,

We would like to thank both reviewers and you for your constructive comments and helpful suggestions that helped to improve the quality of our manuscript entitled “Estimation of subsurface soil moisture from surface soil moisture in cold mountainous areas”.

We have taken into account all the reviewers’ comments and thoroughly revised our manuscript with a major revision. In particular, we have now put a stronger emphasis on restructuring and reorganizing our manuscript logically to improve the scientific quality of our study and reanalyzing the results based on consistent statistics. Revisions following the comments of the reviewers are highlighted in yellow in the revised manuscript.

We are indebted to you and the reviewers for your taking significant amount of time and effort in handling our manuscript and providing detailed comments and suggestions for improving the manuscript. We look forward to your affirmative reply.

Sincerely,

Chansheng He, Ph.D. (on behalf of all co-authors)

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Responses to the comments from reviewers:

The comments of reviewers are in **Bolded Arial font**, while our responses are indicated in Times New Roman font with blue color, and the New text passages are indicated in Times New Roman font with black color.

Comments from Referee #1

The paper explores methods to estimate subsurface soil moisture from surface soil moisture based on an in-situ observations in cold mountainous areas since 2013. This variable is important for different scientific and applied topics. Authors explored the availability of three methods and applied the exponential filter method to the SMAP product. Research showed the improvement of profile soil moisture estimations in the mountainous. Many useful data, figures, and results were shown in the manuscript. I recommend a minor revision.

Response: Thank you for your positive comments.

General comments: The paper is well written, and the results are well presented. Bibliography very exhaustive. The analyzed dataset is interesting, and the results can be useful to improve the estimation of subsurface soil moisture and could be potentially useful for hydrological modelling. The results show that the combination of exponential filter method and satellite surface product can improve the estimation of profile soil moisture, and the availability of the area-generalized Topt in the cold mountainous areas. Related researches in high mountain ranges are limited around the world. Therefore, the presented results add new knowledge on those relevant hydrologic topics.

Response: Thank you for your positive comments. We also think that our work can provide a useful reference for studies in high mountainous areas.

1. Line 111, The half-hourly measurements were averaged to obtain daily SM values that will be used for the estimation of subsurface SM, which cover up the response of soil moisture to precipitation in a day if it's a rainstorm in where are a big soil porosity.

Response: Yes. In this study, the soil moisture data was averaged from half-hourly scale to daily scale, and we neglect short-term effects of rainstorms on the soil moisture dynamics. The exponential filter (ExpF) method assumes that the water flux between two layers is proportional to the difference in soil moisture and that the temporal characteristics of soil moisture can be represented by one parameter (T, time characteristic length) (Albergel et al., 2008; Ceballos et al., 2005). This simplification of the ExpF method ignores the complex relationship between the surface and profile soil moisture during rainstorm events (e.g. Tian et al., 2019). Thus, the ExpF method is typically used at the daily time scale (e.g. Albergel et al., 2008; Ceballos et al., 2005; Ford et al., 2014; Wang et al., 2017).

2. Figure 12, please explain this figure in detail about the temporal variation of soil moisture. It's obvious that SM increased in August. You can link the impact of climate change to moisture source and so on.

Response: We have explained the figure in detail in the revised manuscript (Line 355-360).

"The temporal variation of profile SWI, surface SWI, and precipitation are shown in Fig. S10. Results showed that the temporal variation of profile SM corresponded well with the precipitation. It increased from May (with mean value of 0.27) to September (0.533), then decreased to October (0.304). Profile SWI_{SMAP} was lower than surface SWI_{SMAP} from May to August, while profile SWI_{SMAP} was higher than surface SWI_{SMAP} from September to October. This is attributed to the higher sensitivity of surface SM dynamics to precipitation and evapotranspiration (ET). During September and October, decreased precipitation and increased ET caused the faster decrease of surface SM compared to profile SM."

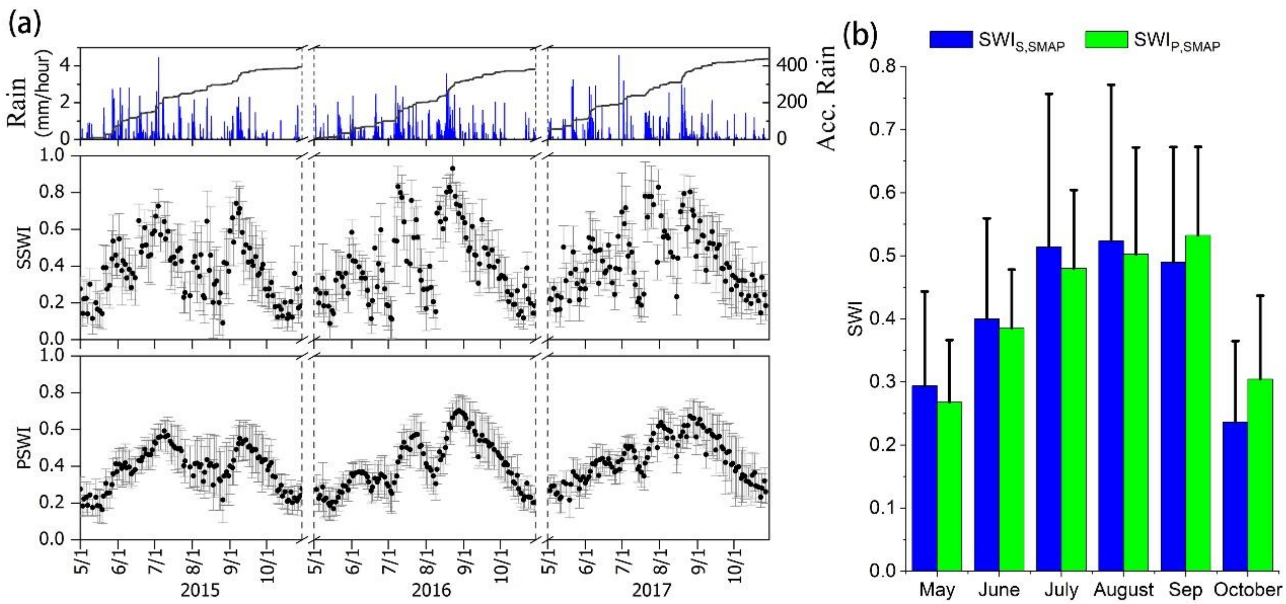

Fig. S10 (a) the temporal variation of precipitation, SSWI and PSWI, and (b) the comparison (bar represents the mean value and error bar means the standard deviation) of the monthly SSWI and PSWI during the growing seasons of 2015-2017.

Specific comments: Line number are related to the authors' line numbers.

3. Line 14, 'statistical' replace with 'multiple'.

Response: We have changed it. (Line 14)

4. Line 15, 'an' replace with 'its'.

Response: We have changed it. (Line 14)

5. Line 15, ’15’ and’ 25’ replace with ’10-20’ and ’20-30’, respectively.

Response: We have changed it. (Line 21)

6. Line 25, ’with’ replace with ’by’.

Response: We have changed it. (Line 22)

7. Line 26, please rewrite this sentence. I would prefer to ’the ExpF method was applied to estimate profile soil moisture using the satellite soil moisture product’.

Response: We have changed it. (Line 23-24)

8. Line 27, the first ’to’ replace with ’with’.

Response: We have changed it. (Line 25)

9. Line 33, please insert ’as’ before ’an’.

Response: We have insert ’to be’ before ’an’. (Line 31)

“Soil moisture (SM) is considered to be an essential climate variable”

10. Line 36, ’included’ replace with ’include’.

Response: We have changed it. (Line 34)

11. Line 41, ’provide’ replace with ’provides’.

Response: We have changed it. (Line 40)

12. Line 48, ’from 0 to 60 cm depth’ replace with ’(from 0 to 60 cm depth) ’.

Response: As the cross-correlation analysis is not connected to the further analysis, we have deleted the part related to the cross-correlation analysis in the revised manuscript.

13. Line 56, please delete ’that’.

Response: We have changed it. (Line 50)

14. Line 59, ’are’ replace with ’is’.

Response: We have changed it. (Line 54)

15. Line 60, ’have’ replace with ’has’.

Response: We have changed it. (Line 54)

16. Line 61, ’on’ replace with ’about’.

Response: We have rewritten the sentence. (Line 56-57)

"The exponential filter (ExpF) method belongs to the semi-empirical modeling approaches and relies on a two-layer SM balance equation (Wagner et al., 1999)."

17. Line 73-74, please re-write this sentence 'In the absence of large-scale networks of in situ SM observations in mountainous areas'.

Response: We have changed it. (Line 67)

"In the absence of large-scale in-situ SM observations networks of mountainous areas"

18. Line 84, delete 'which is'.

Response: We have changed it. (Line 78)

19. Line 106, please put the reference 'Zhang et al., 2017b' at the end of the sentence.

Response: We have changed it. (Line 100)

20. Line 107, ' (González-Zamora et al., 2016) ' replace with 'González-Zamora et al. (2016) '.

Response: We have changed it. (Line 101)

21. Line 109, 'data set' replace with 'dataset'.

Response: We have changed it. (Line 103)

22. Line 118, delete the 'and' after 'bulk density'.

Response: We have changed it. (Line 112)

23. Line 123, I think you use the SMAP products of 2015-2017 in your research, not only 2015-2016.

Response: We have changed the '2015-2016' to '2015-2017'. (Line 117)

24. Line 118, delete 'and' after 'bulk density'.

Response: We have changed it. (Line 112)

25. Line 155, 'tn-1' replace with 'tn-1'.

Response: We have changed it. (Line 146)

26. Line 166, delete ',' before 'The ANN'.

Response: We have changed it. (Line 157)

27. Line 167, delete ’of’ after ’training’.

Response: We have changed it. (Line 164)

28. Line 177, I think the equation (6) is incorrect, please correct it.

Response: We have changed it. (Line 172-173)

$$\hat{\Delta}= K_0 + K_1 \cdot \theta_1 + K_2 \cdot {\theta_1}^2 + K_3 \cdot {\theta_1}^3 \qquad (6)$$

“Where $\hat{\Delta}$ is the predicted difference between surface and subsurface SM, and K_i (i=0,1,2,3) are parameters.”

29. Line 190, please unify the ’lag time’ and ’Lag time’, I think it’s better to use the term ’Lag time’.

Response: As the response for comment 12, we have deleted the contents about the cross-correlation analysis. Thus, the Lag time was also deleted in the revised manuscript.

30. Line 193, ’from 0-70 cm’ replace with ’(from 0-70 cm)’.

Response: We have deleted this part.

31. Line 204, add ’,’respectively at the end.

Response: We have deleted this part.

32. Line 211, I think you mean that ’no significant linear correlations’ rather than ’no linear correlations’.

Response: We have deleted this part.

33. Line 216, delete ’have’ after ‘may’.

Response: We have deleted this part.

34. Line 250, ’season’ replace with ’seasons’.

Response: We have changed it. (Line 212)

35. Line 270, insert ’ranging’ before ’from’.

Response: We have changed it. (Line 229)

36. Line 280, please insert ’ layer’ before both the ’3’ and ’4’.

Response: We have changed it. (Line 238)

37. Line 285, ’Topt’ replace with ’Topt’.

Response: Fig. 5 has been changed and merged with Fig. 4 into a new figure in the revised manuscript. (Fig. 4, Line 234)

38. Line 300, 'suggest' replace with 'suggests'.

Response: As suggested by referee 2, the correlation between ln-transformed LAI and precipitation is significant (Pearson's R=0.80, P<0.01). Furthermore, we tested the partial correlation analysis of the ln-transformed LAI, precipitation and Topt. The results showed that the relationships between ln-transformed LAI and T_{opt} are nonsignificant under the control of precipitation. Meanwhile, the relationships between precipitation and T_{opt} under the control of ln-transformed LAI are not valid for all layers. Thus, this section about the control factors of T_{opt} is not convincing.

Furthermore, as the control factors and regression of Topt are not applied to the further estimation of subsurface soil moisture from the SMAP_L3 product, this part is not important for the manuscript.

Therefore, we have deleted the section about the control factors and regression of T_{opt} in the revised manuscript.

39. Line 310, I think it is negative correlations from Fig. 6.

Response: As the response for comment 38, this part has been deleted in the revised manuscript.

40. Line 356, 'Topt' replace with ' T_{opt} '.

Response: We have changed it. (Line 244)

41. Line 380, insert ' were shown' before both 'in supplementary' and 'in Fig.11'.

Response: We have changed it. (Line 282)

42. Line 380, 'researches' replace with 'research'.

Response: We have changed the sentence as following: (Line 284)

"The poor performance at scrubland sites is consistent with results presented by Zhang et al. (2017b) for this study region"

43. Line 420, '$\mathrm{T_{opt}}$' replace with 'T_{opt}'.

Response: We have changed it. (Line 337)

44. Line 421, insert 'profile SWI' before 'estimation'.

Response: This sentence has been deleted in the revised manuscript as we have rewritten the paragraph (Line 301-307)

"For the estimation of subsurface soil moisture from the SMAP_L3 surface product, the site-specific T_{opt} was calculated based on the best match between SMAP estimations and in-situ observations in terms of NSE. The median values of T_{opt}

for the layers 2, 3, 4, 5 and profile are 7 days, 12 days, 22 days, 35 days and 10 days, respectively. The subsurface SWI estimated from the combination of SMAP surface soil moisture with the ExpF method (with the median values of T_{opt}) were compared with the in-situ observations. A comparison of the subsurface SWI time series for different layers at each station are provided in Fig. S3- S7. Fig.7 shows the scatter plot between measured and predicted SWI, and the performance metrics are summarized in Table 4."

45. Line 430, 'season' replace with 'seasons'.

Response: We have changed it. (Line 309)

46. Line 444, 'soil profile moisture' replace with 'profile soil moisture'.

Response: We have changed it. (Line 346)

47. Line 447, 'SMAP-L4' replace with 'SMAP_L4'.

Response: We have changed it. (Line 349)

48. Line 485, insert 'The' before 'main findings'.

Response: We have changed it. (Line 376)

Comments from Referee #2

General comments:

This manuscript describes a wide-variety of approaches to estimate subsurface and profile soil moisture from surface soil moisture data in the Qilian Mountains of China. Most of the conclusions are well-supported, but the manuscript suffers from statistical inconsistencies. A consistent set of statistical measures should be maintained throughout the manuscript (NSE, RSR, and R). The only exception could be Fig. 10 where the aim is to compare the SMAP ubRMSE to the mission's accuracy requirement.

Response: Thanks for your comments. We have maintained the consistency of the statistics throughout the manuscript, expect for the use of ubRMSE in the evaluation of SMAP product.

Also, 30% of the data should be withheld for validation for all three methods, not only the ANN method.

Response: Thanks for your comments. The T_{opt} parameter of the ExpF method reflects the characteristic length of the temporal dynamics of soil moisture. Earlier studies revealed that T_{opt} is highly dependent on the sampling interval of soil moisture data (De Lange et al., 2008). In our study, we found that when using the random sampling with 70% training data as for the ANN method, T_{opt} was not suitable for the remaining data. Since it was not possible to use the same training method for ExpF method as for ANN, we used the entire soil moisture time series to estimate T_{opt}, which was also the standard procedure in earlier studies (e.g. Wagner et al., 1999; Albergel et al., 2008; De Lange et al., 2008; Ford et al., 2014; Wang et al., 2017).

The performance of the SMAP-based ExpF method for estimating profile soil moisture (i.e., SWI) is overstated, and including the NSE and RSR statistics will likely provide a much more objective view.

Response: Thanks for your comments. In the revised manuscript, the performance of SMAP-based ExpF method for estimating profile soil moisture has been reanalyzed using the metrics of NSE and RSR.

The manuscript also suffers from poor organization in some places and is not well-written.

Response: Thanks for your comments. We have deleted some content that is not important for the analysis and we have reorganized the text to make the revised manuscript easier to understand.

The revised manuscript is now divided into three parts. Firstly, we evaluated the different methods for estimating subsurface soil moisture (SM). The ExpF method was found to be the most suitable method for the further application in the study area.

Secondly, as the ExpF method has only one parameter (T_{opt}), it's importance to analyze the variation of T_{opt}. What's more, as the lack of large-scale SM in-situ observations in the high and cold mountainous areas, there is need to evaluate the alternative methods to estimate $T_{opt.}$ And our results indicate that the median value of

T_{opt} can be used for application of the ExpF method in the study area.

Finally, the ExpF method derived with the median value of T_{opt} was combined with the SMAP_L3 surface SM product to estimate the subsurface SM. The subsurface SM was also compared to the SMAP_L4 root zone SM product (a widely used large-scale root zone SM product). Results indicated that the combination of the ExpF method with the SMAP_L3 surface SM product can significantly improve the estimation of profile SM in mountainous areas. Furthermore, the combination of the SMAP_L3 and ExpF method (with the median value of Topt) were applied to estimate the temporal and spatial distribution of profile SM in the study area.

We think that the revised manuscript is well organization and well written.

Specific comments:

1. line 126. Clarify the meaning of "to consider the assumption of uniform vertical profiles of soil temperature and soil dielectric properties".

Response: For passive microwave soil moisture retrieval soil temperature needs to be known. Considering a temperature gradient in soil and vegetation requires more complex retrieval methods. A gradient is expected during afternoon overpasses when insolation is able to heat the top canopy while shadows and transpiration cools lower vegetation parts. During morning overpasses a uniform temperature gradient can be assumed. However, the gradient in vegetation is mostly more significant than in the upper few soil centimeters. Therefore, we revised this sentence as follows: "to consider the assumption of uniform temperature profiles in the vegetation cover during morning overpasses."

"SMAP descending node observations acquired near 6:00 AM local solar time have been combined to global daily composites in order to reduce the impact of Faraday rotation and to consider the assumption of uniform temperature profiles in the vegetation cover during morning overpasses."

2. Table 1. Results are being reported with too many significant figures. I doubt that the laboratory is able to measure sand and silt content with adequate precision to justify four significant figures. Reduce to a more appropriate level, perhaps three significant figures.

Response: We have reduced the level to three significant figures in the revised manuscript:

Nevertheless, we think that our result about the sand and silt content are precision enough. Our results are measured by the Mastersizer-2000 (Malvern Inc.) The measurements of the grain-size (sand, silt and clay content) analyses were made with a Malvern Mastersizer 2000 laser grain-size analyser with a measurement range of 0.02-2000 μm at a 0.1 Φ resolution and an absolute error of <5%. The measurements are made following the standard procedures of the Mastersizer 2000 laser at the Key Laboratory of Western China's Environmental Systems (Ministry of Education), Lanzhou University. The measurement results are accurate enough to be used for the scientific researches and has been used in many scientific papers (e.g. Sun et al., 2002, *Sedimentary Geology*; Sun et al., 2008, *Palaeogeography, Palaeoclimatology, Palaeoecology*; Zhang et al., 2016, *Quaternary Science Reviews*; Li et al., 2017, *Quaternary Science Reviews*; Guo et al., 2020, *Geophysical Research Letters*).

Table 1. Statistics of the soil physical characteristics at the 35 soil moisture stations: mean (standard deviation)

Layer	Depth (cm)	Bulk Density (g/cm^3)	K_S (cm/hour)	SOC (g/100g)	Sand (%)	Silt (%)	Clay (%)
Layer 1	0-10	1.13(0.28)	3.87(4.11)	4.35(4.11)	26.6(11.9)	66.2(10.9)	7.2(1.6)
Layer 2	10-20	1.14(0.24)	4.61(4.53)	3.9(3.87)	24.5(11.9)	68.6(11.2)	6.9(1.2)
Layer 3	20-30	1.18(0.32)	4.78(6.22)	3.63(3.54)	27.0(15.2)	66.5(14.3)	6.5(1.4)
Layer 4	30-50	1.29(0.3)	3.94(4.68)	2.21(2.28)	29.5(15.3)	63.8(14.5)	6.5(1.6)
Layer 5	50-70	1.34(0.3)	1.85(2.35)	2.34(2.47)	26.9(17.1)	66.5(15.9)	6.7(1.9)

Note: K_S is the Saturated Hydraulic Conductivity; SOC is the Soil Organic Carbon.

3. Section 3.4. Provide more explanation. Was a separate ANN model developed for every depth combination and every site?

Response: Yes. In this study, a separate ANN model was developed for every depth of every site. We have added more details about the set-up of the ANN method in the revised manuscript (Section 3.3, Line 153-165).

