Dear Prof. Na Li,

We thank you very much for the constructive comments and suggestions on our manuscript (hess-2016-617). We have responded to all the questions raised. In the following pages are our point-by-point responses. We hope that our responses are clear enough to all of your questions. Thanks for your consideration, and we are

Sincerely yours

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Responses to comments

General comments:

The manuscript by Gao et al. applied a statistic approach (using observation operators built by Cumulative Distribution Frequency matching method) to multi-station in situ soil moisture observations, aiming to predict profile soil moisture from surface soil moisture. They first investigated the effects of temporal resolution (hourly, daily and weekly) and data length (half year in non-growing season, half year in growing season, one year, two years and four years) on the performance of observation operators. Based on the investigation, daily soil moisture data with two-year duration was then used to test the robustness of observation operators, illustrated in three primary climates (humid con-tinental, humid subtropical and semiarid) of the continental USA. They also compared estimation results with those obtained by the exponential filter method to present the effectiveness of their approach.

Evaluation: The article addresses an important topic in vadose zone research and agricultural management, since such predictions are increasingly being done as the recent advances in soil moisture measurement technology, such as a range of ground-based sensors and remote sensing, providing unprecedented opportunities for mapping moisture dynamics on the soil surface. The Results & Discussion section was described in a clear and concise manner, and the results were presented and illustrated equally good. However, there are some major deficiencies which have to be seriously considered. I will report them in the major comments section. In my opinion, the article deserves publication in HESS however after substantial revision and for this reason I propose major revision.

Major comments

First of all, the structure of the introduction section was in my opinion not good. They have to be accurate and should be focused on their main point.

1) The paper applied a statistic approach to predict profile soil moisture from surface soil moisture. A variety of approaches for the prediction exist, as reviewed by the authors. The authors spent quite a bit of paper (two paragraphs) on the other two kinds of methods - data assimilation methods and analytical methods, which do not directly relevant to this study (except the exponential filter). It is good that the authors cite other's work, however, this could be compressed. Still maintain the citations, but compress the explanations for example.

>> We agree. The sentences in Introduction have been compressed with respect to the methods of data assimilation and analytical methods and these two paragraphs have been merged to one, as follows.

"A variety of approaches for predicting profile soil moisture from surface measurements have been proposed, ranging from simple statistical relationships to physically-based retrieval (Wagner et al., 1999). The primary methods used today can generally be classified into three different types: (1) data assimilation methods; (2) analytical methods; and (3) statistical or computational statistical methods. Data assimilation methods refer to techniques which incorporate surface soil moisture measurements (e.g. remote sensing products) into physically-based hydrologic models to obtain an analysis that best represents profile soil moisture and a number of data assimilation algorithms have been developed (Evensen, 1994; Walker et al., 2002; Heathman et al., 2003; Reichle et al., 2007; Draper et al., 2011; Dumedah et al., 2015). However, its application may be constrained by the required model parameters (soil properties, vegetation features and atmospheric forcing), which are difficult to obtain at larger scales, as well as by uncertainties related to the physical description of soil hydrological processes (Albergel et al., 2008; Hu and Si, 2014). The analytical methods require fewer input parameters and are computationally more efficient than data assimilation methods. They are generally mathematically derived from physically-based relationships of water flows that include some simplification assumptions (Arya et al., 1983; Camillo and Schmugge, 1983; Wagner et al., 1999;

Manfreda et al., 2014). Currently, the exponential filter method introduced by Wagner et al. (1999) is likely the most popular analytical method since it only requires one input parameter, the characteristic time length (T). This method has successfully predicted subsurface soil moisture from surface observations for multiple regions that vary in climatic and/or soil conditions (Ceballos, et al., 2005; Albergel et al., 2008; Brocca et al., 2011; Ford et al., 2014; Peterson et al., 2016). In addition to the two above methods, statistical models are also introduced to do depth scaling of soil moisture due to its simplicity and are completely data driven. These methods include linear and nonlinear regression models (Jackson, 1986; Shi et al., 2014), artificial neural network (Bono and Alvarez, 2012), and time stability analysis (Hu and Si, 2014; Gao et al., 2015) among others. However, the existing statistical methods usually defined surface soil deeper than 20 cm even down to 40 cm which is far beyond the scope of satellite sensors. This restricts the application of statistical methods to profile soil moisture estimation because in many cases only surface measurements (≤ 5 cm) are available. Despite the existing deficiency, robust statistical methods are still appealing in predicting profile soil moisture because of their simplicity and applicability to a wide range of environments."

