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Improving U.S. National Water Model Streamflow with Long Short-Term Memory Networks

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Research Impact Statement: Post-processing the U.S. National Water Model (NWM) with deep learning improves streamflow predictions and identified the NWM channel router as a major source of information loss.

ABSTRACT: Long short-term memory (LSTM) deep learning networks were used to post-process the U.S. National Water Model (NWM) outputs for improved daily averaged streamflow predictions at 531 basins across the continental United States (CONUS). We compared post-processed streamflow against the NWM and a baseline LSTM without NWM outputs. The LSTM post-processors perform better, on average, than the NWM. Overall median NSE scores are 0.62 for the NWM, 0.74 for the standalone LSTM and 0.73 and 0.75 for the two post-processors. The LSTM with NWM inputs was not significantly better than a standalone LSTM, indicating that the NWM provides only situational benefit for LSTM streamflow prediction. Accuracy of predictions in 2 of the 531 basins was severely reduced by post-processing during tests on ungauged basins, and we found no way to identify ahead of time (without streamflow observations and predictions for comparison) basins where this might occur. The baseline LSTM performs well in ungauged basins. The post-processor improves NWM streamflow predictions in all regions within CONUS. A sensitivity analysis was used to diagnose the land surface component of the NWM as the source of mass bias error and the channel router as a source of simulation timing error. Our assessment indicates that the NWM routing scheme should be considered a priority for NWM improvement.

(**KEYWORDS**: National Water Model; theory-guided machine learning; long short-term memory; streamflow; model diagnostics.)

INTRODUCTION

The U.S. National Water Model (NWM), based on WRF-Hydro (Cosgrove *et al.,* 2015), is an emerging large-scale hydrology simulator. Some specific details of the NWM advancements in large scale hydrology are described by Elmer (2019, page 11), including increased resolution and number of stream reaches (2.7 million) for a model covering the continental United States (CONUS). A purported strength of WRF-Hydro is simulating hydrologic dynamics, and specifically timing of hydrological response (Salas *et al.*, 2018). The predictive performance of the NWM (ability to match streamflow observations) has been shown to vary widely. Hansen *et al.* (2019) evaluated the performance of the NWM in the Colorado River Basin in terms of drought and low flows; they found better performance in the Upper Colorado River Basin than in the Lower Colorado River Basin, and attributed this discrepancy to the NWM's ability to simulate snowpack. WRF-Hydro has generally poor performance in the Southwest and Northern Plains (Salas *et al.*, 2018). Salas et al., 2018 hypothesized that error in WRF-hydro might come from lakes, reservoirs, floodplain dynamics and soil parameter calibration.

The NWM version 2.0 was calibrated at 1,457 basins within the CONUS domain. As a point of comparison, the United States Geological Survey (USGS) records daily streamflow at 28,529 basins (https://nwis.waterdata.usgs.gov/nwis, accessed June 2020). Calibrating the model at each stream gauge within the NWM domain is a large computational expense, and while regionalization strategies can be used to improve forecast accuracy without having to calibrate each individual basin, accuracy typically suffers compared to direct calibration. Due to these reasons and others, making accurate hydrological predictions over large scales is a challenging problem, however there are promising results in the machine learning and data science communities that may be directly applicable to improving the NWM.

Machine learning (ML) is a powerful tool for hydrological modeling, and there has been a call to merge ML with traditional hydrological modeling (Reichstein *et al.*, 2019; Nearing et al., 2020). One example of an ML approach that has been effective for hydrological prediction is the "long short-term memory" network (LSTM) (Hochreiter, 1991; Hochreiter and Schmidhuber, 1997). The LSTM is a time series deep learning method that is particularly well suited to model hydrologic processes because it mimics in certain ways the Markovian input-state-ouput structure of a dynamical system (Kratzert *et al.*, 2018). LSTMs have been effective at simulating predictions of surface runoff at the daily time scale (Kratzert *et al.*, 2019a), including in ungauged catchments where traditional methods of calibration do not work (Kratzert *et al.*, 2019b), and also at sub-daily (hourly) timescales (Gauch et al., 2020). One potential problem with ML, however, is that it lacks a physical basis. While there are emerging efforts in hydrology to merge physical understanding with machine learning (Karpatne *et al.*, 2017a; Daw *et al.*, 2020; Pelissier *et al.*, 2019; Chadalawada *et al.*, 2020; Tartakovsky *et al.*, 2020, Read et al., 2019; Nearing et al., 2020; Hoedt et al., 2021), the field of *theory-guided machine learning* (Karpatne *et al.*, 2017b) is still relatively immature in hydrology.

The NWM informs forecasts of many hydrologic conditions, including river ice, snowpack, soil moisture and inundation, which are used for management applications such as transportation, recreation, agriculture and fisheries (NOAA 2019). When ML is to be used in the NWM it should not disrupt the delivery of these hydrologic forecasts, therefore an ML prediction for streamflow that does not also include predictions of the other hydrologic states and variables must be run in parallel with the existing process-based hydrologic model. A natural question arises: does the existing NWM formulation benefit the already highly accurate LSTM predictions of streamflow?

Hydrologic post-processing can remove systematic errors in the model prediction, and has been shown to improve forecast accuracy of both calibrated and uncalibrated basins, particularly in wet basins (Ye *et al.*, 2014). The general methodology of post-processing involves taking the output of a process-based model and feeding it into a data-driven model. In this paper we applied a LSTM-based post-processor for the NWM to improve basin-scale streamflow predictions. This is a straightforward theory-guided machine learning approach. We tested a post-processor that uses dynamic information only from the NWM outputs and compared the results against the NWM itself. We also tested a post-processor that included both the NWM outputs and NLDAS atmospheric forcings as inputs and compared against a 'baseline' LSTM model trained only with atmospheric forcings (no NWM outputs).

We applied the LSTM post-processors to 531 basins across the CONUS. The basins chosen for this large-scale analysis are mostly headwater catchments without engineered control structures, such as dams, canals, and levees. This was a deliberate choice made for the purpose of simulating a close-to-natural rainfall-runoff response. Our goal was to use the post-processor to learn systematic corrections to simulated basin-scale rainfall-runoff processes that can improve forecasts of streamflow, rather than the hydraulic engineering implications resulting from simulated controlled flow, *e.g.,* a reservoir release. Kim *et al.* (2020) showed the limitation of the NWM to predict streamflow in a highly engineered watershed and the need for representing controlled releases. Thus, we are using some of the simplest, and top performing, applications of the NWM for these experiments.

METHODS

Data & Models

CAMELS Catchments. This study used the Catchment Attributes and Meteorological dataset for Large Sample Studies (CAMELS) (CAMELS; Newman *et al.*, 2015; Addor *et al.*, 2017). These data were curated by the US National Center for Atmospheric Research (NCAR; https://ral.ucar.edu/solutions/products/camels, accessed March 2020), and we used the 531 (out of 671) basins that were chosen by Newman *et al.* (2015) for model benchmarking. Newman et al (2015) excluded basins with large discrepancies in different methods for measuring basin area and also basins larger than 2,000 km^2. CAMELS data include corresponding daily streamflow records from USGS gauges, and meteorological forcing data (precipitation, max/min temperature, vapor pressure and total solar radiation) come from North American Land Data Assimilation System (NLDAS; Xia *et al.*, 2012).

National Water Model. We used the National Water Model version 2.0 reanalysis, which contains output from a 25-year (January 1993 through December 2019) retrospective simulation (https://docs.opendata.aws/nwm-archive/readme.html, accessed June 2020). The NWM retrospective ingests rainfall and other meteorological forcings from atmospheric reanalyses (https://water.noaa.gov/about/nwm, accessed June 2020.). NWM reanalysis output includes channel outputs (point fluxes: CHRT) and land surface (gridded states and fluxes: LDAS & RT) outputs. The specific features that we used from the NWM reanalysis are shown in Table 1. To be compatible with the LSTM model, which uses a one-day timestep and was trained using all basins simultaneously, we took the mean values of these model outputs across UTC calendar days (12AM - 11PM) to produce daily records from the hourly NWM when used as input to the LSTM, but for NWM streamflow diagnostics we used the local calendar day (based on U.S. time zone) to be compatible with the USGS gauge records. Channel routing point data

(CHRT) were collected at each individual NWM stream reach that corresponds to the stream gauge associated with each CAMELS catchment. Gridded land surface data (LDAS) was collected from each 1 km^2 Noah-MP cell contained within the boundaries of each CAMELS catchment, and these were averaged to produce a single representative (lumped) value for each catchment. Gridded routing data (RT) were collected from each 250 m^2 cell, and we included the mean and maximum value within the catchment boundary. We did not include lake input and output fluxes because these would be inconsistent across basins (some basins have zero and some basins have multiple lakes). Note that the units of the NWM outputs are not required for the LSTM post-processor.

TABLE 1. National Water Model Output Data

Feature name	**Feature**	NWM model component	**Resolution**
ACCET	Accumulated evapotranspiration	LDAS	1Km
FIRA	Total net long-wave (LW) radiation to atmosphere	LDAS	1Km
FSA	Total absorbed short-wave (SW) radiation	LDAS	1Km
FSNO	Snow cover fraction on the ground	LDAS	1Km
HFX	Total sensible heat to the atmosphere	LDAS	1Km
LH	Latent heat to the atmosphere	LDAS	1Km
SNEQV	Snow water equivalent	LDAS	1Km
SNOWH	Snow depth	LDAS	1Km
SOIL M (4 layers)	Volumetric soil moisture	LDAS	1Km
SOIL W (4 layers)	Liquid volumetric soil moisture	LDAS	1Km
TRAD	Surface radiative temperature	LDAS	1Km
UGDRNOFF	Accumulated underground runoff	LDAS	1Km
streamflow	River Flow	CHRT	point
q_lateral	Runoff into channel reach	CHRT	point
velocity	River Velocity	CHRT	point
qSfcLatRunoff	Runoff from terrain routing	CHRT	point
qBucket	Flux from groundwater bucket	CHRT	point
qBtmVertRunoff	Runoff from bottom of soil to groundwater bucket	CHRT	point
Sfcheadsubrt (mean and max)	Ponded water depth	RTOUT	250Km
Zwattablrt (mean and max)	Water table depth	RTOUT	250Km

Long short-term memory network. The LSTM is a recurrent neural network that is able to maintain a memory of the system state and dynamics through a period of time (in this case 365 days). This recurrent state space is the main advantage for hydrological applications over other types of neural networks. Our LSTM network was developed from Kratzert et al. (2019) using a codebase that is now referred to as NeuralHydrology (https://neuralhydrology.github.io/ accessed March 2021). This research grade codebase was developed in the Python programming language and is based primarily on the Pytorch machine learning library.

The LSTM used two types of inputs: daily meteorological forcings and static catchment attributes. Again, note that the units of the forcing data are irrelevant when used as inputs for the LSTM, which does not include a mass or energy balance. We normalized all inputs to the LSTM, including static and dynamic inputs by subtracting the mean and dividing by the standard deviation of the training data. We used eighteen catchment attributes from the CAMELS dataset related to climate, vegetation, topography, geology, and soils. These are described in more detail by Addor *et al.* (2017) and listed here in Table 2. Catchment attributes are static for each basin (do not change in time). For the post-processing runs we added the states, fluxes, and streamflow predictions from version 2.0 of the NWM.

TABLE 2. LSTM Inputs

Meteorological Forcing Data (used in models denoted with an “A”)	
Maximum Air Temp (TMax)	2-meter daily maximum air temperature
Minimum Air Temp (TMin)	2-meter daily minimum air temperature
Precipitation (PRCP)	Average daily precipitation
Radiation (SRAD)	Surface-incident solar radiation
Vapor Pressure (Vp)	Near-surface daily average
Static Catchment Attributes (used in each of the LSTM models)	
Precipitation Mean	Mean daily precipitation
PET Mean	Mean daily potential evapotranspiration
Aridity Index	Ratio of Mean PET to Mean Precipitation
Precipitation Seasonality	Estimated by representing annual precipitation and temperature as sin waves Positive (negative) values indicate precipitation peaks during the summer (winter).

	Values of approx. 0 indicate uniform precipitation throughout the year.
Snow Fraction	Fraction of precipitation falling on days with temp [C].
High Precipitation Frequency	Frequency of days with ≤ 5x mean daily precipitation. Average duration of high precipitation events (number of consecutive days with ≤ 5x mean daily precipitation).
Low Precipitation Frequency	Frequency of dry days (< 1 mm/day).
Low Precipitation Duration	Average duration of dry periods (number of consecutive days with precipitation < 1 mm/day).
Elevation	Catchment mean elevation.
Slope	Catchment mean slope.
Area	Catchment area.
Forest Fraction	Fraction of catchment covered by forest.
LAI Max	Maximum monthly mean of leaf area index.
LAI Difference	Difference between the max. and min. mean of the leaf area index.
GVF Max	Maximum monthly mean of green vegetation fraction.
GVF Difference	Difference between the maximum and minimum monthly mean of the green vegetation fraction.
Soil Depth (Pelletier)	Depth to bedrock (maximum 50m).
Soil Depth (STATSGO)	Soil depth (maximum 1.5m).
Soil Porosity	Volumetric porosity.
Soil Conductivity	Saturated hydraulic conductivity.
Max Water Content	Maximum water content of the soil.
Sand Fraction	Fraction of sand in the soil.
Silt Fraction	Fraction of silt in the soil.
Clay Fraction	Fraction of clay in the soil.
Carbonate Rocks Fraction	Fraction of the catchment area characterized as “carbonate sedimentary rocks”.
Geological Permeability	Surface permeability (log10).

We trained the LSTM models to make predictions at all 531 CAMELS catchments used in the analysis. We split the data temporally into a training period and testing period, and we present no results from the training period as these results are unrepresentative of the out-of-sample predictions. We trained the LSTMs on water years 2004 through 2014 and tested on water years 1994 through 2002. No spatial splits were included in the training procedure. The LSTMs used a 365-day LSTM look-back period, so a full year gap was left between training and testing to prevent bleedover (*i.e.*, information exchange) between the two periods. We trained separate LSTMs with ten unique random seeds for initializing weights and biases, and calculated benchmarking statistics using the ensemble mean hydrograph. The LSTMs make predictions representing runoff in units [mm], reflecting an area normalized volume of water that moves through a stream at each model timestep. USGS gauge records (and the NWM predictions) are in streamflow units [L^3/T]. We used the geospatial fabric estimate of the catchment area provided in the CAMELS dataset to convert all streamflow to units [L] for our diagnostic comparison. We trained the LSTMs with the protocol and features described in Appendix B of Kratzert et al. (2019b): this includes 30 epochs, a hyperbolic tangent activation function, a hidden layer size of 256 cell states, a look-back of 365 days, variable learning rates set at epoch 0 to 0.001, epoch 11 to 0.005 and epoch 21 to 0.0001, dropout rate of 0.4 and an input sequence length: 270.

Experimental Design

We tested the results from LSTM post-processing against the NWM and also against a baseline LSTM with no inputs from the NWM (referred to as LSTM_A, in which the A stands for atmospheric forcing). Table 3 will guide the reader through the setup of each model.

TABLE 3. Models

Model label	Number of dynamic LSTM inputs	Model description
NWM	N/A	National Water Model mean daily streamflow predictions
LSTM_PP	28	LSTM trained with NWM output for post processing
LSTM_PPA	32	LSTM trained with NWM output and atmospheric forcings for post-processing
LSTM_A	5	LSTM trained with atmospheric forcing conditions.

Simple schematics of the LSTMs used in this study are shown in Figure 1. The LSTM post-processors (LSTM_PP & LSTM_PPA) used NWM outputs as LSTM inputs, and the results were LSTM-based streamflow predictions influenced by the process-based NWM. This is a straightforward method of theory-guided machine learning.

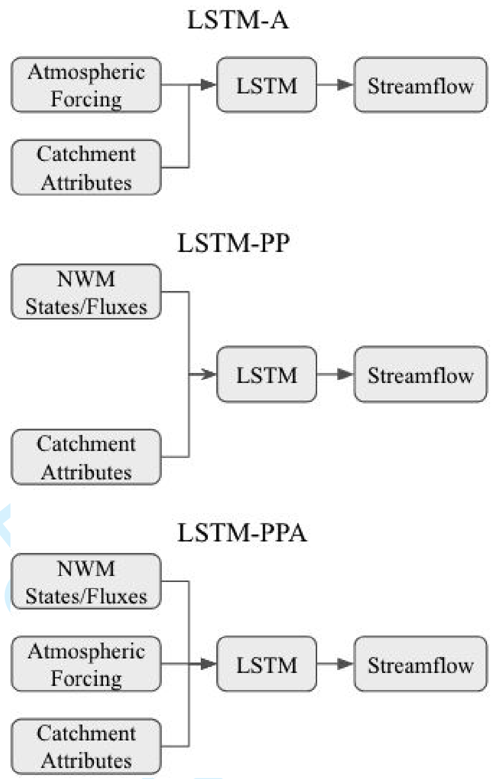

FIGURE 1. Flow chart showing the baseline LSTM (LSTM_A) and the LSTM post-processors with NWM data as inputs (LSTM_PP & LSTM_PPA). LSTM_PP is the post-processor which used only NWM outputs as input to an LSTM, and LSTM_PPA used both the NWM outputs and atmospheric forcings.

As a quality check, we compared the results from each LSTM ensemble member, and found a relative standard error of the mean streamflow about 1%, and relative standard error of the Nash-Sutcliffe Efficiency (NSE) value of about 0.01%. This means that all LSTM solutions are similar between random initialization seeds. Gauch *et al.* (2019) attributed a 0.01 discrepancy in NSE values of the LSTM predictions to non-determinism of the loss function minimization. In our experiments discrepancies in the loss function occur between different random seed initializations, but running the training procedure twice with the same random seed gives an identical solution, satisfying the definition of determinism.

191 **Performance metrics.** We calculated several metrics to evaluate predictive performance,
192 including the NSE and Kling-Gupta Efficiency (KGE) values (Gupta et. al, 2009). The variance,
193 bias and Pearson correlation metrics were calculated separately as components of the NSE
194 (Gupta *et al.*, 2009); these tell us about relative variability, mass conservation and linear
195 correlation between the modeled/observed streamflow values, respectively. Observed streamflow
196 values are from the USGS streamflow gauges associated with each of the CAMELS basins. The
197 metrics were calculated in two ways: 1) at each basin and then averaged together, and 2) using
198 all of the flows from all basins combined.

199 Our graphical results focus on three performance metrics: (i) NSE measures the overall
200 predictive performance as a correlation coefficient for the 1:1 linear fit between simulations and
201 observations, (ii) Peak timing error measures the absolute value of differences (in units days)
202 between simulated and observed peak flows for a given event, and (iii) total (absolute) bias
203 measures the overall bias of the simulated hydrograph relative to observations and represents
204 how well the model matches the total volume of partitioned rainfall that passes through the
205 stream gauge at each basin.

206 We also calculated performance metrics on different flow regimes. Rising limbs and
207 falling limbs were characterized by a one-day derivative, where positive derivatives were
208 categorized as rising limb, and negative derivatives as falling limb. High flows were
209 characterized as all flow above the 80th percentile in a given basin, and low flows as below the
210 20th percentile in a given basin.

211 We tested the performance of the LSTM post-processors in different regions. We split the
212 basins by USGS designated “water resource regions” (https://water.usgs.gov/GIS/regions.html,

accessed July 2020). To analyze the regions individually we averaged the NSE, bias and timing error of the CAMELS basins within each region.

We set an alpha value for statistical significance to $\alpha = 0.05$. To control for multiple comparisons we adjusted the alpha values using family-wise error rate equal to $1-(1-\alpha)^m$, with m being the number of significance tests (86 in total), which brought our effective alpha value down to 0.049. We tested for statistical significance with a Wilcoxon signed-rank test against the null hypothesis that our test models (LSTM post-processors) performance across basins came from the same distribution as our base models (NWM & LSTM_A).

Simulated hydrograph representation of hydrologic signatures. Hydrologic signatures help us understand how well a model represents important aspects of real-world streamflow, and where improvement should be made to the model's conceptualization (Gupta *et al.*, 2008). We analyzed the hydrologic signatures described by Addor *et al.* (2018), and these are listed below in Table 4. We calculated the true signatures with USGS streamflow observations, and calculated model representations with predicted values of daily streamflow. The comparison between true values and predicted values was made with a correlation coefficient (r^2) across basins (one value of the observed and predicted hydrologic signatures were calculated per basin), higher values indicate better representation of hydrologic signature across basins by the model. We used the Steiger method to test for statistically significant improvement (or detriment) between the base models and the LSTM post-processor (Steiger and Browne, 1984).

TABLE 4. Hydrologic signatures (adapted from Addor *et al.* 2018)

Signature description	Signature name
Average duration of low-flow events	low_q_dur
Frequency of days with zero flow	zero_q_freq
Average duration of high-flow events	high_q_dur
Streamflow precipitation elasticity	stream_elas

Frequency of high-flow days	high_q_freq
Slope of the flow duration curve	slope_fdc
Frequency of low-flow days	low_q_freq
Baseflow index	baseflow_index
Runoff ratio	runoff_ratio
Mean half-flow date	hfd_mean
5 percent flow quantile	q5
95 percent flow quantile	q95
Mean daily discharge	q_mean

Identifying basins best suited for post-processing with multi-linear regression. The LSTM post-processors did not improve performance at every basin. It therefore would be valuable to know if a LSTM post-processor will work in any particular basin before implementation. We trained a multi-linear regression, using the Scikit-learn library in Python, to predict the performance changes between the NWM and the LSTM post-processors (LSTM_PP & LSTM_PPA) at each individual basin. The inputs to the regression analysis were the performance score of the NWM streamflow predictions, hydrologic signatures and catchment characteristics. These regressors are useful to help interpret what basins might benefit most from an LSTM post-processor. We trained and tested multi-linear regression models using k-fold cross-validation with 20 splits (k=20) over the 531 basins. We report the correlation (r^2) of out-of-sample regression predictions of post-processing improvements vs. actual post-processing improvements.

Interpretation of LSTM with integrated gradients. We aim to explain the relationship between a model's predictions in terms of its features. This will help us understand feature importance, identifying data issues, and inform NWM process diagnostics from the post-processors. We calculated integrated gradients (Sundararajan *et al.*, 2017) to attribute the LSTM inputs (both atmospheric forcings and NWM outputs) to the total prediction of streamflow.

251 Integrate gradients are a type of sensitivity analysis that are relatively insensitive to low gradients
252 (*e.g.*, at the extremes of neural network activation functions). We calculated integrated gradients
253 separately for each input, at each timestep, for each lookback timestep, in each basin. This means
254 that for 9 years of test data with a 365-day lookback there were about 1.2 million integrated
255 gradients per input, per basin. The unit of the integrated gradient is technically normalized
256 streamflow, but we were mostly interested in the relative values of integrated gradients of each
257 individual LSTM input.

258 **Interpretation of LSTM with correlations between performance and NWM inputs.**
259 We made a direct connection between LSTM post-processor improvements with the NWM
260 outputs using correlation. We calculated Pearson R values between the basin average value of
261 each NWM input feature and the total performance change (NSE, bias and peak timing). These
262 correlations were calculated for different flow regimes (all flows using the whole hydrograph,
263 rising/falling limbs using the single day differentials, and high/low flows using the top 80% and
264 bottom 20%). The strengths of these correlations (positive or negative) indicated which types of
265 basins (via NWM features) are benefiting most from a LSTM post-processor. Results for rising
266 limbs and falling limbs of the hydrograph were qualitatively similar to this figure, and were
267 therefore omitted.

268 **Splitting the CAMELS catchments by calibrated / uncalibrated.** Of the NWM
269 calibrated basins, 480 overlap with the 531 CAMELS catchments used in this study. In a
270 separate set of experiments, we trained the LSTM_A and the LSTM post-processors LSMT_PP
271 and LSTM_PPA) on only the 480 calibrated basins. We then used the full set of 531 catchments
272 to test the performance out-of-sample. We analyzed the 480 in-sample basins and 51 out-of-
273 sample basins separately using the NSE, bias and timing error metrics. This allowed us to

determine if the LSTM is a suitable post-processing method to use in uncalibrated basins. If the post-processors trained only on calibrated basins can improve streamflow predictions at uncalibrated basins, then they would be considered suitable, particularly if there is no statistical difference between the post-processor's performance improvement over the baseline models.

Sensitivity analysis and NWM process diagnostics**.** We trained a set of LSTM post-processors using different combinations of NWM outputs as input to the LSTM, as described in Table 5. To test the sensitivity to the NWM streamflow prediction itself, we trained an LSTM with only streamflow (LSTM_Q_only), and excluded it from another (LSTM_PP_noQ). We tested the sensitivity to the channel routing (LSTM_chrt) and land surface (LSTM_ldas) components of the NWM by training LSTMs with only these dynamic inputs. These modes were trained with the same specifications as the baseline LSTM_A, LSTM_PPA and LSTM_PP.

TABLE 5. Additional models for sensitivity analysis and NWM diagnostics

Model label	Number of dynamic LSTM parameters	Model description
LSTM_PP_noQ	26	LSTM post-processor (LSTM_PP) but without streamflow or velocity.
LSTM_Q_only	1	LSTM trained with NWM streamflow only.
LSTM_chrt	6	LSTM trained with NWM channel routing outputs only.
LSTM_ldas	18	LSTM trained with NWM land surface outputs only.

Each of these models, in addition to the main post-processing models presented above, have a distinct flow of information that we can use to diagnose NWM model processes. Figure 2 shows the information flow of each of the model subcomponents. We used the performance results of the different post-processing models to assess how much information passes between the model components. Nearing et al., (2015) described the method to quantify the information exchange down a modeling chain (i.e., integrating over the expected effect of the conditional probability), but since we used limited outputs from the NWM reanalysis, rather than the full state space, we examined the NWM only qualitatively for information loss between the major NWM sub-components (land surface runoff, overland router and channel router). The LSTM extracts information from its input to make predictions about its target, in our case streamflow, and we assumed higher streamflow prediction accuracy indicated more information is available in the NWM components used as input. If a post-processor made less accurate streamflow predictions than the baseline LSTM, then this indicates that information from the atmospheric forcings was lost along the NWM modeling chain.

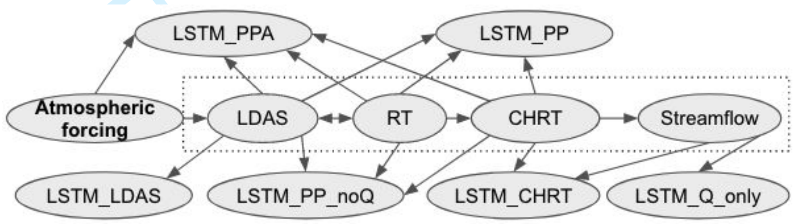

FIGURE 2. Process network diagram showing the information flow of each of these models. Arrows indicate the information flow from one component of the model to another. The NWM components are outlined with the dashed box. This is also a good guide for understanding the inputs to the different post-processing models.

RESULTS

Overall model performance

Post-processing the NWM with LSTMs significantly improved predictive performance, both with or without including the atmospheric forcings as inputs into the model. Figure 3 shows the cumulative distributions of three performance metrics (NSE, peak timing error, and total bias).

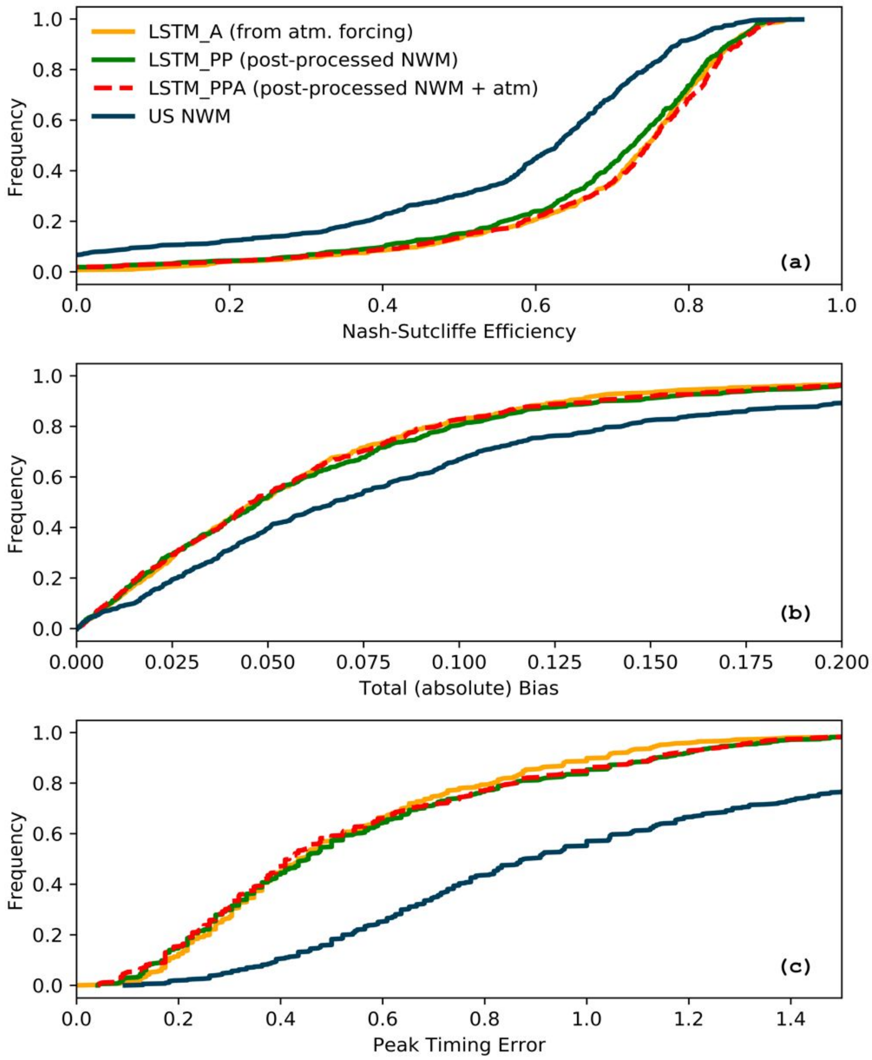

FIGURE 3. Results showing the cumulative distributions of model performance calculated as Nash-Sutcliffe Efficiency (NSE), total bias, and peak timing error over a 10-year test period in 531 CAMELS catchments. The National Water Model (NWM) reanalysis streamflow was averaged daily, long short-term memory (LSTM) networks shown used (i) the original atmospheric inputs (LSTM_A), (ii) NWM states and fluxes only (LSTM_PP), and (iii) both atmospheric forcings and NWM states and fluxes (LSTM_PPA). These figures omit the distribution tails for clarity.

The LSTM_PP improved the NSE score of the NWM mean daily streamflow at a total of 465 (88%) and reduced accuracy in 66 basins (12%) of the total 531 CAMELS basins, improved the total bias of the NWM mean daily streamflow at a total of 325 (61%) of basins and improved the peak timing error at a total of 488 (92%) of basins. The LSTM_PPA post-processor improved the NSE score of the NWM mean daily streamflow at a total of 488 (92%) and reduced accuracy in 43 basins (8%) of the total 531 CAMELS basins. The LSTM_PPA post-processor improved the total bias of the NWM mean daily streamflow at a total of 331 (62%) of basins and improved the peak timing error at a total of 494 (93%) of basins. The LSTM_A (the baseline LSTM without NWM states and fluxes) outperformed the NWM at a total of 473 (89%) and reduced accuracy in 58 basins (11%), improved the total bias of the NWM mean daily streamflow at a total of 339 basins (64%) and improved the peak timing error at a total of 484 basins (91%). The LSTM_PPA improved the greatest number of basins in terms of NSE and peak timing error and the LSTM_A was the best performing model in terms of total bias. Figure 4 shows scatter plots of the post-processor performance at individual basins against the performance of the baseline models.

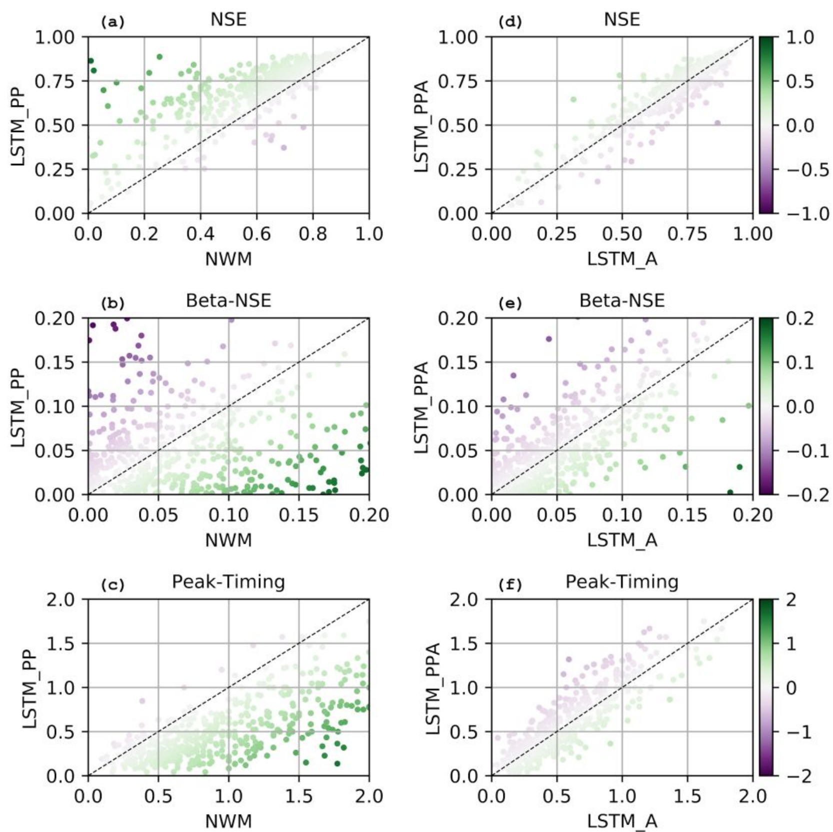

FIGURE 4. Performance differences of the post-processors against the baseline models (NWM and LSTM_A) in 531 CAMELS basins across CONUS. Green indicates basins where post-processing improved performance over the baseline (darker indicates larger relative improvement), and purple indicates basins where there was a decrease in performance (darker indicating worse relative detriment). The first column shows the performance difference between the LSTM_PP and the NWM. The second column shows the performance difference between the LSTM_PPA and the LSTM_A.

The post-processing models (LSTM_PP and LSTM_PPA) improved relative to the NWM in similar basins. The improvements of the two post-processing methods are correlated across all basins ($r^2 = 0.995$). Performance comparisons between the LSTM models and the NWM for each basin are plotted spatially in Figure 5. Notice that some of the highest NSE improvements between the LSTM_PP and the NWM are the worst NSE detriments between the LSTM_PPA and the LSTM_A, particularly in the northern plains. This indicates that although the post-processor greatly improves the NWM, the information from the NWM at bad basins hinders the performance of the LSTM, or in other words, the NWM passes bad information to the LSTM.

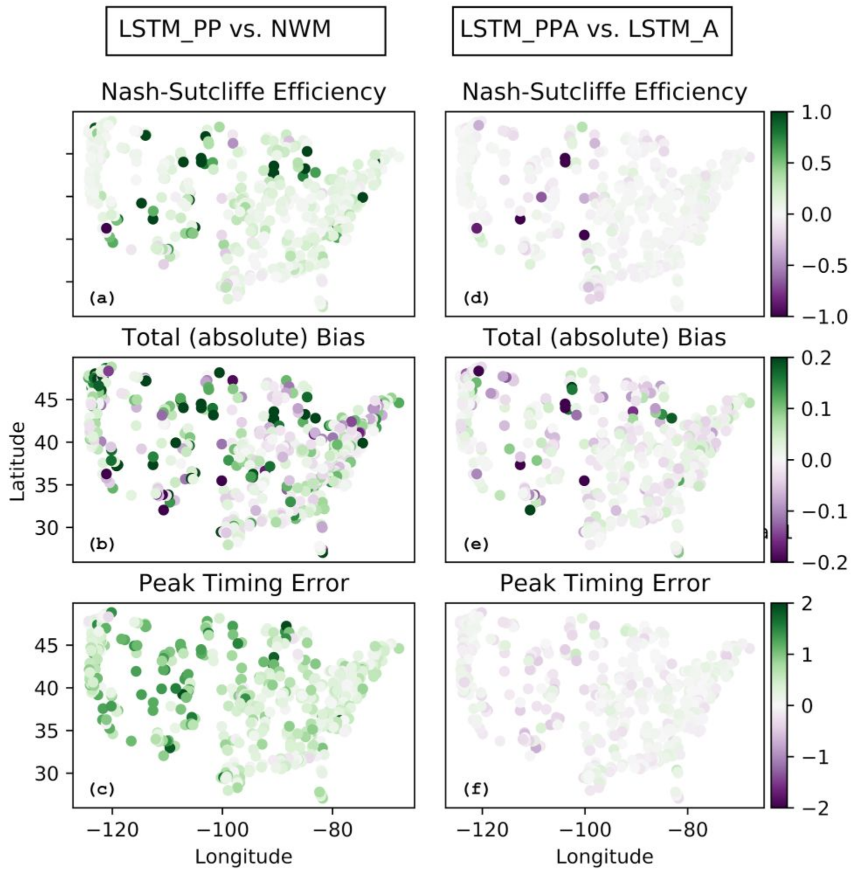

FIGURE 5. Per-basin performance change between the post-processors and baseline models (NWM and LSTM_A) in 531 CAMELS basins across CONUS. Green indicates basins where post-processing improved performance over the baseline (darker indicates larger relative improvement), and purple indicates basins where there was a decrease in performance (darker indicating worse relative detriment). The first column (a-c) shows the performance change between the LSTM_PP and the NWM. The second column (d-f) shows the performance change between the LSTM_PPA and the LSTM_A.

Performance by flow regime

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The LSTM post-processors improved predictive performance of the NWM according to the NSE and KGE metrics, as well as their components (variance and correlation). A full set of performance metrics broken down by flow regime are shown in Table 6. The left side of the table shows the average of metrics calculated individually at each basin, and the right side of the table shows the metrics as calculated combining the flows from all basins. The NSE includes both mean and median averages, but the rest of the metrics are only averaged by median.

TABLE 6. Predictive performance for NWM, LSTM_A and the LSTM Post-processors during various flow regimes. The Nash-Sutcliffe Efficiency (NSE) and Kling-Gupta Efficiency (KGE) are overall performance metrics of prediction quality. Variance, bias and correlation (R) are the components of the NSE. We calculated these in two ways: 1) at each basin and averaged across all basins, and 2) once using the observed and predicted streamflow values from all basins combined. Note that calculations done once across all basins do not include a test of significance.

Flow categories	**Calculated per-basin**						**All basins**			
All flows	**NSE (mean)**	**NSE (median)**	**KGE**	**variance**	**bias**	**R**	**NSE**	**variance**	**bias**	**R**
NWM	0.46	0.62	0.64	0.82	-0.01^	0.82	0.75	0.85	-0.02	0.87
LSTM_PP	0.65*	0.73*	0.74*	0.86	0.02	0.87*	0.81	0.92	0.02	0.90
LSTM_A	0.69	0.74	0.74	0.83	0.02	0.88	0.82	0.89	0.01	0.90
LSTM_PPA	0.67	0.75	0.76	0.87	0.02	0.88	0.82	0.93	0.02	0.91
Rising limbs	**NSE (mean)**	**NSE (median)**	**KGE**	**variance**	**bias**	**R**	**NSE**	**variance**	**bias**	**R**
NWM	0.47	0.60	0.60	0.77	-0.07	0.81	0.73	0.82	-0.05	0.85
LSTM_PP	0.64*	0.70*	0.72*	0.83*	0.00*	0.86*	0.78	0.88	0.00	0.88
LSTM_A	0.66	0.71	0.72	0.80	-0.01	0.86	0.78	0.85	-0.01	0.88
LSTM_PPA	0.65	0.72	0.74	0.85	0.00	0.87	0.79	0.89	0.00	0.89
Falling limbs	**NSE (mean)**	**NSE (median)**	**KGE**	**variance**	**bias**	**R**	**NSE**	**variance**	**bias**	**R**
NWM	0.29	0.62	0.64	0.94	0.03	0.83	0.78	0.90	0.00	0.88
LSTM_PP	0.62*	0.75*	0.76*	0.95*	0.07	0.90*	0.87	0.99	0.04	0.93
LSTM_A	0.69	0.78	0.77	0.92	0.05	0.90	0.87	0.96	0.03	0.93
LSTM_PPA	0.65	0.77	0.77	0.94	0.05	0.90	0.87	0.98	0.03	0.93
Above 80th percentile	**NSE (mean)**	**NSE (median)**	**KGE**	**variance**	**bias**	**R**	**NSE**	**variance**	**bias**	**R**
NWM	0.17	0.41	0.54	0.80	-0.13	0.73	0.69	0.83	-0.10	0.84
LSTM_PP	0.47*	0.57*	0.64*	0.82	-0.08*	0.80*	0.76	0.89	-0.04	0.90
LSTM_A	0.53	0.58	0.67	0.81	-0.08	0.81	0.78	0.86	-0.06	0.88

LSTM_PPA	0.50	0.60	0.69	0.84	-0.07	0.81	0.79	0.90	-0.04	0.89
Below 20th percentile	**NSE (mean)**	**NSE (median)**	**KGE**	**variance**	**bias**	**R**	**NSE**	**variance**	**bias**	**R**
NWM	-18384.37	-17.47	-1.96	3.79	1.89^	0.36	0.37	1.31	0.22	0.81
LSTM_PP	-6941.62*	-15.66*	-1.28*	2.84*	3.21	0.43*	0.53	1.30	0.33	0.90
LSTM_A	-4749.68	-16.35	-1.31	2.85	3.27	0.43	0.56	1.26	0.33	0.89
LSTM_PPA	-5147.62	-14.66	-1.24	2.85	2.87	0.43	0.58	1.28	0.30	0.90

Note: * indicates post-processing significantly helps the NWM

Note: ^ indicates post-processing significantly hurts the NWM

In general Table 6 shows that the LSTM post-processors improved over the NWM in nearly all flow regimes according to most metrics. The LSTM_PPA also improved upon the LSTM_A in more than half the basins, and by most metrics, though not significantly. The rising limb and high flow regimes were improved by the LSTM post-processors according to every metric.

Bias was the only metric that was reduced due to post-processing, and the difference was highest in low flow regimes. Flows below the 20th percentile were poorly predicted by all models. This is likely due to the fact that all models tend to have difficulty predicting zero streamflow, and the 101 basins with periods of zero streamflow affected the average performance metrics. This will be discussed further in terms of hydrologic signatures.

The right side of the table has better performance values than the average of metrics calculated individually at each basin. This is a result of some of the better performing basins compensating for poorer performing basins, or from a different perspective, some basins have relatively poor performance which weighs down the average.

Performance by region

Results from a regional analysis of performance are shown below in Figure 6. The LSTM post-processors significantly improved the NSE over the NWM in fifteen of the eighteen regions, the peak timing error in sixteen regions (all regions with enough basins for a statistical evaluation) and significantly improved bias in only one region. Note that region 9 was represented by only two CAMELS basins, which is not sufficient for statistical evaluation. The bias was better represented by the NWM than the post-processor in five of the eighteen regions, including the entire East Coast (regions 1, 2 & 3), the Pacific Northwest (17) and the Lower-Colorado River (15).

The regional performance of the LSTM post-processors and the regional performance of the baseline LSTM_A were correlated with the regional performance of the NWM in terms of NSE (r2=0.78 for post-processors and 0.63 for LSTM_A) and peak timing error (r2=0.96 for post-processors and 0.92 for LSTM_A), but not in terms of bias (r2=0.24, calculated on bias although absolute bias is plotted for clarity). The post-processors and the baseline LSTM_A are correlated in terms of their bias (r2=0.91). A better model has a higher NSE, bias closer to zero, and a lower timing error.

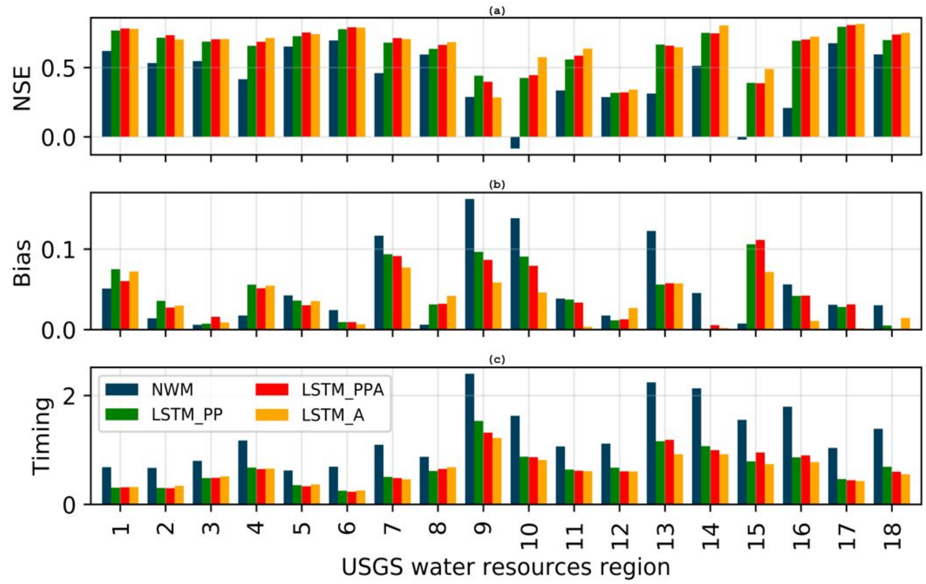

FIGURE 6. Regionally averaged performance metrics for NWM, baseline LSTM_A, and the LSTM post-processors (LSTM_PP & LSTM_PPA) in different USGS water resources regions.

R*egression to predict post-processing performance improvement*

The performance of the baseline LSTM_A was more predictable than the post-processors. We performed a linear regression on the target of performance improvement over the NWM, with inputs being the catchment attributes and hydrologic signatures, as well as the NWM performance itself. Figure 7 shows the results predicting the LSTM improvement over the NWM at each basin with an r^2 value of 0.97, 0.88 and 0.89 for the LSTM_A, LSTM_PPA and LSTM_PP, respectively. The high r^2 value is due in part to the outlier basins with abnormally large performance improvements from the LSTM models (LSTM_A, LSTM_PPA and LSTM_PP). This means that the magnitude of the baseline LSTM_A and post-processors improvement is directly related to the performance of the NWM.

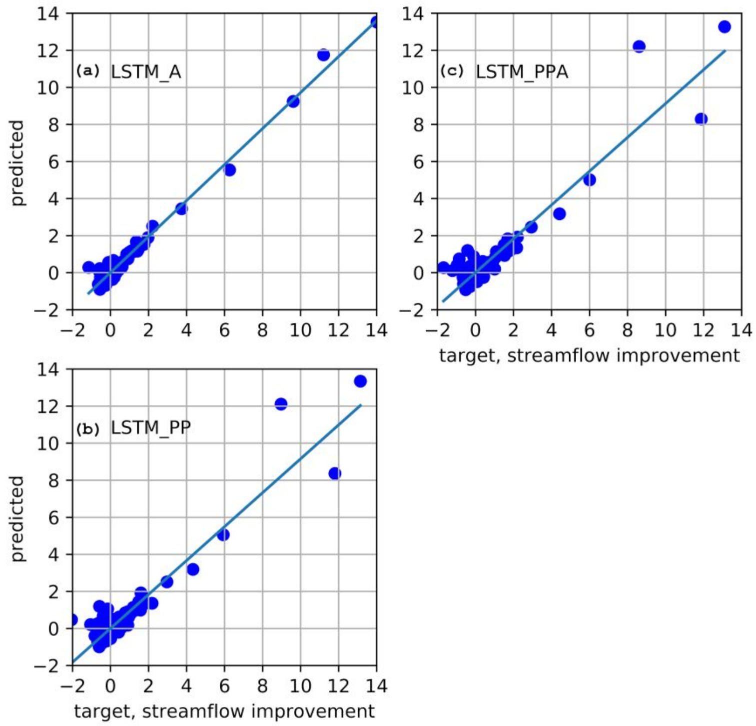

FIGURE 7. Predicting LSTM (baseline and post-processor) performance over the NWM at each basin using a linear regression with NWM performance and hydrologic signatures as inputs. Scatter plots with all of the 531 basins.

The aim of these results is to understand whether it is possible to predict where post-processing might be beneficial (remember that post-processing helped in most basins). Although we found relatively high predictability in the improvement expected from post-processing, a problem is that this requires knowing ahead of time the NWM performance. This prevents us from predicting post-processing improvement in *ungauged* basins, since calculating the NWM performance requires streamflow observations. The correlation analysis below may help inform future efforts to learn general patters of post-processor improvement over both the NWM and the baseline LSTM_A.

Correlations between NWM inputs and improvements

Figure 8 shows correlations (over 531 basins) between the time-averaged NWM inputs and changes in performance metric scores of the post-processor relative to the baseline models. The LSTM_PP was compared against the NWM and the LSTM_PPA was compared against the LSTM_A, although qualitatively both post-processor models were similar. The rows of this figure show that correlation was weaker for differences in NSE score than total bias and peak timing error. Performance differences between the NWM and the post-processor were most strongly (anti)correlated with stream velocity from the channel router and accumulated underground runoff from the land surface model component: basins with lower stream velocity (velocity) and less underground runoff (UGDRNOFF) saw greater performance improvement from (daily) post-processing. This means that in basins with high underground runoff and/or high stream velocity the post-processor improvements were smaller. In contrast, basins with higher total radiation (TRAD) and higher latent heat flux (LH) saw greater improvement due to post-processing. This means that in basins with more radiation and heat flux the post-processor improvements were larger. A direct interpretation of this could be that a flat meandering stream in the Southwest will benefit from post-processing, which is consistent with the findings of Salas et al. (2018) that WRF-Hydro's performance is generally poor in the Southwest. Performance differences between the baseline LSTM_A and the post-processor were most strongly correlated with snow water equivalent and snow depth. This is consistent with the findings of Hansen et al. (2019) that the NWM represents snowpack hydrology well.

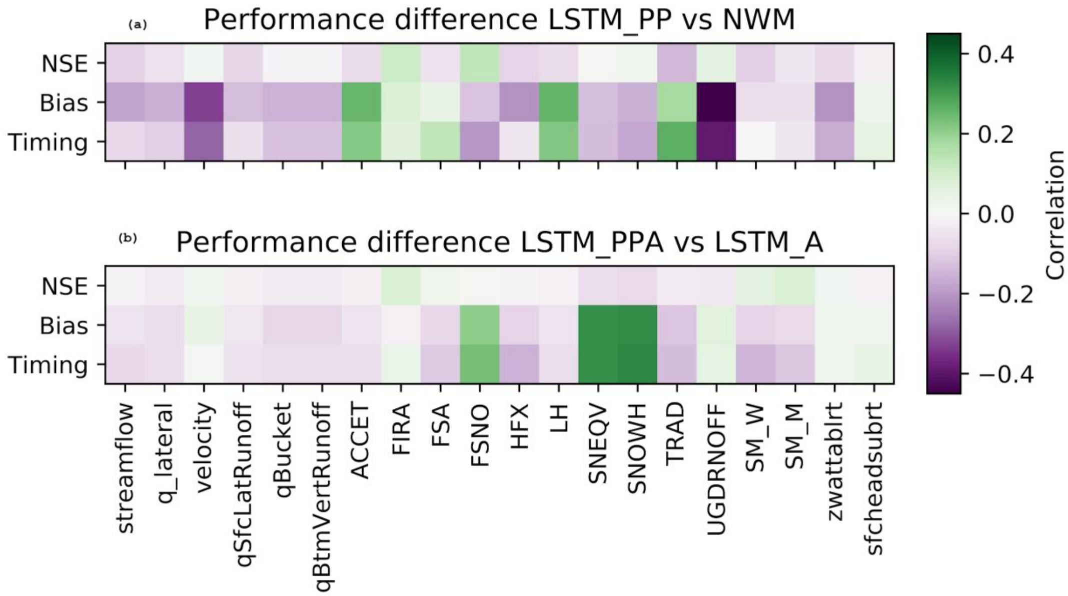

FIGURE 8. Correlations between the time-averaged NWM related inputs vs. performance metric differences between the LSTM post-processors (LSTM_PP & LSTM_PPA) and baseline models (NWM & LSTM_A).

Integrated gradients

Figure 9 shows the relative strength of the total attribution of the dynamic inputs to the LSTM_PPA averaged across the entire validation period and across basins. The ordered magnitudes of the integrated gradients can be interpreted as corresponding to the order of importance of inputs. The most important dynamic features for the LSTM_PPA were: (i) precipitation from NLDAS, and (ii) routed streamflow from the NWM point data. Precipitation inputs were weighted higher than the NWM streamflow output itself, which means that even when NWM streamflow data were available, the LSTM_PPA generally learned to get information directly from forcings rather than from the NWM streamflow output. This indicates that the LSTM_PPA generated a new rainfall-runoff relationship rather than relying on the

NWM, which is consistent with the overall results (Figure 2) that showed similar performance between the LSTM_A and LSTM_PPA.

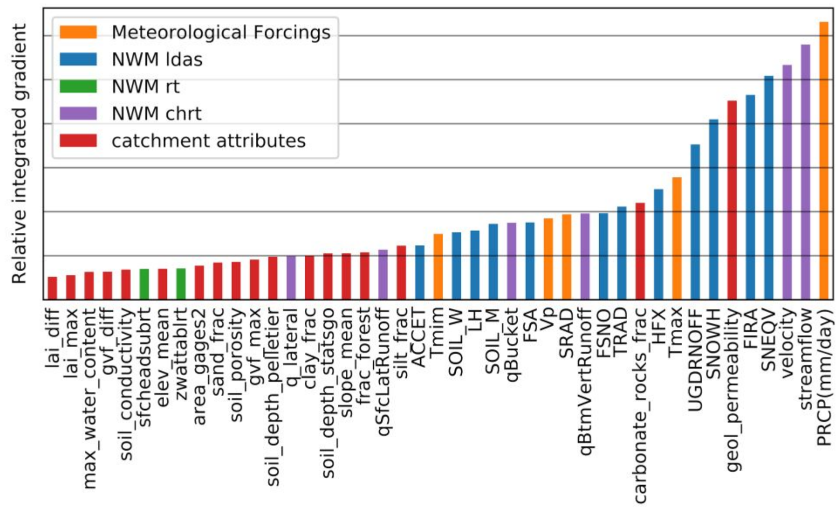

FIGURE 9. Attributions to the LSTM_PPA predictions. The vertical axis shows the relative magnitude of attribution (importance) for each input, with precipitation (PRCP) as the top contributor and NWM-predicted runoff into channel reach (q_lateral) contributing the least.

Figure 10 shows the relative strength of the total attribution of the dynamic inputs to the LSTM_PP. Without the atmospheric forcings included in the post-processor inputs the NWM streamflow output was by far the highest contributing dynamic input feature to the LSTM_PP. The static permeability of the catchment was the next highest.

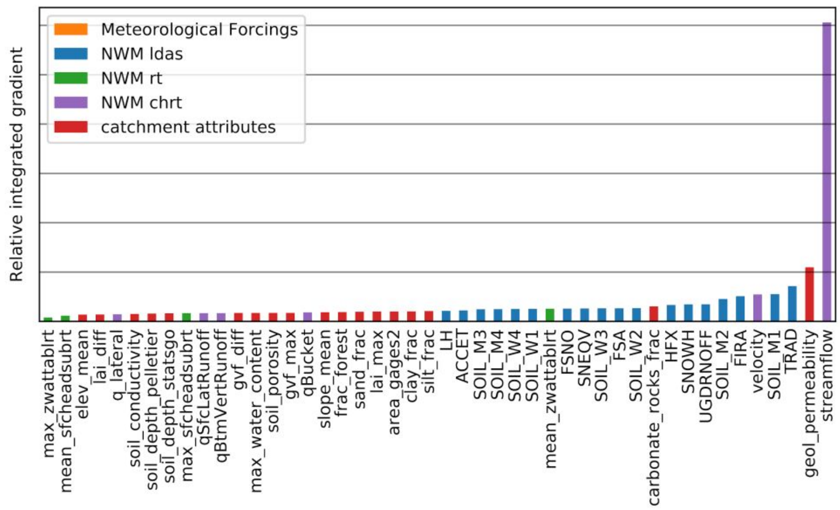

FIGURE 10. Attributions for the LSTM_PP model. Color coded by LSTM input source. The streamflow is overwhelmingly the highest contributor to the post-processed streamflow prediction.

Representations of hydrologic signatures

Results of the analysis of hydrologic signature representation are shown in Figure 11, which also shows that the hydrologic signatures best represented by the NWM were similarly those best represented by the LSTM_PPA. The same was true for the most poorly represented hydrologic signatures in both models.

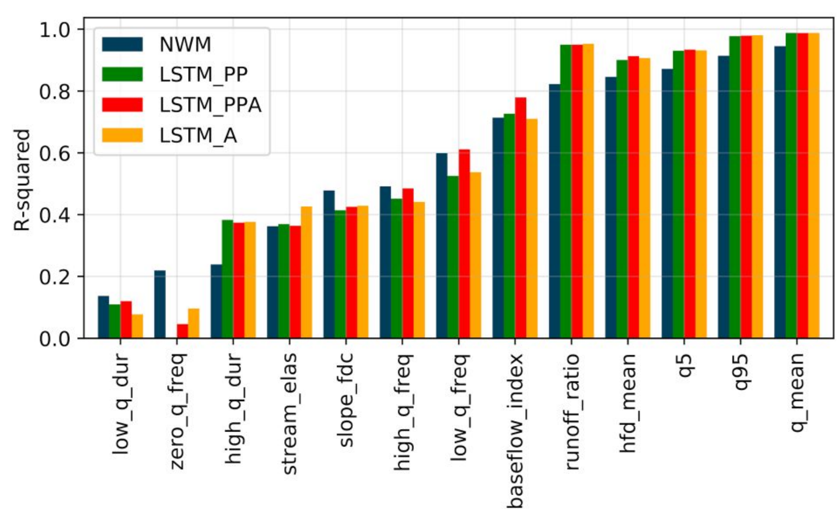

FIGURE 11. Correlation between simulated and observed per-basin hydrologic signatures from the NWM (blue), LSTM_A (orange), LSTM_PPA (green), and LSTM_PP (red). Larger values indicates better performance..

The LSTM post-processors hurt the representation of the frequency of days with zero flow. There were 101 basins with any periods of zero flow. None of these models do well simulating zero flow, but the NWM is better at handling this situation, predicting zero flow periods in 56 of the 101 basins. The LSTM_A, LSTM_PPA and LSTM_PP only predicted periods of zero flows at 35, 29 and 25 basins, respectively. This is an important characteristic in basins in the Southwest, where the NWM could use the benefit of a LSTM post-processor, so this would be a good place to focus future research of theory-guided ML for hydrology.

The LSTM post-processor made a significant improvement over the NWM for several signatures. The improvement to runoff ratio, which is the fraction of precipitation that makes it through the stream gauge at the surface, could be a compensation for the uncalibrated soil parameters in the NWM mentioned by Salas *et al.* (2018). The LSTM post-processor improved both high and low flow predictions (5% & 95% flow quantiles), which are important for natural resources management. Mean daily discharge was the best represented hydrologic signature by all models.

The LSTM_PPA post-processor made significant improvements over the LSTM for baseflow index. This is the only signature that an LSTM post-processor improved over both the NWM and the baseline LSTM_A. This signature estimates the contribution of baseflow to the total discharge, which is computed by hydrograph separation. Klemeš (1986) (summarizing Lindsly's Applied Hydrology) cautioned strongly against using hydrograph separation, because there is no real basis for distinguishing the source of flow in a stream.

Results comparing gauged basins vs. ungauged basins

*R*esults in Table 9 summarize an analysis designed to replicate prediction in ungauged basins. The table has metrics from predictions by the NWM, LSTM_A and the LSTM post-processors (LSTM_PP & LSTM_PPA) calculated only at basins that were either calibrated or uncalibrated, but not both. There was no statistical difference between the calibrated and uncalibrated samples. This indicates that the LSTM post-processor works in uncalibrated basins. When post-processors were trained only in calibrated basins (denoted with a "C" in Table 9), however, the performance in uncalibrated basins significantly deteriorated. But this is true for the baseline LSTM_A as well, so it is not a result of the calibration (as calibration would not influence the baseline LSTM_A), but a result of prediction at ungauged type basins. However, the median performance of the post-processor predictions at ungauged type basins when trained at only calibrated basins was still better significantly than the NWM in the uncalibrated basins.

TABLE 9. Performance of the LSTM and the LSTM post processor split between basins where the NWM was calibrated vs. uncalibrated. The "C" in the model name denotes that the model was trained only on calibrated basins

	Nash-Sutcliffe Efficiency							
	Calibrated basins				Uncalibrated basins			
	mean	median	max	min	mean	median	max	min
NWM	0.49	0.64	0.95	-10.81	0.18	0.48	0.79	-7.10
LSTM_PP	0.65	0.73	0.93	-3.32	0.69	0.71	0.89	0.38
LSTM_A	0.68	0.74	0.93	-0.64	0.73	0.75	0.89	0.43
LSTM_PPA	0.66	0.75	0.93	-3.61	0.71	0.73	0.89	0.42
LSTM_PP(C)	0.65	0.73	0.93	-1.86	0.21	0.57	0.75	-8.12
LSTM_A(C)	0.67	0.74	0.93	-1.13	0.51	0.67	0.84	-2.54
LSTM_PPA(C)	0.67	0.75	0.94	-2.71	0.13	0.58	0.84	-14.07
	Total bias							
	Calibrated basins				Uncalibrated basins			
	mean	median	max	min	mean	median	max	min

NWM	0.01	-0.01	2.57	-0.63	0.00	-0.06	1.84	-0.58
LSTM_PP	0.04	0.02	1.05	-0.24	0.02	0.01	0.27	-0.12
LSTM_A	0.02	0.02	0.56	-0.22	0.02	0.01	0.20	-0.11
LSTM_PPA	0.03	0.02	0.98	-0.21	0.01	0.00	0.22	-0.11
LSTM_PP(C)	0.01	-0.01	0.92	-0.25	0.06	-0.04	2.15	-0.51
LSTM_A(C)	0.02	0.02	0.62	-0.21	0.09	0.04	0.99	-0.20
LSTM-PPA(C)	0.01	0.00	0.95	-0.22	0.06	-0.05	2.89	-0.41

Peak timing error								
	Calibrated basins				Uncalibrated basins			
	mean	median	max	min	mean	median	max	min
NWM	1.06	0.91	3.00	0.10	1.04	0.77	2.70	0.25
LSTM_PP	0.55	0.45	1.95	0.04	0.52	0.35	1.59	0.04
LSTM_A	0.53	0.43	1.76	0.00	0.51	0.41	1.50	0.04
LSTM_PPA	0.54	0.42	1.75	0.04	0.51	0.36	1.45	0.05
LSTM_PP(C)	0.55	0.45	2.10	0.00	0.59	0.41	1.76	0.09
LSTM_A(C)	0.52	0.43	1.77	0.00	0.57	0.50	1.50	0.08
LSTM_PPA(C)	0.54	0.41	1.83	0.04	0.57	0.41	1.65	0.13

The NWM, LSTM_A and the LSTM_PPA had higher NSE scores in calibrated basins than the uncalibrated basins. Note that these results are from the LSTMs (baseline and post-processors) trained on only basins where the NWM was calibrated. In the case of the LSTM post-processors the mean NSE scores in uncalibrated basins were very low for NSE. This is a result of two outlier basins (1466500, MCDONALDS BRANCH, Lat:39.9, Lon:-74.5, Area: 5.7km; and 01484100 BEAVERDAM BRANCH, Lat:38.9, Lon:-75.5, Area: 7.8km)n. Both of those outlier basins are much smaller, and have lower flows, than what were included in the training set. Without these basins the mean NSE scores were 0.32, 0.51, 0.56 and 0.56 for the

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NWM, LSTM_PP, LSTM_A and LSTM_PPA, respectively. Table 9 also shows that the median value of the LSTM_PPA was higher than the NWM, as was the maximum NSE value, but the minimum value was exceptionally low.

The total bias in calibrated basins was generally better (lower) than the uncalibrated basins. The timing error of the NWM was actually better in the uncalibrated basins, but the LSTM_A and LSTM post-processors had better performance in the calibrated basins. The NSE values for the NWM, LSTM_A and the LSTM post-processors (LSTM_PP and LSTM_PPA) were significantly different in the calibrated basins vs. the uncalibrated basins, as were the differences between the LSTM_A and LSTM post-processors (LSTM_PP and LSTM_PPA) compared to the NWM. The bias values were significantly different between the two samples (calibrated vs. uncalibrated), but the differences between LSTM_A and LSTM post-processors vs. the NWM were not statistically different. This means that the LSTM models were successful at predicting streamflow at basins outside of the calibration set.

LSTM post-processor sensitivity to inputs and application for process representation diagnostics.

Figure 12 shows results from the LSTM models with inputs from different parts of the NWM (land surface model only, channel router only, predicted streamflow only, and all states and fluxes. The best performing LSTM models (LSTM_A & LSTM_PPA) were the ones trained with inputs that included the five atmospheric forcing variables with (LSTM_PPA) and without (LSTM_A) the NWM output (these are the same models discussed in previous sections above). This implies that LSTM in general was able to extract more information from the atmospheric forcings than the NWM. Each of the LSTM post-processors made better average daily streamflow predictions than the NWM itself, indicating that information from the atmospheric forcings is lost in the NWM model structure before the streamflow prediction is made. For example, the LSTM that took as inputs only the LDAS model output from the NWM made better predictions than the NWM itself, indicating that there is more information in the LDAS states and fluxes than the NWM is able to translate into streamflow predictions. The same was true for the states and fluxes of the CHRT component of the NWM, meaning that information is also lost in the CHRT component of the NWM model structure.

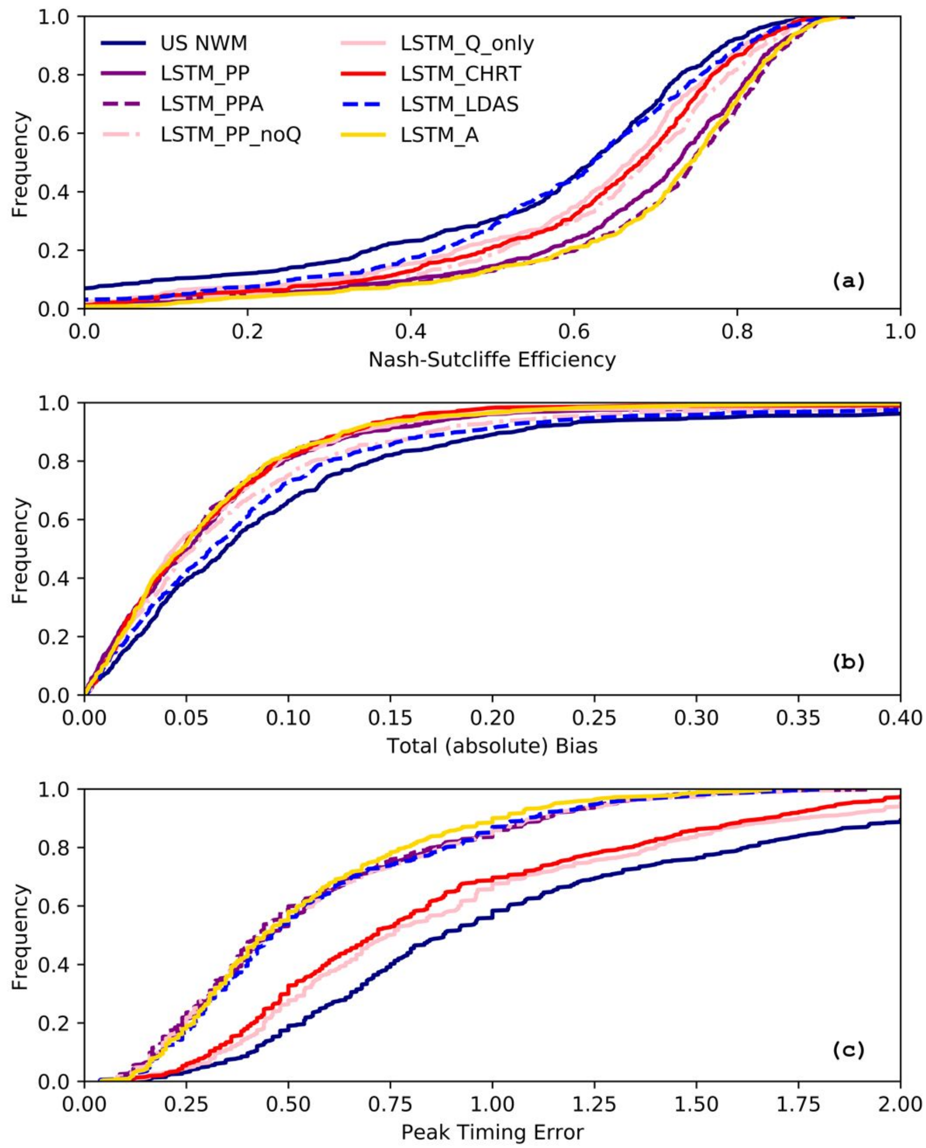

FIGURE 12. Performance of the LSTM post-processor trained with different sets of NWM output. Each of these post-processors outperform the NWM. LSTM_A is the baseline LSTM trained with atmospheric forcings as dynamic inputs. LSTM_PP is the NWM post-processor trained with the outputs of the NWM as dynamic inputs. LSTM_PPA used both the NWM outputs and atmospheric forcings as inputs. LSTM_PP_noQ used all the NWM outputs except for streamflow and velocity from the channel router. LSTM_Q_only used only streamflow from the NWM output. LSTM_chrt used only the NWM channel router outputs. LSTM_ldas used only the land surface fluxes as inputs.

DISCUSSION

Comparison between the baseline LSTM and the post-processors

The baseline LSTM (LSTM_A), trained only on atmospheric forcings as dynamic inputs, was better at extrapolating hydrologic conditions outside the training set than the LSTM post-processors (LSTM_PP & LSTM_PPA). This is shown in the analysis of prediction in ungauged basins, specifically Table 9. The post-processors both failed to make reasonable predictions at two basins that were much smaller than any basins included in the training set. The LSTM_A was able to make good predictions in these basins. Including the NWM output as dynamic inputs to the LSTM constrained the model and prevented it from learning general hydrologic relationships that can be extracted to basins with characteristics that might be unrecognizable.

Potential for improving the performance of both the National Water Model and machine learning

Results presented here show that the LSTM post-processors have potential to improve the daily averaged flow predictions of the NWM. The LSTM post-processors provided significant benefit to the NWM streamflow predictions at almost all (88% & 92% for LSTM_PP & LSTM_PPA, respectively) of the 531 basins analyzed here. In the few basins where this was not the case, it may be possible to use fine tuning a version of the post-processor that is specific to each gauge location (as would be done in traditional model calibration), however the LSTM post-processors used here can be applied to any basin, even ungauged. The post-processors were trained on headwater basins, so further work would be needed to include reservoirs and other management practices. It is worth noting that these LSTM models can be trained on a laptop computer in a few hours, a relatively minor computational cost, and the computational cost of forward prediction is negligible. By comparison the computational cost of calibrating the NWM is much higher - typically requiring HPC or cloud systems.

The NWM performance and the performance improvement from the LSTM post-processors (LSTM_PP & LSTM_PPA) were negatively correlated: basins with low performance by the NWM have the highest performance change from the LSTM post-processors. This means that post-processing can be expected to correct situations where the NWM gives bad predictions. Conversely, the performance of the NWM and the LSTM_A (the baseline LSTM without NWM inputs) were minimally correlated (r-squared = 0.42, 0.30 and 0.67 for NSE, bias and timing, respectively). Considering also that the overall performance of the LSTM_A changed only minimally from the addition of the NWM inputs (as shown in Figures 3-5 and Table 6) and that the LSTM_PPA still preferred to extract more information from precipitation forcings (shown in Figure 9), we might conclude that the LSTM post-processors learned new patterns of the rainfall-runoff response, which are not fully represented by the NWM. The overall improvement in the representation of hydrologic signatures indicates this new rainfall-runoff response is a better representation of physical flow patterns than either the NWM or the LSTM_A. The interpretation of the integrated gradient (Figures 9 & 10) and the correlations between improvement and NWM features (Figure 8) indicate that this improvement of flow patterns comes from information in the NWM representation of streamflow and snow states.

Application to real-time forecasting

The NWM is not simply a rainfall-runoff simulator; it simulates flow through 2.7 million river reaches around CONUS, dam operations, land surface processes, hydraulics, and other complications of large domain hydrology. The nature of the CAMELS catchments selected in these experiments are such that they have few engineered control structures, and are under

20,000 km^2. The results presented in this paper show that the LSTM post-processors improved streamflow predictions in the catchments studied here, which all had limited human disturbance (e.g., dams, reservoirs, *etc.*). Kratzert *et al.* (2019) showed that these predictions extend into ungauged basins. Our results (section "*Results comparing calibrated basins vs. uncalibrated basins*") show that this is true for all but the poorest performing NWM basins. The immediate potential for improving real-time forecasting could be deploying an LSTM for streamflow prediction in undisturbed catchments, and undisturbed sub-catchments upstream of unnatural hydrologic conditions such as dams, agriculture lands and urban centers. This would allow for retaining conceptual representations of lakes and reservoirs that already exist in the NWM.

Diagnosing process-based models, physical processes and data concerns

The sensitivity analysis reported in Figure 12 showed that some components of the NWM caused poor predictions. Specifically, information was lost in channel router (CHRT) component of the model. This diagnostic method could be used to compare different schemes for future versions of the NWM. For instance, changing the routing function might conserve timing information from the land surface fluxes, or modifying the evapotranspiration options in Noah-MP may conserve mass bias information from the NWM forcing engine. Such improvements could be quantified with this post-processing method.

Each of the post-processing models tested for sensitivity (Figure 12) fall, roughly and inclusively, between the NWM and the baseline LSTM_A. Based on the relative positions between those bounding curves, we can identify sources of information loss through the NWM modeling chain:

- The channel routing outputs contain more information of simulation bias than timing, meaning the channel router moves with poor timing, but conserves mass well.
- The land surface outputs contain more information of simulation timing than bias, meaning the land surface component does not conserve mass well, but delivers water to the channel at appropriate times.
- Information is lost during channel routing after the mass is delivered, indicating the channel router is not functioning properly.

There is potential to expand this analysis, breaking down the NWM components even further. Quantification can be done with the full state space from the NWM. Retrospective runs using new versions of the NWM should output the full state space for these types of analysis. This diagnostics analysis using ML post-processing is possible with any physics-based, conceptual or process-based dynamics model.

Moving forward with theory-guided machine learning

The post-processing procedure presented here is one of the cruder techniques currently available for combining process-based and data-driven models. Several other methods of combining the benefits of machine learning (predictability) with the benefits of physically realistic hydrologic theory (robustness) are in development. For example, Pelissier *et al.* (2019) integrated a trained Gaussian Processes into the state-space dynamics of a process-based land surface model for predicting soil moisture time series. Another example is using physical principles to constrain the loss function of an ML model during training - for example Hoedt *et al.* (2020) integrated mass balance constraints into an LSTM and applied this model to the same 531 basins used in this study. Implementing post-processing is relatively straightforward compared to other techniques such as adding physics into ML code or using ML to dynamically update the state variables.

Using ML for post-processing has potential for advancing the explainability of data-driven models. We showed that the LSTM model representation of hydrologic signatures (post-processed and baseline) is highly correlated with the NWM. This indicates that the "learned" functions mapping inputs to streamflow are actually quite similar. We might have trouble expressing the "learned" LSTM with compact formulas (e.g., PDEs), given the high number of trained model weights, but we can use them with confidence knowing their structural similarities with process-based models like the NWM.

CONCLUSION

The LSTM post-processors (LSTM_PPA & LSTM_PP) significantly outperformed the NWM, but only slightly outperformed the LSTM_A (the baseline LSTM without the NWM states and fluxes as inputs). LSTMs, in general, are capable of learning the dynamics of rainfall-runoff processes, gaining little additional information from the conceptualizations coded within the NWM. The "pure" post-processing model (LSTM_PP) outperformed the NWM in terms of bias, and significantly outperformed the NWM in terms of NSE and timing. A decision to use the LSTM as a post-processor for the NWM should be made with professional judgement, considering the comparison of the NWM, LSTM and LSTM post-processor's performance. In locations where the NWM is not calibrated, or the hydrologic conditions are not well understood, it would be best to use the LSTM without the influence from the NWM.

The results indicate that there is more information in the atmospheric forcings about streamflow observations than in the NWM outputs, including the NWM streamflow prediction.

The NWM loses information between the atmospheric forcing inputs and the outputs. The NWM land surface component (LDAS) loses information about mass conservation (shown from the bias error), and the channel router (CHRT) loses information about streamflow timing. The NWM routing scheme should be considered as a priority for improving the NWM.

DATA AVAILABILITY

All data and code used in this paper are publicly available in the following locations:

U.S. National Water Model: https://docs.opendata.aws/nwm-archive/readme.html

CAMELS data: https://ral.ucar.edu/solutions/products/camels

Data processing code: https://github.com/jmframe/nwm-reanalysis-model-data-processing, DOI: 10.5281/zenodo.4642605

LSTM code: https://github.com/kratzert/ealstm_regional_modeling

Post-processing and analysis code: https://github.com/jmframe/nwm-post-processing-with-lstm, DOI: 10.5281/zenodo.4642603

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