"The ANN method is a data-driven method to predict subsurface SM from surface SM (Zhang et al., 2017a). If properly trained, ANN are able to describe nonlinear relationships between dynamics of SM at different depths (Kornelsen and Coulibaly, 2014). The commonly used feed-forward ANN (with one hidden layer and 10 neurons, Levenberg–Marquardt algorithm, Ford et al., 2014) was used in this study and the ANN modelling was carried out using MATLAB (neural network time series tool, R2017b, The MathWorks). The output of the ANN was calculated using:

$$y = f[W_2 g(W_1 X + b_1) + b_2] \tag{7}$$

where y is the output, f and g are the activation functions of the hidden layer and the input layer, respectively, W_1 and W_2 are the weights of the input layer and the hidden layer, respectively, and $b1$ and $b2$ are the biases of the input layer and the hidden layer, respectively. The tangent sigmoid function was used as the activation function as it has shown good performance in hydrological studies (Yonaba et al., 2010). As suggested by Zhang et al. (2017a), 70% of data were randomly selected for training the ANN and the remaining 30% were used for validation. A separate ANN model was developed for every depth combination and every site."

4. Equation 6 is the wrong equation.

Response: We have corrected Equation 6 in the revised manuscript. (Line 173)

$$\hat{\Delta}= K_0 + K_1 \cdot \theta_1 + K_2 \cdot {\theta_1}^2 + K_3 \cdot {\theta_1}^3 \tag{9}$$

Where $\hat{\Delta}$ is the predicted difference between surface and subsurface SM, and K_i (i=0,1,2,3) are parameters.

5. line 196. not "persistent" but "consistent"

Response: As suggested by referee 3, we have deleted this part.

6. line 205-208. This should be moved to the methods section.

Response: As suggested by referee 3, we have deleted this part.

7. line 257. You have not provided any convincing evidence that "For most hydrological researches, the correct temporal variation of SM is more crucial than the exact value, suggesting that more emphasis should be given to R when selecting the most appropriate estimation method." You have presented three statistical measures to evaluate these methods (RSR, R, and NSE). For two out of the three statistical measures (RSR and NSE) the ANN method had the best performance. Therefore, you should include a clear statement that the results from the ANN method were statistically superior to those from the other two methods. You are still free to prefer the ExpF approach if it is simpler to apply than the ANN method. Just don't try to justify that choice on a statistical basis.

Response: Thank you for your comment and suggestion. Yes, the ANN method is statistically superior to those from the other two methods. However, we prefer the ExpF approach as it is simpler to apply and more process-based than the ANN method, thus we can learn much from the ExpF method than the ANN method. We have deleted the statement "For most hydrological researches, the correct temporal variation of SM is more crucial than the exact value, suggesting that more emphasis should be given to R when selecting the most appropriate estimation method" in the revised manuscript. Furthermore, we have included the statement "The results suggested that for two out of the three statistical measures (RSR and NSE), the ANN method was statistically superior to those from the other two methods." in the revised manuscript. (Line 214-223)

"As expected, all metrics showed that the performance decreased with depth. The results indicate that for two out of the three statistical measures (i.e. RSR and NSE), the ANN method was statistically superior to the other two methods. Results also demonstrated that both ANN and ExpF method were able to provide accurate estimates of subsurface SM for layer 2, layer 3 and profile SM. Specifically, the ANN method resulted in the lowest estimation error, while the ExpF method was better able to capture SM dynamics. A similar finding was reported by Zhang et al. (2017a), who found that the ExpF method had a significantly higher correlation coefficient along with a higher mean bias compared to the ANN method. Furthermore, the ExpF method is a simpler approach as it only needs one parameter (T_{opt}), and can thus be easily applied in data-scarce mountainous areas, while the establishment of the ANN method is much more complicated. Besides, the ExpF method is a process-based method, while ANN is the machine learning method. Therefore, the ExpF method was used to estimate subsurface SM in the remainder of this study."

8. Figure 7a is unnecessary and should be deleted. Your results show that "Year" does not have a significant effect, so the data should be presented including all years as done in Fig. 7b.

Response: Thank you for your comment and suggestion. We have now merged Figure 5 into Figure 4 in the revised manuscript (Fig. 4).

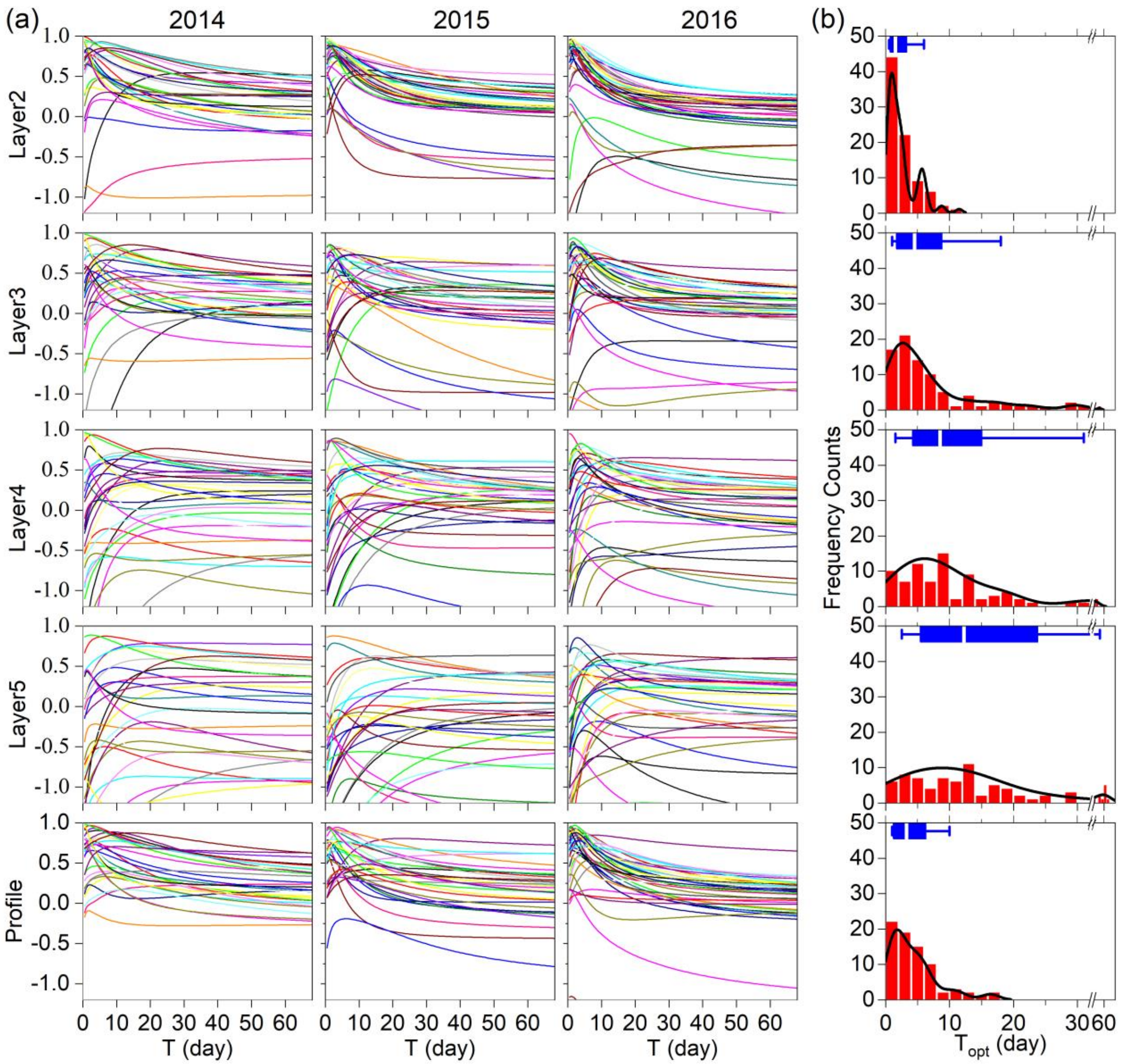

Fig. 4. Variation of NSE with T of the exponential filter method at different layers of each stations during the growing season of 2014, 2015 and 2016. Y axis is the NSE value. Frequency distribution curve and the boxplots to show the distribution of T_{opt} with depth for all stations.

9. line 290-297. This should be moved to the methods section.

Response: Thank you for your comment and suggestion. As suggested in Comment 10, the correlation among variables (e.g. Ln-transformed LAI and precipitation) are strong, and the results of partial correlation analysis among T_{opt} and the variables indicated that the relationship among T_{opt} and variables are not valid. Therefore, the relationships between T_{opt} and variables are not applied in the further analysis. As a result, this part has been deleted in the revised manuscript.

10. line 298-305. This section is not convincing. How strong is the correlation between ln-transformed LAI and precipitation? Perhaps the apparent relationship between Topt and LAI is a spurious result of the correlation between LAI and precipitation.

Response: Thank you for your comment and suggestion. The correlation between ln-transformed LAI and precipitation are significant (Pearson's $R=0.80$, $P<0.01$). Furthermore, we tested the partial correlation analysis of the ln-transformed LAI, precipitation and T_{opt}. The results showed that the relationships between ln-transformed LAI and T_{opt} are non-significant under the control of precipitation. Meanwhile, the relationships between precipitation and T_{opt} under the control of ln-transformed LAI are not valid for all layers. Thus, this section on the control factors of T_{opt} is not convincing and was removed.

Furthermore, as the control factors and regression of T_{opt} are not applied any more to the further estimation of subsurface soil moisture from the SMAP_L3 product.

Thus, we have deleted the content on the control factors and regression of T_{opt} in the revised manuscript.

11. line 319-322. Move to methods.

Response: We have moved it to the Methods section (Section 3.3).

12. line 319-322. What steps were taken to prevent problems due to collinearity of the predictor variables?

Response: Firstly, the regression equation was not used in the further analysis. Secondly, it is difficult to obtain independent variables for the regression equations of T_{opt} in data-scarce mountainous areas. Thus, it's difficult to apply the regression equation for estimating T_{opt} in the data-scarce mountainous areas. Therefore, we have deleted this part in the revised manuscript.

13. Table 4. Is "ln ln (sand)" correct in the last row?

Response: As stated in the reply for comment 10, this part has been deleted in the revised manuscript.

14. Fig. 9. Present RSR instead of RMSE to be consistent with the rest of the manuscript.

Response: We have changed the RMSE with RSR in the revised manuscript. (Fig. 5)

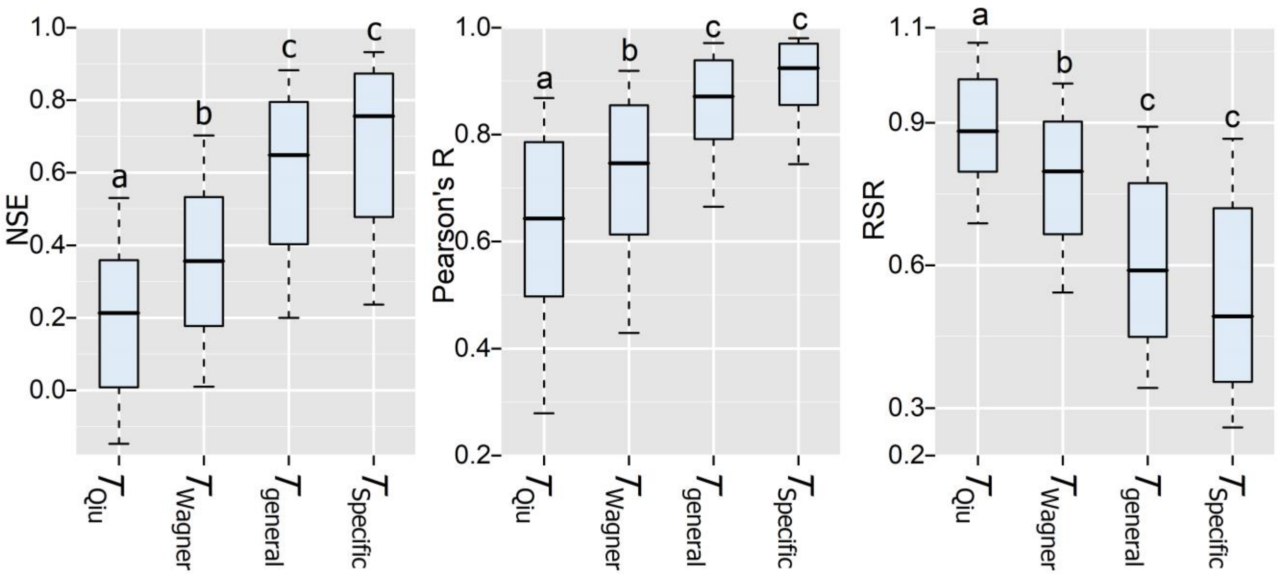

Fig. 5. The boxplot of NSE, Pearson's R, and RMSE for the T_{opt} generated from different schemes. The different letters above box indicate the significant difference for different schemes.

15. line 380. Not "persistent" but "consistent".

Response: We have changed it. (Line 283)

16. Section 4.4.1. You should note an important limitation of this analysis. There is a huge scale mismatch between the 9 km SMAP data and the in situ sensors which measure at a single point. This will likely degrade the agreement between the two data sets.

Response: We agree that there is a large scale-disparity between our point measurements and the 9 km resolution of SMAP. Nevertheless, many studies have successfully compared point scale in-situ data with remote sensing information (e.g. Chen et al., 2017; Ford et al., 2014; González-Zamora et al., 2016; Paulik et al., 2014; Pablos et al., 2018; Ullah et al., 2018; Zhang et al., 2017). Some studies were able to downscale the SMAP soil moisture data to higher resolution with the aid of high resolution soil maps (Montzka et al. 2018). However, due to the harsh natural environment of the Qilian Mountain region, there is still lack of high-precision soil properties data (Li et al. 2017; Li et al., 2018; Tian et al. 2017; Zhao et al. 2018), precluding such downscaling treatments. Nevertheless, we used an extensive in-situ soil moisture station network with 36 soil moisture stations to cover the main vegetation, elevations and soil properties of the Qilian Mountain region. Therefore, we believe that our point scale measurement results are still providing sufficient spatial representativeness of the study area. Nevertheless, we have added a discussion on the potential influence of the scale mismatch between our datasets in the revised manuscript (Line 281-284).

"The relationship between the SMAP_L3 SM data product and the in-situ observations a 5 cm depth is presented in

Fig.6. Clearly, the part of the scatter in the relationship is due to the scale discrepancy between the satellite and the in-situ SM sensor data. Nevertheless, the statistical metrics still indicate a significant relationship between the SMAP_L3 SM data product and the in-situ observations a 5 cm depth."

17. line 394-399. Move this to methods.

Response: We have moved it to Data and Methods section (Section 3.1). (Line 122-124)

"SMAP_L3 surface soil moisture product was also used to estimate the subsurface soil moisture (Layer 2: 10-20 cm, Layer 3: 20-30 cm, Layer 4: 30-50 cm, Layer 5: 50-70 cm) and profile soil moisture (0-70 cm) during the growing seasons of 2015 and 2016 in the mountainous area."

18. line 394-399. Why did you even bother all the effort to determine Topt from the in situ stations in the prior sections? Now you are not using those Topt values but instead finding new ones based on comparison of the SMAP data with the in situ data. This does not make sense in the flow of the manuscript.

Response: On the one hand, the ExpF method only need one parameter (T_{opt}) to estimate the subsurface soil moisture. In order to use the exponential filter method in areas with limited or no soil moisture observations, especially in high and cold mountainous areas, it is necessary to understand the variation and the alternative estimations of T_{opt}. And this analysis showed that the median value of T_{opt} is robust in the study area.

On the other hand, earlier studies revealed that T_{opt} highly depended on the sampling interval of soil moisture data (De Lange et al., 2008). As data with the longer time interval typically have higher T_{opt} values, T_{opt} of in-situ data are mostly lower than satellite retrievals (Albergel et al. 2008; Ford et al., 2014; González-Zamora et al., 2016). In this study, the in-situ soil moisture observations are daily scale (the mean and standard deviation of the time interval for the 35 sites are 1 days and 0.3 days, respectively). However, as SM estimation from spaceborne sensors is still challenging for the high and cold mountainous regions, data gaps exist for the SMAP_L3 data in our study area (the mean and standard deviation of the time interval for the 35 sites are 2.3 days and 1.6 days, respectively). Thus, the time interval of the SMAP_L3 data is larger than the in-situ observations. Thus, the T_{opt} of SMAP is different from the T_{opt} of in-situ observations. Consequently, to get the best estimation of subsurface soil moisture at large scale, the subsurface SWI was estimated through combination of SMAP surface soil moisture with the ExpF method (with the site-specific T_{opt} based on the best match between observations in terms of NSE).

19. line 400-406. Include NSE and RSR measures here. They are crucial for quantifying the mismatch between the SMAP SWI and the observed SWI values as shown in Fig. 11.

Response: We have included the NSE and RSR here. (Line 311-318)

"As expected, the estimation accuracy of subsurface SM decreased with depth. The ANOVA results showed that the subsurface SM estimation accuracy for layer 2 (median value of RSR=0.92, R=0.69, NSE=0.18) and profile SM (RSR=0.92, R=0.65, NSE=0.14) were significantly higher than for layer 4 (RSR=1.12, R=0.31, NSE=-0.13) and layer 5 (RSR=1.17, R=0.34, NSE=-0.15) ($p<0.05$). The NSE values were positive for layer 2 and profile SM, while the NSE values for the other layers were negative. The negative MBE showed that subsurface SM was underestimated. The relationship between SMAP-derived and in-situ observed subsurface SM for layer 2 and profile SM was significant ($p<0.01$) at all but one station (D15). Thus, the SMAP surface product and ExpF method can be used to estimate the subsurface SM in the study area, especially for layer 2 (10-20 cm) and profile (0-70 cm) SM."

20. line 425-428. This point should also have been made in Section 4.4.1.

Response: We have added the error caused by the scale mismatch between point measurements and satellite footprints in Section 4.3.1 of the revised manuscript. (Line 281-284).

"The relationship between the SMAP_L3 SM data product and the in-situ observations a 5 cm depth is presented in Fig.6. Clearly, the part of the scatter in the relationship is due to the scale discrepancy between the satellite and the in-situ SM sensor data. Nevertheless, the statistical metrics still indicate a significant relationship between the SMAP_L3 SM data product and the in-situ observations a 5 cm depth."

21. Tables 5 and 6. Replace RMSE with RSR. Add NSE.

Response: We have replaced the RMSE with RSR and added the NSE in Tables 4 and 5. The analysis of the results was also changed according to the metrics of RSR, R and NSE in the revised manuscript. (Table 4 and Table 5, as the original Table 4 is the results of regression equation for T_{opt}, it has been deleted in the revised manuscript).

"**Table 4.** Statistics of the metrics (RSR, R, NSE) of the comparisons of SMAP estimated and observed SWI at different layers for the 35 stations during the growing seasons of 2015-2016.

Layer	RSR		R		NSE	
	Mean±Std	Median	Mean±Std	Median	Mean±Std	Median
Layer 2 a	1.21±1.27	0.90	0.64±0.24	0.73a	0.04±0.49	0.19
Layer 3 ab	1.27±0.93	1.06	0.55±0.31	0.64ab	-0.05±0.46	0.05
Layer 4 b	1.53±1.49	1.10	0.43±0.38	0.52b	-0.22±0.53	-0.08
Layer 5 b	2.03±3.48	1.16	0.41±0.39	0.55b	-0.27±0.61	-0.14
Profile a	1.18±0.74	0.88	0.63±0.27	0.72a	0.12±0.38	0.19

Note: the different letters after the layers indicate that the difference is significant at $p<0.05$ (Kruskal-Wallis ANOVA)

"**Table 5.** Statistics of the metrics (RSR, R, NSE) of the comparisons of estimated-observed profile SWI datasets, SMAP_L3-observed surface SWI datasets, SMAP_L3-observed profile SWI datasets, and SMAP_L4-observed profile SWI datasets for the 35 stations during the growing season of 2015-2016.

Comparisons	RSR		R		NSE	
	Mean±std	Med	Mean±std	Med	Mean±std	Med
Estimated-observed PSWI	0.86±1.00	0.68	0.88±0.11	0.9	0.56±0.32	0.64
SMAP_L3-observed SSWI	1.13±0.49	1.01	0.57±0.17	0.59	-0.09±0.52	-0.07
SMAP_L3-observed PSWI	1.18±0.74	0.88	0.63±0.27	0.72	0.12±0.38	0.19
SMAP_L4-observed PSWI	1.42±0.76	1.25	0.47±0.31	0.55	-0.49±0.68	-0.3

Note: e.g. Estimated-observed PSWI means the comparison of the estimated profile SWI and observed profile SWI. Med represents the median value.