2) Further, the authors spent one paragraph to list several statistical approaches such as linear and multivariate regression methods and pointed drawbacks of these methods. Two points should be explained: Is these methods directly relevant to the CDF matching method employed in this paper (if not, this paragraph also needs to be compressed); Does the CDF matching method employed by the authors overcome those drawbacks? In any case, I suggest the authors pay more attention to the development and application of the CDF methods.

>> We agree. We have integrated this part with those words with respect to data assimilation and analytical models. Please see the above response. Yes, this study overcomes the shortcomings of these statistical methods. Because this is the first study of using CDF matching method in soil moisture depth scaling, the details of development and application of this method is given in Methods part.

3) With regard to the CDF match method, I didn't really understand what other studies exist which deal with the same or similar topic (application of CDF matching method to predict profile soil moisture from surface moisture) and in what way this

study is different and/or better. This is very crucial for the impact of the article. Furthermore, if similar studies exist I believe that the authors should point out what are the benefits of this method in comparison with existed studies.

>> To the best of our knowledge, this is the first study of using CDF matching method in the depth scaling of soil moisture. The CDF matching method is usually used to adjust the systematic difference of soil moisture between different data sources (e.g., model outputs, remote sensing products, and *in situ* measurements) or spatial locations and generally very good results are reported (Reichle and Koster, 2004; Drusch et al., 2005; Han et al., 2012; Gao et al., 2013). This idea is from that soil moisture at different layers can be regarded as belonging to different spatial domains or sources. In this sense, the CDF matching method can be used directly to adjust the difference of soil moisture between surface and profile soils.

References

Reichle, R.H., and Koster, R.D.: 2004. Bias reduction in short records of satellite soil moisture, Geophys. Res. Lett., 31 (19).

Drusch, M., Wood, E.F., and Gao, H.: Observation operators for the direct assimilation of TRMM microwave imager retrieved soil moisture. Geophys. Res. Lett. 32 (15), 2005.

Han, E., Heathman, G.C., Merwade, V., and Cosh, M.H.: Application of observation operators for field scale soil moisture averages and variances in agricultural landscapes, J. Hydrol., 444-445, 34-50, 2012.

Gao, X., Wu, P., Zhao, X., Zhou, X., Zhang, B., Shi, Y., and Wang, J.: Estimating soil moisture in gullies from adjacent upland measurements through different observation operators, J. Hydrol., 486, 420-429, 2013.

4) Further, what is the scientific merit and what is the main contribution of this study?

>> First of all, the CDF matching method is used for the first time in soil moisture depth scaling. Furthermore, we demonstrate the feasibility and robustness of this method in depth scaling of profile soil moisture by using the exponential filter as a reference method of which the robustness has been demonstrated widely. Therefore, the findings here have the potential in the prediction of profile soil moisture from surface measurements obtained *via* various means, including remote sensing techniques.

5) The authors stated that one of the advantages of the statistical methods is their computational efficiency compared to other two kinds of methods (line 15 in page 3). But this is confused and seems not consistent with previous statement that the analytical methods require fewer input parameters and are computationally efficient. Did the authors compare the computational express between the exponential filter and the CDF methods? Additionally, the first sentence (lines 15-18 in page 3) should be rewritten and more accurate. Actually, in my opinion, it is better to move this sentence to other place, e.g., prior to the introduction of the statistical methods.

>> We agree. In fact, both the statistical and analytical methods have high computation efficiency. The text with respective statistical methods has been changed. Please see our response to the first comment in page 3.

6) Lines 28-30 in page 3, to my understanding, this study applied the CDF method to 12 stations respectively. Although they chose these stations on the basis of some differences between them, cross-relations between these stations are not considered. Thus, the sentence (lines 28-30 in page 3) should be rephrased to avoid confusion.

>> We agree. These 12 stations are distributed in three varying climates in the USA. They have distinctive precipitation regimes and soils.

My second concern has to do with the methodology which they used.

1) The CDF matching method developed and applied in this study was not well explained. The authors just described the technical procedure (lines 25-30 in page 4 with a concept map in figure 1, it is better to demonstrate the method in detail. I noted that the authors presented the detailed formula of the exponential filter method instead.

>> We agree. More details have been added in the text.

The technical procedure of this method progressed as follows:

(I) The *in situ* measured surface (θ_s) and profile (θ_p) soil moisture datasets were ranked.

