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Error distribution modelling of satellite soil moisture measurements for hydrological applications

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Abstract

Satellite-based soil moisture data accuracies are of important concerns by hydrologists because they could significantly influence hydrological modelling uncertainty. Without proper quantification of their uncertainties, it is difficult to optimise the hydrological modelling system and make robust decisions. Currently, the satellite soil moisture data uncertainty has been limited to summary statistics with the validations mainly from the in-situ measurements. This study attempts to build the first error distribution model with additional higher order uncertainty modelling for satellite soil moisture observations. The methodology is demonstrated by a case study using SMOS (the Soil Moisture and Ocean Salinity) satellite soil moisture observations. The validation is based on soil moisture estimates from hydrological modelling which is more relevant to the intended data use than the in-situ measurements. Four probability distributions have been explored to find suitable error distribution curves using the statistical tests and bootstrapping resampling technique. General Extreme Value is identified as the most suitable one among all the curves. The error distribution model is still in its infant stage which ignores spatial and temporal correlations, and nonstationarity. Further

improvements should be carried out by the hydrological community by expanding the methodology to a wide range of satellite soil moisture data using different hydrological models.

Keywords: error distribution model, uncertainty modelling, satellite soil moisture, hydrological modelling, Soil Moisture and Ocean Salinity (SMOS), Xinanjiang (XAJ)

1 Introduction

Soil moisture is crucial to the improvement of most water-related systems, including real-time hydrological modelling at catchment scales (Brocca et al., 2010; Guingla et al., 2012; Merlin et al., 2006; Ottlé and Vidal-Madjar, 1994). This is because real-time hydrological modelling suffers from the accumulation of errors in evapotranspiration and soil moisture. This shortcoming can often result in poor performance of flow prediction after some dry periods due to the inaccurate calculation of the antecedent soil moisture (Brocca et al., 2008; Ottlé and Vidal-Madjar, 1994).

The in-situ measurements, remote sensing and land surface models are the main sources of soil moisture estimation for hydrological applications. Soil moisture has a high variability in both space and time, so it is difficult to estimate accurately (Walker et al., 2004; Wang and Qu, 2009). The majority of the available ground-based soil moisture observations are sparsely distributed, and hence are not able to provide sufficient information at a catchment-scale (Al‐Shrafany et al., 2013; Srivastava et al., 2013b). Another technique to obtain catchment-scale soil moisture relies on land surface modelling (e.g., Noah MP and VIC models) or utilising data assimilation to integrate land surface models with ground measurements. However model-based soil moisture estimation tends to suffer from time drifts problem (e.g., error accumulation over times). Alternatively, remote sensing is a feasible way to monitor catchment-scale soil moisture information since it provides integrated estimation over pixel scales (Engman and

Chauhan, 1995). Optical and thermal infrared remote sensing (Hain et al., 2011; Hulley et al., 2010), as well as passive and active microwave remote sensing techniques (Kerr et al., 2010; Sánchez-Ruiz et al., 2014) have been extensively used for soil moisture monitoring over various conditions of topography and vegetation.

These data products have the potential to be used in real-time flood forecasting systems. However, those measurements can be affected by several error sources (e.g., algorithms, sensors, and physical processes) (Dorigo et al., 2010). Quantification of such uncertainties is particularly important for applying the soil moisture datasets in real-time flood forecasting systems (Brocca et al., 2010). More importantly, this is the foundation to the optimal modelling performance in using such soil moisture datasets. Since satellite soil moisture data are global and widely available, they are of great interest to the hydrological community. Although there are many studies on exploring the uncertainty of satellite soil moisture estimates in hydrological applications, they are mainly represented as summary statistics (such as root mean square error (*RMSE*), correlation or Nash-Sutcliffe Efficiency (*NSE*)) (Al Bitar et al., 2012; Albergel et al., 2012; Albergel et al., 2011; Collow et al., 2012; Lacava et al., 2012b; Panciera et al., 2008; Piles et al., 2011; Srivastava et al., 2014; Srivastava et al., 2013a; Srivastava et al., 2013b), and there is a lack of attention on the error distribution model (such as probability density function, spatial and temporal correlation, nonstationarity).

It is recognised that due to the complexity of soil moisture in the field, no reference dataset can provide the absolute truth (Wagner, 2008) so it is important that the assessment of soil moisture products should be based on different benchmarks (such as in-situ measurements, modelled soil moisture data from land surface model or hydrological model, different sensors, etc.) according to their applications. Conventionally, satellite soil moisture data have been mainly validated using in-situ measurements, which are useful in many applications, but it should not

be considered as the only benchmark. For example, Dorigo et al. (2010) used three independent satellite soil moisture datasets to derive their error characterisations (albeit only summary statistics such as *RMSE* are derived) without using ground based estimates (the so called 'triple collocation error estimation'). The reason is explained by the authors as 'a spatially coherent assessment of the quality of the various globally available datasets is often hampered by the limited availability over space and time of reliable in-situ measurements.' As Wagner, (2008) has explained that 'there is no universal remote sensing method (= sensor + algorithm) that satisfies all user requirements', an excellent performance of the soil moisture data in one application field may have a poor performance in another field. For example, in climate change modelling, the global climate models usually have spatial resolutions in hundreds of kilometres, so a soil moisture product suitable for such applications may not be optimal for studies in crop growth monitoring in agriculture, and vice versa. Since this study aims at hydrological modelling applications, the benchmark is based on the effective catchment soil moisture data estimated from a well-known operational hydrological model Xinanjiang (XAJ).

In contrast to previous studies which have only focused on summary statistics, in this study we aim to build the first error distribution model of satellite soil moisture estimates. The SMOS (the Soil Moisture and Ocean Salinity) level-3 soil moisture product is used as a case study (Kerr et al., 2001). SMOS satellite is chosen because it is the first mission dedicated to monitoring direct surface soil moisture on a global scale (Kerr et al., 2010) and owns a higher soil penetrating capability (~ 5 cm of soil surface at 1.4 GHz) due to its longer wavelength (L-band). Another dedicated soil moisture satellite called SMAP (the Soil Moisture Active/Passive mission (1.20-1.41 GHz; (Entekhabi et al., 2010)) was only launched in early 2015 which is not suitable due to its short record. Long-term satellite and model datasets are processed (i.e., four consecutive years). Four traditional probability distributions are introduced to identify the optimal error distribution model(s) to describe the features of the SMOS soil moisture

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uncertainty, by employing the statistical tests and bootstrapping resampling technique. The optional error distribution models are then quantified further by second-order error distribution modelling.

2 Data, catchment and methodologies

2.1 Study area and datasets

The chosen catchment (Pontiac, 1500 km^2) is a part of the Vermilion River situated in the central Illinois of the United States (U.S.) (40.878°N, 88.636°W). This region is influenced primarily by hot summer continental climate (Peel et al., 2007) and covered mainly by cropland (Bartholomé and Belward, 2005; Hansen, 1998) on Mollisols soil type (Webb et al., 2000). The average altitude of the catchment is 188 m above mean sea level and its average annual rainfall is 867 mm. The layout of the Pontiac catchment is shown in Fig. 1 along with the location of its flow gauge, the National Aeronautics and Space Administration (NASA) Land Data Assimilation Systems 2 (NLDAS-2) grids, and distribution of the river network.

The NLDAS-2 (Mitchell et al., 2004) precipitation (P) and potential evapotranspiration (PET) at 0.125° spatial resolution and daily temporal resolution (converted from hourly resolution) are used to drive the XAJ model. More detail about the NLDAS-2 datasets can be found in Xia et al. (2012) and Zhuo et al. (2015b). Only the NLDAS-2 grid points within the catchment area are selected. As a result there are a total of 20 grid points covering the whole area. Furthermore the selected PET and P datasets have been converted into one catchment-scale dataset using the weighted average method for the usage in the lumped XAJ model. The U.S. Geological Survey daily flow data from January 2010 to April 2011 have been chosen for the calibration of the XAJ model and the period of May 2011 to December 2011 is used for the validation. The two year data restriction is due to the unavailability of the flow data in the catchment.

However, the short data length can still serve the purpose of this study due the reason as follows. The beauty of the XAJ model is that its calibration can be based on short data period. A study on calibration data selection of a XAJ like model (i.e., PDM) has shown that even a six-month data can be sufficient for excellent model calibration (Liu and Han, 2010). The reason is that the information content in the calibration data is a key factor instead of the length of the data period. As long as there is enough perturbation to model parameters, it is not necessary to have a much longer calibration time period. We have found that the one year calibration data has sufficient information to properly derive the effective model parameters, and the validation result has also demonstrated the effectiveness of the model. The level-3 SMOS soil moisture dataset is obtained from the SMOS Barcelona Expert Centre (SMOS-BEC, http://cp34-bec.cmima.csic.es), and has been processed for the period from January 2010 to December 2013. In addition, the soil moisture dataset under frozen condition has been removed (i.e., air temperature below zero). This is because SMOS is incapable of retrieving good quality soil moisture measurements under frozen weather (Al-Yaari et al., 2014; Lacava et al., 2012a; Wagner et al., 2014; Zhuo and Han, 2015). It has been further averaged into one catchment-scale dataset by applying the weighted average method. The Matlab code has been used for all the modelling works carried out in this study.

2.2 Uncertainty and its quantification methods

In a hydrological model, the soil moisture input can be described by ensembles with stochastic elements and the usage of error distribution modelling allows us to better understand the system (Beven, 2006; Jain and Singh, 2003). By analysing the error distribution models of the input dataset, a decision can be made based on a range of possible outcomes instead of a fixed dataset; this is rather important in water resources management (Jain and Singh, 2003).

As aforementioned, there exist many error sources in satellite soil moisture measurements. However in real life, it is extremely difficult to investigate these error sources separately and discover their interdependencies. The statistical error distribution model of satellite soil moisture established with the assistance of hydrological model could be a practical and efficient solution. The error distribution model may change with time (i.e., nonstationarity), but it is more challenging to build such a model from the start. In this study, the model will be built by exploring the significant characteristics of satellite soil moisture errors from the long-time historical records without considering the nonstationarity. One of the simplest empirical based error distribution modelling is via the systematic error analysis. It collects the information of differences or ratios between satellite estimated and hydrological modelled soil moisture pairs. This methodology has been proven to be effective and time efficient in numerous studies (Anagnostou et al., 1998; Borga and Tonelli, 2000; Seo et al., 1999; Smith and Krajewski, 1991) and provides a fundamental framework for more complex error distribution models (Dai et al., 2014b).

In quantifying the uncertainty of SMOS soil moisture estimates, it is assumed that the 'true' soil moisture (S_T) for assessing the observed satellite soil moisture (S_S) is based on the XAJ soil moisture simulations (S_X) which is used as the hydrological benchmark. The 'true' soil moisture can be described by the following equation:

$$S_T = \{S_X | S_S\} \tag{1}$$

In another word, the probable true soil moisture corresponds to a realisation of the distribution of the XAJ soil moistures depending on the given satellite estimates. Based on this, the satellite soil moisture uncertainty can be shown as:

$$S_T = M(S_S) + \varepsilon(S_S) \hspace{4cm} (2)$$

where $M(S_S)$ stands for the systematic errors of satellite estimates and $\varepsilon(S_S)$ represents the random error component.

In this study, it is mainly focused on quantifying the total error observed when comparing SMOS and XAJ soil moisture values and optimising it with potential theoretical models, so that the main parameters and statistical characteristics of the observed error distribution model can be derived. Four commonly used probability distributions are explored to represent the error distribution of the SMOS soil moisture estimates.

2.3 The SMOS soil moisture product

The SMOS satellite was launched at the end of 2009 and has been providing soil moisture data for more than five years. SMOS acquires brightness temperature at the frequency of 1.4 GHz (near surface soil moisture (approximately 5 cm)). The spatial resolution of the SMOS products is 35-50 km (Kerr et al., 2010; Kerr et al., 2001) with soil moisture retrieval unit in m^3/m^3. SMOS offers a global coverage at the equator crossing the times of 6 am (local solar time (LST), ascending) and 6 pm (LST, descending) (Kerr et al., 2012).

SMOS-BEC provides soil moisture measurements at various temporal resolutions: daily, 3-days, 9-days, monthly and annually. The BEC soil moisture products comes in two formats: the ISEA 4H9 grid (Icosahedral Snyder Equal Area projection with aperture 4, resolution 9) with its shape of cells as hexagon (Pinori et al., 2008), and the EASE grid (Equal Area Scalable Earth grid) with a spatial resolution of ~25 km x 25 km. In this study the daily soil moisture dataset with the EASE grid is chosen, because it is more widely used. The main algorithms in generating the BEC level-3 surface soil moisture is the same as the one utilised by the European

Space Agency (ESA) for retrieving the standard level-2 soil moisture products (Kerr et al., 2012). In this study only the descending SMOS data is used, because we have found that the performance of descending retrievals is much better than ascending's in this catchment (Zhuo and Han, 2015; Zhuo et al., 2015a). This could be partly explained by the fact that this area is highly affected by radio frequency interference, which preferentially affects the ascending retrievals because of the SMOS antenna pattern (Collow et al., 2012).

2.4 The XAJ hydrological model

There are many hydrological models available globally and in this study, a widely used model called XAJ is employed. It is a fairly general conceptual lumped rainfall-runoff model, which is capable of simulating flows at a variety of catchment scales over the globe (Khan, 1993; Wang, 1991; Zhao, 1992; Zhao et al., 1995; Zhuo et al., 2014). Moreover its model concept and structure are representative to many typical conceptual hydrological models. It is able to account for soil water content in the system with a suitable time step and easy access of data inputs (i.e., P and PET only) (Peng et al., 2002). In hydrology, soil moisture deficit (SMD) or depletion is a significant indicator of soil water content, which stands for the amount of water to be added to a soil profile to bring it to the field capacity (Calder et al., 1983; Rushton et al., 2006). It has been shown by considerable number of studies that the three-layer XAJ model is very effective in generating SMD from the hydrological forcing (Zhao, 1992; Zhao et al., 1995; Zhuo et al., 2014). The main concept of XAJ is the runoff generation on repletion of storage, which indicates that runoff is not emerged until the soil water content of its aeration zone reaches the field capacity. As shown in Fig. 2, the structure of the XAJ model comprises an evapotranspiration module, a runoff production module and a runoff routing module. The XAJ model has 16 parameters which are calibrated in this study by finding the optimal performance in flow simulation (Zhao, 1980; Zhao, 1992). The three-layer SMDs are estimated to determine

the effect of drying and wetting on the catchment soil storage, and in this study only the SMD from the surface layer is used because it is more scale-matched with the satellite surface soil moisture retrieval.

2.5 Bootstrapping resampling

Bootstrapping is a random sampling technique firstly presented in Efron, (1979), and a very informative and readable account is given by Efron and Tibshirani, (1986). It has been used widely in systematic and clinical studies (Hillis and Bull, 1993; Sauerbrei and Schumacher, 1992). The reason for using bootstrapping is that it is able to provide an indirect way of assessing the characteristics of the distribution underlying the sample data (Adèr and Mellenbergh, 2008). Moreover bootstrapping is capable of controlling and checking the stability of the results, yet it only requires simple computing procedures. The general idea of bootstrapping is the usage of 'sampling with replacement' and more details regarding bootstrapping can be found in Efron, (1979).

2.6 Performance indicators

NSE (Nash and Sutcliffe, 1970) is used to assess the performance of the XAJ model as well as to select the suitable error distribution curves during bootstrapping resampling process. *NSE* is the most common and important performance measure used in hydrology and it is calculated using the following equation:

$$NSE = 1 - \frac{\sum_{i=1}^{n}(y_i - x_i)^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \tag{3}$$

where x_i is the observed values and y_i is the simulated values. *n* is the number of data pairs.

Chi-square test is a statistical test commonly used to compare the observed data (e.g., cumulative distribution function (CDF) of the observed error) with the data which would be expected to obtain according to a specific hypothesis (Mantel, 1963). The formula for calculating chi-square (χ^2) is:

$$\chi^2 = \sum_{i=1}^{n} \frac{(x_i - y_i)^2}{y_i} \tag{4}$$

Pearson product moment correlation coefficient (r) is used to evaluate the linear relationship between two variables, which is defined as:

$$r = \frac{n(\sum x_i y_i) - (\sum x_i)(\sum y_i)}{\sqrt{[n\sum x_i^2 - (\sum x_i)^2][n\sum y_i^2 - (\sum y_i)^2]}} \tag{5}$$

Spearman rank correlation coefficient (r_{sp}) is a nonparametric method for evaluating the degree of correlation between two independent variables (Chen et al., 2013; Dai et al., 2014a). Due to its ability to cope with nonlinear correlation as well as linear correlation, it is used in addition to r to check the existence of nonlinearity between two sets of data. Its formula is:

$$r_{sp} = 1 - \frac{6\sum_{i=1}^{n} d_i^2}{n^3 - n} \tag{6}$$

where d_i is the difference between ranks for each data pair (x_i, y_i).

3 Results

3.1 SMD estimated from XAJ model

First, the surface SMD is simulated by driving the XAJ model. When running the XAJ model, the initial two thirds of the data from the period of January 2010 to December 2011 is used for model calibration while the rest one third of the data is utilised for validation; this is a common procedure used in hydrological modelling. Since the XAJ model has been proven as quite reliable (Zhao, 1992; Zhao et al., 1995), this allows us to confidently apply the model for the periods different from those used for calibration. The calibration procedure focuses especially on the modelling of three-layer SMDs and the distribution of the total runoff (e.g., surface runoff, interflow and groundwater), as well as a good agreement between the modelled flow and measured flow. The performance of the model is judged by the *NSE* indicator as its objective function. The optimal values of the XAJ parameters, along with their initialisation values used in this study are shown in Table 1. The overall performance shows a *NSE* value of 0.806 for the calibration and 0.804 during the validation, which reveals that the model works very well. The time series plots of rainfall and flow during the calibration and validation periods are illustrated in Fig. 3. Further details on calibration and validation of the XAJ model in this catchment are discussed by Zhuo et al., (2015a).

3.2 SMD derived from SMOS soil moisture

In order to model the error distribution of the SMOS soil moisture estimates for hydrological applications, the four-year SMOS volumetric soil moisture dataset needs to be converted into the hydrological SMD initially. First the correlation between the SMOS volumetric soil moisture and the XAJ SMD is studied. As shown in Fig. 4(a), the Spearman r_{sp} and Pearson r correlation statistics between the SMOS soil moisture estimates and XAJ SMD are calculated, which yield almost the same values, indicating that there is no strong nonlinearity. For this reason a linear fitting method is used for the derivation of SMOS SMD. As seen in Fig. 4(a), the upper part of the XAJ SMD represents the wilting point, while the lower range represents

the field capacity point of the soil. The values depend on the soil properties and vegetation cover. The comparison result between the derived SMOS SMD and the XAJ SMD is presented in Fig. 4(b), with *NSE* calculated as 0.492. It can be seen that there is an overestimation of the SMOS SMD when surface soil is relatively wetter (i.e., smaller XAJ SMD) and a slight underestimation when surface soil dries out (i.e., larger XAJ SMD). This observed error (i.e., the differences between the XAJ SMD and the SMOS SMD) is then investigated further by first-order and second-order uncertainty modelling. For the XAJ SMD, there is also an issue with the maximum ceiling at 0.047 where many points are concentrated. We will explore it in the discussion.

3.3 First-order error distribution modelling

This section is carried out to find the most representative curves to describe the observed discrepancy between the SMOS SMD and the XAJ SMD. Here the observed discrepancy is fit with four well known distributions in hydrology: Gaussian, Extreme Value (EV), General Extreme Value (GEV), and Logistic distributions. Distribution formulas together with their parameters are shown in Table 2. More details about these four distributions can be found in Walck, (2007). It can be seen that almost all the selected distributions are formed by two parameters: a scale parameter and a location parameter, except the GEV. The GEV introduces an additional parameter called the shape parameter, which is able to further describe the tail behaviour of a distribution.

The fitted results of the four distributions can be observed from their histograms and CDFs plotted in Fig. 5. The skewness of the observed error is calculated as 0.339, so it is right-tailed. In Fig. 5(a), it is clear to see that EV is more left-skewed than others. For the simulation of peak occurrence, the Logistic shows the highest value, while the Gaussian and GEV give lower

peaks (but very close to each other). The CDF plots are also presented in Fig. 5(b). It shows that the Gaussian, Logistic and GEV curves are all very close to the observation; however it is difficult to judge which one is the best based on visual inspection. Therefore the chi-square test is implemented and the results are shown in Table 3. It is noted that a 5% level of statistical significance is adopted in this study and curves with chi-square p value bigger than 5% are acceptable (i.e., the observed error is truly from that distribution). It is noted that since a right-tailed chi-square distribution is adopted, the larger the p value, the better the curve fits to the observation. In general, GEV achieves the best performance ($p = 0.359$), followed by Logistic ($p = 0.165$) and Gaussian ($p = 0.129$) curves. This result may be partially explained by the number of parameters used in different curves, because GEV is controlled by three parameters while Logistic and Gaussian are only governed by two parameters.

3.4 Error distribution modelling by bootstrapping resampling technique

Although in previous section the GEV is found to be the optimal curve to describe the uncertainty of SMOS soil moisture, it is still necessary to check the reliability and stability of this outcome. Therefore the bootstrapping resampling technique is employed. The observed SMD errors are analysed by bootstrapping with 10,000 replicates. For each bootstrapping replicate, *NSE* is used to measure the agreement between the expected and the observed CDFs.

The 10,000 curve fitting results of *NSE* using the bootstrapping technique is shown in Fig. 6(a). In addition, the CDFs of the *NSE* performances are also derived for a better visual inspection, as presented in Fig. 6(b). It is clear to see that although there are some overlaps of the *NSE* performance among the curves (e.g., the GEV curve is not always better than the Logistic curve), the GEV is generally the best curve. On the other hand, the performance of EV is the poorest, which also gives the widest *NSE* range. Moreover from the CDF plots it can be seen

that the performances of Gaussian, GEV and Logistic curves are again rather close. The statistical calculation of the overall *NSE* performance (Table 4) indicates that GEV is indeed the best and most stable error distribution model of all, which gives the highest *NSE* at 0.992, as well as the lowest standard deviation value (0.003). The *NSE* result for the Logistic and Gaussian curves are also acceptable (with the mean *NSE* of 0.987 and 0.982, respectively). The performance of EV is the poorest (mean $NSE = 0.945$).

3.5 Second-order error distribution modelling

From the above analysis, the GEV, Logistic and Gaussian are the preferred error distribution models to describe the uncertainty of the satellite observed soil moisture. However these models themselves are uncertain and it is important to estimate those uncertainties which are usually neglected in error distribution modelling. For example if a weather forecast reports there is 40% chance of rain, a question is how accurate is this 40% (e.g., maybe between 30% - 50%)? Therefore the uncertainty of the 40% chance is also important and should be questioned (Wagner and Gorelick, 1987). The uncertainty of the error distribution model is based on its parameters. Hence a second-order error distribution modelling is needed for each parameter of the error distribution models. The values of these parameters are calculated from each of the bootstrapping resampled dataset. As a result there are a total of 10,000 values for each of the error distribution model parameter. Furthermore the chi-square test is again used to statistically find the best models to describe the uncertainty of these parameters. The Gaussian, EV, GEV and Logistic curves are used for the fitting.

The histograms together with the coefficients of skewness of the model parameter uncertainties are illustrated in Fig. 7. It is noted that all the distributions tend to be right-skewed slightly (i.e., positive skewness). Since the Logistic scale parameter s is proportional to the standard

deviation, it shows a very similar distribution to the Gaussian σ, but with smaller magnitude (about six times less). The chi-square test is calculated as shown in Table 5. It is not surprising to see that in almost all the cases, Gaussian is the only curve that passes the chi-square test (because all the calculated Gaussian p values are above the 5% level of statistical significance), except for the GEV scale parameter σ, where the GEV curve also fits. Generally speaking Gaussian is the most suitable curve for describing the second-order uncertainties for the selected Gaussian, Logistic and GEV error distribution models. This is different to the first-order error distribution modelling where GEV is better than Gaussian.

4 Discussion and conclusions

Soil moisture is an essential variable in hydrological processes and plays a significant role in hydrological modelling. However, it is impractical to use in-situ sensors to obtain soil moisture over a catchment-scale. Remote sensing with its advantages of providing near-real-time global-coverage soil moisture dataset has gradually been accepted as an important data source for hydrological applications. Since it measures soil moisture remotely and indirectly, the quality of its retrievals can be affected by several sources. Understanding its uncertainty can help the hydrological modelling community to better use the data in addressing other uncertainties of hydrological systems. A proper error distribution model beyond summary statistics is useful in generating input ensembles for Monte Carlo simulations in uncertainty analysis of hydrological modelling. In this study we attempt to explore the uncertainty quantification of the SMOS soil moisture estimates hydrologically, at a medium-sized catchment in the central U.S. This study focuses on the satellite soil moisture products usage in hydrological modelling, therefore depending on the research purpose the XAJ estimated effective catchment soil moisture (i.e., SMD) is used as a hydrological benchmark.

In this study, four commonly used probability distributions (Gaussian, EV, GEV, and Logistic) are adopted to describe the uncertainties of satellite soil moisture data, which are extensively evaluated by using the chi-square statistical test and the bootstrapping resampling technique. From the analysed results, it can be concluded that GEV is the best curve in describing the uncertainty of the SMOS soil moisture estimates, without considering the complexity of its formation. In addition, the performances of the Logistic and Gaussian are also acceptable based on a 5% level of statistical significance. Since both Logistic and Gaussian only require two parameters, they have a clear advantage over the GEV in their simplicity. However, the extra usage of a shape parameter in the GEV may be significant when extreme soil moisture conditions are considered because it controls the tail behaviour (relevant to extreme hydrological events such as floods). During the second-order error distribution modelling, Gaussian is the most suitable curve for describing the uncertainty of the GEV error distribution model. This result is preferable, because Gaussian is a relatively simple probability distribution and could be easily applied in a hydrological model. However, it is debateable and still a research question on how to use the second-order error distribution model in hydrology (Pearl, 1987).

The uncertainty of a conceptual hydrological model is caused by three sources: model parameter uncertainties, model structure uncertainty, and input data uncertainty. To work out the impact of those uncertainty sources, a huge number of ensembles are required. However there are no commonly agreed methods for generating those ensembles because the perturbation of the model parameters depends on the PDF of individual parameters. Currently there are no practical and consensual ways to derive the model parameter PDFs. One of the popular methods is suggested by Keith Beven in his GLUE methodology which is not generally agreed and adopted by the community because it is based on the uniform perturbation of the model parameters using subjective criteria of behaviour model parameters. Furthermore, the

model structure uncertainty requires the utilisation of different hydrological models such as XAJ, PDM, VIC etc. However some models own common features, hence they duplicate results with restricted ensemble range. Ideally we want a large number of models which are distinct with a broad range of model structures. Currently, there are no convincing research publications to provide useful guidance on model structure uncertainty analysis. Therefore we focus on the third uncertainty as discussed in this study.

Proper identification of satellite soil moisture uncertainty in runoff modelling is relevant for flow ensemble studies (e.g., error propagation). For example, if the observed flow falls outside the forecasted ensembles, then further revisions are required in the formulation of the hydrological model, its states or inputs. However if the chosen error distribution model is wrong (i.e., flow uncertainty bands become too wide or too narrow), it can lead to false conclusions regarding the adequacy of the input datasets, the hydrological model and its parameters. Furthermore understanding the uncertainty features of remote sensed soil moisture is also useful in controlling and correcting the soil moisture status in a hydrological model after dry periods, so that error accumulation impact can be reduced. Therefore error distribution modelling of satellite soil moisture measurements is vital to the data application in the hydrological community. This paper demonstrates the first attempt in modelling satellite soil moisture error distribution in hydrological applications, therefore, there are many rooms for improvements.

For example, there is one clear issue with the current XAJ model's maximum ceiling as shown in Fig 4. This shows the weakness with the XAJ model's soil moisture accounting component. Such a problem is common in the current conceptual hydrological models and further work is needed in this area. However, the error distribution modelling is still useful despite such an issue because those hydrological models need ensemble inputs based on them for sensitivity

analysis and uncertainty analysis. In addition, more detailed studies such as the spatial and temporal dependence analysis should be conducted in the future. Studies are also needed to consider soil moisture information from other satellite missions over a wider range of catchment conditions with different hydrological models in order to find generalisation patterns of the error distribution models (this is especially important for ungauged catchments). However this is a huge task that cannot be achieved by a single study. The key mission for this paper is to attract attention by the hydrological community on this important issue which has been largely neglected, so that a great deal of hydrological models, satellite soil moisture observations and various catchments could be further explored by the community. We hope this study will raise the awareness on the importance of satellite soil moisture error distribution modelling so that such useful data source could be fully utilised in future hydrological modelling.

Acknowledgments

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