Fig. S8 and Table 5 show that the SMAP-observed SWI comparisons had lower performance metrics for surface SWI (median value of RSR, R and NSE are 1.01, 0.59 and -0.07, respectively) than for profile SWI (median value of RSR, R and NSE are 0.88, 0.72 and 0.19, respectively). A possible reason for this is that the profile SWI was estimated based on the SMAP surface SWI and T_{opt}. The latter was determined by optimization using the maximum NSE, which improved the performance of profile SWI estimation. In addition, the performance metrics for SMAP–observed SWI comparisons for both surface and profile SWI were significantly ($p<0.001$) lower than those of estimated–observed profile SWI (median value of RSR, R and NSE are 0.68, 0.90 and 0.64, respectively). Thus, the major error in SMAP-based profile SWI estimates stems from the SMAP satellite product and is not derived from ExpF method, which is also supported by other researches (e.g. Ford et al., 2014; Pablos et al., 2018). Notably, the scale mismatch between point measurements and satellite footprints will introduce additional errors in the validation of the satellite estimated subsurface products (Jin et al. 2017)."

22. line 436. Your results (Fig. 11) show that the performance of the SMAP profile SWI estimates is relatively poor. This is being partly obscured by the omission of the NSE and RSR statistics.

Response: Thank you for your comments and suggests. We have added NSE and RSR in the revised manuscript. As shown in Tables 4 and 5, the SMAP estimated profile SWI has a median value of RSR=0.88, R=0.72 and NSE=0.19, respectively. For the estimation of profile soil moisture using the satellite surface soil moisture product and ExpF method in the previous studies: González-Zamora et al. (2016) found a mean R ranged from 0.6 to 0.8 (12 soil moisture stations of REMEDHUS network) for estimating the 0-50 cm soil moisture from the SMOS surface soil moisture. Ford et al. (2014) found a mean R=0.49 (0~0.71) and mean NSE=0.22 (-0.99~0.54) for the root zone soil moisture estimation from SMOS surface soil moisture at Nebraska station, USA. Thus, our results are comparable with the previous studies. Furthermore, although the NSE in this study is low, its performance is significantly ($p<0.001$) higher than the SMAP_L4 profile SWI (a widely-used root zone soil moisture product) in our study area.

23. line 451-452. Here on the 22nd page of the manuscript a completely new data set is introduced. This is inappropriate. If this section is important to the manuscript, then take the time to justify it in the introduction and describe it in the methods.

Response: We have deleted this part in the revised manuscript.

24. line 465. Interpolated how? What evidence do you have that the interpolation is statistically valid? What is the associated uncertainty? This again should be justified in the introduction and described in the methods.

Response: As suggested in comment 25, we can use the median value of T_{opt} instead of using the site-specific T_{opt} value. Thus, the median value of T_{opt} (T_{opt}=10 days) was used to derive ExpF method in estimating the profile SWI in the study area in the revised manuscript. We have deleted the content related to the interpolation of T_{opt} and the Fig. S14 (spatial distribution of T_{opt}).

25. line 465. Also, why bother to spatially interpolate Topt? You have just argued that Topt defined in one region (Heihe) is valid in another region (Maqu).

Response: As argued in Section 4.3.3, the median value of T_{opt} can be used to derive the ExpF method for estimating profile soil moisture. For the estimation of profile SWI from SMAP surface product, we used the median value of T_{opt} (T_{opt}=10 days) instead of the interpolated T_{opt} to derive the ExpF method in the revised manuscript.

26. line 495. The data in Fig. 11 show that the accuracy is relatively poor. Relying on the R value alone is clearly misleading in this case where there is a substantial bias. Including the NSE and RSR as suggested above will likely show that the performance is not very good.

Response: We have included NSE and RSR in the analysis (Tables 4 and 5 in the revised manuscript). This is now mentioned in the revised manuscript accordingly. (Line 383-384)

"4) Subsurface SM derived from the SMAP_L3 surface SM product using the ExpF method showed less deviation from the in-situ observations compared to the SMAP_L4 root zone product for the study area."

Comments from Referee #3

This manuscript describes three approaches (ANN, Exponential filter, and CDF) to estimate subsurface soil moisture from surface soil moisture data in the Qilian Mountains of China. Authors identified the Exponential filter as the best model and applied this model in different ways throughout the manuscript. The topic is of great interest, but I think that the manuscript requires a significant restructuring in order to be considered acceptable for publication on HESS. My major concerns are:

Response: Thanks for your comments. We have made a significant restructuring in the revised manuscript.

1. The organization of the manuscript and its presentation is not fluent. It seems that a series of tests and analysis have been listed one after the other without a logic.

Response: Thanks for your comments. In the revised manuscript, we have deleted some contents that are not important for the analysis, and we made a drastic restructuring and reorganization to make the revised manuscript easier to understand.

The revised manuscript is now divided into three parts. Firstly, we evaluated the different methods for estimating subsurface soil moisture (SM). The ExpF method was found to be the most suitable method for further application in the study area.

Secondly, as the ExpF method has only one parameter (T_{opt}), it's importance to analyze the variation of T_{opt}. What's more, as the lack of large-scale SM in-situ observations in the high and cold mountainous areas, there is need to evaluate the alternative methods to estimate $T_{opt.}$ And our results indicate that the median value of T_{opt} can be used for application of the ExpF method in the study area.

Finally, the ExpF method derived with the median value of T_{opt} was combined with the SMAP_L3 surface SM product to estimate the subsurface SM. The subsurface SM was also compared to the SMAP_L4 root zone SM product (a widely used large-scale root zone SM product). Results indicated that the combination of the ExpF method with the SMAP_L3 surface SM product can significantly improve the estimation of profile SM in mountainous areas. Furthermore, the combination of SMAP_L3 and the ExpF method (with the median value of Topt) was applied to estimate the temporal and spatial distribution of profile SM in the study area.

2. For instance, I do not see any added value in the preliminary analysis of the soil moisture data. It is quite obvious that surface and subsurface soil moisture are linked or coupled. Remove this part or avoid stating that it is an outcome of the study.

Response: We have deleted this part in the revised manuscript.

3. Second step in the manuscript is the intercomparison of different models. In this step, it seems that the use of ANN is made just applying a matlab tool without providing enough details about the

approach adopted.

Response: We have added the details of the ANN in the revised manuscript. (Line 154-165)

"The ANN method is a data-driven method to predict subsurface SM from surface SM (Zhang et al., 2017a). If properly trained, ANN are able to describe nonlinear relationships between dynamics of SM at different depths (Kornelsen and Coulibaly, 2014). The commonly used feed-forward ANN (with one hidden layer and 10 neurons, Levenberg–Marquardt algorithm, Ford et al., 2014) was used in this study and the ANN modelling was carried out using MATLAB (neural network time series tool, R2017b, The MathWorks). The output of the ANN was calculated using:

$$y = f[W_2 g(W_1 X + b_1) + b_2] \tag{7}$$

where y is the output, f and g is the activation function of the hidden layer and the input layer, respectively. W_1 and W_2 are the weights of input layer and hidden layer, respectively. b1 and b2 are the bias of input layer and hiden layer, respectively. The tangent sigmoid function was choiced as the activation function as it has the good performance in the hydrological studies (Yonaba et al., 2010). As suggested by Zhang et al. (2017a), 70% of data were randomly selected for training the ANN and the remaining 30% were used for validation. A separate ANN model was developed for every depth combination and every site."

4. The intercomparison may be influenced by the different approaches used for the calibration of the methods. In fact, authors states that 70% of the data was used for validation of ANN and CDF, but they do not provide such indication for the exponential filter. If they used the entire database for this last, this may affect the results.

Response: The T_{opt} parameter of the ExpF method reflects the characteristic length of the temporal dynamics of soil moisture. Earlier studies revealed that T_{opt} is highly dependent on the sampling interval of soil moisture data (De Lange et al., 2008). In our study, we found that when using the random sampling with 70% training data as for the ANN method, T_{opt} was not suitable for the remaining data. Since it was not possible to use the same training method for ExpF method as for ANN, we used the entire soil moisture time series to estimate T_{opt}, which was also the standard procedure in earlier studies (e.g. Wagner et al., 1999; Albergel et al., 2008; De Lange et al., 2008; Ford et al., 2014; Wang et al., 2017).

5. I personally do not understand the need to include a section of the cross-correlation analysis. It seems out of the scope of the manuscript. Moreover, no significant results are discussed herein. Please remove this section.

Response: We have deleted the part of cross-correlation analysis in the revised manuscript.

6. Authors proposed some multilinear functions to describe relative value of T, which is fine, but it is not connected with anything else in the manuscript. It is another element somewhat independent from the main objective of the manuscript. Consider to

Response: We have changed the manuscript. We deleted the regression equation for T_{opt} that is not connected with the further analysis any more. Meanwhile, the evaluations of the other four methods for estimating T_{opt} were kept, as the results indicated the usability of the median value of T_{opt} for the ExpF method, which is important for data-scarce mountainous areas. What's more, the median value of T_{opt} was used to derive the ExpF method to estimate the subsurface soil moisture from the SMAP_L3 surface product in the revised manuscript (Section 4.3.2). Thus, this part was connected to the further analysis in the revised manuscript.

7. In the last section, we start another new section where SMAP is used first in comparison with the observation revealing some limitation for higher values. Such statement should take into consideration the existing gap in the spatial resolution of the two measurements. Rough resolution tend to smooth out higher values. This is quite obvious.

Response: We agree that there is a large scale-disparity between our point measurements and the 9 km resolution of SMAP. Nevertheless, many studies have successfully compared point scale in-situ data with remote sensing information (e.g. Chen et al., 2017; Ford et al., 2014; González-Zamora et al., 2016; Paulik et al., 2014; Pablos et al., 2018; Ullah et al., 2018; Zhang et al., 2017). Some studies were able to downscale the SMAP soil moisture data to higher resolution with the aid of high resolution soil maps (Montzka et al. 2018). However, due to the harsh natural environment of the Qilian Mountain region, there is still lack of high-precision soil properties data (Li et al. 2017; Li et al., 2018; Tian et al. 2017; Zhao et al. 2018), precluding such downscaling treatments. Nevertheless, we used an extensive in-situ soil moisture station network with 36 soil moisture stations to cover the main vegetation, elevations and soil properties of the Qilian Mountain region. Therefore, we believe that our point scale measurement results are still providing sufficient spatial representativeness of the study area.

Nevertheless, we have added the discussion about the introduced error from the scale mismatch in the revised manuscript. (Line 281-284)

"The relationship between the SMAP_L3 SM data product and the in-situ observations a 5 cm depth is presented in Fig.6. Clearly, the part of the scatter in the relationship is due to the scale discrepancy between the satellite and the in-situ SM sensor data. Nevertheless, the statistical metrics still indicate a significant relationship between the SMAP_L3 SM data product and the in-situ observations a 5 cm depth."

8. Finally, authors close with a comparison of exponential filter applied on SMAP. The regression are not used for this scope, other methods are not considered in this section, cross-correlation and spatial dynamics also neglected. I reached this point and I realized that authors are following a random walk of activities and I felt confused and disoriented.

Response: We have made a drastic restructuring and reorganization in our revised manuscript. In the revised manuscript, we deleted the content related to the cross-correlation analysis and the regression analysis of Topt, which were not connected to the further analysis. After establishing that the median value of T_{opt} can be used for the

ExpF method, further calculation of subsurface soil moisture from SMAP_L3 surface soil moisture used the median value of T_{opt} in the revised manuscript. As stated in detail in comment 1.

This manuscript requires a DRASTIC RESTRUCTURING and REORGANIZATION before being considered for publication. It will also benefit of a significant shortening of useless contents.

Response: As stated in detail in comment 1, we have revised the manuscript with a drastic restructuring and reorganization.

Short Comments

1. The aim of this study is ambiguous. Is it comparison of different methods, improvement of methods, or evaluation of satellite products?

Response: The aim of this study is to use multi-station in situ SM observations and remotely sensed SM data from the Qilian Mountains, a prime example of a high and cold mountainous area, to characterize the relationship between surface SM and deeper SM in order to obtain the spatial distribution of profile SM.

In the revised manuscript, we have deleted some contents that are not important for the analysis, and we made a drastic restructuring and reorganization to make the revised manuscript easier to understand.

The revised manuscript is now divided into three parts. Firstly, we evaluated the different methods for estimating subsurface soil moisture (SM). The ExpF method was found to be the most suitable method for further application in the study area.

Secondly, as the ExpF method has only one parameter (T_{opt}), it's importance to analyze the variation of T_{opt}. What's more, as the lack of large-scale SM in-situ observations in the high and cold mountainous areas, there is need to evaluate the alternative methods to estimate $T_{opt.}$ And our results indicate that the median value of T_{opt} can be used for application of the ExpF method in the study area.

Finally, the ExpF method derived with the median value of T_{opt} was combined with the SMAP_L3 surface SM product to estimate the subsurface SM. The subsurface SM was also compared to the SMAP_L4 root zone SM product (a widely used large-scale root zone SM product). Results indicated that the combination of the ExpF method with the SMAP_L3 surface SM product can significantly improve the estimation of profile SM in mountainous areas. Furthermore, the combination of SMAP_L3 and the ExpF method (with the median value of Topt) was applied to estimate the temporal and spatial distribution of profile SM in the study area.

2. Does the ExpF method with optimum Topt perform better than the ANN? If not, why does the author apply the ExpF method to expand SMAP?

Response: Thank you for your comment and suggestion. The ANN method is statistically superior to those from the other two methods. However, we prefer the ExpF approach as it is simpler to apply and more process-based than the ANN method. in the revised manuscript. (Line 214-223)

"As expected, all metrics showed that the performance decreased with depth. The results indicate that for two out of the three statistical measures (i.e. RSR and NSE), the ANN method was statistically superior to the other two methods. Results also demonstrated that both ANN and ExpF method were able to provide accurate estimates of subsurface SM for layer 2, layer 3 and profile SM. Specifically, the ANN method resulted in the lowest estimation error, while the ExpF method was better able to capture SM dynamics. A similar finding was reported by Zhang et al. (2017a), who found that the ExpF method had a significantly higher correlation coefficient along with a higher mean bias compared to the ANN method. Furthermore, the ExpF method is a simpler approach as it only needs one parameter (T_{opt}), and can thus be easily applied in data-scarce mountainous areas, while the establishment of the ANN method is much more complicated. Besides, the ExpF method is a process-based method, while ANN is the machine learning method. Therefore, the ExpF method was used to estimate subsurface SM in the remainder of this study."

3. In the introduction, the author mentions there are four groups of methods, what are their advantages and disadvantages? Why did the author choose the three methods in this study?

Response: In the introduction, we introduced five groups of methods, which are data assimilation of remote sensing data into land surface model (Han et al., 2013), physically-based methods (Manfreda et al., 2014), (semi-) empirical approaches (Albergel et al., 2008), data-driven methods (Kornelsen and Coulibaly, 2014; Zhang et al., 2017a), and statistical methods (Gao et al., 2019). Among them, the application of both data assimilation and physically based methods are limited due to the large amount of required input data, e.g. soil properties, which are often not available for data-scarce mountainous areas (Jin et al., 2015; Li et al., 2017; Dai et al., 2019). As we want to evaluate the methods that can be used in data-scarce mountainous areas, we exclude both data assimilation and physically based methods, and evaluated the other three methods in this study.

4. In section 4.1, there are lag time between soil moisture data at different layers and at surface. How did the author consider the impacts of the lag time in applications of these methods?'

Response: Thanks for your suggestion. We wanted to evaluate the coupling strength between surface soil moisture and subsurface soil moisture. However, there is no satisfying criterion to conclude whether the coupling strength is strong or not according to the results of the cross-correlation analysis. Thus, we have deleted the contents related to the cross-correlation analysis in the revised manuscript. So, we didn't consider the lag time in the applications of methods.

5. The performance of the ANN method is significantly related to the training data. In this study, 70 % data was used as training data according to Zhang's study. However, Zhang's study focused on the US., is 70 % suitable for the high mountainous area? Moreover, even with a ratio of 70%, there are lots of data combinations, what's the principle to choose these data? Does the author compare the performance of the ANN method with different data combinations?

Response: Firstly, for the ANN method, the sample number of training has no relation with the location, and 70% is usually selected as the number of the training samples (e.g. Kornelsen and Coulibaly, 2014; Zhang et al., 2017; ter Braak and Vrugt, 2008). The training with 70% of the data was also used in the estimation of soil moisture time series from passive microwave data using the ANN method in the Heihe River watershed (Lu et al., 2017).

Secondly, we used random sampling with uniform distribution in this study, which can best balance the induced error by data sampling (Vrugt et al., 2011). Then, the combination with the best metric (minimum RMSE) was selected for the ANN method.

6. In section 4.3.2, Topt is estimated by precipitation and clay ratio. However, the main advantage of the RBF method is its requirement of few data in introduction. Thus, the improvement in this study is meaningless. What's the insight of this improvement in other regions?

Response: The correlation between ln-transformed LAI and precipitation is significant (Pearson's $R=0.80$, $P<0.01$). Furthermore, we tested the partial correlation analysis of the ln-transformed LAI, precipitation and Topt. The results showed that the relationships between ln-transformed LAI and T_{opt} are nonsignificant under the control of precipitation. Meanwhile, the relationships between precipitation and T_{opt} under the control of ln-transformed LAI are not valid for all layers. Thus, this section about the control factors of T_{opt} is not convincing. Furthermore, as the control factors and regression of Topt are not applied to the further estimation of subsurface soil moisture from the SMAP_L3 product, this part is not important for the manuscript. Therefore, we have deleted the section on the control factors and regression of T_{opt} in the revised manuscript.

We improved the estimation of profile soil moisture in data-scarce mountainous areas as follows. Our study evaluates four methods to estimate T_{opt} in the data-scarce Qilian mountains, and the results show that the area-specific estimation of T_{opt} (site-specific T_{opt}, area-generalized T_{opt}) has significantly higher performance than the widely-used T_{opt} (T_{Warger} and T_{Qiu}), which has been applied in cold mountainous areas (e.g. the utility of T_{opt}=20 days for profile SM estimation in east Asia in Muhammad et al. (2017)).

Furthermore, the results indicate that there is a non-significant difference between the performance of a site-specific T_{opt} and an area-generalized T_{opt}. Thus, the area-specific Topt can be combined with ExpF method to estimate profile soil moisture with good performance. The reference T_{opt} for the estimation of profile and subsurface soil moisture in the study area are provided in the manuscript, and provide a reference for future studies in similar areas.

Finally, we compared the estimation of profile soil moisture based on the combination of the SMAP_L3 surface product and the ExpF method (with a median value of T_{opt} of SMAP) with a widely-used profile soil moisture product (SMAP_L4 root zone product). Results showed that our method can improve the profile soil moisture estimation significantly in our study area. Thus, based on the large-scale in-situ observations, we believe that our study improves the estimation of profile soil moisture in cold mountain areas, which will be useful for water resources management in inland river basins.

7. The author evaluates both SMAP_L3 and SMAP_L4 products against in situ observations. The SMAP_L4 is the assimilation results of satellite data and model simulation. What's the impacts of their original biases of SMAP_L3 and SMAP_L4 respectively? What's the impacts of scale-mismatch between footprint scale of satellite products and point scale of in situ observations?

Response: In this study, we have we partitioned the bias in the SMAP-based estimation of profile SWI ("SMAP-observed profile SWI", Fig. S8(c)) in bias associated with the ExpF method and bias due to SMAP original differences to get insight into the major source of error in SMAP-based estimates of profile SWI. Results showed that the major bias stems from the SMAP_L3 product.

The SMAP_L4 product is widely-used large-scale root zone soil moisture product. It is used as reference to test whether our method can improve profile soil moisture estimation. The results indicate that the ExpF method combined with the SMAP_L3 can significantly improve profile soil moisture estimation.

We have noted the problem of scale mismatch between the in-situ observations and the SMAP product. We have added a discussion about the introduced error from the scale mismatch in the revised manuscript (Line 281-284).

"The relationship between the SMAP_L3 SM data product and the in-situ observations a 5 cm depth is presented in Fig.6. Clearly, the part of the scatter in the relationship is due to the scale discrepancy between the satellite and the in-situ SM sensor data. Nevertheless, the statistical metrics still indicate a significant relationship between the SMAP_L3 SM data product and the in-situ observations a 5 cm depth."

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Estimation of subsurface soil moisture from surface soil moisture in cold mountainous areas

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Abstract. Profile soil moisture (SM) in mountainous areas is important for water resources management and ecohydrological studies of downstream arid watersheds. Satellite products are useful in providing spatially distributed SM information, but only have limited penetration depth (e.g. top 5 cm). In contrast, in situ observations can provide multi-depth measurements, but only with limited spatial coverage. Spatially continuous estimates of subsurface SM can be obtained from surface observations using multiple methods. This study evaluates methods to calculate subsurface SM from surface SM and its application to satellite SM products based on a SM observation network in the Qilian Mountains (China) established since 2013. First, three different methods were tested to estimate subsurface (10-20, 20-30, 30-50, 50-70 cm, and profile of 0-70 cm) SM from in-situ surface SM (0-10 cm): the exponential filter (ExpF), the artificial neural network (ANN) and the cumulative distribution function matching (CDF) methods. The results showed that both ANN and ExpF methods were able to provide accurate estimates of subsurface soil moisture at 10-20 cm, 20-30 cm, and for the profile of 0-70 cm using surface (0-10 cm) soil moisture only. Specifically, the ANN method had the lowest estimation errors (RSR) of 0.42, 0.62 and 0.49 for depths of 10-20 and 20-30 cm and profile SM, respectively, while the ExpF method best captured the temporal variation of subsurface soil moisture. Furthermore, it was shown that the performance of profile SM estimation was not significantly worse when an area-generalized T_{opt} (optimum T) was used instead of station-specific T_{opt} for the Qilian Mountains. In a final step, the ExpF method was applied to obtain profile soil moisture from the SMAP_L3 surface soil moisture product, and the resulting profile SM was compared with in situ observations. The results showed that the ExpF method was able to estimate profile SM from SMAP_L3 surface data with reasonable accuracy (median R of 0.65). It was also found that the combination of ExpF method and SMAP_L3 surface product can significantly improve the estimation of profile SM in mountainous areas compared to the SMAP_L4 root zone product. Overall, it was concluded that the ExpF method is useful and has potential for estimating profile SM from SMAP surface products in the Qilian Mountains.

1. Introduction

Soil moisture (SM) is considered to be an essential climate variable (Bojinski et al., 2014) because of its critical role in the water, energy (Jung et al., 2010) and carbon cycle (Green et al., 2019). In particular, knowledge of profile SM is important for runoff modeling (Brocca et al., 2010), water resources management (Gao et al., 2018), drought assessment (Jakobi et al., 2018), and climate analysis (Seneviratne et al., 2010). Methods for SM measurements include ground-based measurements and satellite-based methods (Dobriyal et al., 2012). Most ground-based methods enable the determination of SM changes with high temporal resolution at different depths, but with limited spatial coverage (Jonard et al., 2018). Especially in mountainous regions, in situ SM measurements at large scales are difficult to obtain and thus scarce (Ochsner et al., 2013). In addition, strong SM heterogeneity in complex mountainous areas makes SM estimation at large scales more difficult (Williams et al., 2009). By comparison, satellite estimates of SM, such as those from the Soil Moisture Active & Passive (SMAP) mission, provides spatial SM coverage at large scale (Entekhabi et al., 2014; Brocca et al., 2017). Unfortunately, SMAP and other microwave-based SM products from spaceborne sensors only provide SM estimates for a limited depth up to ~5 cm (Escorihuela et al., 2010). Thus, a gap exists with respect to the availability of deeper SM information with adequate spatial coverage.

Previous studies have shown that subsurface SM is often related to surface-near SM (Mahmood and Hubbard, 2007; Wang et al., 2017). A variety of approaches for estimating deep SM from surface SM information has been developed, including data assimilation of remote sensing data into land surface models (Han et al., 2013), physically-based methods (Manfreda et al., 2014), (semi-) empirical approaches (Albergel et al., 2008), data-driven methods (Kornelsen and Coulibaly, 2014; Zhang et al., 2017a), and statistical methods (Gao et al., 2019). Among them, the application of both data assimilation and physically based methods are limited to data-rich areas due to the large amount of required input data, e.g. soil properties, which are often not available for data-scarce mountainous areas (Jin et al., 2015; Li et al., 2017; Dai et al., 2019). The Cumulative Distribution Function (CDF) matching approach is a statistical method developed to adjust systematic differences in different SM datasets (e.g. in-situ observations and satellite products) based on observation operators (Drusch et al., 2005; Peng et al., 2017). CDF matching can also be used for upscaling of SM (Han et al., 2012) and estimating subsurface SM from surface SM (Gao et al., 2019). Artificial neural network (ANN) is effective and powerful data-driven tools for nonlinear estimation problems, and has been widely used to estimate subsurface SM from surface SM measurements (Kornelsen and Coulibaly, 2014; Pan et al., 2017). The exponential filter (ExpF) method belongs to the semi-empirical modeling approaches and relies on a two-layer SM balance equation (Wagner et al., 1999). This method has been widely applied with both in situ observations and satellite products, and the performance of the ExpF method for estimating subsurface SM varied considerably over regions with different environmental conditions (Ford et al., 2014; González-Zamora et al., 2016; Tobin et al., 2017; Wang et al., 2017; Zhang et al., 2017a). Ford et al. (2014) found that root zone SM estimated from SMOS satellite products had a mean R^2 of 0.57 (ranging from 0.00 to 0.86) and 0.24 (ranging from 0.00 to 0.51) for SM networks in Oklahoma and Nebraska, respectively. In addition to surface SM data, the ExpF method requires only one additional parameter (T, the characteristic time) that reflects the joined influence of local conditions on the temporal characteristics of SM (Albergel et al., 2008; Ceballos et al., 2005). Previous studies have shown that T varied among different stations and several methods have been developed to estimate T (Wagner et al., 1999; Albergel et al., 2008; Brocca et al., 2010; Qiu et al., 2014).

Methods for estimating deeper SM from surface SM have not been evaluated for high and cold mountainous areas using large scale in-situ SM observations. In the absence of large-scale in-situ SM observation networks, satellite SM products can be an alternative for providing large scale surface SM information (Ochsner, et al., 2013). Although SM estimation from spaceborne sensors is especially challenging for mountainous regions, some validation activities have shown adequate accuracy (Pasolli et a., 2011; Rasmy et al., 2011; Zhao et al., 2014; Zeng et al., 2015; Zhao and Li, 2015; Colliander et al., 2017; Ullah et al., 2018; Qu et al., 2019; Liu et al., 2019). Nevertheless, the accuracy of profile SM estimation from remotely sensed SM products is currently unknown for mountainous regions.

In this study, we focus on the Qilian Mountains, which is a water source for several key inland rivers with terminal lakes in Northwest China, including the Heihe, Shiyang, and Shule Rivers (He et al., 2018). Water scarcity threatens both food and ecosystem security in these endorheic basins (Feng et al., 2019). At the northeastern border of the Tibet-Qinghai plateau with its significant role in the Asian monsoon, profile water content in the Qilian Mountains is a key variable in ecohydrological studies on water resources and exchange processes in these basins (Zhao et al., 2013). Therefore, the aim of this study is to use multi-station in situ SM observations and remotely sensed SM data from the Qilian Mountains, a prime example of a high and cold mountainous area, to characterize the relationship between surface SM and deeper SM in order to obtain the spatial distribution of profile SM. We first evaluated the performance of the different methods for estimating subsurface SM. Subsequently, the best method was employed with SMAP surface SM products to evaluate its utility for estimating profile SM in mountainous regions.

2. Study Area

This study was carried out in the upland area of the Heihe River Basin, which is a typical terminal lake basin of the arid regions (Liu et al., 2018) (Fig 1). It is located in the Qilian Mountains at the Northeastern border of the Qinghai-Tibet plateau. It covers approximately 2.7×10^4 km^2 and the elevation ranges from about 2000 to 5000 m (Yao et al., 2017). The region has an annual precipitation ranging from 200 to 500 mm (Luo et al., 2016), annual potential evapotranspiration ranging from 700 to 2000 mm, and an annual mean temperature ranging from -3.1 °C to 3.6 °C during 1960-2012 (He et al, 2018). The main land covers are grassland, forestland and sparsely vegetated land (Zhou et al., 2016). The main soil types are Calcic Chernozems, Kastanozems, and Gelic Regosols. The main soil texture classes are silt loam, silt and sandy loam (Tian et al., 2017; 2019).

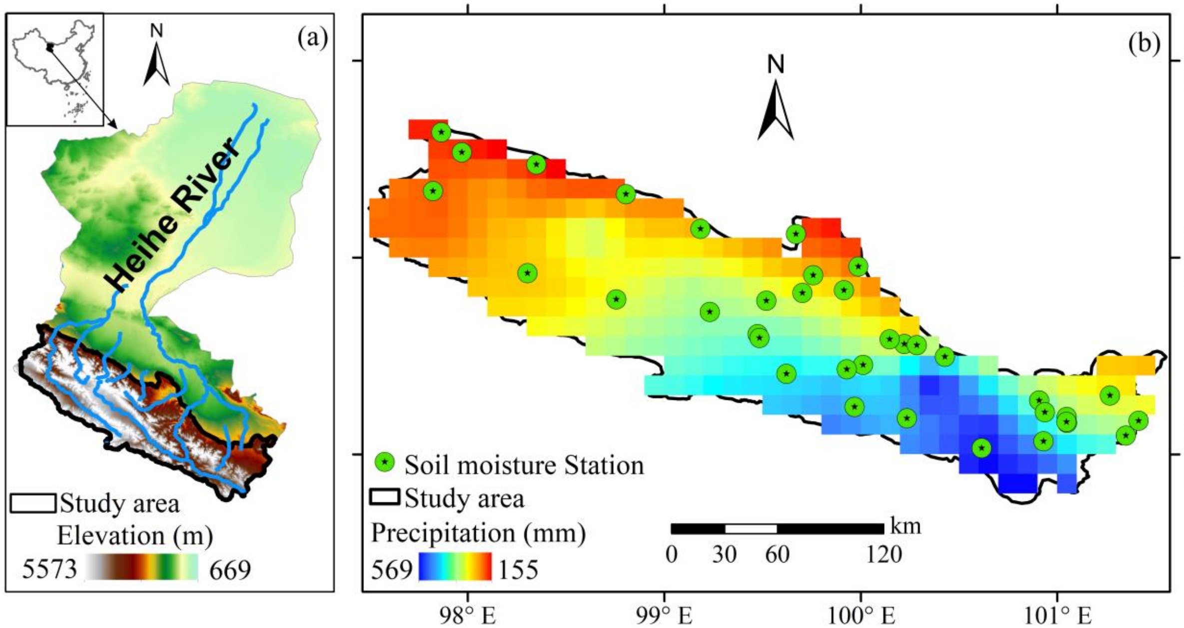

Fig. 1. (a) Study area and **(b)** distribution of the SM stations with spatial distribution of annual average precipitation from 2014 to 2016.

3. Data and Methods

3.1. Datasets

A SM monitoring network was set up in September 2013 in the Qilian Mountains. The network is composed of 35 SM stations distributed over the entire study area (Fig. 1). At each station, SM profiles from 0 to 70 cm were measured by soil moisture probes (ECH2O 5TE, METER Group Inc., USA) installed at depths of 5 (representing depth of 0-10 cm, $SM_{5\ cm}$), 15 (10-20 cm, $SM_{15\ cm}$), 25 (20-30 cm, $SM_{25\ cm}$), 40 (30-50 cm, $SM_{40\ cm}$) and 60 cm (50-70 cm, $SM_{60\ cm}$) below the soil surface at 30 min intervals. Soil-specific sensor calibrations were performed with the direct calibration method using soil samples taken from each station (Cobos and Chambers, 2010; Zhang et al., 2017b). The profile integrated SM ($SM_{0\text{-}70\ cm}$) was calculated by the method of González-Zamora et al. (2016):

$$\mathrm{SM}_{0-70\ cm} = \frac{\mathrm{SM}_{5\ cm}\times 10+\mathrm{SM}_{15\ cm}\times 10+\mathrm{SM}_{25\ cm}\times 10+\mathrm{SM}_{40\ cm}\times 20+\mathrm{SM}_{60\ cm}\times 20}{70} \tag{1}$$

The entire data set used in this study thus consists of six in situ SM time series at depths of 5, 15, 25, 40, 60 cm, and 0-70 cm for each of the 35 stations. Due to the influence of soil freezing in winter, the soil moisture time series were limited to the growing seasons (May to October, Tian et al., 2019) of 2014, 2015 and 2016. The half-hourly measurements were averaged to obtain daily SM values for the estimation of subsurface SM (Wagner et al., 1999). Data quality management was performed for each station, and data gaps existed in the harsh mountainous environment, as described in detail in Tian et al. (2019). Time series where the amount of missing values exceeded 50% were excluded in the analysis. The final dataset after processing is presented in Fig. 2. The surface SM measured at 5 cm was used to predict the subsurface SM at depths of 15, 25, 40, 60 cm and the profile average (0-70 cm).

Soil cores were taken to measure soil properties including soil organic carbon (SOC), saturated hydraulic conductivity (K_S), soil particle composition and bulk density for each layer during the sensor installation. Detailed descriptions of the soil properties can be found in Tian et al. (2017; 2019). The statistics of the soil physical characteristics are provided in Table 1. Daily precipitation from reanalysis (Chen et al., 2011), Landsat-based continuous monthly 30m×30m resolution NDVI data for the period 1986-2017 (Cihlar et al., 1994; Huete et al., 2002; Wu et al., 2019) were acquired from the National Tibetan Plateau Data Centre (https://data.tpdc.ac.cn/en/).

The widely used higher level SMAP_L3 Global Daily 9 km product for the growing seasons of 2015 to 2017 were used in this study (O'Neill et al., 2018). This product is distributed by NASA (http://nsidc.org/). SMAP descending node observations acquired near 6:00 AM local solar time have been combined to global daily composites in order to reduce the impact of Faraday rotation and to consider the assumption of uniform temperature profiles in the vegetation cover during morning overpasses. It has to be noted that the data are provided on a 9 km grid, but that this is a result of a Backus-Gilbert optimal interpolation at brightness temperature level. The actual spatial resolution is coarser (O'Neill et al., 2018). SMAP_L3 surface soil moisture product was also used to estimate the subsurface soil moisture (Layer 2: 10-20 cm, Layer 3: 20-30 cm, Layer 4: 30-50 cm, Layer 5: 50-70 cm) and profile soil moisture (0-70 cm) during the growing seasons of 2015 and 2016 in the mountainous area.

SMAP_L4 provides estimates of both surface and root zone SM products based on the assimilation of brightness temperature into the NASA land-surface model, and it has a spatial and temporal resolution of 9 km and 3 h, respectively, (Reichle et al., 2017). SMAP_L4 is a widely used root zone SM product (Pablos et al., 2018). Here, the SMAP_L4 data were averaged to a daily resolution in order to compare it with the profile SM estimates from the SMAP_L3 surface product obtained in this study. In particular, the SMAP_L4 SM product with both surface (0-5 cm, sm_{0-5}) and root zone (0-100 cm, sm_{0-100}) information were used to calculate SM of the 0-70 cm profile (sm_{0-70}) using:

$$sm_{0-100} = (5 * sm_{0-5} + 95 * sm_{5-100})/100 \tag{2}$$

$$sm_{0-70} = (5 * sm_{0-5} + 65 * sm_{5-100})/70 \tag{3}$$

Table 1. Statistics of the soil physical characteristics at the 35 soil moisture stations: mean (standard deviation)

Layer	Depth (cm)	Bulk Density (g/cm^3)	K_S (cm/hour)	SOC (g/100g)	Sand (%)	Silt (%)	Clay (%)
Layer 1	0-10	1.13(0.28)	3.87(4.11)	4.35(4.11)	26.6(11.9)	66.2(10.9)	7.2(1.6)
Layer 2	10-20	1.14(0.24)	4.61(4.53)	3.9(3.87)	24.5(11.9)	68.6(11.2)	6.9(1.2)
Layer 3	20-30	1.18(0.32)	4.78(6.22)	3.63(3.54)	27.0(15.2)	66.5(14.3)	6.5(1.4)
Layer 4	30-50	1.29(0.3)	3.94(4.68)	2.21(2.28)	29.5(15.3)	63.8(14.5)	6.5(1.6)
Layer 5	50-70	1.34(0.3)	1.85(2.35)	2.34(2.47)	26.9(17.1)	66.5(15.9)	6.7(1.9)

Note: K_S is the Saturated Hydraulic Conductivity; SOC is the Soil Organic Carbon.

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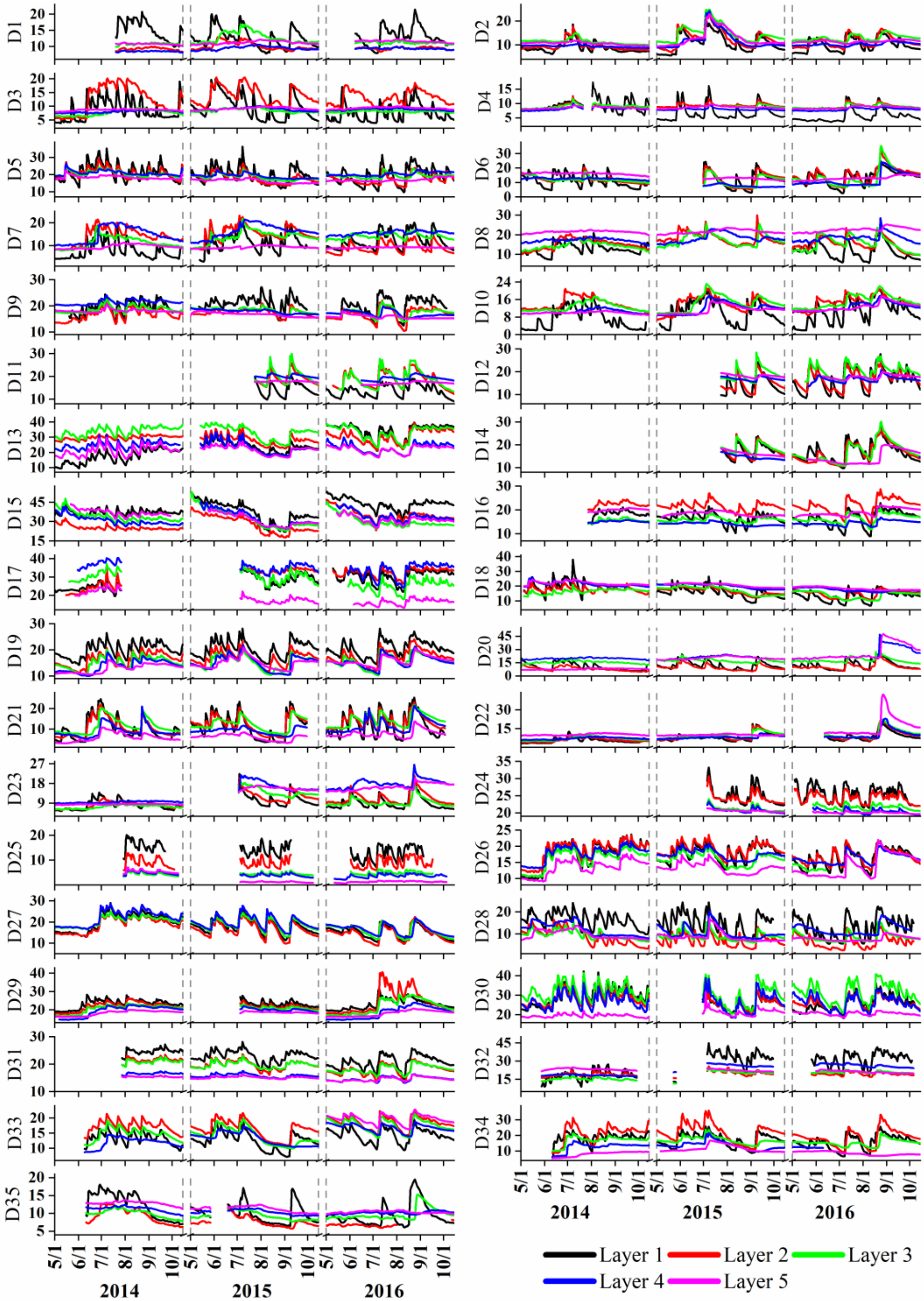


Fig. 2. Daily soil moisture (vol. %) time series during the growing season of 2014 to 2016 for the 5 layers (layer 1, 0-10 cm; layer 2, 10-20 cm; layer 3, 20-30 cm; layer 4, 30-50 cm; layer 5, 50-70 cm) in the 35 soil moisture stations. Gaps exist for some stations due to missing data.

3.2. Exponential Filter (ExpF) method

The ExpF method predicts the dynamics of subsurface SM using an exponential filter function of the surface SM dynamics (Wagner et al., 1999; Albergel et al., 2008). First, SM (cm^3/cm^3) is transformed into a soil water index (SWI) with:

$$SWI_i = \frac{\theta_i - \theta_{i,min}}{\theta_{i,max} - \theta_{i,min}} \tag{4}$$

where $\theta_{i,min}$ and $\theta_{i,max}$ are the minimum and maximum SM in the time series collected since installation for each layer of each station (Ford et al., 2014). The ExpF method then estimates subsurface SM from surface SM using:

$$SWI_{m,t_n} = SWI_{m,t_{n-1}} + K_{t_n}(ms_{t_n} - SWI_{m,t_{n-1}}) \tag{5}$$

where $SWI_{m,t_{n-1}}$ and SWI_{m,t_n} are the predicted subsurface SWI at time t_{n-1} and t_n, respectively. ms_{t_n} is the observed surface SWI at time t_n, and K_{t_n} represents the gain at time t_n calculated by:

$$K_{t_n} = \frac{K_{t_{n-1}}}{K_{t_{n-1}} + e^{-\frac{t_n - t_{n-1}}{T}}} \tag{6}$$

where $K_{t_{n-1}}$ is the gain at time t_{n-1} and T is the characteristic time length in days. The equation was initialized with $SWI_{m,t_1} = ms_{t_1}$ and $K_{t_1} = 1$ (Albergel et al., 2008). This method is particularly useful as T is the only unknown parameter. The optimum T (T_{opt}) was determined by optimization using the highest Nash-Sutcliffe score for each specific depth at each station.

3.3. Artificial Neural Network (ANN) method

The ANN method is a data-driven method to predict subsurface SM from surface SM (Zhang et al., 2017a). If properly trained, ANN are able to describe nonlinear relationships between dynamics of SM at different depths (Kornelsen and Coulibaly, 2014). The commonly used feed-forward ANN (with one hidden layer and 10 neurons, Levenberg–Marquardt algorithm, Ford et al., 2014) was used in this study and the ANN modelling was carried out using MATLAB (neural network time series tool, R2017b, The MathWorks). The output of the ANN was calculated using:

$$y = f[W_2 g(W_1 X + b_1) + b_2] \tag{7}$$

where y is the output, f and g are the activation functions of the hidden layer and the input layer, respectively, W_1 and W_2 are the weights of the input layer and the hidden layer, respectively, and $b1$ and $b2$ are the biases of the input layer and the hidden layer, respectively. The tangent sigmoid function was used as the activation function as it has shown good performance in hydrological studies (Yonaba et al., 2010). As suggested by Zhang et al. (2017a), 70% of data were randomly selected for training the ANN and the remaining 30% were used for validation. A separate ANN model was developed for every depth combination and every site.

3.4. Cumulative Distribution Function matching (CDF) method

In this study, the following procedure for CDF matching was used:

1) Rank the surface (θ_1) and the subsurface SM (θ_2) time series;

2) Calculate the difference between the two observation time series:

$$\Delta_i = \theta_{1,i} - \theta_{2,i} \tag{8}$$

3) Use a cubic polynomial fit to relate the difference (Δ) to surface SM (θ_1) as recommended by Gao et al. (2019):

$$\hat{\Delta} = K_0 + K_1 \cdot \theta_1 + K_2 \cdot {\theta_1}^2 + K_3 \cdot {\theta_1}^3 \tag{9}$$

where $\hat{\Delta}$ is the predicted difference between surface and subsurface SM, and K_i (i=0,1,2,3) are parameters.

4) Calculate CDF-matched subsurface SM (θ_{CDF}) with:

$$\theta_{CDF} = \theta_1 - \hat{\Delta} \tag{10}$$

Similar to the ANN method, 70% of the data were used to calibrate the approach and the remaining 30% of the data were used for validation of the CDF matching method.

3.5. Statistical analysis

Boxplots were used to show the scatter of the data. The difference between data in different groups was examined using a one-way analysis of variance (ANOVA) with the post-hoc Bonferroni test when the normality and homogeneity of variance of the datasets were satisfied. The Kruskal-Wallis ANOVA with a post-hoc Dunn's test was used in case these conditions were not satisfied (Lange et al., 2008). The statistical analysis was performed in SPSS (SPSS 18.0, SPSS Inc.) and Matlab (R2017b, The MathWorks). The significance level was 0.05 for all statistical tests.

4. Results and discussion

4.1. Evaluation of different methods

The ExpF method estimates subsurface SM based on SWI, while the ANN and CDF methods are based on volumetric soil moisture. Following Moriasi et al. (2007), the Nash-Sutcliffe efficiency (NSE), the ratio of RMSE to the standard deviation of the observations (RSR, an error statistic that normalizes the RMSE), and Pearson correlation coefficient (R) were used to evaluate the performance of different methods with different units. Fig. 3, Table 2 and Fig. S1 summarize the metrics (NSE, RSR, and R) for subsurface SM estimates at different depths obtained using different methods for the growing season of 2014, 2015 and 2016. Fig. 3 shows that there were significant differences for the NSE of different methods for all layers ($p<0.05$). The ANN had the highest NSE with a median value of 0.82, 0.56, 0.35, 0.35 and 0.76 for layers 2, 3, 4, 5 and profile SM, respectively. There were no significant differences between the ExpF and the CDF matching method for layer 2, layer 3 and the profile SM. The CDF matching method showed the lowest NSE for layers 4 and 5. Overall, both the ANN and ExpF methods showed good performance in terms of NSE for layer 2, layer 3 and profile SM (median NSE > 0.5), and the CDF matching method showed a good performance in terms of NSE for layer 2 and profile SM (median NSE > 0.5).

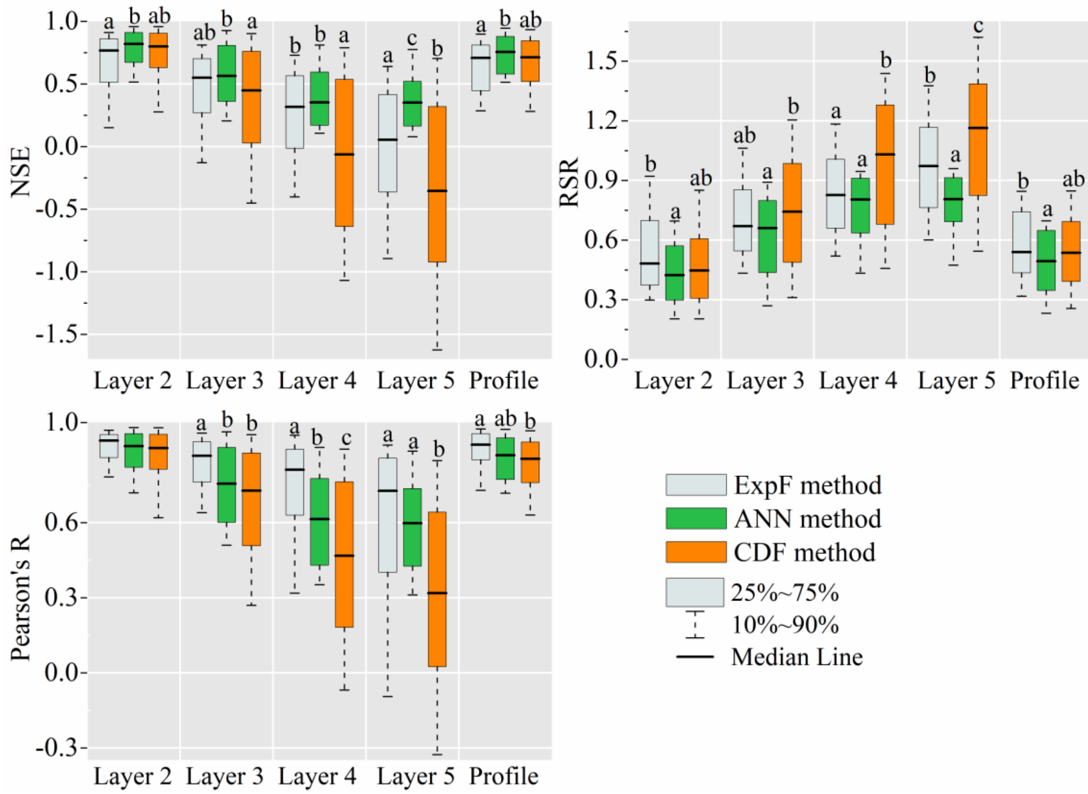


Fig. 3. Boxplot of the metrics (NSE, RSR, R) to compare the subsurface SM estimation using surface SM through the three methods (ExpF, ANN, CDF) with the observations for the 35 stations during the growing seasons of 2014 to 2016. Different letters above the box indicate the significant difference ($p<0.05$) among different methods.

Similar to the results for NSE, Fig. 3 shows that the ANN method resulted in a significantly lower RSR ($p<0.01$) for all depths. There were no significant differences between the ExpF and CDF matching method for layer 2, layer 3 and profile SM, and the CDF matching method showed a significantly higher RSR for layer 4 and layer 5. The ExpF method had a similar estimation error as the CDF matching method for layer 2, layer 3 and profile SM. Both the ANN and ExpF methods showed satisfactory results (RSR<0.7) for layer 2, layer 3 and profile SM, and the CDF matching method showed satisfactory results for layer 2 and profile SM (Moriasi et al., 2007).

Fig. 3 shows that the ExpF method resulted in the highest R for all layers (with a median value of 0.93, 0.87, 0.81, 0.73 and 0.91 for layers 2, 3, 4, 5 and profile SM, respectively), while the CDF matching method resulted in the lowest R for all layers (with a median value of 0.90, 0.73, 0.47, 0.32 and 0.86 for layers 2, 3, 4, 5 and profile SM, respectively). The good performance for R suggests that the ExpF method had the best ability to describe the temporal variability in SM.

Table 2. The statistics (mean±standard deviation) of the performance (RSR, R and NSE) of different methods (ExpF, ANN, and CDF) for estimating subsurface SM using surface SM for each layer of 35 stations during the growing seasons of 2014, 2015, and 2016

Layer	RSR			R			NSE		
	ExpF	ANN	CDF	ExpF	ANN	CDF	ExpF	ANN	CDF
Layer 2	0.55±0.25	0.44±0.20	0.50±0.27	0.89±0.10	0.87±0.13	0.84±0.19	0.63±0.36	0.76±0.21	0.68±0.37
Layer 3	0.72±0.27	0.62±0.23	0.75±0.34	0.81±0.19	0.74±0.18	0.66±0.29	0.41±0.50	0.56±0.28	0.33±0.56
Layer 4	0.83±0.27	0.75±0.22	0.99±0.37	0.70±0.31	0.61±0.21	0.44±0.37	0.24±0.47	0.40±0.29	-0.11±0.71
Layer 5	0.97±0.29	0.77±0.19	1.11±0.38	0.57±0.39	0.58±0.22	0.3±0.41	-0.03±0.61	0.37±0.26	-0.38±0.82
Profile	0.58±0.22	0.49±0.19	0.54±0.22	0.88±0.11	0.85±0.11	0.83±0.13	0.61±0.32	0.73±0.18	0.66±0.26

As expected, all metrics showed that the performance decreased with depth. The results indicate that for two out of the three statistical measures (i.e. RSR and NSE), the ANN method was statistically superior to the other two methods. Results also demonstrated that both ANN and ExpF method were able to provide accurate estimates of subsurface SM for layer 2, layer 3 and profile SM. Specifically, the ANN method resulted in the lowest estimation error, while the ExpF method was better able to capture SM dynamics. A similar finding was reported by Zhang et al. (2017a), who found that the ExpF method had a significantly higher correlation coefficient along with a higher mean bias compared to the ANN method. Furthermore, the ExpF method is a simpler approach as it only needs one parameter (T_{opt}), and can thus be easily applied in data-scarce mountainous areas, while the establishment of the ANN method is much more complicated. Besides, the ExpF method is a process-based method, while ANN is the machine learning method. Therefore, the ExpF method was used to estimate subsurface SM in the remainder of this study.

4.2. Evaluation of T_{opt} for the ExpF method

4.2.1. Variation of T_{opt} with depth

It was found that the accuracy of the ExpF method varied with the selected T value, and that higher T values resulted in more stable estimation of SM time series (Wagner et al., 1999; Albergel et al., 2008). Furthermore, it was found that each station had an optimum T (T_{opt}) as determined based on the best match with observations in terms of NSE. The variation of NSE with T (ranging from 0 to 68 days) for different layers for each station is shown in Fig. 4 and Table 3. It can be seen that the sensitivity of high values of NSE to changes in T decreased with increasing depth, indicating that the range of T values with high NSE was larger deeper in the soil. This was also observed in previous studies (e.g. Wang et al., 2017).

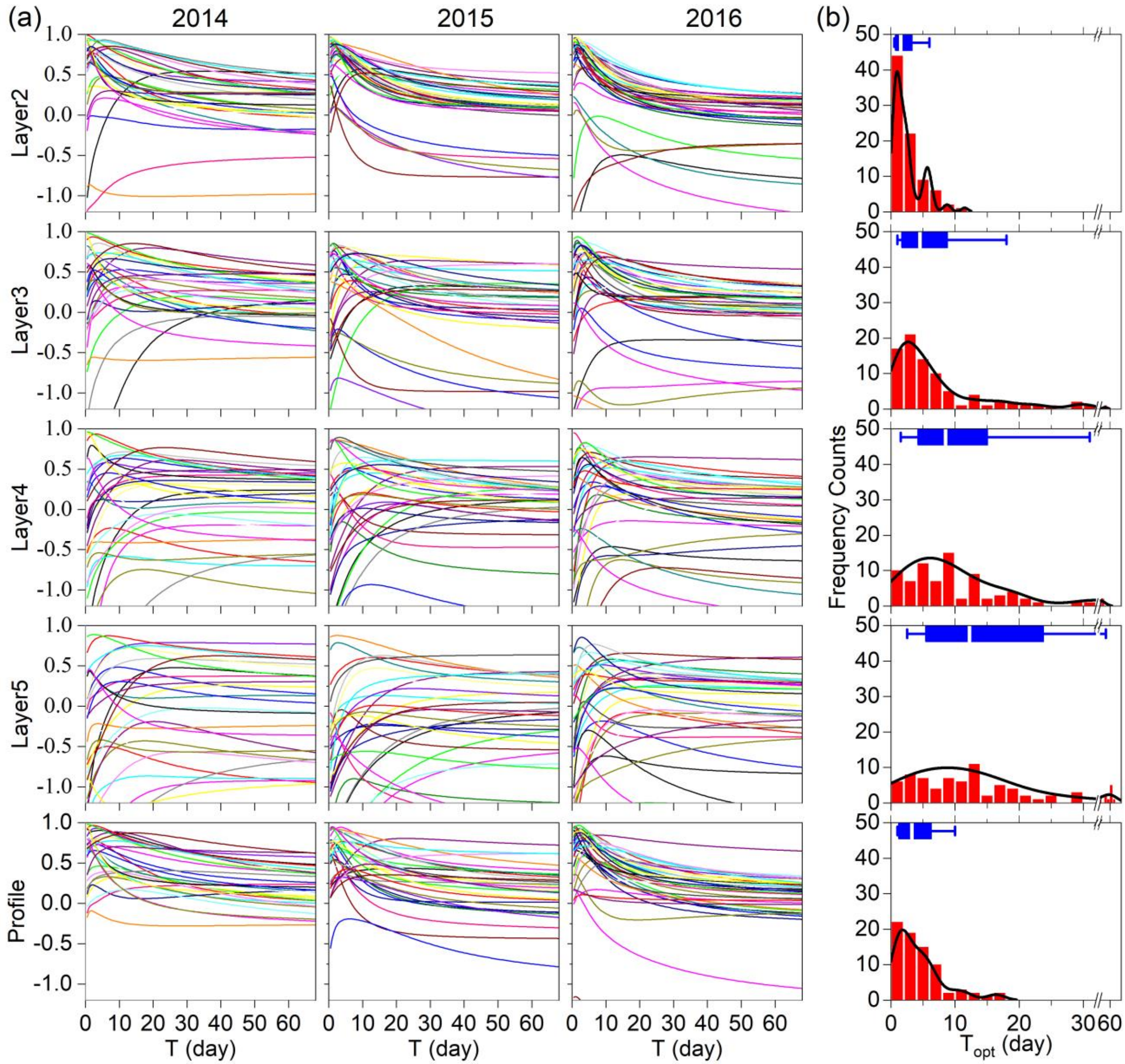


Fig. 4. Variation of NSE with T of the exponential filter method at different layers of each stations during the growing season of 2014, 2015 and 2016. Y axis is the NSE value. Frequency distribution curve and histogram to show the distribution of T_{opt} with depth for all stations.

Results of a two-way ANOVA showed that the difference of T_{opt} is not significant between different years (p=0.06) while differences were significant between layers (p<0.001). Furthermore, it can be seen that T_{opt} increased with depth from layer 2 to 5. The median of T_{opt} ranged from 1.5 for layer 2 to 12.5 days for layer 5. The median T_{opt} for profile SM was 3.5 days. Significant differences in T_{opt} were obtained for layer 2, layer 3, and layer 4, but the difference between layers 4 and 5 was not significant. The increase of T_{opt} with depth has already been observed in many studies, and is related to the greater temporal stability of SM in deeper soil layers (Wang et al., 2017; Tian et al., 2019).

Table 3. The statistics of T_{opt} (day) for different layers and different years for all stations.

Year	Statistics	Layer 2	Layer 3	Layer 4	Layer 5	Profile
2014	mean (std)	2.72 (2.22)	8.32 (8.39)	13.18 (12.52)	16.81 (16.70)	4.73 (4.16)
	median	2.00	5.50	9.50	12.75	4.00
2015	mean (std)	2.56 (2.54)	7.78 (8.04)	15.77 (15.87)	23.15 (19.61)	5.23 (4.51)
	median	1.50	5.00	9.00	12.00	3.75
2016	mean (std)	2.23 (2.13)	6.13 (9.80)	9.26 (9.43)	17.74 (18.93)	3.32 (2.56)
	median	1.50	4.00	6.50	12.50	2.75
Summary	mean (std)	2.48(2.26)[a]	7.29(8.85)[b]	12.37(12.67)[c]	18.93(18.43)[c]	4.32(3.77)[ab]
	median	1.50	4.50	8.50	12.50	3.50

Note: std represents the standard deviation. Summary represents the statistics results of the three years. Different letters in Summary row indicate significant differences among different layers ($p<0.05$), while the same letter indicates that the difference is nonsignificant.

4.2.2 Evaluation of alternative methods for T_{opt} estimation

Previous studies have used various methods to estimate T_{opt}. For example, it was found that using a single representative value for T_{opt} (e.g. average or median) for all stations did not significantly reduce the accuracy of the SM estimates (Albergel et al., 2008; Ford et al., 2014). Wagner et al. (1999) recommended a common value of T_{opt} = 20 (days) to estimate root zone SM, and this value has been widely adopted (e.g. Lange et al., 2008; Muhammad et al., 2017). Qiu et al. (2014) proposed to estimate T_{opt} using the station-specific long-term mean NDVI using $T_{opt} = -75.263 \times \mathrm{NDVI} + 68.171$ (R=0.5, $p<0.01$). This approach has also been applied in other studies (Tobin et al., 2017).

Here, we evaluated four different methods to estimate T_{opt} in our study region for estimating profile soil moisture (0-70 cm, SWI) from surface soil moisture (5 cm, SWI). In the first method, T_{opt} was estimated from the NDVI-based regression of Qiu et al. (2014) to provide T_{Qiu}. In the second method, T_{opt} was set to 20 days as recommended by Wagner et al. (1999) to provide T_{Wagner}. In the third method, an area-generalized T_{opt} was obtained from the median value for the profile SM in our study region (3.5 days) to provide $T_{general}$. In the fourth and final method, the original station-specific T_{opt} parameter for profile SM was used ($T_{specific}$). The accuracy of the SM estimates obtained using the different methods to estimate T_{opt} was again evaluated using NSE, R and RMSE (Fig. 5). The performance metrics show that $T_{specific}$ performed best (mean RSR of 0.58, R of 0.88, and NSE of 0.61) followed by $T_{general}$ (mean RSR of 0.61, R of 0.85, and NSE of 0.58), T_{Wagner} (mean RSR of 0.79, R of 0.69, and NSE of 0.32) and T_{Qiu} (mean RSR of 0.89, R of 0.59, and NSE of 0.17). However, the difference in performance between $T_{specific}$ and $T_{general}$ is not significantly different. The T_{Wagner} and the T_{Qiu} approach performed less well, and the metrics (NSE, R, RSR) are significantly ($p<0.001$) lower than those of the $T_{general}$ and $T_{specific}$ methods. Our results suggest that a site-specific T_{opt} significantly improves the performance of the ExpF method compared to the use of the universal T_{opt} recommended by Wagner et al. (1999) or the regression of Qiu et al. (2014). Similarly, Lange et al. (2008) also found a significant improvement when using a station-specific T_{opt} instead of T_{opt} = 20 days. It should be mentioned that the estimation depth in the method of Wagner et al. (1999) was 0-100 cm, while that of our study was 0 - 70 cm. This may partly explain the poor performance of the T_{Wagner} approach in this study. The use of an area-generalized T_{opt} (3.5 days) is a suitable alternative for T_{opt} estimation in our study area, and provides similar estimation performance. Other studies have also found a good performance when using an area-generalized T_{opt} (e.g. Albergel et al., 2008; Brocca et al., 2010; Ford et al., 2014).

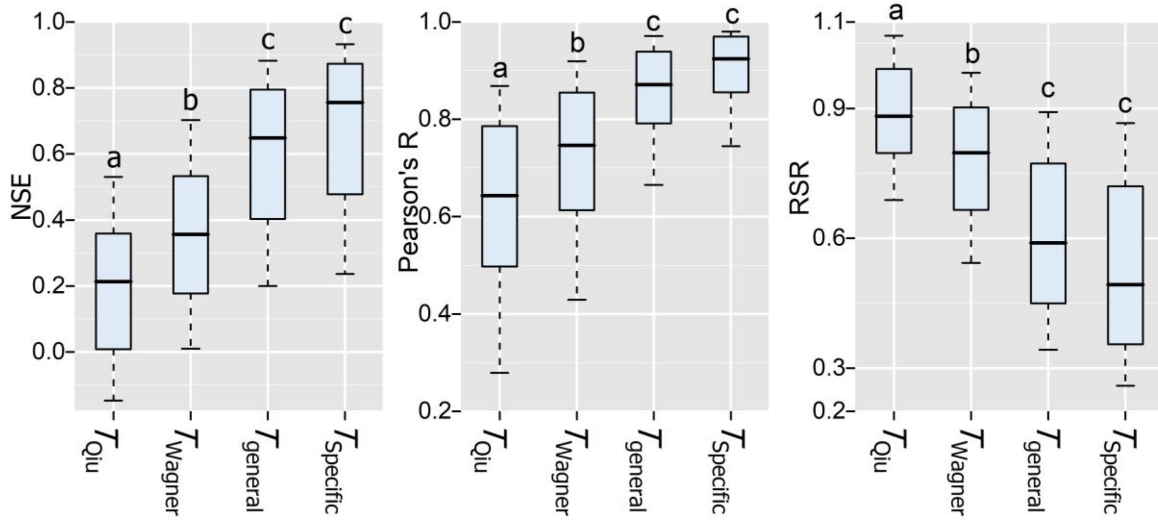


Fig. 5. The boxplot of NSE, Pearson's R, and RSR for the T_{opt} generated from different schemes. The different letters above box indicate the significant difference for different schemes.

4.3 Estimating profile soil moisture using SMAP

The results have shown that the ExpF method is suitable to estimate profile SM from surface SM. Moreover, the evaluation of methods for T_{opt} estimation concluded that the median value of T_{opt} is suitable for estimation of subsurface soil moisture. Thus, in this section, we evaluate the utility of the ExpF method (with the median value of T_{opt} of SMAP) in combination with SMAP surface products for estimating subsurface SM in mountainous areas.

4.3.1 Assessment of SMAP surface SM product

The observed surface SM of each station was compared with the SMAP_L3 soil moisture product that overlapped with the corresponding station for the growing seasons of 2015 and 2016 for all stations to evaluate the accuracy of the SMAP measurements (Pablos et al., 2018). The root mean square error (RMSE), mean bias error (MBE), unbiased RMSE (ubRMSE) and R were adopted as metrics to evaluate accuracy. The relationship between the SMAP_L3 SM data product and the in-situ observations a 5 cm depth is presented in Fig.6. Clearly, the part of the scatter in the relationship is due to the scale discrepancy between the satellite and the in-situ SM sensor data. Nevertheless, the statistical metrics still indicate a significant relationship between the SMAP_L3 SM data product and the in-situ observations a 5 cm depth. Time series of the two datasets for each station are provided in the supplementary Fig. S2. Figs. 6 and S2 show that the performance was low at two stations (D13 with R of 0.18, D15 with R of 0.08) with scrubland and relatively high soil moisture. The poor performance at scrubland sites is consistent with results presented by Zhang et al. (2017b) for this study region. Results showed that the MBE varied from -0.23

to 0.07 cm^3/cm^3 with a median of -0.021 cm^3/cm^3. This indicates that SMAP underestimated surface SM over the study region, which is consistent with previous studies in the area (Chen et al., 2017; Zhang et al., 2017b). The RMSE varied between 0.026 and 0.250 cm^3/cm^3 between sites with a median value of 0.052 cm^3/cm^3. After removing the bias, the SMAP product had a median ubRMSE of 0.036 cm^3/cm^3 (range from 0.024 to 0.083 cm^3/cm^3). Therefore, the SMAP product achieved the accuracy requirement of 0.04 cm^3/cm^3 (Chan et al., 2016) in this study area. The R value ranged from 0.075 to 0.81 with a median value of 0.59. The relationship between SMAP-derived and in-situ observed surface SM was significant ($p<0.05$) at all but one station. This suggests that the SMAP surface product can represent the temporal dynamics of the observed surface SM time series.

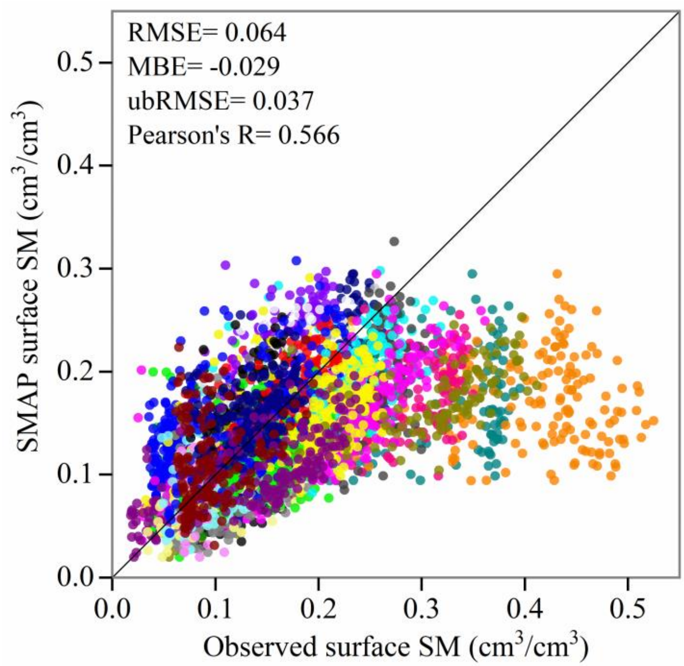


Fig. 6. Scatterplot of the SMAP_L3 surface SM (cm^3/cm^3) with in-situ observations at the surface (5 cm) of the 35 soil moisture stations. Each color indicated one station. Averaged metrics (RMSE, MBE, R, ubRMSE) of 35 stations during the growing seasons of 2015 and 2016 were showed in the plot.

4.3.2 SMAP-based estimation of subsurface soil moisture

For the estimation of subsurface soil moisture from the SMAP_L3 surface product, the site-specific T_{opt} was calculated based on the best match between SMAP estimations and in-situ observations in terms of NSE. The median values of T_{opt} for the layers 2, 3, 4, 5 and profile are 7 days, 12 days, 22 days, 35 days and 10 days, respectively. The subsurface SWI estimated from the combination of SMAP surface soil moisture with the ExpF method (with the median values of T_{opt}) were compared with the in-situ observations. A comparison of the subsurface SWI time series for different layers at each station are provided in Fig. S3- S7. Fig.7 shows the scatter plot between measured and predicted SWI, and the performance metrics are summarized in Table 4.

Table 4. Performance metrics (RSR, R, NSE) for the comparison of SMAP estimated and observed SWI at different layers for the 35 stations during the growing seasons of 2015-2016.

Layer	RSR		R		NSE	
	Mean±Std	Median	Mean±Std	Median	Mean±Std	Median
Layer 2 a	1.24±1.31	0.92	0.58±0.28	0.69	0.06±0.37	0.18
Layer 3 ab	1.28±0.83	1.11	0.45±0.35	0.55	-0.08±0.41	-0.02
Layer 4 b	1.49±1.21	1.12	0.28±0.46	0.31	-0.18±0.37	-0.13
Layer 5 b	1.96±3.43	1.17	0.24±0.5	0.34	-0.15±0.39	-0.15
Profile a	1.22±0.82	0.92	0.55±0.3	0.65	0.08±0.41	0.14

Note: the different letters after the layers indicate that the difference is significant at $p<0.05$ (Kruskal-Wallis ANOVA)

As expected, the estimation accuracy of subsurface SM decreased with depth. The ANOVA results showed that the subsurface SM estimation accuracy for layer 2 (median value of RSR=0.92, R=0.69, NSE=0.18) and profile SM (RSR=0.92, R=0.65, NSE=0.14) were significantly higher than for layer 4 (RSR=1.12, R=0.31, NSE=-0.13) and layer 5 (RSR=1.17, R=0.34, NSE=-0.15) ($p<0.05$). The NSE values were positive for layer 2 and profile SM, while the NSE values for the other layers were negative. The negative MBE showed that subsurface SM was underestimated. The relationship between SMAP-derived and in-situ observed subsurface SM for layer 2 and profile SM was significant ($p<0.01$) at all but one station (D15). Thus, the SMAP surface product and ExpF method can be used to estimate the subsurface SM in the study area, especially for layer 2 (10-20 cm) and profile (0-70 cm) SM.

As suggested by Ford et al. (2014), we partitioned the error in the SMAP-based estimation of profile SWI ("SMAP-observed profile SWI", Fig. S8c) in errors associated with the ExpF method and errors due to SMAP observation differences to gain some insight into the error sources of SMAP-based estimates of profile SWI. For this, profile SWI estimated using the ExpF method from observed surface SWI was compared with in-situ observed profile SWI ("estimated-observed profile SWI") to assess errors of the ExpF method (Fig. S8(a)). In addition, SMAP-based and in-situ observed surface SWI ("SMAP-observed surface SWI") were compared to assess inherent errors of the SMAP product (Fig. S8 (b)). RMSE, R and MAE were used as the metrics to assess accuracy. The results of this analysis are summarized in Table 5.

Table 5. Statistics of the metrics (RSR, R, NSE) of the comparisons of estimated-observed profile SWI datasets, SMAP_L3-observed surface SWI datasets, SMAP_L3-observed profile SWI datasets, and SMAP_L4-observed profile SWI datasets for the 35 stations during the growing seasons of 2015-2016.

Comparisons	RSR		R		NSE	
	Mean±std	Median	Mean±std	Median	Mean±std	Median
Estimated-observed PSWI	0.86±1.00	0.68	0.88±0.11	0.9	0.56±0.32	0.64
SMAP_L3-observed SSWI	1.13±0.49	1.01	0.57±0.17	0.59	-0.09±0.52	-0.07
SMAP_L3-observed PSWI	1.22±0.82	0.92	0.55±0.3	0.65	0.08±0.41	0.14
SMAP_L4-observed PSWI	1.42±0.76	1.25	0.47±0.31	0.55	-0.49±0.68	-0.3

Note: e.g. Estimated-observed PSWI means the comparison of the estimated profile SWI and observed profile SWI.

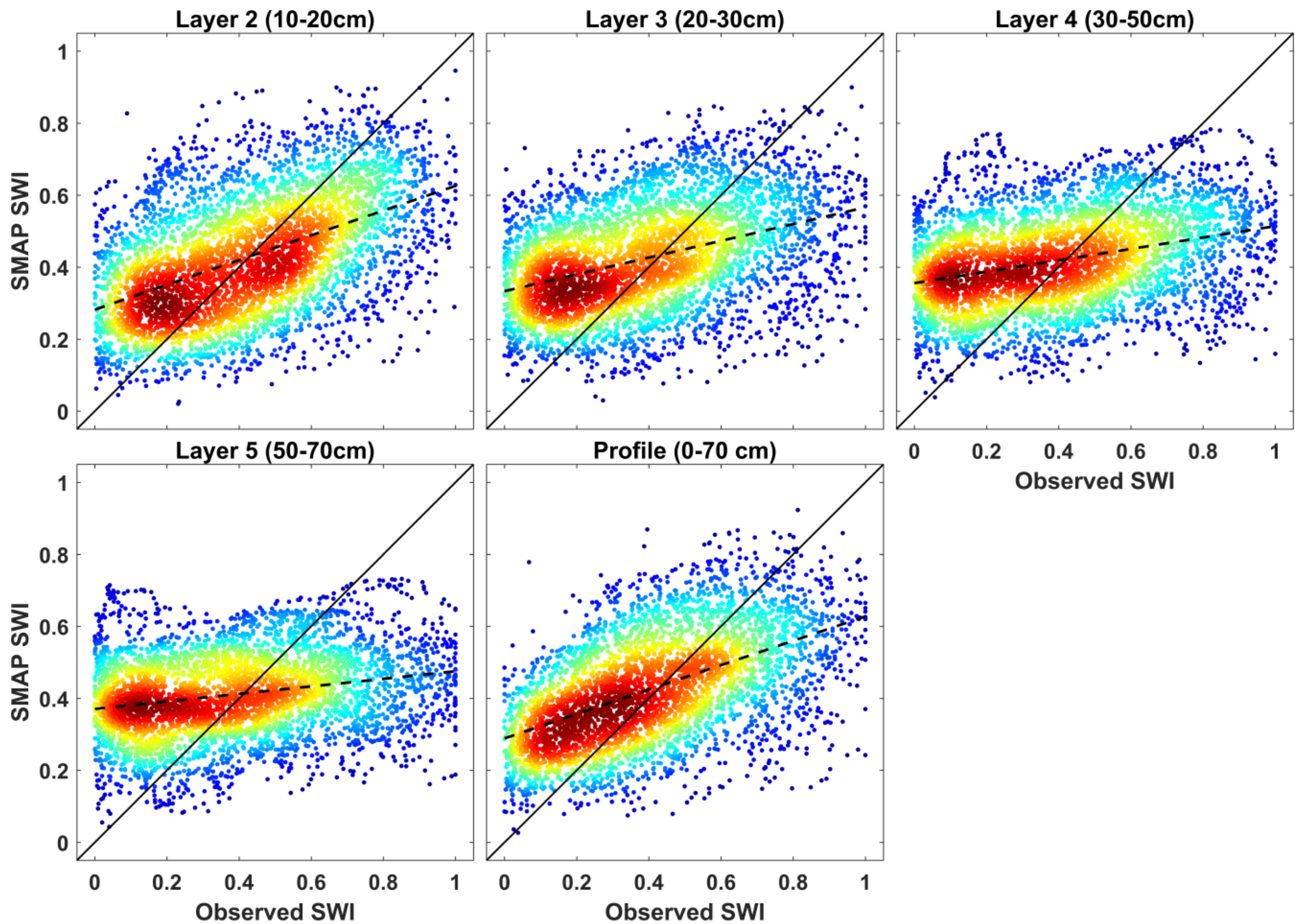


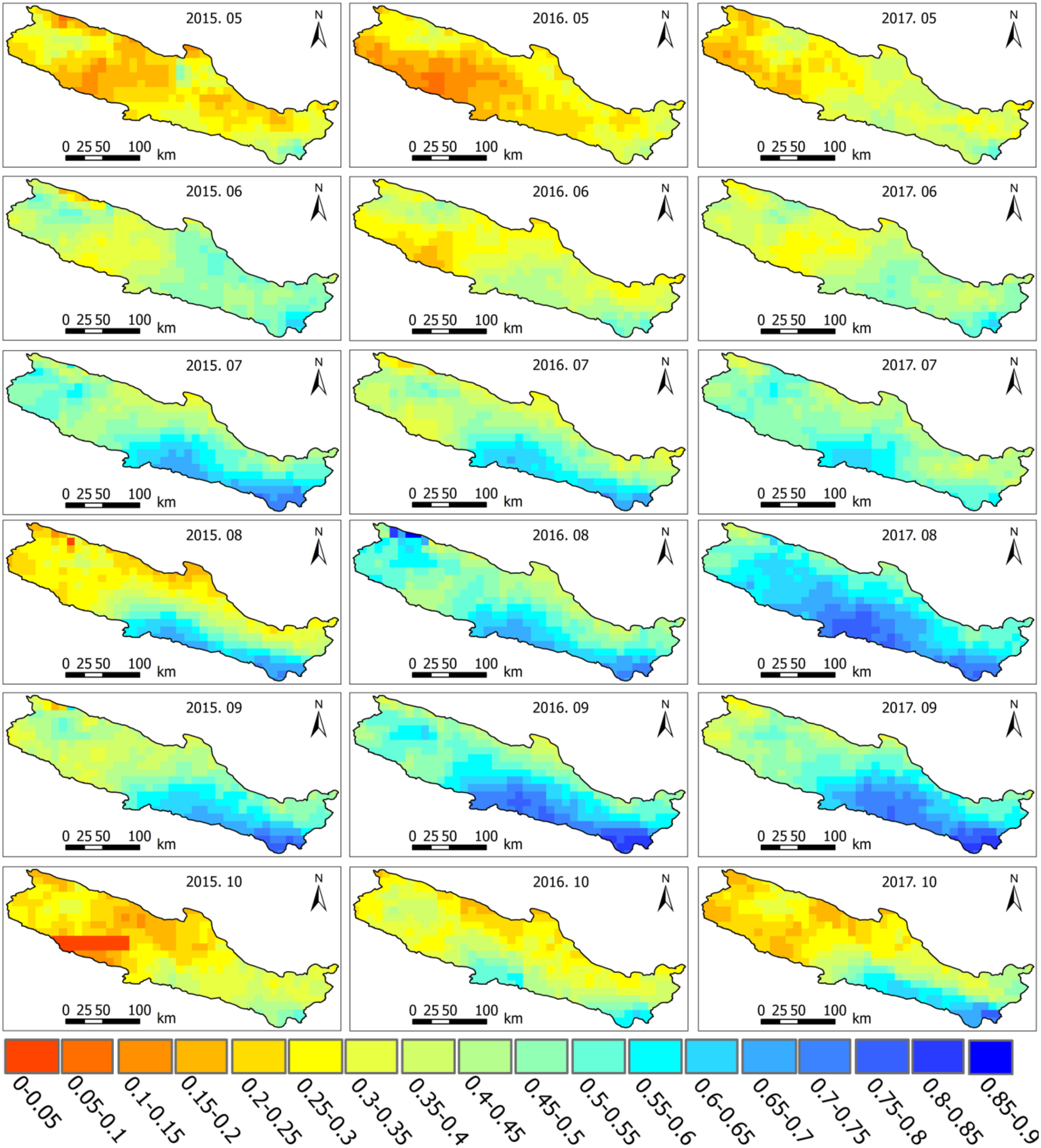
Fig. 7. Scatterplot of the comparisons of SMAP_L3 estimated-observed subsurface SWI for all stations during the growing seasons of 2015-2016. The representation is a smoothed color density of a scatter plot to make a quantity of points visual. The dash and solid line are the best-fitted curve and "y=x" line, respectively.

Fig. S8 and Table 5 show that the SMAP-observed SWI had lower performance metrics for surface SWI (median value of RSR, R and NSE are 1.01, 0.59 and -0.07, respectively) than for profile SWI (median value of RSR, R and NSE are 0.88, 0.72 and 0.19, respectively), which was similar to the results obtained from the Nebraska SM network (Ford et al., 2014). This may be because the profile SWI was estimated based on the SMAP surface SWI and T_{opt}, which was determined by optimization using the maximum NSE. This may have improved the performance of profile SWI estimation. In addition, the performance metrics for SMAP–observed SWI comparisons for both surface and profile SWI were significantly ($p<0.001$) lower than those of estimated–observed profile SWI (median value of RSR, R and NSE are 0.68, 0.90 and 0.64, respectively). Thus, the major error in SMAP-based profile SWI estimates stems from the SMAP satellite product and is not derived from the ExpF method, which is also supported by previous studies (e.g. Ford et al., 2014; Pablos et al., 2018). As mentioned before, the scale mismatch between point measurements and satellite footprints will introduce additional errors in the validation of the satellite-derived subsurface products (Jin et al. 2017).

Subsequently, the SMAP_L4 and SMAP_L3 estimated profile SWI were compared to the in situ observed profile SWI (see Fig. S10 and Table 5). From these results, we can see that the performance of profile soil moisture estimation using the SMAP_L3 surface product and the ExpF method (median RSR, R and NSE of 0.92, 0.65 and 0.14, respectively) was significantly ($p<0.01$) better than that of the SMAP_L4 product (median RSR, R and NSE of 1.25, 0.55 and -0.3, respectively). The low performance of the SMAP_L4 profile product may be associated with uncertainty in the meteorological driving forces and the soil parameters in the NASA catchment model for cold mountainous areas (Reichle et al., 2017; Zhao et al., 2018; Dai et al., 2019). Thus, our results suggest that combining the exponential filter method with the SMAP_L3 product improves the estimation of profile SM for the data-scarce cold arid mountainous areas significantly.

Finally, the spatial distribution of profile soil moisture during the growing season of 2015, 2016 and 2017 was obtained using the median value of T_{opt} and the SMAP_L3 product to get the spatial distribution of profile SM in the study area (Fig. 8). The spatial distribution of the profile SM shows higher values in the southeast, while lower values were obtained in the northwestern part of the study area. This distribution coincides with the spatial distribution of precipitation and surface SM. The temporal variation of profile SWI, surface SWI, and precipitation are shown in Fig. S10. Our results show that the temporal variation of the SM profile corresponded well with the occurrence of precipitation: Profile SM increased from May (mean SM of 0.27) to September (0.533) and then decreased until October (0.304). Profile SWI_{SMAP} was lower than surface SWI_{SMAP} from May to August, while profile SWI_{SMAP} was higher than surface SWI_{SMAP} from September to October. This can be attributed to the higher sensitivity of surface SM dynamics to precipitation and evapotranspiration (ET). During the months of September and October, less precipitation and higher ET caused a faster decrease in surface SM compared to profile SM.

Previous studies have shown the difficulty of applying the ExpF method to satellite products in mountainous area, where complex topography (Paulik et al., 2014), snow and soil freezing (Ford et al., 2014; Pablos et al., 2018) cause large errors and poor performance of the filtering method (Albergel et al., 2008). Ford et al. (2014) found an improvement of performance after removing the effects of snow from the data in the SCAN network, USA. Based on in situ SM observations, this study showed that the ExpF method is useful in estimating profile SM from SMAP surface products in the growing season in high and cold mountainous areas.



370 **Fig. 8.** The spatial distribution of the monthly averaged profile SWI product estimated from SMAP_L3 surface product during the growing season from 2015 to 2017. The title of each subplot provides the month and year.

5. Conclusions

In this study three methods (the exponential filter (ExpF), the artificial neural network (ANN) and the cumulative distribution function matching (CDF) methods) were used to calculate subsurface SM from in-situ surface SM observations at 5 cm depth in the Qilian Mountains (China). We also evaluated the utility of the ExpF method to estimate profile SM from SMAP surface products in the study area. Our main findings are:

1) With increasing depth of the predicted soil layer, the accuracy of all three methods decreased. Both the ANN and ExpF methods showed good performance for the estimation of SM down to 30 cm.

2) The ANN method exhibited the lowest estimation error, while the ExpF method was able to better capture the temporal variation of subsurface SM.

3) The area-generalized T_{opt} value of the ExpF method can be used in the study area to estimate the subsurface SM without significantly reducing the performance compared to a station-specific T_{opt}.

4) Subsurface SM derived from the SMAP_L3 surface SM product using the ExpF method showed less deviation from the in-situ observations compared to the SMAP_L4 root zone product for the study area.

We anticipate that our findings can improve the large-scale estimation of subsurface SM in mountainous areas, which in turn will support ecohydrological research and water resources management in inland river basins.

Data availability. All the data used in this research are available upon request.

Author contributions. BZ and CH prepared the research project. JT, ZH, CH, HB and JH conceptualized the methodology. JT, ZH and CM collected the data. JT, ZH and HB developed the code and performed the analysis. JT prepared the manuscript with contributions from all co-authors.

Competing interests. The authors declare that they have no conflict of interest

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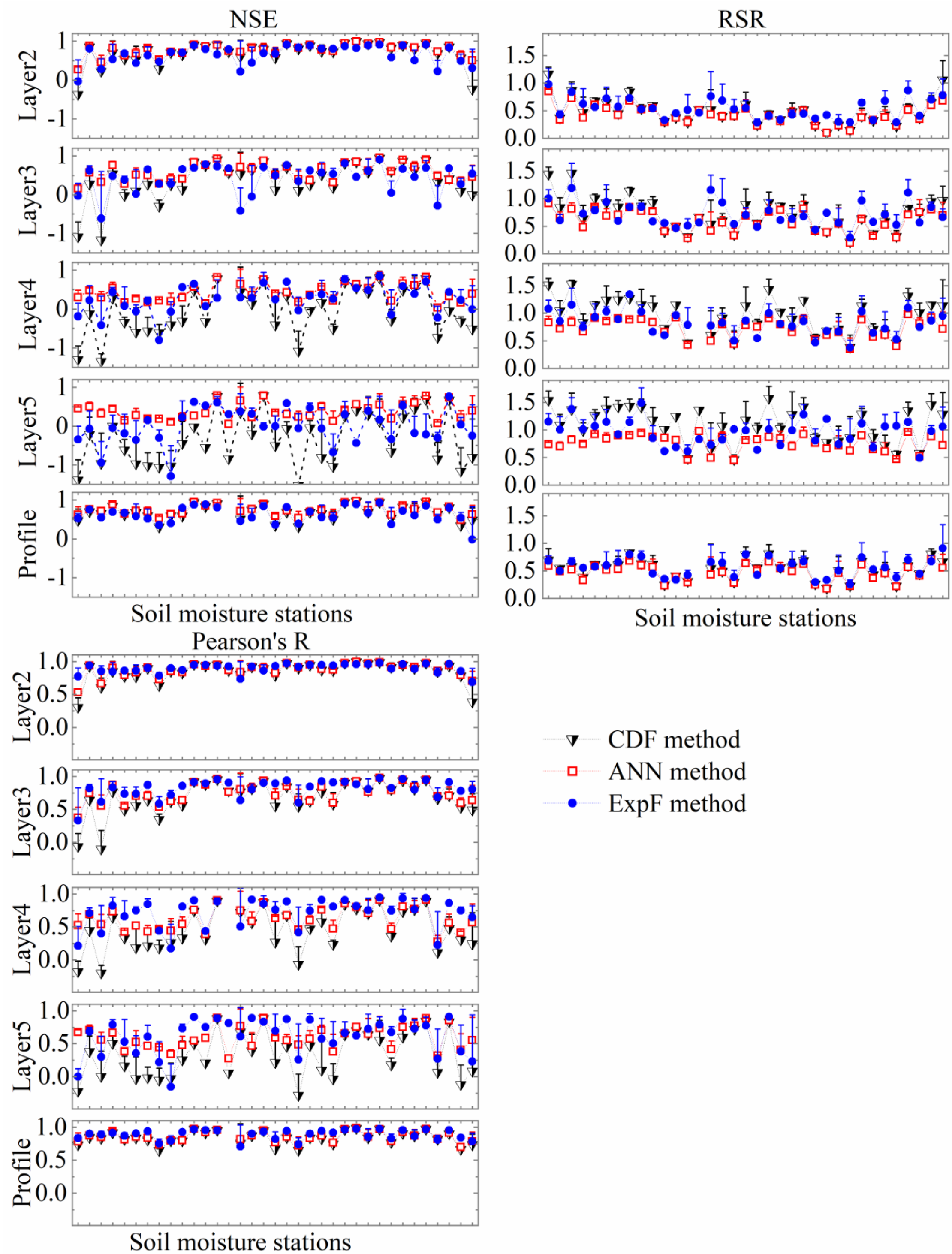
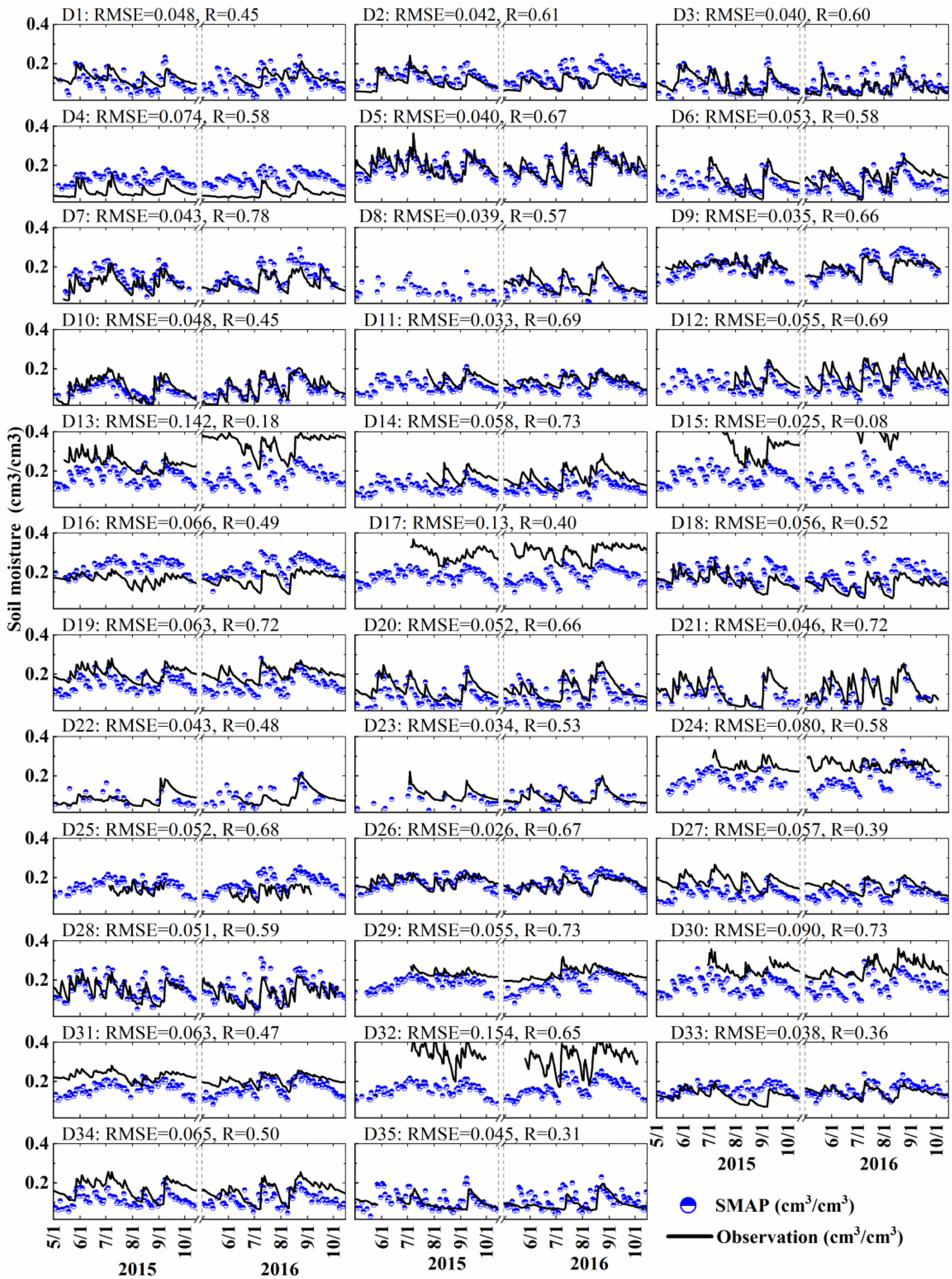


Fig. S1. Metrics (NSE, RSR, and Pearson's R) of the different methods for the estimation of subsurface soil moisture from surface soil moisture for each layer of all soil moisture stations. Plot shows the mean value with the error bar of the standard deviation.



5 **Fig. S2.** Comparison of the SMAP and in-situ observations of surface soil moisture (cm^3/cm^3) data during the growing season of 2015-2016 for the 35 stations. Also with the RMSE and R of the comparisons of the two datasets for each station during the growing season of 2015-2016.

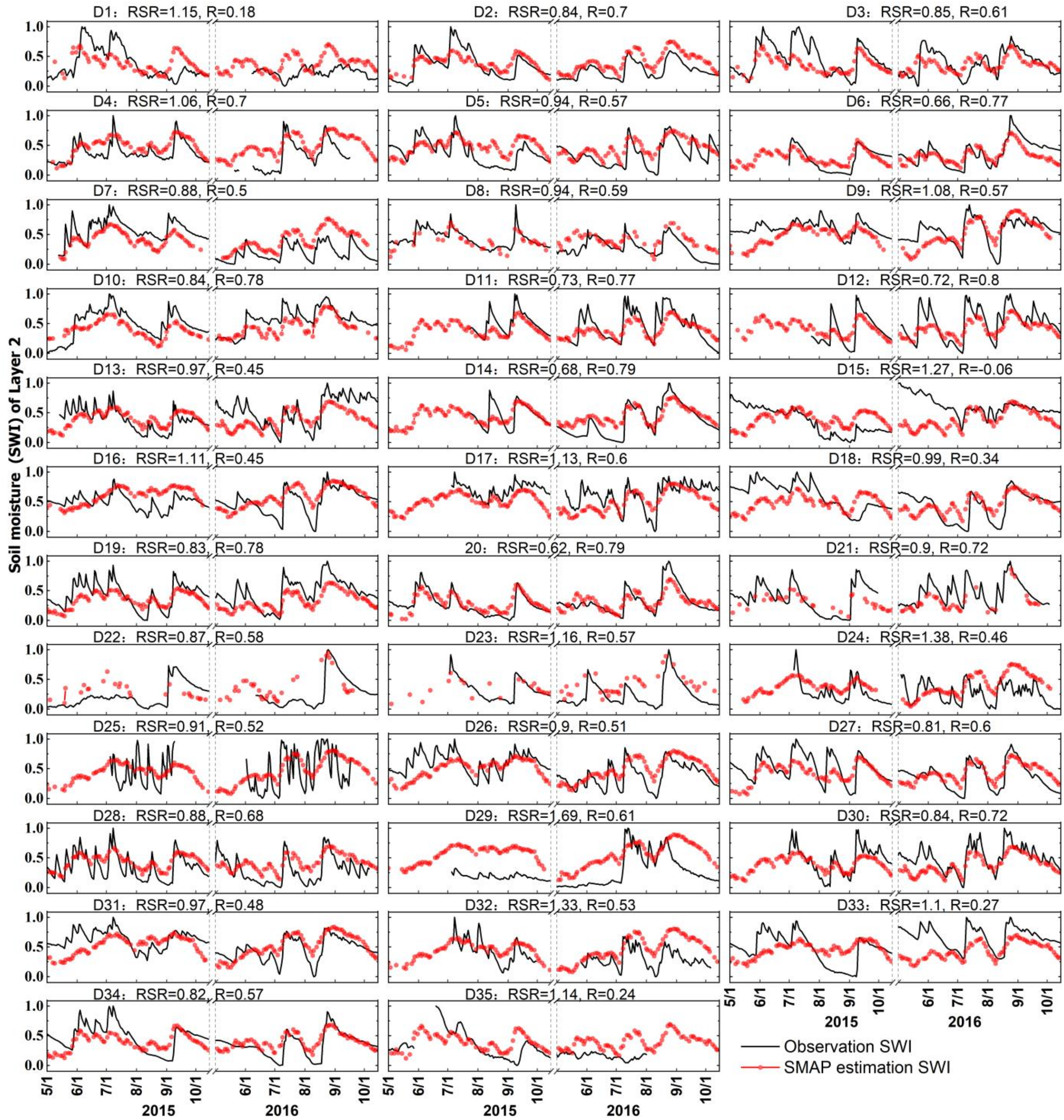


Fig. S3. Comparison of the SMAP estimation and in-situ observation of layer 2 SWI time series during the growing season of 2015-2016 for the 35 stations. Also with the RMSE and R of the comparisons of the two datasets for each station during the growing season of 2015-2016.

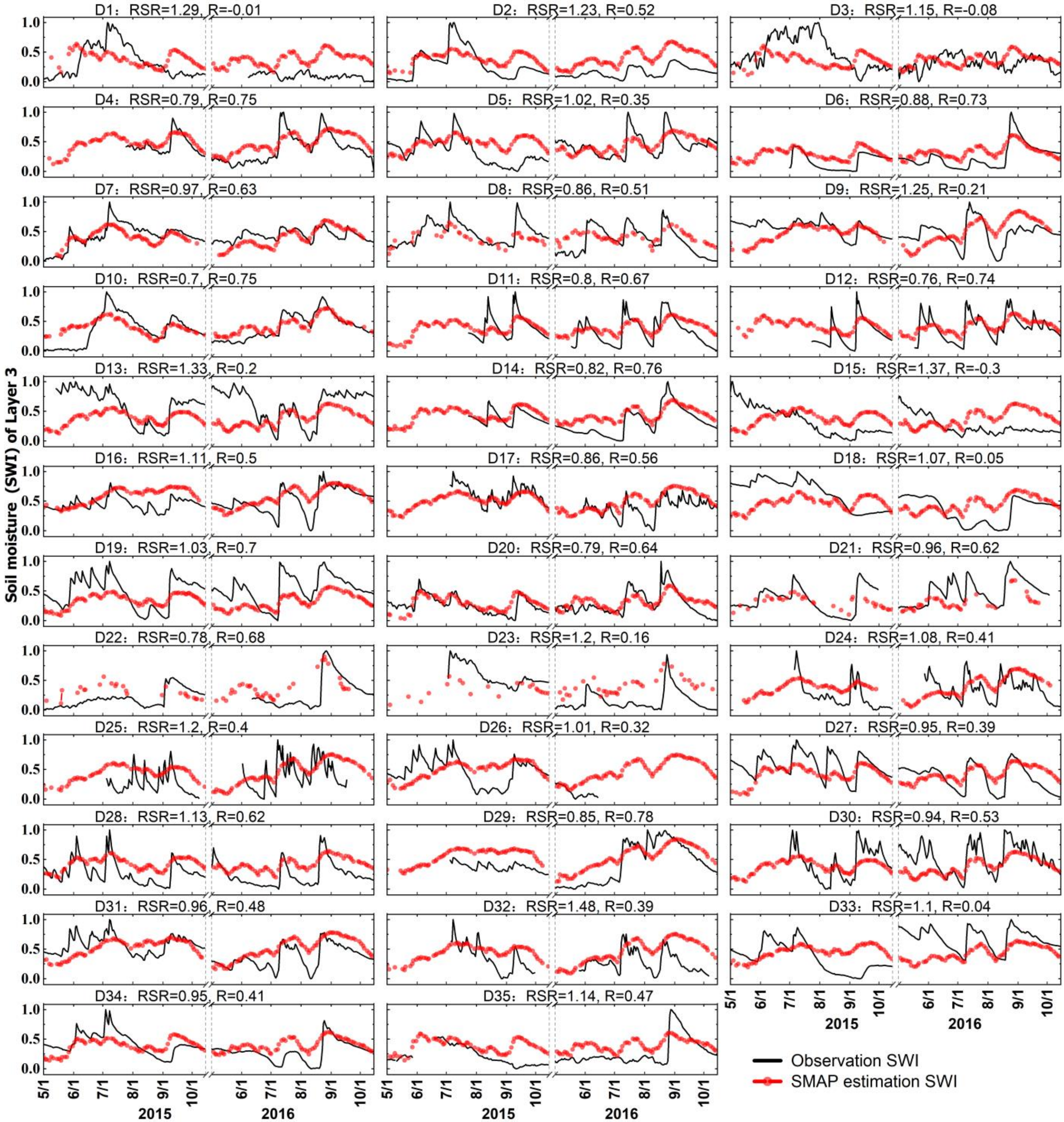


Fig. S4. Comparison of the SMAP estimation and in-situ observation of layer 3 SWI time series during the growing season of 2015-2016 for the 35 stations. Also with the RMSE and R of the comparisons of the two datasets for each station during the growing season of 2015-2016.

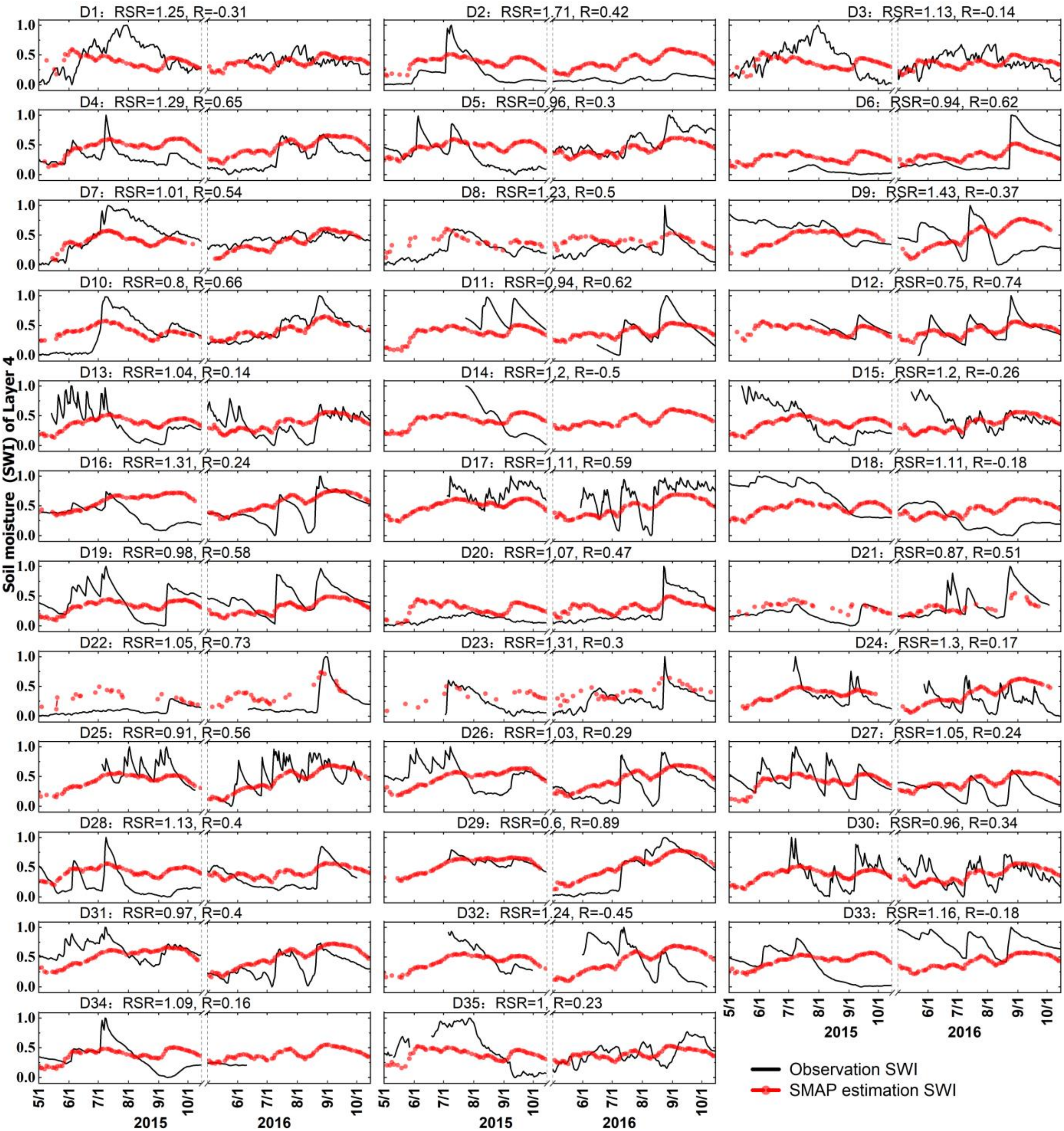


Fig. S5. Comparison of the SMAP estimation and in-situ observation of layer 4 SWI time series during the growing season of 2015-2016 for the 35 stations. Also with the RMSE and R of the comparisons of the two datasets for each station during the growing season of 2015-2016.

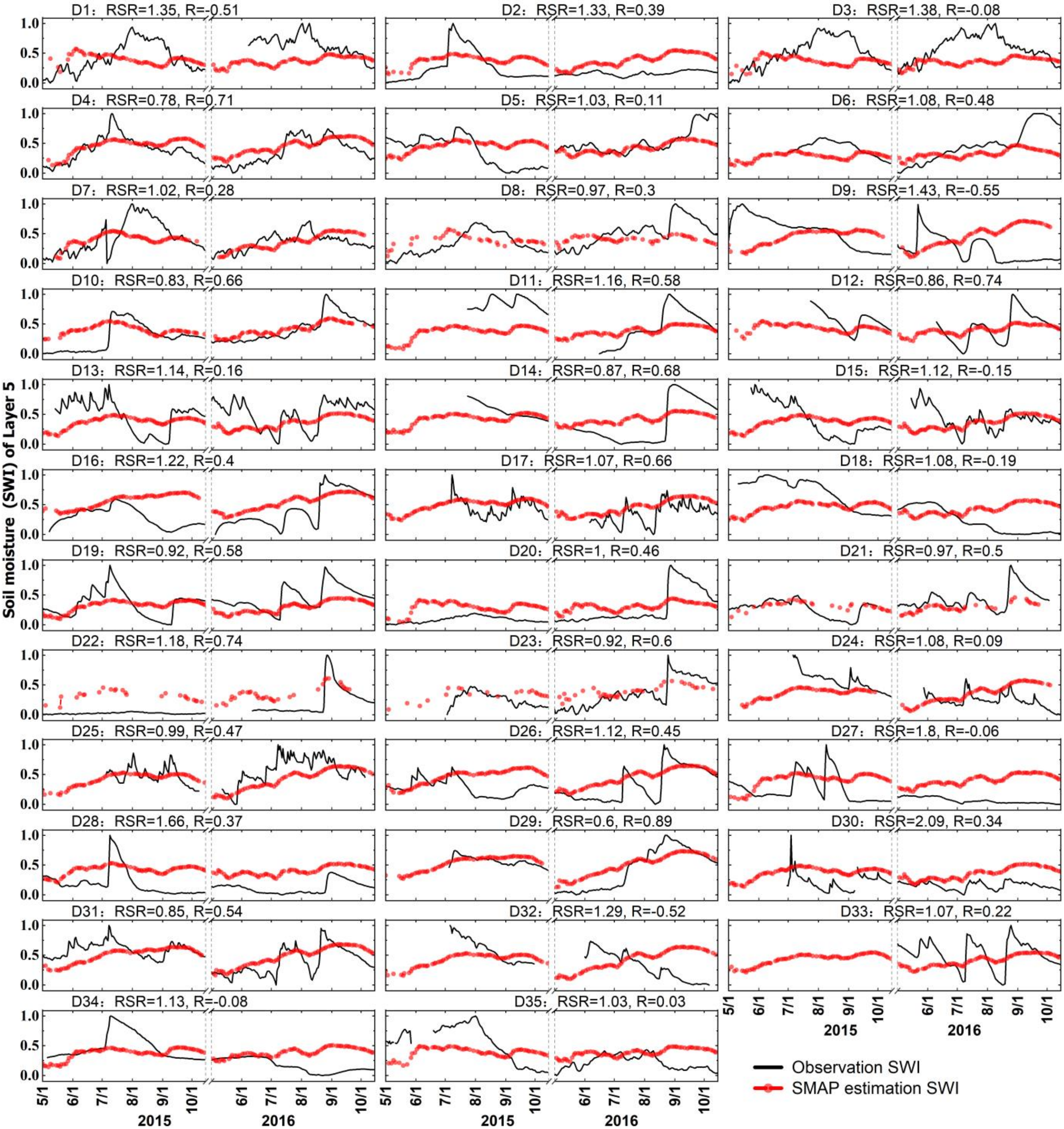


Fig. S6. Comparison of the SMAP estimation and in-situ observation of layer 5 SWI time series during the growing season of 2015-2016 for the 35 stations. Also with the RMSE and R of the comparisons of the two datasets for each station during the growing season of 2015-2016.

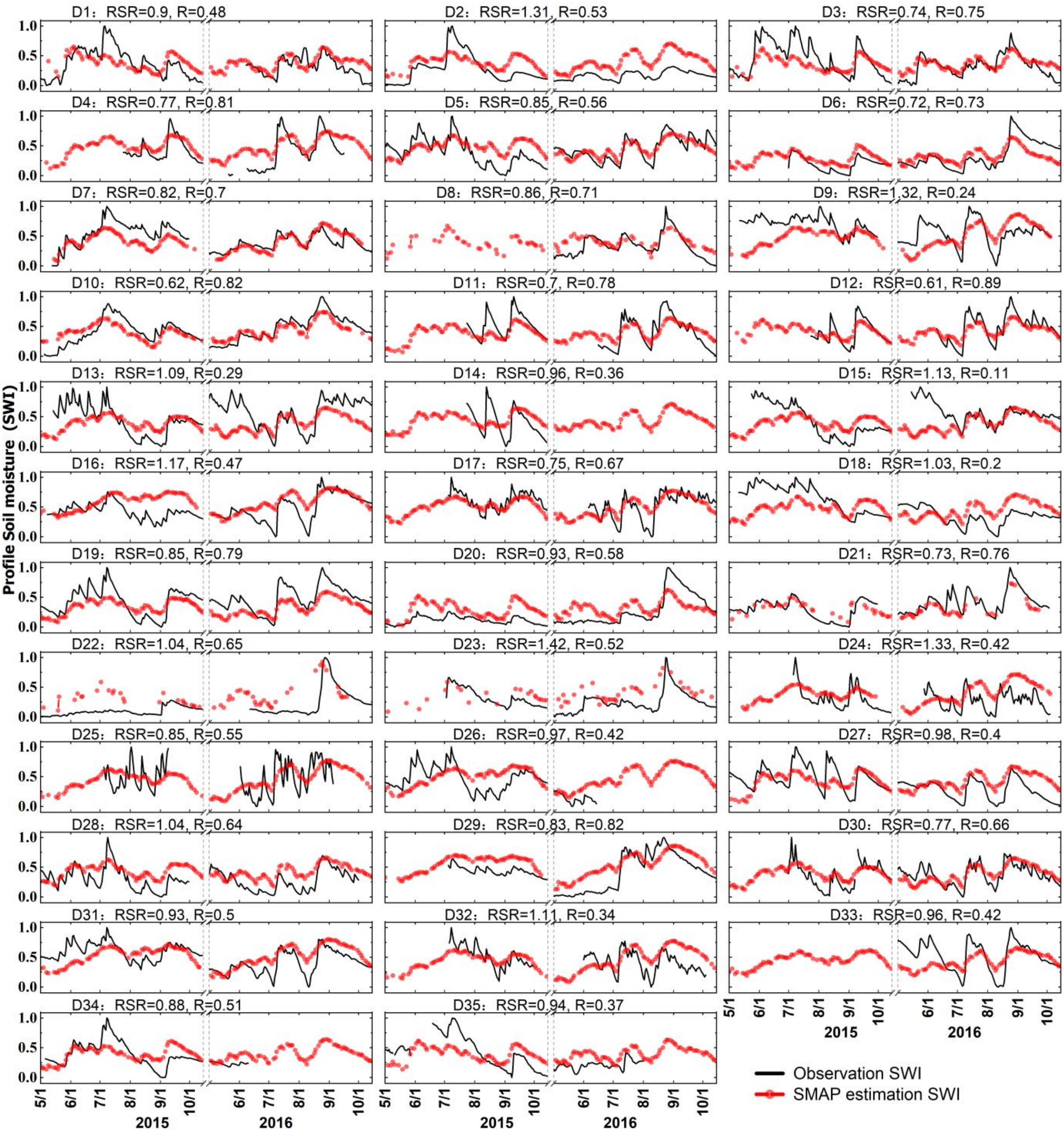


Fig. S7. Comparison of the SMAP estimation and in-situ observation of profile SWI time series during the growing season of 2015-2016 for the 35 stations. Also with the RMSE and R of the comparisons of the two datasets for each station during the growing season of 2015-2016.

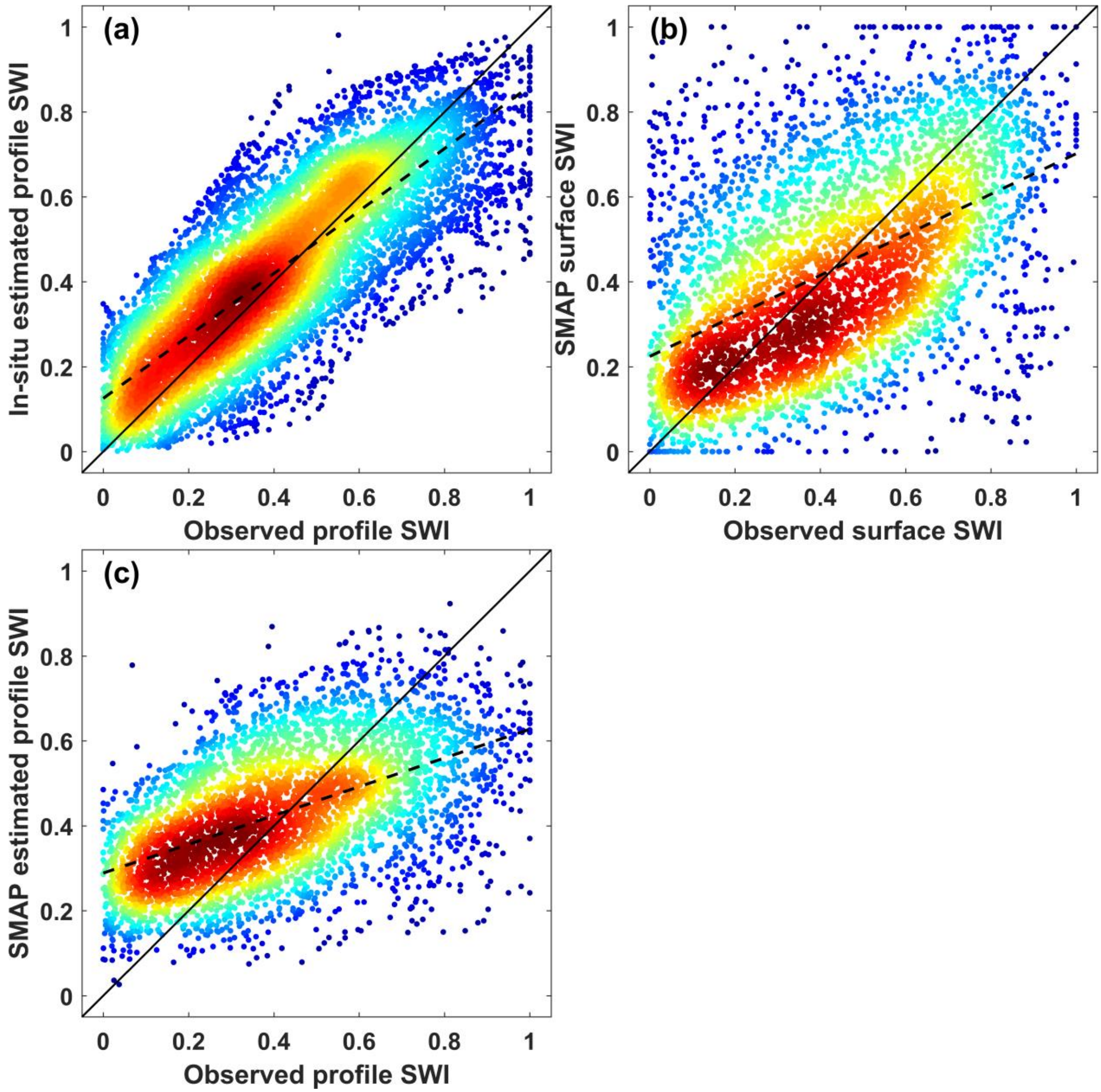


Fig. S8. Scatterplot of the comparisons of (a) estimated-observed profile SWI, (b) SMAP-observed surface SWI, and (c) SMAP-observed profile SWI for the 35 stations during the growing seasons of 2015-2016.

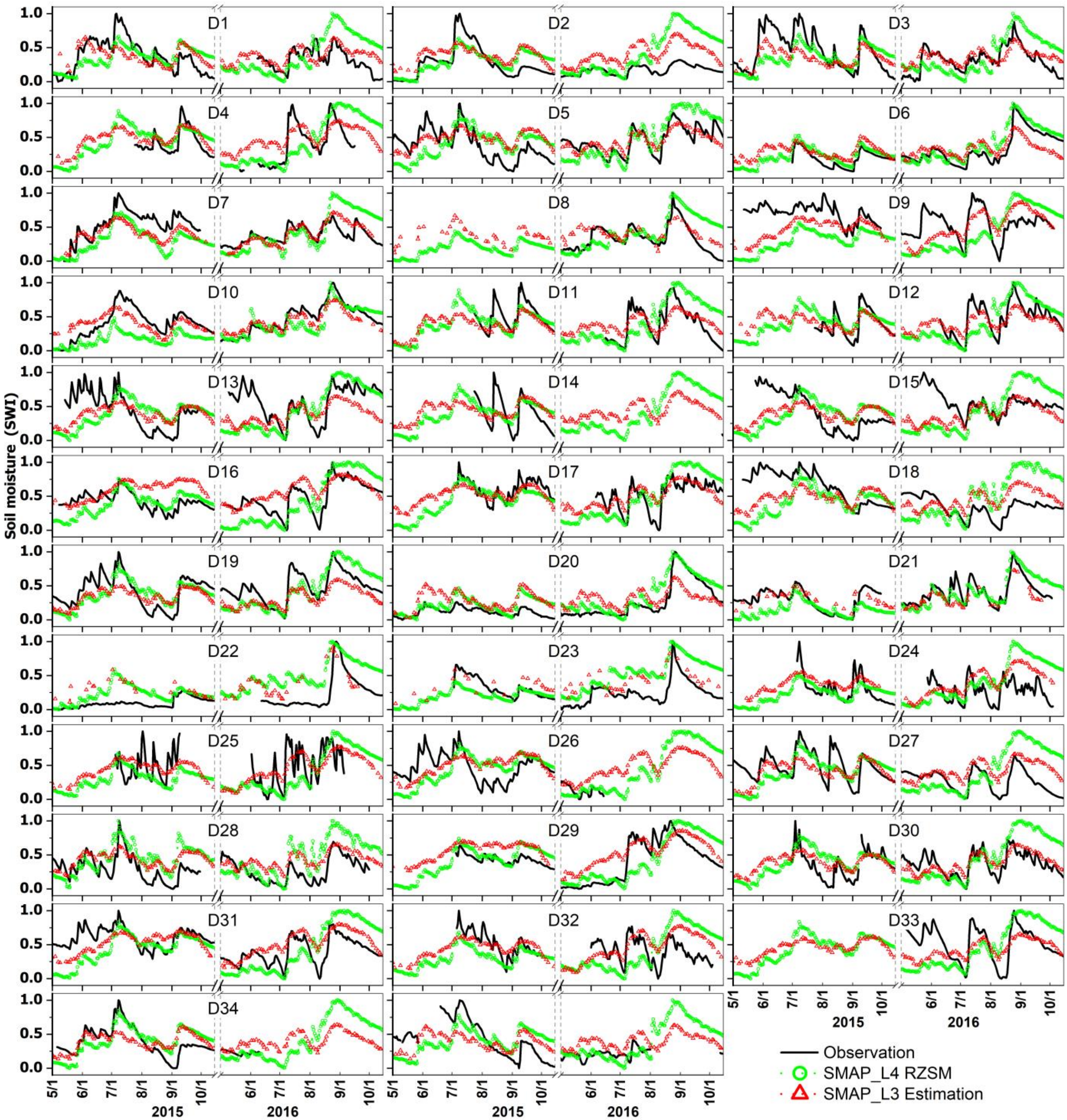


Fig. S9. Comparison of the SMAP_L3 estimated PSWI, SMAP_L4 PSWI and in-situ observation of PSWI time series during the growing season of 2015-2016 for the 35 stations.

35

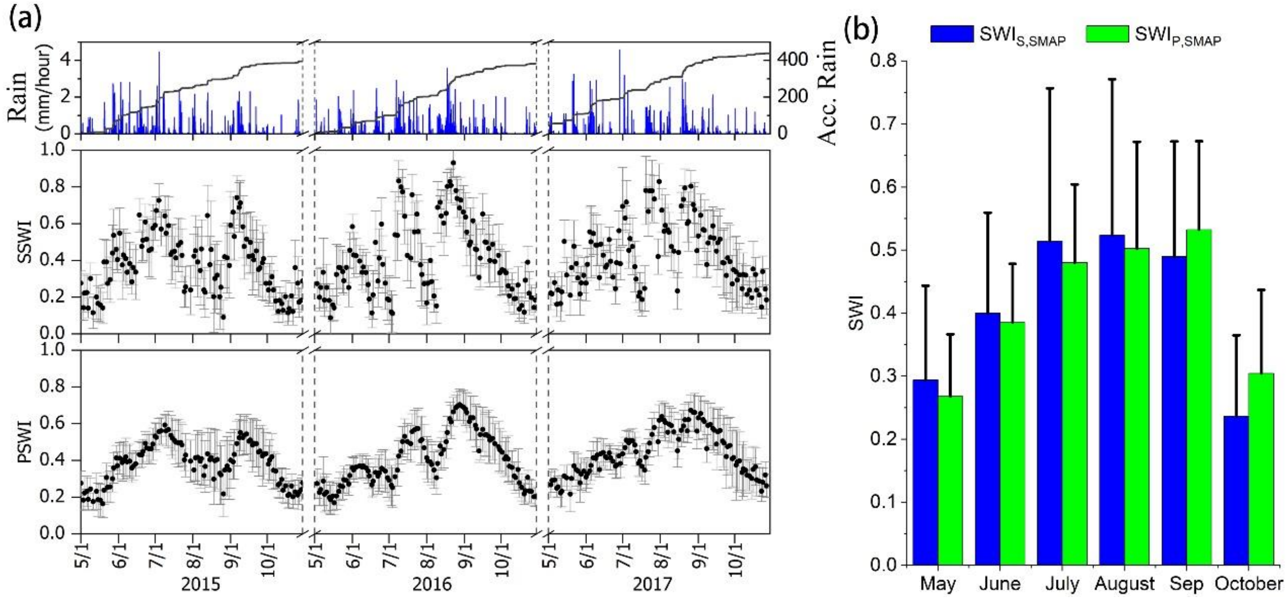


Fig. S10. (a) the temporal variation of precipitation, SSWI and PSWI, and (b) the comparison (bar represents the mean value and error bar means the standard deviation) of the monthly SSWI and PSWI during the growing seasons of 2015-2017.