(II) Next the differences (Δ) in soil moisture between corresponding elements in the surface and profile datasets were calculated as:

$$\Delta = \theta_s - \theta_p \quad (1)$$

(III) A polynomial fit was then used to quantify the relationship between θ_s and Δ. This study employed pre-experiments to identify the optimal order, and a fifth-order polynomial was finally used when considering the accuracy of fitting and the principle of parsimony.

$$\hat{\Delta} = k_0 + k_1 \cdot \theta_s + k_2 \cdot \theta_s^2 + k_3 \cdot \theta_s^3 + k_4 \cdot \theta_s^4 + k_5 \cdot \theta_s^5 \quad (2)$$

where $\hat{\Delta}$ is the predicted difference of Δ, and k_0, k_1, k_2, k_3, k_4 and k_5 are parameters. The polynomial Eq. (5) serves the observation operators here to eliminate the systematic difference between θ_s and θ_p.

(IV) Profile soil moisture could then be estimated by using the observation operators to rescale surface measurements.

$$\hat{\theta}_p = \theta_s - \hat{\Delta} \quad (3)$$

where $\hat{\theta}_p$ is the predicted profile soil moisture.

2) Further, as stated by the authors, the CDF method was first calibrated and then validated in different time period, but which parameters and functions are calibrated? This could be explained in section 2 (Methodology) and the calibration results could be presented in section 3.

>> We agree. Calibration here means to determine the parameters in the observation operators by five-order polynomial fitting, i.e., k_0, k_1, k_2, k_3, k_4 and k_5 in the equation (2) above.

3) With regard to the outliers excluded (Lines 13-18 in page 4), some values of the moisture in one given layer were identified as outliers when their variations were inconsistent with values at adjacent depths and rainfall events. Generally, lagged relations exist between the rainfall events and the variation of the soil moisture, especially the subsurface soil moisture.

>> We agree that subsurface soil moisture has delayed response to rainfall events. Here we mean that if soil moisture in one layer increases with time during a time period but at adjacent layers soil moisture decreases and meanwhile there is no rainfall event occurs, then we argue that the soil moisture values in this layer is

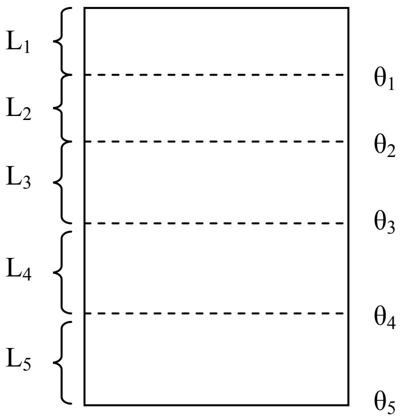
outliers during this period. The text has been edited as follows for clarity.

"To identify outliers in one layer, soil moisture at this depth was linked to values at adjacent depth(s) and rainfall events. On the one hand, if soil moisture in one layer clearly increased during some period but no rainfall events occurred before and meanwhile the soil moisture in adjacent layers did not show clear increase, the soil moisture values in this layer during this period were identified as outliers. On the other hand, if soil moisture in one layer clearly decreased whereas soil moisture in adjacent layers showed no clear decrease, then these soil moisture values were also identified as outliers. The outliers were then excluded from the analyses."

4) Is it a novelty to use fifth-order polynomial instead of third-order. And is this the only difference compared with previous CDF matching method (Lines 2-5 in page 5)?
>> Using the fifth-order polynomial fitting is not the novelty of this study. To the best of our knowledge, this is the first study of using the CDF matching method to predict profile soil moisture from surface measurements. Furthermore, we tested the effects of data resolutions and lengths on the performance of this method and demonstrated its feasibility by applications under varying climates.

5) Section 2.2.3, did the four replicates be conducted in all three stations?
>> Yes, they did.

Lastly, simulations conducted in the manuscript are not explained explicitly.
1) It was not explained explicitly soil moisture in which layers are considered in the calibration and validation. Did the soil moisture at all depths of 5, 10, 20, 50, and 100 cm be used to calculate the observation operators? Was the near-surface (5 cm) soil moisture data regarded as the input (surface soil moisture)? Which layer was the "profile" referred to in this study?
>> In this study, surface soil moisture refers to soil moisture in the 5 cm, and the profile soil moisture refers to that in the 0-100 cm. The profile soil moisture is a depth-weighted mean of the values in the 5, 10, 20, 50 and 100 cm. It is calculated as follows:



$$\theta_p = \frac{(\theta_1 \times L_1 + \frac{(\theta_1+\theta_2)}{2} \times L_2 + \frac{(\theta_2+\theta_3)}{2} \times L_3 + \frac{(\theta_3+\theta_4)}{2} \times L_4 + \frac{(\theta_4+\theta_5)}{2} \times L_5)}{(L_1+L_2+L_3+L_4+L_5)} \qquad (1)$$

where θ_p refers to the profile soil moisture content (m^3 m^{-3}); θ_i (i=1, 2, …, 5) refer to soil moisture content at the five different layers (m^3 m^{-3}); and L_i (i=1, 2, …, 5) refer to the depth of different soil layers (m). It has been edited in the text.

2) To this reviewer's understanding, the authors used soil moisture with daily resolution to calculate the observation operators (line 23 in page 8) and then used these observation operators to predict daily soil moisture in profile. Is it true?

>> Yes, only daily soil moisture is used for analyses in the sections following 3.1 because time series resolution has negligible effect on prediction accuracy.

3) The authors listed the soil texture in different stations (Table 1). Does the texture impact the prediction results, besides the type of climate.

>> The effects of texture on prediction accuracy are not within the scope of this study. The texture are presented here are used as basic data to show the difference in soils of the stations.

4) I cannot understand why does figure 5 illustrate the effects of data length on performance of observation operators. Which level of data length is indicated in figure 5?

>> The Figure 5 showed the prediction metrics including RMSE, R^2 and NSC (NSC is replaced by mean bias error, MBE, in the revised paper) under five different data lengths (DL1 to DL5) for three stations. It can be seen clearly that as data length

increased the values of these metrics changed correspondingly. Therefore, this figure can reflect the effects of data length on the performance of observation operators.

5) I guess the authors omitted one figure, maybe figure 11 (mentioned in line 9 in page 11).

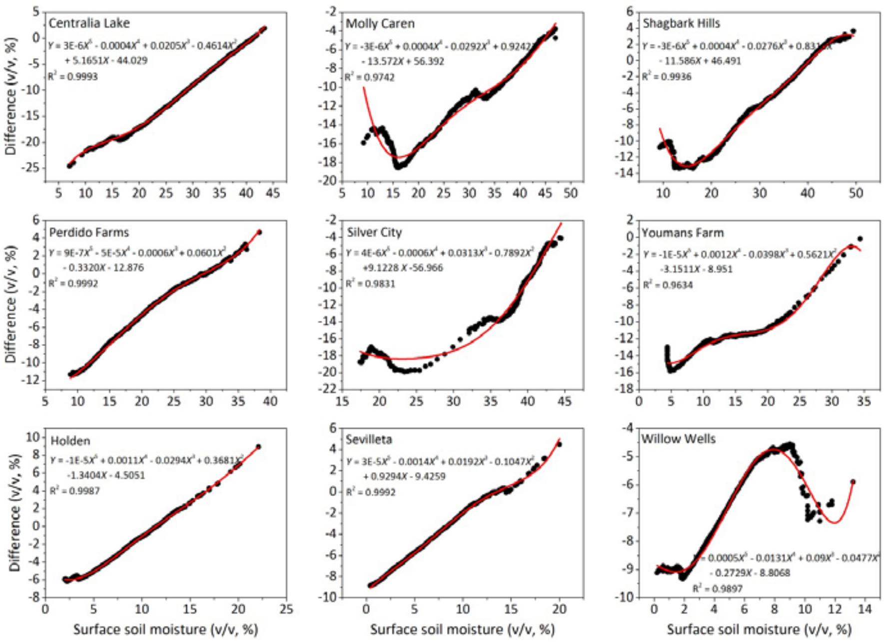
>> Sorry for the confusion. Actually, it is the Figure 10 in the original paper.

6) Did the same input (surface and profile soil moisture data) be used when the CDF and the exponential filter methods were employed respectively to do calibration and validation?

>> Yes, the same data was used as input of the CDF matching and exponential filter methods under each of the 12 stations.

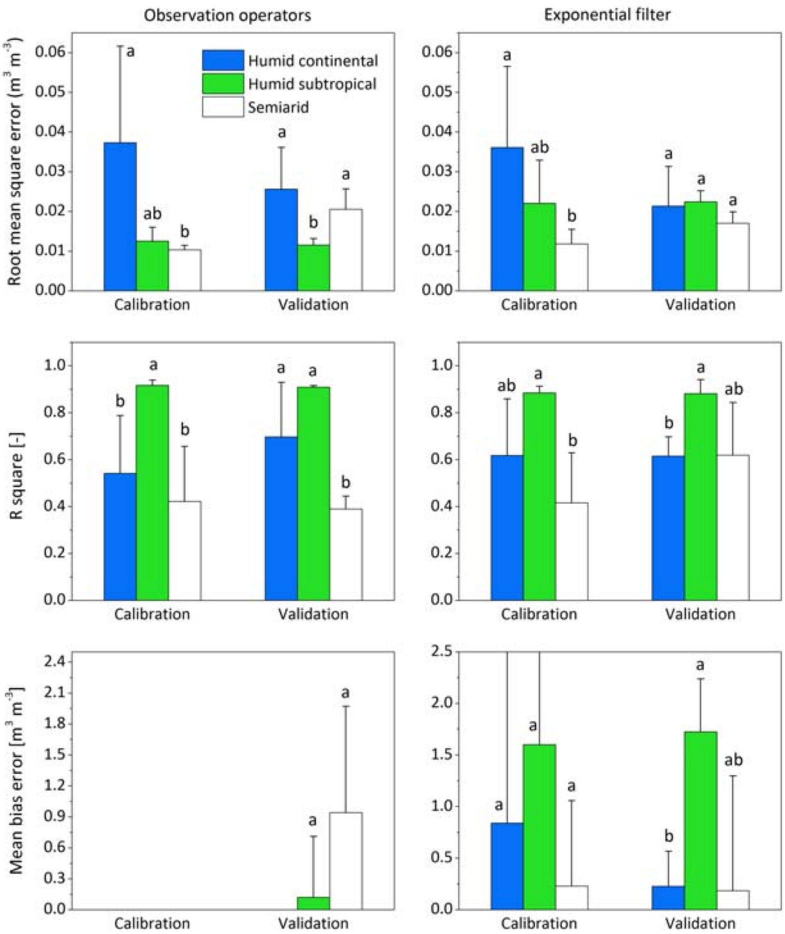
7) Uncertainty is one of the main issues when statistical methods are applied. Could the authors explore possible sources of uncertainties for the prediction.

>> We agree. In calibration, the primary uncertainty can be attributed into the fitting curves. As shown in the figure below, the fitting curve can not completely match the relationship between surface moisture content (θ_s) and the difference ($\Delta\theta$) between surface and profile soil moisture. In validation, the relationship between θ_s and $\Delta\theta$ can deviate to some extent with respect to that in calibration, and this deviation is expected to increase the prediction error.



8) Lines 13-16 in page 11. I am not sure whether it is reasonable and substantiated enough to conclude that the CDF matching method is more robust than the exponential filter method based on the application of this study. It is better to constrain such conclusion in specific conditions considered in this study.

>> We agree. In fact, there was a mistake in the procedure of the CDF matching method in the original paper and this resulted in the agreement degree was unrealistic high between measured and predicted profile soil moisture. The mistake has been corrected in the revised paper. The updated calculations indicate that the CDF matching method performed almost equally well with the exponential filter (please see the figure below). Based on this result, the conclusion has been changed accordingly.



Minor comments

1) Title, why use "upscaling" in the title? The main point of the method is to use

surface soil moisture to predict profile soil moisture based on a prior calibration using available surface and profile soil moisture data in other time period. I think this procedure is not relevant to upscaling.

>> We agree. The title has been changed into “Depth scaling of soil moisture from surface to profile: multi-station testing of observation operators”.

2) Line 6 in page 3, "found that multivariate regression and artificial neural network was able to produce reliable profile soil moisture estimations, but required ...", "was" should be "are", "required" should be "require".

>> We respectfully disagree. We consulted Dr. John Blackwell from the sees-editing Ltd, and he told me that verb tense should be consistent within sentences. But we find that “was” is wrong here and has been changed into “were”. Thanks all the same for your suggestion.

3) Line 1 in page 5, "profile" instead of "Profile".

>> We agree. We have rewritten the sentence including this word.

4) Line 5 in page 5, replace "when considering the accuracy of fitting and the principle of parsimony" by "when the accuracy of fitting and the principle of parsimony are considered".

>> We agree. We have rewritten the sentence including this sentence.

5) Line 18 in page 9, "soil moisture time series data length" needs to be rephrased.

>> We agree. It has been changed into “data length of soil moisture time series”.

6) What do the symbols "a", "b", "ab" mean in figure 10? The authors should present the explanation in the caption of this figure.

>> The figure caption gave the explanation. It is that “Different lowercase letters above bars indicate significant ($P<0.05$) differences between climates in either calibration or 5 validation period.”