

1                   **Improved Accuracy of Watershed-Scale General Circulation Model**

2                                   **Runoff Using Deep Neural Networks**

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11   **Key Points:**

- 12       • We used a deep neural network (DNN) to predict watershed-scale runoff from gridded,  
13       downscaled general circulation model (GCM) outputs.
- 14       • The DNN reduced the error of runoff predictions from 51% for gridded GCM runoff to  
15       29% for DNN watershed-scale runoff.
- 16       • The DNN outperformed other modeling methods used to convert downscaled GCM  
17       outputs to watershed-scale runoff.

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22 **Abstract**

23 Projecting impacts of climate change on water resources is a vital research task, and general  
24 circulation models (GCMs) are important tools for this work. However, the spatial resolution of  
25 downscaled GCMs makes them difficult to apply to non-grid conforming scales relevant to water  
26 resources management: individual watersheds. Machine learning techniques like deep neural  
27 networks (DNNs) may address this issue. Here we use a DNN to predict monthly watershed-  
28 scale runoff (i.e., stream discharge divided by watershed area) from monthly gridded and  
29 downscaled Coupled Model Intercomparison Project Phase 5 (CMIP5) GCM hydroclimatic  
30 fluxes (i.e., precipitation, evapotranspiration, and temperature). We used hydroclimatic fluxes,  
31 biotic, and abiotic characteristics from 2,731 watersheds in the conterminous United States to  
32 train and test a DNN that can predict watershed-scale runoff. The DNN described 93%  
33 (Pearson's correlation coefficient = 0.962) of the variability in observed runoff and was  
34 temporally and spatially robust. The median absolute error (MAE) of DNN predictions was  
35 approximately 25 percentage points lower than that of gridded, downscaled GCM runoff or  
36 monthly normal runoff (i.e., 30-year average of runoff observations at the watershed-outlet).  
37 DNN monthly runoff predictions had the lowest MAE of all the grid-to-watershed-scale  
38 conversion approaches we tested, including: linear ridge regression, support vector machines,  
39 extreme gradient boosting, and artificial neural networks. We demonstrated why using DNNs to  
40 convert gridded GCM hydroclimatic fluxes to watershed-scales is relevant to water resources  
41 research and management. We also provided a methods guide for hydrologists interested in  
42 implementing machine learning techniques.

43 **Plain Language Summary**

44 Environmental scientists use runoff from general circulation models (GCM) to study the impacts  
45 of climate change on water resources. One GCM grid square may represent runoff for a large  
46 area on Earth’s surface (e.g., a 100km by 100km square). This coarse resolution and gridded  
47 nature of GCM outputs make them difficult to use at the watershed-scale because watersheds are  
48 rarely square-shaped. There are many ways to convert gridded GCM runoff to the watershed-  
49 scale, and machine learning techniques such as deep neural networks (DNNs) have yet to be  
50 applied to this task. Thus, we used a large, publicly available dataset to train a DNN to convert  
51 GCM outputs to watershed-scale runoff for 2,731 watersheds in the USA. The DNN accurately  
52 predicted watershed-scale runoff even when the runoff varied in space and time. The DNN  
53 outperformed all the grid-to-watershed-scale conversion approaches we tested. In summary,  
54 machine learning techniques like DNNs may help improve runoff predictions. These improved  
55 predictions may be especially helpful in regions of the USA experiencing climate change-  
56 induced drought (e.g., Colorado, USA) and flooding (e.g., North Carolina, USA). Finally, we  
57 discussed modeling best practices that may help environmental scientists interested in  
58 implementing DNN techniques.

59

60 **Keywords**

61 machine learning, deep neural networks, deep learning, downscaling, general circulation models,  
62 runoff

63

64

65 **1 Introduction**

66 Water is a critical resource for human society and ecosystems (Oki & Kanae, 2006; Zhao &  
67 Running, 2010; Srinivasan et al., 2017) and projecting the impacts of future climate change on  
68 water resources is a fundamental task for hydrologists and the larger scientific community  
69 (Vorosmarty et al., 2000; NRC, 2012; Blöschl et al., 2019). Tools such as general circulation  
70 models (GCM) help researchers investigate how watersheds respond to climate change (Chiew et  
71 al., 2009; Alkama et al., 2013; Zhang et al., 2014; Bring et al., 2015; Knighton et al., 2019).  
72 However, GCM outputs (e.g., precipitation, temperature, runoff) are gridded and typically have  
73 spatial resolutions measured on the order of degrees (e.g., 1.4° x 1.4° or ~150 km x ~120 km for  
74 the MIROC5 model at the T85 gridded resolution at 40°N 100°W; ENES, 2016), which may be  
75 too coarse for many watershed-scale investigations (Chiew et al., 2009). To overcome this issue,  
76 researchers rely on various methods to resolve—or downscale—coarser resolution GCM data to  
77 finer spatial resolutions (Fowler et al., 2007). To date, machine learning techniques such as deep  
78 neural networks (DNNs) have played a limited role in downscaling GCM outputs.

79

80 Downscaling techniques are typically grouped into either dynamical or statistical approaches  
81 (Hewitson & Crane, 1996; Fowler et al., 2007; Schoof, 2013). Dynamical downscaling nests  
82 higher resolution, physically-based, regional models within lower resolution GCMs where  
83 regional (or finer) observations constrain GCM boundary conditions (Hewitson & Crane, 1996;  
84 Chiew et al., 2009; Schoof, 2013). Dynamical downscaling requires considerable computational  
85 demand (Fowler et al., 2007; Chiew et al., 2009; Arritt & Rummukainen, 2011; Schoof, 2013)  
86 and outputs are often still gridded, albeit, at a finer resolution than the original GCM grid.  
87 Statistical downscaling uses regression models to relate lower resolution GCM output to higher

88 resolution observations (Charles et al., 2004; Fowler et al., 2007; Chiew et al., 2009). Besides  
89 regression models, statistical downscaling methods may also include weather classifications and  
90 weather generators (Fowler et al., 2007; Schoof, 2013). Statistical downscaling can be less  
91 computationally demanding than dynamical downscaling and can generate downscaled GCM  
92 outputs at any grid scale as well as the (non-gridded) watershed-scale (Wilby & Wigley, 1997;  
93 Fowler et al., 2007). However, statistical downscaling requires data records of substantial length,  
94 can poorly predict extreme events, and can be hindered by non-stationarity (Wilby, 1997; Wilby  
95 & Wigley, 1997; Fowler et al., 2007).

96

97 Machine learning methods are not new to statistical GCM downscaling; however, there has been  
98 limited application of DNNs in this research area. Previous studies have used three major  
99 machine learning methods to downscale GCM data. They include support vector machines  
100 (SVMs; Tripathi et al., 2006; Ghosh et al., 2008; Guo et al., 2009), relevance vector machines  
101 (RVMs; Ghosh et al. 2008), and artificial neural networks (ANNs; Hewitson & Crane, 1996;  
102 Trigo & Palutikof, 1999; Cavazos, 2000; Sheridan & Lee 2011; Ramseyer et al., 2018). SVMs  
103 map input data into a high dimensional feature space and then classify data into groups by  
104 minimizing classification error to hyperplanes within this high dimensional space (Raghavendra  
105 et al., 2014). RVMs are similar to SVMs but rely on probabilistic Bayesian learning to classify  
106 data into groups (Ghosh et al., 2008). ANNs consist of layers of nodes (also called cells or  
107 neurons) and edges where each layer of nodes and edges represents a linear or non-linear input-  
108 output mapping (Shen, 2018). The values of ANN nodes and edges are adjusted during training  
109 to minimize a loss function that compares the ANN predicted output to the observed output  
110 (Dawson & Wilby, 1998; Shen, 2018). Besides being used to downscaled climate predictions via

111 a regression-style approach (e.g., Trigo & Pulutikof; 1999), ANNs are used to develop self-  
112 organizing maps that aid statistical downscaling via weather typing schemes (e.g., Ramseyer et  
113 al., 2018). ANNs have up to four layers (Figure S1a) including an input layer, two hidden layers,  
114 and an output layer. In contrast, DNNs are extensions of ANNs containing more than two hidden  
115 layers (Figure S1b). We know of one study using convolutional neural networks (CNNs)—a  
116 class of DNNs applied to multiple two-dimensional inputs such as images—to develop seasonal  
117 and regional extreme weather classifications from gridded GCM outputs (Knighton et al., 2019).  
118 To the best of our knowledge, no studies have used DNNs to downscale gridded GCM runoff to  
119 the watershed-scale.

120

121 Machine learning-based downscaling methods offer benefits over other downscaling methods.  
122 Machine learning techniques such as DNNs are agnostic to the mathematical parameterization of  
123 physical processes, even though they may effectively recreate those processes from related data  
124 or be used in coordination with physically-based models (Shen, 2018; Shen et al., 2018). Rather,  
125 machine learning techniques assume that mathematical parameterizations of physical  
126 relationships are represented in observational data themselves (LeCun et al., 2015; Goodfellow et  
127 al., 2016; Shen, 2018; Shen et al., 2018). Consequently, DNNs may enable researchers to  
128 identify hydrologic processes that remain poorly characterized or even undiscovered, generate  
129 hypotheses, and conduct targeted field and/or physically-based hydrologic modeling studies  
130 based on these hypotheses (Shen et al., 2018). Given sufficiently large training datasets and  
131 model regularization—a process that relies on a loss function to simultaneously reward model  
132 accuracy and flexibility (Goodfellow et al., 2016)—DNNs can be more robust compared to other  
133 statistical approaches (i.e., regularized linear regression; Shen, 2018; Shen et al., 2018). In the

134 context of GCM downscaling, a robust DNN is one that accurately predicts watershed-scale  
135 runoff from a test set of gridded GCM outputs across a spatio-temporal gradient. The test set  
136 includes observational data that was not used to train the model (see *Sections 2.2* and *4.5*).

137

138 Specific to downscaling, machine learning techniques offer a flexible approach to explore  
139 complex relationships between gridded GCM outputs, watershed characteristics, and watershed-  
140 scale runoff. DNNs, in particular, are well suited for downscaling because they have more  
141 hidden layers than ANNs. These extra hidden layers enable DNNs to (1) represent complex, non-  
142 linear relationships between inputs and outputs and (2) identify relationships in a high-  
143 dimensional space given limited initial parameterization (LeCun et al., 2015; Goodfellow et al.,  
144 2016; Knighton et al., 2019). The number of hidden layers (i.e., increased model depth) is not the  
145 only reason why DNNs are well suited for representing complex relationships between inputs  
146 and outputs; diverse model architectures, unsupervised pretraining, and weight sharing improve  
147 computational convergence in DNNs (Shen, 2018). Furthermore, neural network-based  
148 approaches may overcome temporal and spatial non-stationarity by enabling the incorporation of  
149 additional variables (Wilby & Wigly, 1997) such as time-lagged climate variables.

150

151 Machine learning techniques such as DNNs are not without limitations: time-efficient  
152 development require specialized computing resources (e.g., graphical processing units; GPUs),  
153 large amounts of data are a prerequisite, and machine learning techniques can be difficult to train  
154 due to vanishing gradients and the potential for model overfitting (Glorot & Bengio, 2010;  
155 Sutskever et al., 2013; Srivastava et al., 2014; He et al., 2015; Ioffe & Szegedy, 2015;  
156 Schmidhuber, 2015; Shen et al., 2018). In the case of GCMs, certain hydrologic processes may

157 not be represented within the data and data may be temporally or spatially incomplete (Shen et  
158 al., 2018). Last, DNNs are often criticized for treating physical processes and/or relationships  
159 between variables as a black box (Shen et al., 2018). Despite these issues, a number of  
160 techniques can be implemented to achieve efficient DNN training and accurate DNN test set  
161 predictions (Goodfellow et al., 2016; Shen, 2018; Shen et al., 2018). Some of these techniques  
162 include: dropout (Srivastava et al., 2014), batch normalization (Ioffe & Szegedy, 2015), variance  
163 scaling of initial weights (He et al., 2015), early stopping (Goodfellow et al., 2016), and the use  
164 of semi-random sampling when holding out data for the test set (Rice et al., 2019). We discuss  
165 each in *Section 2.2*. Recent advances in optimization algorithms, computer hardware (e.g.,  
166 GPUs), computer software (e.g., Google TensorFlow), and cloud computing services (e.g.,  
167 Amazon Web Services' Sage Maker) have also made the utilization of machine learning methods  
168 readily feasible for applications in hydrology and other areas (LeCun et al., 2015; Schmidhuber  
169 et al., 2015; Shen et al., 2018). Furthermore, explanation techniques such as local interpretable  
170 model-agnostic explanations (LIME; Ribeiro et al., 2018; Worland et al., 2019), can help model  
171 developers assess the trustworthiness of their machine learning algorithm results.

172

173 Given the limited use of DNNs in hydrologic science and the practical need to generate  
174 watershed-scale runoff from GCMs, this study aims to demonstrate the application of DNNs to  
175 the practical problem of downscaling GCM runoff from grid cells to watersheds, which are  
176 fundamental units of hydrologic analysis. The objectives of this study are to: (1) train and test a  
177 DNN that accurately predicts watershed-scale runoff from gridded, downscaled GCM data and  
178 (2) compare DNN performance to alternative grid-to-watershed-scale conversion techniques.



179 This study also serves as a guide to hydrologists and other earth systems scientists who are  
180 interested in applying DNNs and other machine learning tools to their work.

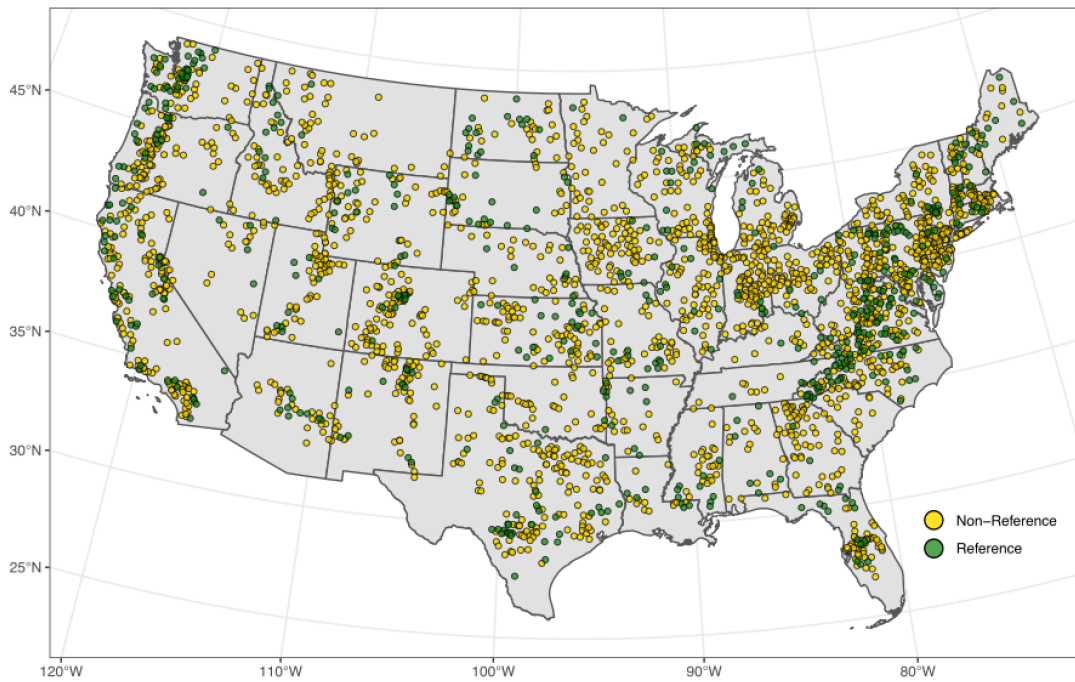
181

## 182 **2 Methods**

### 183 *2.1 Data Overview*

184 We used the United States Geological Survey Geospatial Attributes of Gages for  
185 Evaluating Streamflow version II (GAGES-II) dataset, which provides standardized, continuous,  
186 long-term streamflow records and watershed characteristics (e.g., mean elevation and mean  
187 percent developed land cover) for watersheds across the United States (Falcone et al., 2010). We  
188 downloaded GAGES-II data from  
189 [https://water.usgs.gov/GIS/metadata/usgswrd/XML/gagesII\\_Sept2011.xml#stdorder](https://water.usgs.gov/GIS/metadata/usgswrd/XML/gagesII_Sept2011.xml#stdorder). More  
190 specifically, we identified 2,731 reference (i.e., un-disturbed watersheds,  $n = 558$ ) and non-  
191 reference (i.e., human-disturbed,  $n = 2,173$ ) watersheds in the conterminous United States  
192 (CONUS) with corresponding GAGES-II mean daily streamflow records that were  $\geq 99\%$   
193 complete from January 1970 - December 1999 (Figure 1). We included both reference and non-  
194 reference watersheds to better reflect the increasingly pervasive effects of human activity on the  
195 hydrologic cycle (Dynesius & Nilsson, 1994; Nilsson et al., 2005; Villarini & Smith, 2010; Rice  
196 et al., 2015; Emanuel et al., 2015; Munoz et al. 2018). We downloaded streamflow data from  
197 <https://water.usgs.gov> and skipped approximately 10,200 observations at the beginning of the  
198 streamflow data time series in order to incorporate time-lagged features as discussed below. This  
199 resulted in a total of 972,960 monthly runoff observations from 2,731 separate watersheds. We  
200 converted daily streamflow from the GAGES-II dataset from discharge to runoff (i.e., mm) by

201 dividing daily discharge by the watershed area, which we obtained from the GAGES-II dataset.  
202 We aggregated observed runoff from a daily mean, as provided in the GAGES-II dataset, up to a  
203 monthly mean and then used this monthly runoff as a response variable when training and testing  
204 the DNN (Figure S2).  
205



206  
207 **Figure 1.** Location (centroid) of non-reference and reference watersheds included in this study.  
208

209 We used GAGES-II watershed characteristics as DNN features (i.e., predictor variables) when  
210 training and testing the DNN; these variables addressed themes of climate, watershed  
211 topography, geomorphology, soil properties, and land cover. For a full description of the  
212 watershed characteristics included in this study, see Table S1. In addition to GAGES-II data, we  
213 downloaded monthly, gridded, downscaled precipitation, temperature, evapotranspiration, and  
214 runoff GCM outputs for each of the 2,731 study watersheds at a spatial resolution of  $1/8^\circ \times 1/8^\circ$

215 (14 km x 11 km at 40°N 100°W) for the previously mentioned 30-year study period for an  
216 ensemble of 18 (model abbreviations: bcc\_csm1-1, ccsm4, cesm1-cam5, csiro-mk3-6-0, fio-esm,  
217 gfdl-cm3, gfdl-esm2g, gfdl-esm2m, giss-e2-r, hadgem2-ao, hadgem2-es, ipsl-cm5a-lr, ipsl-cm5a-  
218 mr, miroc-esm, miroc-esm-chem, miroc5, noresm1-m, and noresm1-me) CMIP5 GCMs (Maurer  
219 et al., 2007; Taylor et al., 2012). We downloaded CMIP5 data from [http://gdodcp.ucllnl.org/downscaled\\_cmip\\_projections/](http://gdodcp.ucllnl.org/downscaled_cmip_projections/). We used temperature data from all 18 CMIP5  
220 GCMs. For precipitation, evapotranspiration, and runoff data, we excluded ipsl-cm5a-lr and  
221 noresm1-me GCMs because they only provided annual averages over the study period (i.e.,  
222 1970-1999) and hydroclimatic fluxes (i.e., runoff) needed for model comparisons were not  
223 available. We used each watershed boundary to calculate a watershed areal average value (i.e.,  
224 area weighted average of gridded GCM data falling within the watershed boundary) for each  
225 CMIP5 variable (i.e., temperature, precipitation, evapotranspiration, runoff) and each GCM. We  
226 then calculated the mean CMIP5 variable across GCMs for each watershed. This resulted in a  
227 monthly ensemble value, which we used for all remaining analyses. We also calculated the one-,  
228 two-, and three-month time lags in monthly average GCM ensemble precipitation, temperature,  
229 and evapotranspiration using a similar areal average approach (Table S1). We used the ArcGIS  
230 (version 10.4.1; ESRI, 2011) arcpy Python library to calculate watershed areal averages. Similar  
231 to the watershed characteristics discussed previously, we used the ensemble monthly average  
232 precipitation, temperature, and evapotranspiration (i.e., unlagged and lagged) as continuous  
233 features when training and testing the DNN (Figure S2). We compared model runoff predictions  
234 to ensemble monthly average runoff; thus, ensemble monthly average runoff served as a control  
235 (see *Section 2.4*).  
236  
237

238 *2.2 Deep Neural Network Development, Architecture, & Testing*

239 The combination of a 30-year study period and 2,731 study watersheds resulted in a total of  
240 972,960 monthly observations of runoff that were  $\geq 99\%$  complete. We constructed the DNN  
241 train set by randomly sampling (i.e., 75% of observations from each ecoregion and either  
242 reference/non-reference class) observations at each time step (i.e., monthly) over the 30-yr study  
243 period. We refer to this grouped random selection as semi-random sampling; its purpose is to  
244 ensure that the trained DNN model can accurately represent non-random spatio-temporal  
245 autocorrelation in the original dataset by explicitly forcing consistent and complete spatio-  
246 temporal coverage (Rice et al., 2019). We used the remaining 25% of the data as a test set to  
247 assess model performance (i.e., DNN testing). For a complete breakdown of data included in the  
248 train and test sets see Figure S3. We used an NVIDIA GeForce GTX 1070 GPU (NVIDIA, Santa  
249 Clara, CA) on a desktop PC with a 3.5 GHz Intel Core i7-5820K central processing unit (CPU;  
250 Intel, Santa Clara, CA) and 32GB of memory to train the DNN. We carried out DNN training  
251 and testing in Python (version 3.7.1; Python Software Foundation, 2018) using the open source  
252 TensorFlow (version 1.12.0, <https://www.tensorflow.org/>, Abadi et al., 2015) and Keras (version  
253 2.2.4, <https://github.com/fchollet/keras>, Chollet et al., 2015) software libraries.

254

255 We applied a number of techniques to counter issues such as poor network initializations and  
256 data over-fitting, which can both limit DNN performance. These techniques included: dropout,  
257 batch normalization, variance scaling of initial weights, and early stopping. *Dropout* is a  
258 computationally efficient way to combine many network structures and prevent over-fitting; it  
259 adds noise and limits co-dependencies between neurons during DNN training (Srivastava et al.,  
260 2014; Goodfellow et al. 2016). It involves temporarily removing randomly selected neurons

261 during DNN training (Srivastava et al., 2014; Goodfellow et al., 2016; Worland et al. 2019).  
262 *Batch normalization* helps improve DNN training efficiency and increases DNN model  
263 generalizability beyond the training by normalizing the distribution of each DNN layer's inputs  
264 such that training between upstream and downstream DNN layers converges more efficiently  
265 (Ioffe & Szegedy, 2015). Specifically, batch normalization uses the mean and variance of each  
266 activation layer with each training mini-batch to normalize the network activation functions so  
267 they have a mean of zero and variance of one (Ioffe & Szegedy, 2015). *Variance scaling of*  
268 *initial weights* helps initialize DNN weights and protect against exploding or vanishing  
269 gradients; therefore, reducing DNN training time and improving DNN performance (He et al.,  
270 2015). It is implemented by determining the variance of output values from each DNN layer and  
271 then scaling initial DNN weights such that they share the same distribution (He et al., 2015).  
272 *Early stopping* constrains the potential number of training iterations so the optimization process  
273 will iteratively check model error from one training step to the next (Goodfellow et al, 2016).  
274 This optimization process can be implemented by saving a copy of the model parameters for  
275 every DNN training step where model error decreases; when model error does not decrease after  
276 a pre-specified number of steps, training is stopped (Goodfellow et al., 2016). Dropout, batch  
277 normalization, variance scaling of initial weights, and early stopping can all be implemented  
278 using built-in functions in the Keras and TensorFlow libraries. See the Python scripts associated  
279 with this study and available on GitHub for further details.

280

281 Throughout DNN training, we maintained an input layer of 62 nodes (i.e., one neuron for each  
282 feature in Table S1) and one output layer node to represent the regression output of watershed-  
283 scale runoff predictions (Table 1). However, to arrive at the final DNN hidden layer architecture,

284 our basic approach was to start with a large number of hidden layers with many nodes and prune  
 285 both down based on DNN training loss performance (i.e., overall prediction accuracy as well as  
 286 the time it takes for the DNN to converge to a solution). More specifically, we initialized the  
 287 DNN architecture with a large number of hidden layers, where the first hidden layer had  
 288 approximately 10x more nodes than the input layer. Subsequent hidden layers had approximately  
 289 half as many nodes as the previous hidden layer. Hidden layers 2 and 3 were an exception to this  
 290 because we observed that slowing down the node “size decay” reduced training loss (i.e.,  
 291 improved DNN predictions). The initial DNN architecture contained 14 hidden layers but we  
 292 trimmed it down to 7 after monitoring training loss and the DNNs ability (or inability) to  
 293 converge in a reasonable amount of time. This is one of several suggested approaches for  
 294 determining DNN hyperparameters such as the number of hidden layers and hidden layer nodes.  
 295 Beginners may look to established guides that discuss these approaches in more detail (e.g.,  
 296 Nielsen, 2015; Goodfellow et al., 2016; Brownlee, 2018; Chollet & Allaire, 2018; Kim, 2019).  
 297

298 **Table 1.** Summary of the final deep neural network architecture used to predict monthly  
 299 watershed-scale runoff for the conterminous United States. Input and hidden layers were  
 300 initialized using the “he\_normal” method and used the PReLU activation function.

Layer	Description	Number of Nodes	Number of Parameters
0	Input	62	N/A
1	Hidden, Dense with Batch Normalization (30% dropout)	1000	68000
2	Hidden, Dense with Batch Normalization (30% dropout)	800	804800
3	Hidden, Dense with Batch Normalization (30% dropout)	600	483600
4	Hidden, Dense with Batch Normalization (30% dropout)	400	242400
5	Hidden, Dense with Batch Normalization (30% dropout)	200	81200
6	Hidden, Dense with Batch Normalization (30% dropout)	100	20600
7	Hidden, Dense with Batch Normalization (30% dropout)	50	5300
8	Output, Dense	1	51

301

302

303 The final DNN developed here consisted of 7 hidden layers with a varying number of neurons  
304 per layer: 1000, 800, 600, 400, 200, 100, and 50 neurons for hidden layers 1 to 7, respectively  
305 (Table 1). The input layer consisted of 62 nodes (i.e., one for each of the 62 watershed  
306 characteristics; Table S1) and the final layer consisted of one node with a linear output given the  
307 regression task (i.e., predicting watershed-scale streamflow). For all layers, we initialized  
308 weights using the ‘he\_normal’ method (He et al., 2015). For all the hidden layers, we set the  
309 dropout rate to 30% and used a Parametric Rectified Linear Unit (PReLU) activation function  
310 (He et al., 2015). Additionally, we set the training batch size to 4,096, the number of epochs (i.e.,  
311 training time steps) to 2,500, and early stopping to 50 time steps. As mentioned previously, we  
312 used a 75:25 training:testing split for model development and testing. In model training, we used  
313 a Nesterov Adam (i.e., ‘nadam’) optimizer with mean absolute error (in mm units) as the loss  
314 function (Kingma & Ba, 2014; Sutskever et al., 2013). The parameters in Table 1 refer to tunable  
315 weights and biases of DNN nodes and edges that are optimized during model fitting. These  
316 parameters effectively control non-linear mapping used to relate DNN input and output  
317 variables. The number of parameters represents flexibility in this non-linear mapping rather than  
318 the dimensionality of the data space. This is in contrast to, for example, linear regression where  $p$   
319 variables are used to fit a line passing through each of  $p$  points. Best practices such as model  
320 evaluation using an independent test sets help reduce the risk of DNN model overfitting.

321

322 We used bias (i.e., y-axis intercept), slope, Pearson’s correlation coefficient (PCC), and median  
323 absolute error expressed as a percentage (MAE) to test DNN performance. We obtained bias,  
324 slope, and PCC from the (linear) line-of-best-fit between observed versus modeled watershed-  
325 scale runoff. We bootstrapped 95% confidence intervals ( $n = 1000$ ) for MAE and PCC using

326 SciPy (Virtanen et al., 2019), Pandas (McKinney et al. 2010), and NumPy (van der Walt et al.,  
327 2011) Python libraries to determine whether these metrics were statistically meaningful. In  
328 addition to determining DNN performance metrics for the test set, we also calculated them for  
329 extreme monthly runoff events including those in the test set that were below the 10<sup>th</sup> percentile  
330 (Q10) or above the 90<sup>th</sup> percentile (Q90). Q10 and Q90 events were calculated from the entire  
331 dataset and labeled in the test set. We also calculated DNN performance metrics for non-  
332 reference and reference watersheds as well as for each of the nine GAGES-II watershed  
333 ecoregions (i.e., Central Plains, East Highlands, Mixed Wood Shield, Northeast, Southeast  
334 Coastal Plain, Southeast Plain, West Mountains, West Plains, and West Xeric; Figure S4). In  
335 addition to determining overall (i.e., CONUS-scale) DNN testing metrics, we assessed DNN  
336 performance at the watershed-scale by calculating the median residual as a percentage for each  
337 of the 2,731 watersheds and plotted the result on a CONUS map. We also plotted DNN residuals  
338 versus spatio-temporal variables such as time (i.e., month), watershed area, watershed longitude  
339 determined at the watershed centroid, and watershed latitude determined at the watershed  
340 centroid to evaluate DNN temporal and spatial robustness. For each spatio-temporal variable, we  
341 calculated PCC and bootstrapped 95% confidence intervals as discussed above to evaluate  
342 whether model residuals lacked robustness.

343

### 344 *2.3 Development, Architecture, and Testing of Other Downscaling Approaches*

345 We tested the ability of four other grid-to-watershed-scale conversion approaches to predict  
346 observed monthly runoff at the watershed-scale (Table 2). These included: linear ridge  
347 regression, SVM, extreme gradient boosting (XGBoost), and ANN modeling approaches. Similar  
348 to the DNN, we tested the performance of these four approaches using bias, slope, MAE, and



349 PCC (*Section 2.2*). The linear ridge regression model used an L1 regularization penalty applied  
350 to the loss function (squared error) to impose sparsity on model features (i.e., parameters for  
351 variables in Table S1 should not get too large). SVM, described previously (*Section 1*), utilized a  
352 linear SVM with L1 regularization (Drucker et al., 1997). XGBoost is a more advanced version  
353 of gradient boosting (Friedman; 2001) that incorporates model regularization, parallel  
354 processing, and a number of algorithmic innovations that improve model development efficiency  
355 and model prediction accuracy (Chen & Guestrin, 2016). Specifically, we used XGBoost to train  
356 an ensemble of gradient boosted regressions. The ANN had two hidden layers (Figure S1a). We  
357 developed the linear ridge regression, SVM, and XGBoost models via  $k$ -fold cross-validation  
358 coupled with a randomized search process for hyperparameter tuning as described previously by  
359 Rice & Emanuel (2017). We used the scikit-learn (version 0.21.2) and XGBoost (version 0.90)  
360 Python libraries to train these four models (Pedregosa et al., 2011; Chen & Guestrin, 2016). We  
361 used the same computer hardware as described in *Section 2.2*; we trained the ANN and DNN on  
362 a GPU and all other models were trained on a CPU.

363

364 **Table 2.** Model performance comparisons relative to observed, monthly runoff at the watershed-scale for the test set. Abbreviations:  
 365 Generalized Circulation Model (GCM), median absolute error (MAE), Pearson’s correlation coefficient (PCC), support vector  
 366 machine (SVM), extreme gradient boosting (XGBoost), artificial neural network (ANN), deep neural network (DNN), graphics  
 367 processing unit (GPU), central processing unit (CPU), and not-applicable (N/A). MAE and PCC are reported with the lower and upper  
 368 95% confidence intervals in parentheses.

Method	MAE (%)	PCC	Bias (mm)	Slope	Processor	Computing Time (min)
GCM Runoff	49.97 (49.74, 50.2)	0.811 (0.806, 0.815)	6.82	0.85	NA	NA
Monthly Normal Runoff	50.36 (50.10, 50.60)	0.812 (0.809, 0.815)	0.04	1.01	NA	NA
Linear Ridge Regression	>1000	0.155 (0.152, 0.159)	42.68	4.00E-14	CPU	17
SVM	110.11 (109.03, 111.18)	0.772 (0.768, 0.776)	-18.84	1.31	CPU	20
XGBoost	40.28 (40.05, 40.51)	0.933 (0.931, 0.935)	-0.19	1.01	CPU*	300
ANN	35.57 (35.41, 35.73)	0.916 (0.913, 0.917)	-0.29	1.19	GPU	18
DNN	24.31 (24.18, 24.46)	0.962 (0.961, 0.963)	2.36	0.94	GPU	110

369 \* Six cores in parallel

370

371

372

373 *2.4 Comparing Downscaling Approaches*

374 We used three approaches to comparatively assess the predictive power of the five models  
375 presented here (i.e., linear ridge regression, SVM, XGBoost, ANN, and DNN). First, we  
376 compared observed monthly runoff at the watershed outlet (i.e., the USGS gage) to modeled  
377 watershed-scale runoff from the test set. We included comparisons with the test set, with Q10  
378 and Q90 events in the test set, with non-reference and reference watersheds in the test set, and  
379 with watersheds in the nine GAGES-II watershed ecoregions in the test set. For these  
380 comparisons, we used bias, slope, PCC, and MAE metrics as described in *Section 2.2*. Second,  
381 we tested model performance by comparing bias, slope, PCC, and MAE metrics between  
382 observed monthly runoff at the watershed outlet and the monthly ensemble of areal averaged  
383 GCM runoff (see *Section 2.1* for a full description), which we refer to henceforth as ‘GCM  
384 runoff’. Third, we assessed model performance by comparing bias, slope, PCC, and MAE  
385 metrics between observed monthly runoff and the average of monthly runoff (i.e., observed  
386 streamflow at the watershed outlet divided by watershed area) over the 30-year study period,  
387 which we refer to henceforth as ‘monthly normal runoff’. As with computing GCM runoff,  
388 monthly normal runoff was estimated at the watershed extent as described in *Section 2.1*. This  
389 process was implemented on a monthly time-step prior to computing 30-year means. We note  
390 that monthly normal runoff only relies on three features while the five models mentioned  
391 previously rely on 62 features (see Table S1). As a result, GCM runoff and monthly normal  
392 runoff serve as model comparison controls.

393

394 *2.5 Data and Script Availability*

395 We analyzed these data using Python (version 3.7.1, Python Software Foundation, 2018) and R  
396 (version 3.4.3; R Core Team, 2017). All model development code, data, trained model weights  
397 (i.e., parameters), and scripts associated with this publication are available on GitHub at [insert  
398 link here upon manuscript acceptance] and Zenodo (DOI: [insert link here upon manuscript  
399 acceptance]).

400

401 **3 Results**

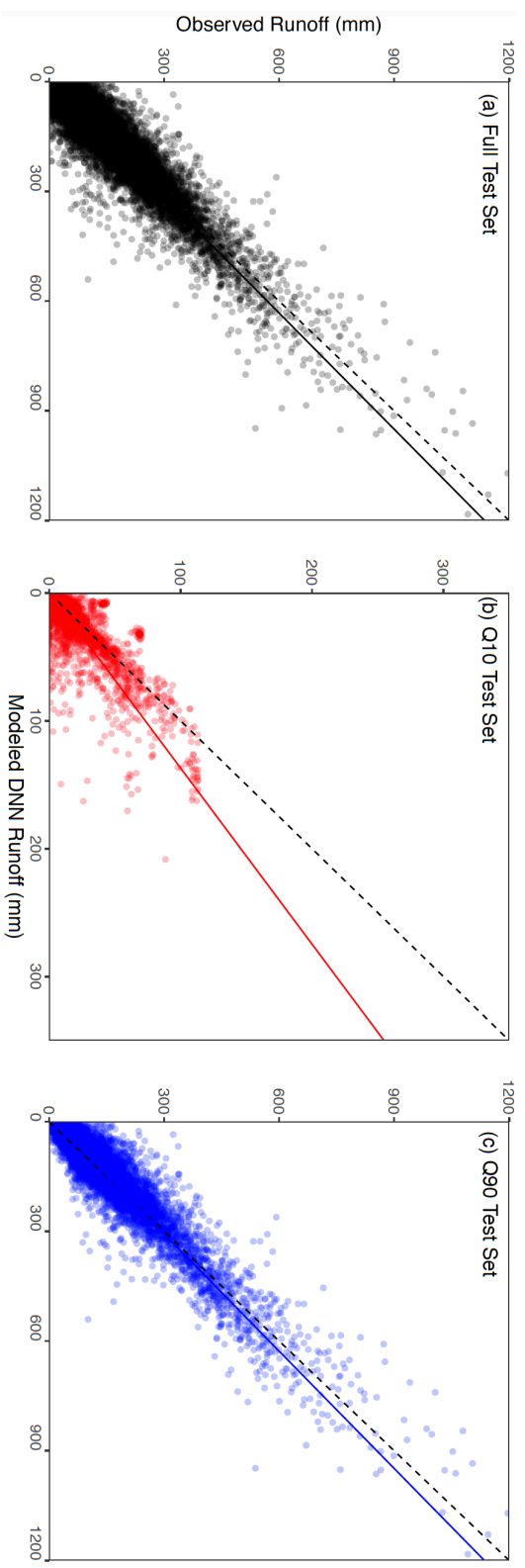
402 *3.1 Deep Neural Network Testing*

403 At the CONUS-scale, the DNN explained 92.5% (PCC = 0.962) of the variation in observed  
404 monthly test set runoff ( $p < 0.0001$ ; Figure 2a). Test set DNN residuals were close to zero and  
405 roughly symmetric around zero (Figures S5a). DNN MAE was 24.31%, bias was 2.36, and slope  
406 was 0.94 for the test set (Table 2). For Q10 events, the DNN explained 77.4% (PCC = 0.880) of  
407 variation in observed monthly runoff (Figure 2b). The MAE, bias, and slope were 50.87%, 0.52,  
408 and 0.73, respectively for Q10 events (Table S2). For Q90 events, the DNN explained 91.4%  
409 (PCC = 0.956) of variation in observed monthly runoff (Figure 2c). The MAE, bias, and slope  
410 were equal to 15.96%, 12.94, and 0.94, respectively for Q90 events (Table S2). The DNN  
411 explained 91.0% (PCC = 0.954) and 94.3% (PCC = 0.971) of the variation in observed monthly  
412 runoff for non-reference and reference watersheds in the test set, respectively (Table S3). The  
413 bias of non-reference watersheds in the test set was 2.36 and the slope was 0.94. For the  
414 reference watersheds in the test set the bias was 2.60 and the slope was 0.95. When separating  
415 out test set results by ecoregion for the DNN, bias ranged from 0.83 to 7.31 (Table S4), slope

416 ranged from 0.87 to 1.08 (Table S5), and PCC ranged from 0.80 to 0.97 (Table S6). DNN  
417 residuals were spread around zero when plotted against spatio-temporal variables such as time,  
418 latitude, longitude, and watershed area (Figures S5d-S5f, and S6). PCCs between DNN residuals  
419 and spatio-temporal variables were close to zero (Figures S5d-S5f, S6, and S10); they ranged  
420 from -0.05 to 0.04 (Table 3). At the watershed-scale, DNN median residuals were distributed  
421 around zero for test set (Figures 3, S5a, and S7a). The same was true for Q10 and Q90 events  
422 (Figures S7b, S7c, S8, and S9). Last, DNN test set median watershed residuals grouped by  
423 month were close to zero (Figure S10).

424

425



426

427 **Figure 2.** Comparison of deep neural network predicted (a) test set runoff (black,  $n = 243,376$ ), (b) Q10 test set runoff (red,  $n =$

428 24,928), and (c) Q90 test set runoff (blue,  $n = 24,362$ ) versus observed monthly runoff from the GAGES-II dataset. Dashed lines

429 represent 1:1 line and solid lines represent linear regression line-of-best-fit. Note that the x-axis and y-axis scales in (b) are different

430 from (a) and (c).

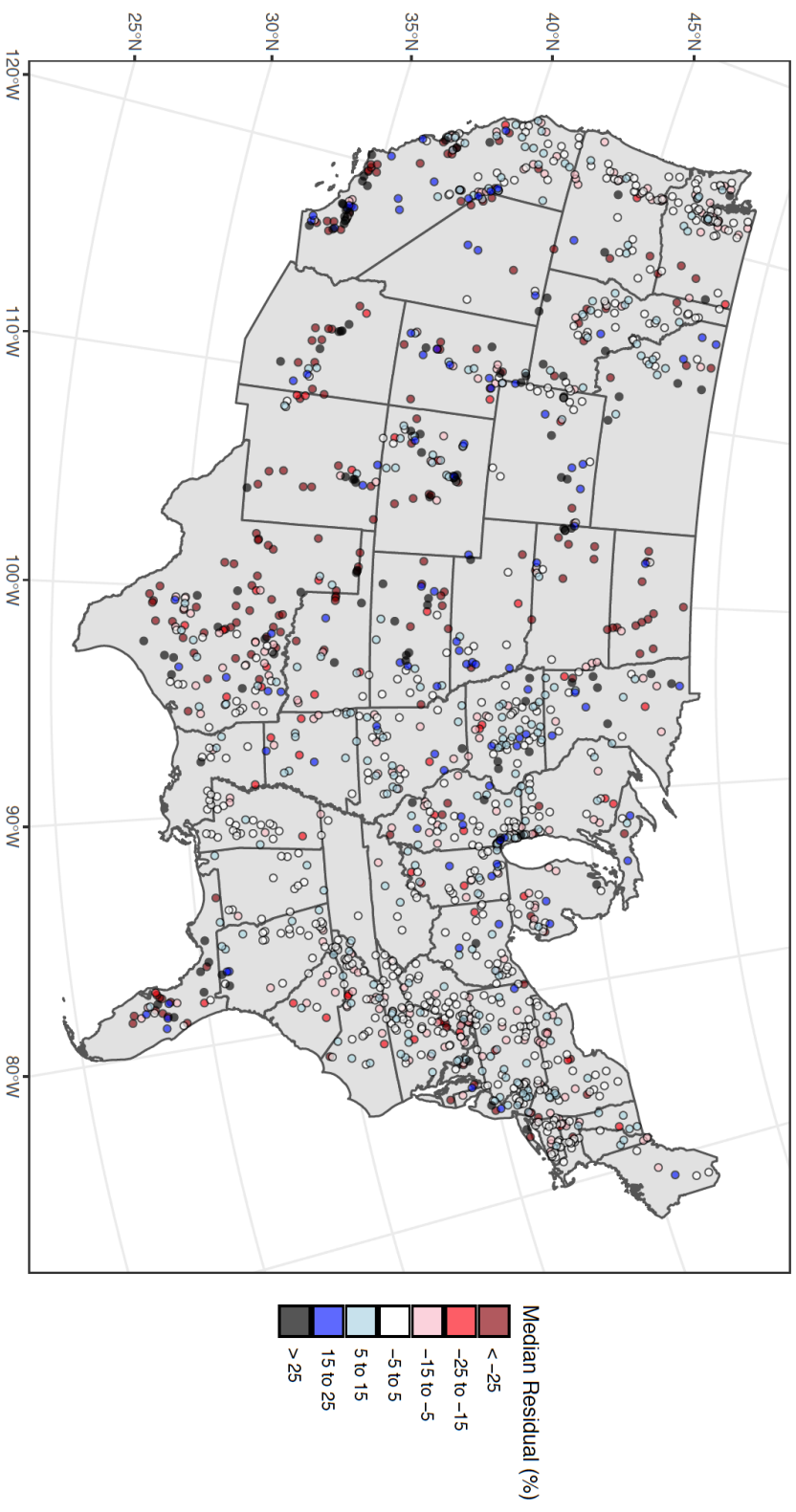
431

432 **Table 3.** Pearson's correlation coefficient (PCC), bootstrapped lower 95% confidence intervals  
433 (CIs), and bootstrapped upper 95% CIs between DNN residuals and spatio-temporal variables.

Variable	PCC	Lower CI	Upper CI
Time (month)	-0.003	-0.008	0.001
Watershed Area	-0.003	-0.005	-0.001
Latitude	0.040	0.035	0.045
Longitude	-0.050	-0.055	-0.045

434

435



436  
437 **Figure 3.** Deep neural network test set median watershed residuals. Point location represents the watershed centroid. Median  
438 watershed residuals are expressed as a percent relative to observations.  
439



440

441 *3.2 Model Performance Comparisons*

442 We included two model controls in this study: GCM runoff and monthly normal runoff. GCM  
443 runoff explained 65.8% (PCC = 0.811) and monthly normal runoff explained 65.9% (PCC =  
444 0.812) of the variation in observed monthly test set runoff (Table 2). GCM runoff MAE was  
445 49.97% and monthly normal runoff MAE was 50.36% for the test set. For Q10 events, GCM  
446 runoff explained 25.6% (PCC = 0.506) of the variation in observed monthly runoff and had a  
447 MAE of 149.05% (Table S2). Monthly normal runoff explained 62.7% (PCC = 0.792) of the  
448 variation in observed monthly runoff for Q10 events and had a MAE equal to 293.91% (Table 3).  
449 For Q90 events, GCM runoff and monthly normal runoff explained 58.8% (PCC = 0.767) and  
450 75.9% (PCC = 0.871) of variation in observed monthly runoff, respectively (Table S2). GCM  
451 runoff MAE was 35.36% and monthly normal runoff was 48.45% for Q90 events; both were  
452 lower than the MAE of Q10 events (Table S2). For non-reference watersheds in the test set,  
453 GCM runoff and monthly normal runoff had lower PCCs compared to the full test set (Tables 2  
454 and S3). Conversely, for reference watersheds in the test set, GCM runoff and monthly normal  
455 runoff had a higher PCC compared to the full test set (Table S3). When looking at test set results  
456 by ecoregion, GCM runoff bias ranged from 0.55 to 13.56 (Table S4), slope ranged from 0.56 to  
457 1.07 (Table S5), and PCC ranged from 0.58 to 0.86 (Table S6). For monthly normal runoff test  
458 set results analyzed by ecoregion bias ranged from -0.1 to 0.4 (Table S4), slope ranged from 0.99  
459 to 1.03 (Table S5), and PCC ranged from 0.58 to 0.86 (Table S6).

460

461 In addition to model controls, we compared DNN performance to four other grid-to-watershed-  
462 scale conversion techniques: linear ridge regression, SVM, XGBoost, and ANN (Table 2). Of the

463 four methods, XGBoost explained the most variation in observed monthly test set runoff  
464 followed by (in order of decreasing PCC) ANN, SVM, and linear ridge regression techniques  
465 (Table 2). For the test set, MAE was smallest for the ANN followed by (in order of increasing  
466 MAE) XGBoost, SVM, and linear ridge regression techniques (Table 2). Slopes for the four  
467 techniques were all greater than one except for linear ridge regression, which was close to zero  
468 (Table 2). For Q10 events, XGBoost explained the most variation in observed monthly test set  
469 runoff followed by (in order of decreasing PCC) ANN, SVM, and linear ridge regression  
470 techniques (Table S2). MAE was smallest for the ANN followed by (in order of increasing  
471 MAE) XGBoost, SVM, and linear ridge regression for Q10 events. Like Q10 events, model  
472 results for Q90 events have a similar PCC ranking. XGBoost explained the most variation in  
473 monthly observed runoff (Table S2). For Q90 events, MAE was smallest for XGBoost followed  
474 by (in order of increasing MAE) ANN, SVM, and linear ridge regression. For non-reference  
475 watersheds in the test set, XGBoost followed by (in order of decreasing PCC) ANN, SVM, and  
476 linear ridge regression explained the most variation in observed monthly runoff (Table S3). For  
477 reference watersheds in the test set, a similar PCC ranking held. When looking at test set results  
478 by ecoregion, slopes for the four techniques were typically  $> 1.0$ , except for linear ridge  
479 regression (Table S5) and PCCs were typically  $> 0.7$  except for in a few cases for SVM and in all  
480 cases for linear ridge regression (Table S6).

481

482 We assessed model training efficiency by comparing computer processor requirements and  
483 computing time. For the DNN and the four alternative grid-to-watershed-scale conversion  
484 techniques, the ANN and DNN were the only models requiring a GPU. The DNN took  $\sim 10$   
485 times more computing time than the ANN. Of the techniques using a CPU (i.e., linear ridge

486 regression, SVM, XGBoost), XGBoost took the longest to train; about three times as much time  
487 as the DNN. Of all the techniques we tested, linear ridge regression took the least amount of time  
488 to train.

489

## 490 **4 Discussion**

### 491 *4.1 Deep Neural Network Testing*

492 The trained DNN predicted monthly runoff more accurately than controls (i.e., GCM runoff and  
493 monthly normal runoff) and was able to effectively translate gridded GCM outputs into  
494 watershed-scale runoff as demonstrated by several key results. First, the DNN explained more  
495 variation in observed monthly runoff and had a lower MAE compared to any other methods that  
496 we considered (Table 2). Second, the DNN runoff predictions approximated observed runoff  
497 with little bias (Figure 2a). Third, DNN residuals were close to zero and were relatively  
498 symmetric (Figures S5a, S5b, and S7a). This indicates the absence of a systematic tendency for  
499 the DNN to overestimate or underestimate watershed-scale runoff. Fourth, we observed a near-  
500 zero correlation between DNN residuals and variables related to time, location, or watershed size  
501 (i.e., time, longitude, latitude, and watershed area; Table 3, Figures S5d-S5f, S6, S7, S10). This  
502 indicates that the DNN was generally robust to spatio-temporal variation. However, we observed  
503 that the DNN overpredicted monthly runoff in California, Texas, and Florida as indicated by  
504 large negative (i.e.,  $< -25\%$ ) median watershed residuals (Figure 3). Future studies may use local  
505 interpretable model-agnostic explanations (LIME; Ribeiro et al., 2018) and other machine  
506 learning interpretation techniques to further explain these patterns in model residuals (e.g.,  
507 Worland et al., 2019).

508

509 The trained DNN adequately predicted monthly Q10 and Q90 runoff events, although, Q90  
510 events tended to be more accurately predicted than Q10 events. More specifically, the DNN  
511 explained a larger percentage of variation (i.e., higher PCC) in observed monthly runoff test set  
512 Q90 events compared to Q10 events (Table S2). Also, the scatter plot of observed versus  
513 modeled runoff for Q90 events tracked the 1:1 line closer than that for Q10 events (Figures 2b  
514 and 2c). Points below the 1:1 line support the finding that the DNN tended to overpredict Q10  
515 events (Figure 2b). We also observed a higher MAE for Q10 events compared to Q90 events  
516 (Table S2). Compared to GCM runoff and monthly normal runoff, the DNN was more effective  
517 at predicting Q10 and Q90 monthly runoff events as supported by a consistently higher PCC and  
518 lower MAE.

519

520 In addition to scale (i.e., CONUS- and watershed-scale) and extreme events, the DNN accurately  
521 predicted monthly runoff for non-reference as well as reference watersheds and across all nine  
522 GAGES-II watershed ecoregions. More specifically, PCC for non-reference watersheds in the  
523 test set was 0.954 and 0.971 for reference watersheds in the test set (Table S3). Bias was less  
524 than 8, slope was close to one, and PCC was  $> 0.8$  for watersheds in all ecoregions. We observed  
525 the largest PCC in the West Mountains (Table S6). Compared to GCM runoff and monthly  
526 normal runoff, the DNN was better at predicting non-reference and reference site monthly runoff  
527 as supported by a consistently higher PCC and lower MAE (Table S3).

528

529 *4.2 Model Performance Comparisons*

530 Compared to the four other grid-to-watershed-scale conversion techniques, the DNN explained  
531 the most variation in observed monthly runoff (i.e., highest PCC) and had the lowest MAE  
532 (Table 2). We found that linear ridge regression and SVM methods all had higher MAE, higher  
533 bias (either negative or positive), and lower PCC than the control methods (i.e., GCM runoff and  
534 monthly normal runoff; Table 2). Therefore, we do not recommend using these methods for  
535 converting gridded, downscaled monthly GCM hydroclimatic fluxes to watershed-scale monthly  
536 runoff for the CONUS. The ANN, which represents a simpler neural network structure compared  
537 to the DNN (Figure S1a), could adequately predict monthly runoff, albeit not as well as the DNN  
538 (Table 2). This finding is likely explained by the difference in hidden layers between the ANN  
539 and DNN. The DNN has more hidden layers, which enable it to represent more complex  
540 relationships between data inputs and outputs (Shen, 2018). XGBoost predicted monthly runoff  
541 better than controls, had a higher PCC and MAE than the ANN, but underperformed relative to  
542 the DNN (Table 2).

543

544 The DNN outperformed the model controls as well as the four alternative techniques when it  
545 came to predicting Q10 and Q90 monthly runoff, non-reference and reference monthly runoff,  
546 and monthly runoff in various ecoregions. Similar to the results discussed above, we do not  
547 recommend the linear ridge regression because this technique tended to perform worse than  
548 model controls for Q10 and Q90 events; it had a higher MAE and lower PCC (Table S2). Linear  
549 ridge regression also had a lower PCC than the controls for non-reference and reference  
550 watersheds (Table S3) as well as for watersheds in all ecoregions (Table S6). SVM sometimes  
551 outperformed the model controls for Q10 and Q90 events, but there were some exceptions to this

552 finding (e.g., the MAE for Q10 events was 736%; Table S2). SVM tended to have a lower PCC  
553 compared to the model controls for non-reference and reference watersheds (Table S3) as well as  
554 for watersheds in some ecoregions (e.g., West Mountains). While not as accurate as the DNN,  
555 XGBoost and ANN consistently had a lower MAE and higher PCC for Q10 and Q90 monthly  
556 runoff compared to model controls (Table S2). Additionally, compare to model controls,  
557 XGBoost and ANN had a higher PCC for non-reference and reference watersheds as well as  
558 watersheds in all ecoregions.

559

560 When it came to computing power, we found that the DNN required the second longest  
561 computing time and a GPU compared to all the other grid-to-watershed-scale monthly runoff  
562 conversion methods tested (Table 2). However, other well performing approaches required either  
563 a GPU (i.e., ANN) or parallel computing on a CPU (i.e., XGBoost; Table 2). This finding  
564 highlights a potential limitation of DNN-based methods; hydrologists interested in using  
565 machine learning methods to convert gridded GCM hydroclimatic fluxes to watershed-scale  
566 runoff may wish to consider available computing resources before implementing DNNs. DNNs  
567 can be trained on a single desktop workstation in less than a day using open-source software or  
568 users may seek out cloud-based computing methods to carry out analyses if research budgets are  
569 more limited. Based on these results, DNNs hold great promise as a tool for improving the  
570 accuracy of GCM-derived runoff estimates for watershed-scale research.

571

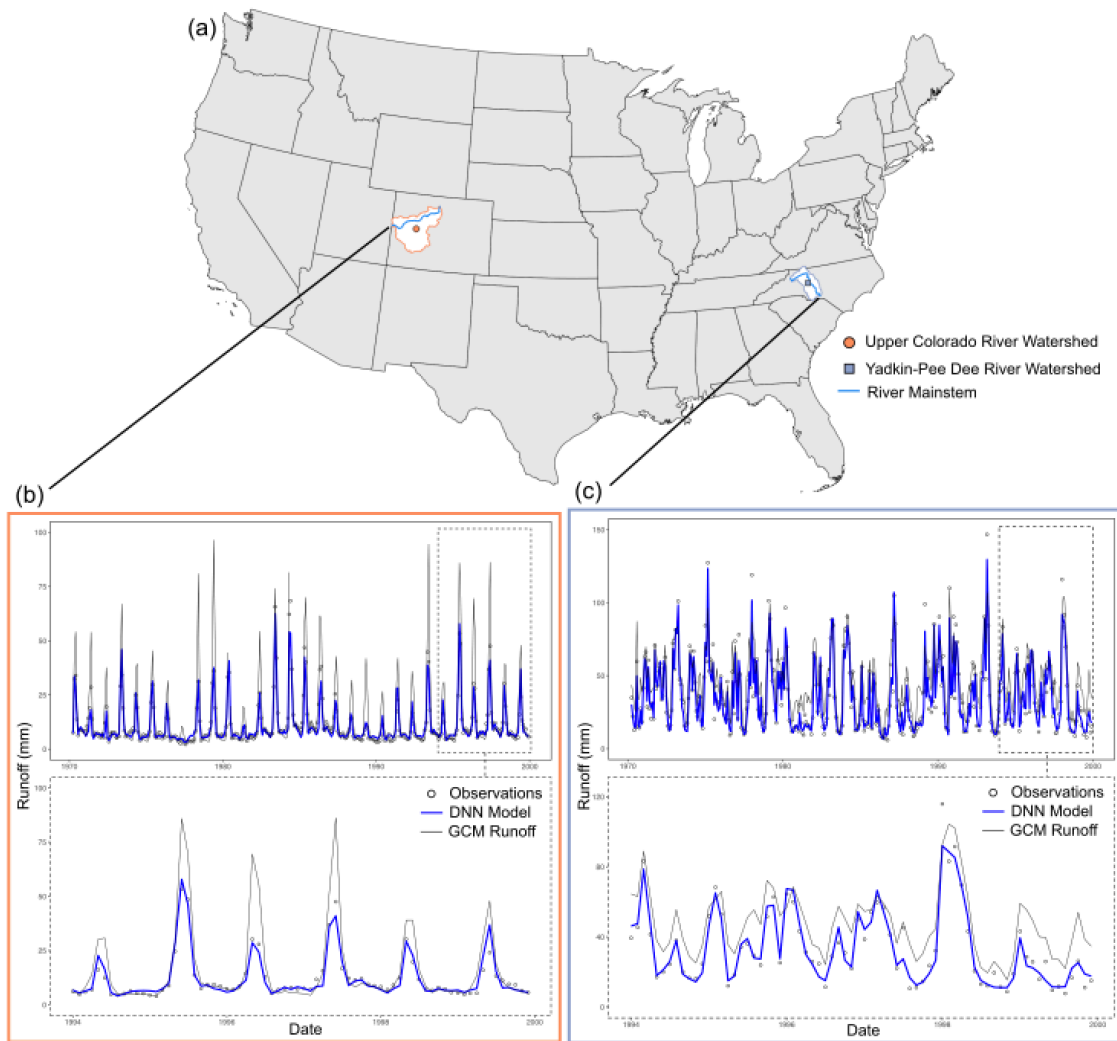
572 *4.3 Applying Deep Learning to Climate Model Downscaling: Examples in Colorado and North*  
573 *Carolina, USA*

574 To illustrate the efficacy of using the DNN to convert gridded, downscaled GCM outputs to  
575 watershed-scale runoff, we consider two example watersheds (Figure 4a). USGS stream gage  
576 number 09163500 measures runoff for the portion of the Colorado River that flows through  
577 Colorado, USA (henceforth referred to as the Upper Colorado River Watershed; UCR) and  
578 USGS stream gage number 02129000 measures runoff for the Yadkin-Pee Dee River Watershed  
579 (YPD). The UCR an area of 46,300 km<sup>2</sup> and the YPD has an area of 17,800 km<sup>2</sup>. Both are  
580 characterized as non-reference (i.e., human-disturbed) watersheds (Falcone et al., 2010).

581

582

583



584

585 **Figure 4.** Examples of the Upper Colorado River Watershed (UCR) in the Southwest United  
 586 States and Yadkin-Pee Dee River Watershed (YPD) in the Southeast United States. (a) Location  
 587 of UCR centroid (orange circle) and boundary and YPD centroid (blue square) and boundary. (b)  
 588 Comparison of UCR observed runoff (empty circles), DNN modeled runoff (thick blue solid  
 589 line), and GCM runoff (thin black solid line) versus time. (c) Comparison of the same results for  
 590 the YPD. Bottom plot of (b) and (c) includes the five most recent years of the time series.

591



592 In 2006, the UCR consisted of primarily (53.8%) forest land cover, followed by 24% shrubland,  
593 9.9% grassland, 4.1% agriculture, 3.8% barren, 1.7% wetlands, and 1.5% development, and  
594 1.1% water (including snow and ice; Falcone et al., 2010; Fry et al., 2012). While the fraction of  
595 development within the watershed is low, it is a key water source for ecosystems and  
596 downstream residents in the southwestern US (McCabe & Wolock, 2007; Udall & Overpeck,  
597 2017). Climate change is projected to increase temperatures by 2-4°C in the Southwest United  
598 States by 2050, leading to decreases in snowpack, increases in drought duration, and decreases in  
599 runoff (Seager & Vecchi, 2010; Hayhoe et al., 2018; Gonzalez et al., 2018). Consequently,  
600 climate change will likely stress regional water supplies that are already very sensitive to  
601 changes in runoff (McCabe & Wolock, 2007; Christensen & Lettenmaier, 2006; Woodhouse et  
602 al., 2016, Udall & Overpeck 2017).

603

604 Given these sensitivities in water resources management to changes in UCR runoff, it is important  
605 to accurately downscale GCM results to the watershed-scale. Compared to observations, GCM  
606 runoff predictions for the UCR had a MAE of 25.2%. Using the DNN developed by this study,  
607 the MAE of monthly runoff for the UCR was 12.2%; nearly 50 percentage points better. More  
608 specifically, many of the monthly runoff peaks were overpredicted by GCM runoff (Figure 4b).  
609 To put these numbers into perspective, mean monthly runoff from this basin during the study  
610 period was 11.0 mm, or 511 million m<sup>3</sup>. Using that value as a guideline, the reduction in error  
611 associated with applying the correction model to monthly, gridded GCM runoff for the UCR  
612 equates to an improvement in accuracy on the order of 66 million m<sup>3</sup> of water per month (i.e.,  
613 511 million m<sup>3</sup> x 0.252 minus 511 million m<sup>3</sup> x 0.122), which is 2.8-5.6% of the total monthly

614 water withdrawals for Colorado in 2015 (Dieter et al., 2018). For the UCR, the DNN enhanced  
615 the accuracy of GCM runoff and GCM output applicability to water resources management.

616

617 In 2006, the YPD consisted of mainly (53.8%) forest land cover, followed by 24.8% agriculture,  
618 12.5% developed, 4.8% grassland, 1.8% shrubland, 1.3% water, 1% wetlands, and <1% barren  
619 lands (Falcon et al., 2010; Fry et al., 2012). Compared to UCR, the YPD has more development  
620 which is projected to increase 101-192% in the Southeast United States by 2060 (Terando et al.,  
621 2014). This development will largely replace forested land cover (USFS, 2012; Wear, 2013).  
622 Climate change is projected to increase regional temperatures 2.2-2.6°C by 2100 and future  
623 precipitation is likely to be more extreme, including more intense events and longer periods  
624 between events (O’Gorman & Schneider 2009; Laseter & others 2012; IPCC 2014; Walsh et al.  
625 2014; Carter et al. 2018). In the YPD, these land cover and climate changes may combine to  
626 increase peak flows and reduce groundwater recharge (Ogden et al., 2011; Hamel et al., 2013;  
627 Walsh et al., 2014; Martin et al., 2017; Carter et al., 2018; Suttles et al., 2018). This increase  
628 number of future high flow events may negatively impact vulnerable communities in the YPD  
629 (Saia et al., 2019).

630

631 Compared to observations, GCM runoff predictions for the YPD had a MAE of 46.1%. Using the  
632 DNN developed by this study, the MAE of monthly runoff for the YPD was 9.58%; nearly 80  
633 percentage points better. Unlike the UCR where monthly runoff peaks were overpredicted, GCM  
634 runoff seemed to overpredict peaks as well as time points between peaks for the YPD (Figure  
635 4c). Mean monthly runoff from this basin during the study period was 36.4 mm, or 647 million  
636 m<sup>3</sup>. Using that value as a guideline, the reduction in error associated with applying the correction

637 model to monthly, gridded GCM runoff for the UCR equates to an improvement in accuracy on  
638 the order of 236 million m<sup>3</sup> of water per month (i.e., 647 million m<sup>3</sup> x 0.461 minus 647 million  
639 m<sup>3</sup> x 0.0958), which is about 10-20% of the total monthly water withdrawals for North Carolina  
640 in 2015 (Dieter et al., 2018). Many studies conducted in and around YPD region (e.g., Martin et  
641 al., 2018 and Suttles et al., 2018) note the importance of managing forest land cover in the face  
642 of projected climate and land use change. More accurate runoff predictions may improve forest  
643 land cover management, and ultimately, water resources (Vose, 2018).

644

#### 645 *4.4 Implications and Future Directions*

646 To the best of our knowledge, this study was the first to combine watershed characteristics from  
647 a large publicly available dataset with gridded GCM hydroclimatic fluxes (i.e., precipitation,  
648 temperature, and evapotranspiration) to develop a DNN that accurately predicted monthly runoff  
649 for watersheds across the CONUS (Figure S2). The trained DNN was robust to spatio-temporal  
650 changes in monthly runoff, accounted for non-reference and reference site characteristics, and  
651 was robust across the nine GAGES-II watershed ecoregions. Additionally, the trained DNN  
652 adequately predict Q90 events; however, it had a more difficult time predicting Q10 events. We  
653 also compared DNN runoff predictions to two controls (i.e., GCM runoff and monthly normal  
654 runoff) and four statistical grid-to-watershed-scale conversion techniques. The DNN  
655 outperformed all alternative techniques but required more computing power and computing time  
656 than some alternatives. This work highlights key benefits of DNNs as well as future  
657 opportunities for the application of DNNs to statistical GCM downscaling.

658

659 In addition to key benefits discussed in *Section 1*, DNN structure—including input, hidden, and  
660 output layers (Figure S1b)—conserves the conceptualization of watersheds as spatio-temporal  
661 filters (e.g., Weiler et al., 2003; Nippgen et al., 2011; Emanuel et al., 2014; Rice et al., 2015;  
662 Rice & Emanuel, 2019). The concept underpins the Geomorphic Instantaneous Unit Hydrograph  
663 (GIUH; Rodriguez-Iturbe & Valdes, 1979; Gupta et al., 1980; Rinaldo et al., 1995; Nippgen et  
664 al., 2015) and hydrologic similarity (Beven & Kirkby, 1979; Brutsaert, 1994; Lyon & Troch,  
665 2007). In the context of this study, watersheds translate hydroclimatic input signals into runoff  
666 output signals given interaction between internal watershed characteristics (e.g., soil saturation)  
667 that occurs in the context of external hydroclimatic inputs. As an example, geomorphic and  
668 topographic landscape structures (Emanuel et al., 2010; Jencso & McGlynn, 2011; Nippgen et  
669 al., 2011) and patterns in vegetation and land cover (Rodriguez-Iturbe, 2000; DeFries &  
670 Eshlemann, 2004; Piao et al., 2007; Emanuel et al., 2010; 2014; Nippgen et al., 2015) control the  
671 movement of water through watersheds. Although hidden layers may or may not represent  
672 recognizable hydrologic processes, the DNN effectively learns a representation of the  
673 overarching conceptualization of watersheds as filters from the data.

674

675 Using DNNs to represent watershed signal filtering is also consistent with current understanding  
676 of watersheds as complex systems comprising non-linear feedbacks and other interactions  
677 (McDonnell et al., 2007). We suggest that DNNs can account for non-linear interactions between  
678 spatial biotic, abiotic, endogenous, and exogenous features that yield watershed-scale memory  
679 effects, and ultimately, result in emergent streamflow responses (Nippgen et al., 2016) and land-  
680 atmosphere biogeochemical fluxes (Emanuel et al., 2011; Riveros-Iregui et al., 2012; Reyes et  
681 al., 2017). Existing governing equations may represent some of these behaviors, but machine

682 learning models such as DNNs have the ability to independently uncover previously  
683 unrecognized or unparameterized feedbacks contained within large datasets publicly available to  
684 hydrologists. When adequate training data and training time are available, DNNs serve as  
685 universal function approximators (LeCun et al., 2015; Goodfellow et al., 2016; Rolnick &  
686 Tegmark, 2017; Knighton et al., 2019); where in the case of watershed-scale runoff prediction,  
687 the universal function likely describes some of these non-linear feedbacks occurring within the  
688 watershed. A deeper look at these universal functions may confirm or challenge aspects of our  
689 existing conceptual understanding of watersheds and runoff processes. Thus, probing of DNN  
690 results may help hydrologists (1) develop hypotheses concerning understudied or unidentified  
691 interactions between hydroclimatic fluxes, watershed characteristics, and runoff and (2) test  
692 these hypotheses using physically-based modeling and field studies (Shen et al., 2018).

693

694 While this study does not attempt to characterize the filtering processes of watersheds across the  
695 CONUS, future studies may apply tools such as partial response functions (Rice et al., 2016;  
696 Rice & Emanuel, 2017) and local interpretable model-agnostic explanations (Worland et al.,  
697 2019) to explore the impact of GCM inputs and watershed characteristics on watershed-scale  
698 runoff. Also, these statistical model interpretation methods may be used to open up the machine  
699 learning “black box” by generating hypotheses that can be tested using physically-based  
700 hydrology models and field experiments (Shen et al., 2018; Rice and Emanuel 2019). For  
701 example, one study combined XGBoost results with the Budyko framework (Budyko, 1974) to  
702 assess the impact of forest land cover on watershed storage (Rice & Emanuel, 2019). Another  
703 study used gridded GCM climate variables to develop a convolutional neural network—a  
704 specific type of DNNs that relies on 2D inputs such as images—and then to interpret seasonal

705 extreme precipitation patterns in the Eastern United States using archetypal analysis (Knighton et  
706 al., 2019). We incorporated methods to improve model training and testing when it comes to  
707 temporal changes in runoff (i.e., semi-random sampling and residual trend analysis); however,  
708 additional opportunities exist to train and test DNN model response to non-stationary processes.  
709 This may include the use of covariate shift adaptation (Sugiyama et al., 2007) in hydrological  
710 science machine learning applications and long short-term memory (LSTM) neural networks  
711 (Shen, 2018).

712

#### 713 *4.5 Recommendations for DNN Applications in the Hydrologic Sciences*

714 With the growing emergence of big data and machine learning methods, this study serves as a  
715 guide to hydrologists interested in implementing machine learning techniques such as DNNs. In  
716 this study we applied a DNN to convert GCM runoff to the watershed-scale but DNNs could be  
717 used more broadly to convert other gridded data products (e.g., Gravity Recovery and Climate  
718 Experiment; GRACE, Moderate Resolution Imaging Spectroradiometer-Evapotranspiration;  
719 MODIS-ET, Coupled Model Intercomparison Project Phase 6; CMIP6) to the watershed-scale.  
720 Below we note a few practical experimental design considerations for hydrologic scientists and  
721 researchers; however, we also suggest recent publications by Shen (2018), Shen et al. (2018),  
722 and Worland et al. (2019) for didactic texts on deep neural network applications in hydrology.

723

- 724 • *training and test splits* - Similar to standards methods for hydrology model evaluation  
725 (i.e., Moriasi et al., 2007), researchers designing DNN-based experiments should separate  
726 full datasets up into a train and test sets. Typical splits are 75:25 (75% training and 25%  
727 testing) or 80:20, but the exact split is less important as ensuring the creation of an

728 independent test set to evaluate model performance. As in other types of model training,  
729 DNN training uses only the train set and is evaluated based on the independent test set,  
730 which it has never “seen”. Ideally, the DNN may also be evaluated based a separate  
731 validation set that includes newly generated data. For example, this may include using  
732 current precipitation and temperature data as inputs to the model. Researchers may also  
733 wish to consider their method for splitting up data (i.e., random sampling or semi-random  
734 hold out). Here, we used semi-random sampling because we wanted to make sure the  
735 DNN was robust in time and space. Thus, we are choosing which input variables are  
736 important for the DNN to represent.

- 737 • *model evaluation metrics* - Consider using multiple model evaluation metrics when  
738 assessing DNN performance. These may include bias, slope,  $R^2$ , and MAE as well as  
739 others we do not use here (e.g., Nash- Sutcliffe Efficiency). For a thorough review of  
740 standard hydrology model evaluation metrics see Moriasi et al. (2007).
- 741 • *residual analysis* - Residual analysis including the plotting of residuals versus  
742 observations, and in this case, important spatio-temporal variables is an important  
743 statistical evaluation technique to assessing whether or not the DNN is robust to changes  
744 in model inputs.
- 745 • *architecture* - Researchers should consider whether they will start simply and add layers  
746 and nodes or start with a large model and remove layers and nodes. Both approaches can  
747 lead to useful capabilities, as we discussed in *Section 2.2*.
- 748 • *model training improvement techniques* - In this study, we implemented a number of  
749 techniques to improve model training accuracy and reduce model training time (e.g.,  
750 early stopping). Researchers should consider including some of these; fortunately, many

751 are easily implemented using existing Python and R libraries. For a thorough description  
752 of these techniques, look to Goodfellow et al. (2016).

753 • *data quality and research framing* - The old adage “garbage in, garbage out” is important  
754 to consider when it comes to implementing machine learning methods. If your data are  
755 biased, the machine learning model may learn to reproduce those biases. For example, if  
756 a DNN model is conditioned only on water samples collected after a precipitation event,  
757 the model may have a hard time predicting water quality metrics before or during a  
758 storm. Just as importantly, it is key to be mindful that machine learning, while powerful,  
759 is simply another tool for extracting insights from data. Therefore, machine learning is  
760 best used in combination with well-framed research questions and relevant, high quality  
761 data.

762

## 763 **5 Conclusions**

764 We used a large publicly available dataset from the United States Geological Survey combined  
765 with monthly, gridded, downscaled, general circulation model (GCM) hydroclimatic fluxes (i.e.,  
766 precipitation, evapotranspiration, and temperature) to train and test a deep neural network (DNN)  
767 capable of predicting monthly runoff at the watershed-scale for 2,731 watersheds across the  
768 conterminous United States. We also compared DNN performance to the performance of four  
769 other grid-to-watershed-scale conversion techniques, including: linear ridge regression, support  
770 vector machine, extreme gradient boosting, and an artificial neural network. Of all these  
771 modeling approaches, the DNN had the lowest median absolute error, the lowest bias, and  
772 explained the most variation in observed monthly runoff. Furthermore, the DNN was temporally  
773 and spatially robust and represented extreme low (i.e., monthly runoff events in the 10<sup>th</sup>



774 percentile or lower; Q10) and extreme high (i.e., monthly runoff events in the 90<sup>th</sup> percentile or  
775 higher; Q90) relatively well compared to the four other grid-to-watershed-scale conversion  
776 techniques. However, of all the approaches we tested, the DNN took the second longest to train  
777 using specialized computing hardware (i.e., a graphical processing unit; GPU). Finally, we  
778 presented example results in the Upper Colorado River Watershed and Yadkin-Pee Dee River  
779 Watershed to demonstrate how the DNN improved upon raw, gridded GCM runoff data and why  
780 this improvement is relevant for water resources management in these regions. Overall, this  
781 study highlights the emerging role of machine learning techniques such as DNNs for hydrologic  
782 and environmental science research.

783

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788

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Supporting Information for

**Improved Accuracy of Watershed-Scale General Circulation Model**

**Runoff Using Deep Neural Networks**

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**Contents of this file**

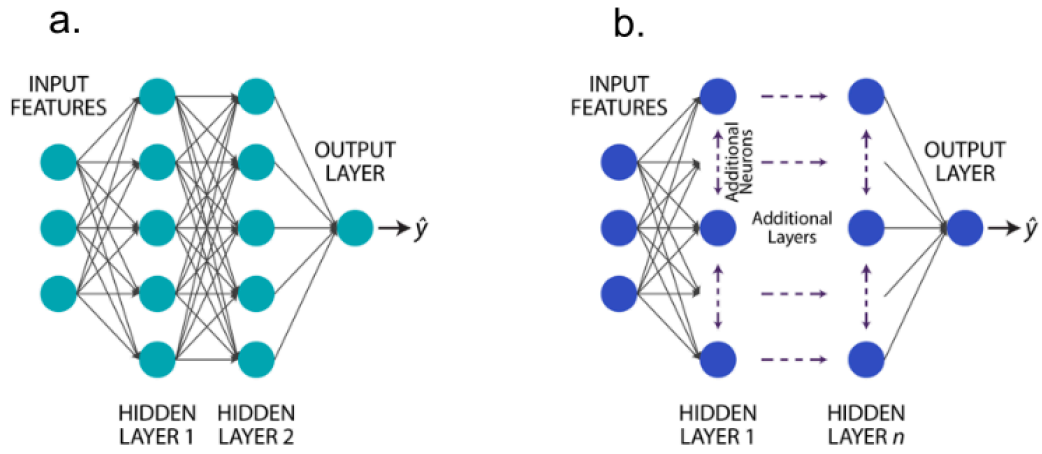
Figures S1-S10, