Comments/Text of Anonymous Referee 2 (AR2) posted in blue, our text in black with old passages in red and the new passage in green.

Artificial neural networks (ANN) enjoyed great popularity in the late 1990s and – as other data driven modeling techniques – are now part of the standard toolbox in rainfall-runoff modeling. Thus, it is surprising enough, that a limited number of studies can be found in the hydrologic literature which are applying the latest developments of the artificial intelligence research, such as e.g. deep learning.

This paper provides a first step into this direction and introduces Long-Short-Term-Memory (LSTM) networks for the task of rainfall-runoff modeling. In a comprehensive comparative study the proposed method is applied to the CAMELS data set and is compared with the conceptional SAC-SMA model which was complemented by the Snow-17 routine. The study comprises 3 numerical experiments starting with the application to single catchments and ending with the test of potential applications for ungauged catchments using a regionalisation approach.

The paper is reasonably well written and a novel contribution for assessing the predictive performance of LSTM networks in rainfall-runoff modeling. This makes the study very interesting for scientists who did not use a LSTM networks before. Since it is a first application, the paper should describe more systematically the training procedure and characteristics of the LSTM network which in the present version turned out to be more art than science. In addition and although I am enthusiastic about the work, I think a balanced discussion of the new approach should also include limitations, especially in the "Summary and conclusion" chapter. I encourage the authors to make following major modifications as they prepare their manuscript for revision:

We thank the Anonymous Referee 2 (AR2) for his comments and suggestions. In the revised manuscript, we will systematically address the issue of training a LSTM in more detail. We will also discuss some of the limitations of our approach in the the "Summary and Conclusion" section. Generally, we are grateful for the detailed comments and suggestions raised by AR2 and believe that the input has significantly helped to improve the manuscript.

### Comments:

1. Please check carefully the recent literature for applications of deep learning in water resources and discuss those, there are more than cited, e.g. ().

We agree that a careful examination of the recent literature (for applications of deep learning and LSTM) will improve the quality of the publication. Currently there exist many applications of classical neural networks, so that a general review would be difficult (therefore we cited the two review paper in the original manuscript (Abrahart et al. (2012); ASCE Task Committee on Application of Artificial Neural Networks (2000)). Thus, we believe that the focus should lie especially on LSTM applications in hydrology only, to prevent an escalation of the review-size. To provide some context: A quick

search in the Journal of Hydrology reveals 3 publication with LSTM as keyword (we found 1 in WRR and ours in HESS). Similarly 171 matches exist for the keyword "deep learning" (1 in WRR, and 233 in HESS). The numbers of the latter are however strongly inflated because of the fuzzy search which also includes matches for the keyword learning into the query. This is of course not a comprehensive review, but gives an indication about the sparsity of publication that fit the just outlined narrow domain we are interested in.

Nevertheless, as proposed by AR2 we conducted an additional literature research and added the following references to the review part: Assem et al. (2017), Shen (2017), Zhang et al. (2018 a), Zhang (2018 b). For a short summary, see the new passage below.

We did not include the following contributions, but would like to mention them here for the sake of transparency:

- Bai et al. (2016). The authors developed a multi-scale wavelet-based ANN approach for forecast daily reservoir inflow. This would fit to the general topic, but the developed approach seemed too different from a methodological point of view
- Wu et al. (2015). The authors conceptualize how deep learning in general and deep belief network in special, can be used as forecasting tasks within of smart water network. To us the contribution seemed to be quite theoretical from a method standpoint and topic-wise only marginally relevant.

This addition lead to the following adoptions for the manuscript:

### Old passage (P2, L22ff):

In recent years, neural networks have gained a lot of attention under the name of Deep Learning (DL). As in hydrological modelling, the success of DL approaches is largely facilitated by the improvements in computer technology (especially through graphic processing units or GPUs (Schmidhuber, 2015) and the availability of huge datasets (Halevy et al., 2009; Schmidhuber, 2015). While most well-known applications of DL are in the field of computer vision (Farabet et al., 2013; Krizhevsky et al., 2012; Tompson et al., 2014), speech recognition (Hinton et al., 2012) or natural language processing (Sutskever et al., 2014) few attempts have been made to apply recent advances in DL to hydrological problems. Shi et al. (2015) investigated a deep learning approach for precipitation nowcasting. Tao et al. (2016) used a deep neural network for bias correction of satellite precipitation products. Recently, Fang et al. (2017) investigated the use of deep learning models to predict soil moisture in the context of NASA's Soil Moisture Active Passive (SMAP) satellite mission. In general, the potential use and benefits of DL approaches in the field of hydrology and water sciences has only recently come into the focus of discussion (Marçais and de Dreuzy, 2017; Shen et al., 2018).

#### New passage:

In recent years, neural networks have gained a lot of attention under the name of Deep Learning (DL). As in hydrological modelling, the success of DL approaches is largely facilitated by the improvements in computer technology (especially through graphic processing units or GPUs (Schmidhuber, 2015) and the availability of huge datasets (Halevy et al., 2009; Schmidhuber, 2015). While most well-known applications of DL are in the field of computer vision (Farabet et al., 2013; Krizhevsky et al., 2012; Tompson et al., 2014), speech recognition (Hinton et al., 2012) or natural language processing (Sutskever et al., 2014) few attempts have been made to apply recent advances in DL to hydrological problems.

Shi et al. (2015) investigated a deep learning approach for precipitation nowcasting. Tao et al. (2016) used a deep neural network for bias correction of satellite precipitation products. Fang et al. (2017) investigated the use of deep learning models to predict soil moisture in the context of NASA's Soil Moisture Active Passive (SMAP) satellite mission. Assem et al. (2017) compared the performance of a deep learning approach for water flow level and flow predictions for the Shannon river in Ireland with multiple baseline models. They reported that the deep learning approach outperforms all baseline models consistently. More recently, Zhang et al. (2018a) compared the performance of different neural network architectures for simulating and predicting the water levels of a combined sewer structure in Drammen (Norway), based on online data from rain gauges and water level sensors. They confirmed that LSTM (as well as another recurrent neural network architecture with cell memory) are better suited for for multi-step-ahead predictions than traditional architectures without explicit cell memory. Zhang et al. (2018b) used an LSTM for predicting water tables in agricultural areas. Among other things, the authors compared the resulting simulation from the LSTM based approach with that of a traditional neural network and found that the former outperforms the latter. In general, the potential use and benefits of DL approaches in the field of hydrology and water sciences has only recently come into the focus of discussion (Marcais and de Dreuzy, 2017; Shen 2017; Shen et al., 2018). In this context we would like to mention Shen (2017) more explicitly, since he provides an ambitious argument for the potential of DL in earth sciences/hydrology. In doing so he also provides an overview of various applications of DL in earth sciences. Of special interest for the present case is his point that DL might also provide an avenue for discovering emergent behaviours of hydrological phenomena.

2. I have concerns about the reproducibility of the performance of the LSTM network since the training is done by trial and error and it is not very systematically evaluated. But it is an important issue, because the number of free parameters of the LSTM network is huge and as I understand a gradient-based error backpropagation method is used for training. As a reference for the state of the art evaluation of data driven models I recommend () where a stochastic procedure, involving random sampling for training, cross-validation, and testing, is proposed.

We have to admit that we do not fully understand this statement. It is true that the LSTM is trained by a form of gradient-based error back propagation (called backpropagation through time, a standard method for training recurrent neural networks). To us it is not apparent how this is related to "trial and error" (or to systematic evaluation as such). We agree that the form of evaluation is not typical for data-driven modelling approaches. It was chosen so that the model performance of the LSTM can be compared to the baseline model of the CAMELS data set, i.e. SAC-SMA + Snow-17. If the intent of AR2 was to point out that this is an unusual evaluation/diagnostic for a data-driven model, then we fully agree with him. However, a more specifically geared performance evaluation (say, a three way splitting of the data and training-, validation- and test-data and 10 to 20 repeated executions of the training with different random seeds) would make it more difficult or even impossible to compare the two different modelling approaches.

In this context it is also worth noting that even more (than an "extended" evaluation) can be undertaken to search for the best possible realization of the LSTM. E.g., one could also tune the hyperparameters to each catchment, train more models (with different random seeds) for each one and choose the best performing LSTM per catchment. If, AR2 wanted to indicate that, then we agree that this could be an interesting study by itself.

Maybe we did not communicate this clear enough, but the goal of our study was to investigate the (general) potential of LSTMs for rainfall-runoff modelling and not to search for the best possible performing (data-driven) model for each catchment. We defined the simulation setup in such a way that the results can be used as a comparison in the context of the modelling capabilities of a well established hydrological model. Since major parts of the manuscript are devoted to this comparison (between SAC-SMA and the LSTM), we prefer to keep the model calibration/evaluations as comparable as possible. In this context, it is probably also worth mentioning that we believe that the size of the used data-set (241 catchment) is large enough to infer the representative properties of the LSTM model.

We therefore added a discussion to the revised conclusions-section (see answer to C3 AR#2) and added the following passage to the new section 2.5 (former 2.4 Experimental

design) so that it is clear that we chose our calibration scheme for a specific purpose (and that one needs to adapt it if the aim is best model performance):

### New passage:

We want to mention here that our calibration scheme (see description in the three experiments below) is not the standard way for calibrating and selecting data-driven models, especially neural networks. As of today, a widespread calibration strategy for DL models is to subdivide the data into three parts, referred to as training-, validation- and test-data (see Goodfellow et al. 2016). The first two splits are used to derive the parametrization of the networks and the remainder of the data to diagnose the actual performance. We decided to not implement this splitting strategy, because we are limited to the periods Newman et al. (2015) used so that our models are comparable with their results. Theoretically, it would be possible to split the 15 year calibration period of Newman et al. (2015) further into a training and validation set. However, this would lead to (a) a much shorter period of data that is used for the actual weight updates or (b) high risk of overfitting to the short validation period, depending one how this 15 year period is divided. In addition to that, LSTMs with a low number of hidden units are quite sensitive to the initialization of their weights. It is thus common practice to repeat the calibration task several times with different random seeds to select the best performing realisation of the model (Bengio, 2012). For the present purpose we decided not to implement these strategies, since it would make it more difficult or even impossible to compare the LSTM approach to the SAC-SMA + Snow-17 reference model. The goal of this study is therefore not to find the best per-catchment model but rather to investigate the general potential of LSTMs for the task of rainfall-runoff modelling. However, we think that the sample size of 241 catchment is large enough to infer some of the (average) properties of the LSTM based approach.

3. Finally, more information and discussion about limitations of the new approach would be helpful, e.g. the computational effort, extrapolation behavior, performance for extreme events (floods) etc.

Because of this comment, as well as minor comment 11, AR2 and comment 11, AR1 we decided to rewrite the entire conclusion and to add a more extended discussion about limitation and advantages of our approach.

To address some of the specific points mentioned in this comment:

 Computational effort: LSTMs of this size do not have any special computational requirements and can be trained and used on any modern computer on the CPU. However, most modern deep learning libraries allow to train on graphic cards (CUDA accelerated NVIDIA cards). Using graphic cards increases the performance and can be especially useful for large hyperparameter searches. All experiments of this study however have been made purely on a common computers CPU.

- Extreme events (floods): This is discussed to some point in the "Results & Discussion" sections of the experiments (especially Experiment 1 & 2). We believe that these comments sufficiently cover the topic (considering that 241 catchments where analyzed). However, if LSTMs are trained using MSE as loss functions they generally underestimate peak flows because the MSE encourages models with low variance (which is the same reason as for hydrological models, for a principled discussion see Gupta et al. (2009)).
- Extrapolation performance: As for any data driven approach, doing extrapolations with LSTMs is difficult. As a side note: This might also be a reason, why pre-training one network for a large amount of data (Experiment 2 & 3) can be useful, since it increases the amount of data "seen" by the network. With this, we are not sure what more to add.

While rewriting the conclusion we kept the points made in this comment in mind. We therefore included additional sections about the network-limitations (data need, black-box-ness, transferability) into the new version of the discussion. Additionally, a different point was added to the new passage regarding the calibration scheme (i.e. sensitivity of weights initialization, see comment 2 of this review).

### New conclusion:

This contribution investigated the potential of using long short-term memory networks (LSTMs) for simulating runoff from meteorological observations. LSTMs are a special type of recurrent neural networks with an internal memory that has the ability to learn and store long-term dependencies of the input-output relationship. Within three experiments, we explored possible applications of LSTMs and demonstrated that they are able to simulate the runoff with competitive performance compared to a baseline hydrological model (here the SAC-SMA + Snow-17 model). In the first experiment we looked at classical single basin modelling, in a second experiment we trained one model for all basins in each of the regions we investigated, and in a third experiment we showed that using a pre-trained model helps to increase the model performance in single basins. Additionally, we showed an illustrative example, why traditional RNNs should be avoided in favor of LSTMs, if the task is to predict runoff from meteorological observations.

It bears repeating that the goal was to explore the potential of the method and not to obtain the best possible realisation of the LSTM model per catchment (see Sect. 2.5). It is therefore very likely that better performing LSTMs can be found by an exhaustive (catchment-wise) hyperparameter search. However, with our simple calibration approach, we were already able to obtain comparable (or even slightly higher) model performances compared to the well established SAC-SMA + Snow-17 model.

In summary, the major findings of the present study are:

- (a) LSTMs are able to predict runoff from meteorological observations with accuracies comparable to the well established SAC-SMA + Snow-17 model.
- (b) The 15 years of daily data used for calibration seem to constitute a lower bound as of data-requirements.
- (c) Pretrained knowledge can be transferred into different catchments, which might be a possible approach for reducing the data-demand and/or regionalization applications, as well as for prediction in ungauged basins or basins with few observations.

The data intensive nature of the LSTMs (as for any deep learning model) is a potential barrier for applying them in data scarce problems (e.g. for the usage within a single basin with limited data). We do believe that the use of "pre-trained LSTMs" (as explored in Experiment 3) is a promising way to reduce the large data-demand for an individual basin. However, further research is needed to verify this hypothesis. Ultimately however, LSTMs will always strongly rely on the available data for calibration. Thus, even if less data is needed, it can be seen as a disadvantage in comparison to physically based models, which - at least in theory - are not reliant on calibration and can thus be applied with ease to new situations or catchments. However, more and more large-sample data sets are emerging which will catalyze future applications of LSTMs. In this context, it is also imaginable, that adding physical catchment properties as an additional input layer into the LSTM may enhance the predictive power and ability of LSTMs to work as regional models and to make predictions in ungauged basins. An entirely justifiable barrier of using LSTMs (or any other data-driven model) in real world applications is their black-box nature. Like every common data-driven tool in hydrology, LSTMs have no explicit internal representation of the water balance. However, for the LSTM at least, it might be possible to analyze the behaviour of the cell-states and link them to basic hydrological patterns (such as the snow accumulation melt processes) as we showed briefly in Sect. 3.4. We hypothesize that a systematic interpretation or the interpretability in general of the network internals would increase the trust in data-driven approaches, especially those of LSTMs, leading to their use in more

### Minor Comments:

### 1. page 4,Eq. 1 Uf is not correct.

The error will be corrected in the revised manuscript.

2. page 4 Give an equation for the calculations of the dense layer.

(novel) applications in environmental sciences in the near future.

Thank you for this comment, we also think that it is helpful to include the calculation for the dense layer. We therefore added the following new passage to the revised manuscript:

### Old passage (P6 L18-19):

The output from the last LSTM layer at the last time step is connected through a traditional dense layer to a single output neuron, which computes the final discharge prediction (see Fig. 1 for a schematic image of the network).

### New passage:

The output  $h_t$  from the last LSTM layer at the last time step (here t = n) is connected through a traditional dense layer to a single output neuron, which computes the final discharge prediction (as shown schematically in Fig. 1). The calculation of the dense layer is given by the following equation:

 $y = W_d h_n + b_d,$ 

Where y is the final discharge,  $h_n$  is the output of the last LSTM layer at the last time step derived from Eq. (7),  $W_d$  is the weight matrix of the dense layer and  $b_d$  the bias term.

### 3. page 5, Fig. 2 Add bias b. Why c is capital letter?

Regarding the addition of the bias b to the figure: We did not include any model parameter to the figure (e.g. W<sub>c</sub>, W<sub>f</sub>, W<sub>i</sub>). The reason for this is that the intention of the figure is to show the information flow through the RNN and LSTM cell. Thus, we believe that the bias term should not be added neither.

Regarding the capitalized c: This is correct, it should be lowercase c, since it is a vector. This will be changed in the revised manuscript.

# 4. page 5 Please give the reference on which the theory is based when starting with the description of the LSTM network – around Eq. 2.

In the revised manuscript we added the original publication of the LSTM (Hochreiter and Schmidhuber, 1997) at the beginning of page 3 (where we start with the formal description of the LSTM). Albeit the key-citation was already given earlier in the text, we agree that it is helpful to refer to it throughout the document. We therefore added the following citations to the revised manuscript:

Old passage (P3 L28):

In this section, we introduce the LSTM architecture in more detail.

### New passage:

In this section, we introduce the LSTM architecture in more detail, using the notation of Graves et al. (2013).

### Old passage (P2 L6-7):

In comparison, the LSTM has (i) an additional cell state or cell memory ct in which information can be stored, and (ii) three gates that control the information flow within the LSTM cell (three encircled letters in Fig. 2b). The first gate is the forget gate, introduced by Gers et al. (2000)

### New passage:

In comparison, the LSTM has (i) an additional cell state or cell memory Ct in which information can be stored, and (ii) gates (three encircled letters in Fig. 2b) that control the information flow within the LSTM cell (Hochreiter and Schmidhuber, 1997). The first gate, the forget gate, was later introduced by Gers et al. (2000).

5. page 6 I. 17 "For this study, we used a 2-layer LSTM network, with each layer having a cell/hidden state length of 20." First, I would split the theory and the setup of the LSTM for the numerical experiment. So move all the specific details to section 2.4. In addition, I would expect a table with all the specifications of the used LSTM including number of the parameters in Wc, Wf, Wi, Wo, Uc, Uf, Ui, Uo, bc, bf, bi, bo and hyperparameters. Second, I do not understand that the LSTM has a number of 365 inputs and the "hidden state length of 20". Please explain this!

Thank you for this recommendation. We agree that it is better to split the theory of the LSTM functionality and our specific setup into different sections. Therefore, we moved the part dealing with our specific network architecture to section of the experimental design, as suggested by AR2.

We are also thankful for the suggestion of listing the parameters and their sizes in a table, and believe that this will indeed help to better understand the calculations in Eq. (2-8). Consequently, we added a table with the specifications of all parameters to the revised manuscript.

Regarding the last part of the comment: It could be that we did not explain the terms input length, number of inputs and the nature of the hidden state well enough, as the question indicates a potential confusion. There are 5 inputs to the LSTM. These are the 5 meteorological variables, which are are presented sequentially to the network. This means that we show the network the 5 meteorological variables of e.g. the first day of the sequence and compute equations 2-7, before the next day of meteorological variables are presented (For the next day equations 2-7 are then computed again, and

so on...see Figure 1 and 2 of the original manuscript). Since our sequence is 365 days long, this computation is repeated for 365 days before the final output is calculated. The hidden state length of 20 is a hyperparameter and defines how much capacity we give the network to learn from the data (similarly, the number of LSTM layers - i.e. 2 - is an other hyperparameter which influences the capacity). The hidden state length can be compared to the number of hidden neurons in a single layer within traditional feed forward networks).

To avoid confusions for future readers we added, the algorithm of the LSTM as pseudocode to section 2.1, beside the table with the parameters and their respective shapes (in section 2.4); and added further descriptions to the end of section 2.1. We hope that this helps further with understanding the LSTM.

(Screenshot of parameter table, which will be inserted into Section 2.4, where the network architecture is presented in the revised manuscript.):

 Table 2. Shapes of learnable parameters of all layer.

Layer	Parameter	Shape
1 <sup>st</sup> LSTM layer	$\mathbf{W}_f, \mathbf{W}_{\widetilde{c}}, \mathbf{W}_i, \mathbf{W}_o$	[20, 20]
	$\mathbf{U}_f, \mathbf{U}_{\widetilde{c}}, \mathbf{U}_i, \mathbf{U}_o$	[20, 5]
	$oldsymbol{b}_f,oldsymbol{b}_{\widetilde{c}},oldsymbol{b}_i,oldsymbol{b}_o$	[20]
2 <sup>nd</sup> LSTM layer	$\mathbf{W}_f, \mathbf{W}_{\widetilde{c}}, \mathbf{W}_i, \mathbf{W}_o$	[20, 20]
	$\mathbf{U}_f, \mathbf{U}_{\widetilde{c}}, \mathbf{U}_i, \mathbf{U}_o$	[20, 20]
	$oldsymbol{b}_f,oldsymbol{b}_{\widetilde{c}},oldsymbol{b}_i,oldsymbol{b}_o$	[20]
Dense layer	$\mathbf{W}_{d}$	[20, 1]
	$oldsymbol{b}_d$	[1]

(Screenshot of LSTM pseudocode):

Algorithm 1 Pseudocode of LSTM layer

- 1: Input:  $x = [x_1, ..., x_{365}], x_i \in \mathbb{R}^n$
- 2: Given parameters:  $\mathbf{W}_f, \mathbf{U}_f, \mathbf{b}_f, \mathbf{W}_{\widetilde{c}}, \mathbf{U}_{\widetilde{c}}, \mathbf{b}_{\widetilde{c}}, \mathbf{W}_i, \mathbf{U}_i, \mathbf{b}_i, \mathbf{W}_o, \mathbf{U}_o, \mathbf{b}_o$
- 3: Initialize  $h_0, c_0 = \overrightarrow{0}$
- 4: for t=1, ..., 365 do
- 5: Calculate  $f_t$  (Eq. 2),  $\tilde{c}_t$  (Eq. 3),  $i_t$  (Eq. 4)
- 6: Update cell state  $c_t$  (Eq. 5)
- 7: **Calculate**  $o_t$  (Eq. 6),  $h_t$  (Eq. 7)
- 8: end for
- 9: **Output:**  $h = [h_1, ..., h_{365}], h_i \in \mathbb{R}^m$

New passage (will be added together with the pseudo code at the end of section 2.1 after the insertion of minor comment #2):

To conclude, Algorithm 1 shows the pseudocode of the entire LSTM layer. As indicated above and shown in Fig. 1, the inputs for the complete sequence of meteorological observations  $x = [x_1, ..., x_{365}]$ , where  $x_t$  is a vector containing the meteorological inputs of time step t, is processed time step by time step and in each time step Eq. (2-7) are repeated. In the case of multiple stacked LSTM layers, the next layer takes the output  $h = [h_1, ..., h_{365}]$  of the previous layer as input. The final output, the discharge, is then calculated by Eq. (8), where  $h_{365}$  is the last output of the second LSTM layer.

6. I would skip section 2.1.1 or move this to the discussion since this is hypothetical and no mathematical equivalence is shown.

See answer to comment #3 of AR1.

### 7. page 7 I. 10 Is the LSTM limited to MSE when backpropagation is used?

The LSTM is not limited to MSE, when backpropagation is used. It is able to use any loss function that can be utilized for any other neural network. That is, any loss function that can be differentiated. A common way to derive the loss function is to use the principle of maximum likelihood in conjunction with the output layer. For the case at hand this is a dense layer, yielding the MSE as loss function, which is also the most common loss for regression tasks such as this one (see Goodfellow et al. 2016). If the task of interest is e.g. a classification problem, different output layers and loss functions would be used (such as the binary cross entropy or the negative log likelihood).

### 8. page 7 I. 19 spelling->"iteration"

Thank you very much for this finding. Word will be corrected in the revised manuscript.

# 9. page 11 Please give more information about the calibration of the SAC-SMA model and the computational effort.

Sadly, we do not have any information on the computational effort it took the CAMELS authors to calibrate the SAC-SMA + Snow-17 models for all basins (and no information is given in their publication). Regarding the calibration process, we added the following sentences to section 2.3, because we see that this summary also helps explaining why we trained the models the way we did (see comment #2, AR2).

### Old passage:

Additionally, the CAMELS data set contains time series of simulated discharge from the calibrated Snow-17 models coupled with the Sacramento Soil Moisture Accounting Model (see Newman et al. (2015) for further details). The models were calibrated with the first 15 hydrological years for which streamflow data is available (in most cases 1 October 1980 until 30 September 1995). We use the exact same period for the training of the LSTM, while the remaining data (in most cases 1 October 1995 until the end of 2014) is used for model validation.

### New passage:

Additionally, the CAMELS data set contains time series of simulated discharge from the calibrated Snow-17 models coupled with the Sacramento Soil Moisture Accounting Model. Roughly 35 years of meteorological observations and streamflow records are available for most basins. The first 15 hydrological years with streamflow data (in most cases 1 October 1980 until 30 September 1995) are used for calibrating the model, while the remaining data is used for validation. For each basin 10 models were calibrated using the shuffled complex evolution algorithm by Duan et al. (1993), starting with different random seeds. The objective Newman et al. (2015) used, was minimizing the root mean squared error (RMSE). As final model (and as the model we used for comparison), the model with the lowest RMSE in the calibration period is chosen. For further details see Newman et al. (2015).

10. page 13 Explain, why the LSTM network is better for the mean, but not for the median NSE (see Fig.6b). From my point of view, it is not surprising that the LSTM network performance better for mean flows. So discuss in detail also the behavior for high flows.

We are not completely sure whether we understood the comment correctly. In our view, the performance difference between mean and median NSE is not associated with the "better performance for mean flows". From Figure 7a and the sentences below one can see that the NSE values of the SAC-SMA have large negative deviations (see also our answer to minor comment #11 to AR#1), while the ones for the LSTM network do not. The mean is influenced by these outliers, while the median is not. The lack of robustness of the mean is in this case an advantage, as it does not hide bad model performances.

11. page 15 "However, we want to highlight again that achieving the best model performance possible was not the aim of this study, rather testing the general ability of the LSTM in reproducing runoff processes."<-Since we already know that data driven techniques are able to reproduce runoff processes, the authors of the paper should be

more ambitious and give some more details and discussion about advantages and disadvantages of the LSTM network.

In the revised manuscript, we rewrote the entire conclusion (see also our answer to comment 3 of AR2). The new conclusion contains a broader discussion about limitations and advantages of LSTMs.

12. page 21 I would skip Fig. 21 or would present a more detailed analysis of internal states and combine this with the hypothesis described in section 2.1.1.

See answer to comment #3 of AR1

## References:

- Abrahart, R. J., Anctil, F., Coulibaly, P., Dawson, C. W., Mount, N. J., See, L. M., Shamseldin, A. Y., Solomatine, D. P., Toth, E., and Wilby, R. L.: Two decades of anarchy? Emerging themes and outstanding challenges for neural network river forecasting, Progress in Physical Geography, 36, 480–513, 2012.
- 2. ASCE Task Committee on Application of Artificial Neural Networks: Artificial Neural Networks in Hydrology. Ii: Hydrologic Applications, Journal Of hydrologic engineering, pp. 124–137, 2000.
- 3. Assem, Haytham, et al. "Urban Water Flow and Water Level Prediction Based on Deep Learning." *Joint European Conference on Machine Learning and Knowledge Discovery in Databases*. Springer, Cham, 2017.
- 4. Bai, Yun, et al. "Daily reservoir inflow forecasting using multiscale deep feature learning with hybrid models." *Journal of hydrology* 532 (2016): 193-206.
- 5. Bengio, Yoshua. "Practical recommendations for gradient-based training of deep architectures." Neural networks: Tricks of the trade. Springer, Berlin, Heidelberg, 2012. 437-478.
- Duan, Q. Y., Vijai K. Gupta, and Soroosh Sorooshian. "Shuffled complex evolution approach for effective and efficient global minimization." *Journal of optimization theory and applications* 76.3 (1993): 501-521.
- 7. Graves, Alex, Abdel-rahman Mohamed, and Geoffrey Hinton. "Speech recognition with deep recurrent neural networks." *Acoustics, speech and signal processing (icassp), 2013 ieee international conference on.* IEEE, 2013.
- 8. Gupta, H. V., Kling, H., Yilmaz, K. K., and Martinez, G. F. "Decomposition of the mean squared error and NSE performance criteria: Implications for improving hydrological modelling" *Journal of Hydrology*, 377, 80–91, 2009.
- 9. Shen, Chaopeng. "A trans-disciplinary review of deep learning research for water resources scientists." *arXiv preprint arXiv:1712.02162* (2017).

- 10. Wu, Zheng Yi, Mahmoud El-Maghraby, and Sudipta Pathak. "Applications of deep learning for smart water networks." *Procedia Engineering* 119 (2015): 479-485.
- Zhang, Duo, Geir Lindholm, and Harsha Ratnaweera. "Use long short-term memory to enhance Internet of Things for combined sewer overflow monitoring." *Journal of Hydrology* (2018 a): 409-418.
- 12. Zhang, Jianfeng, et al. "Developing a Long Short-Term Memory (LSTM) based model for predicting water table depth in agricultural areas." *Journal of Hydrology* 561 (2018 b): 918-929.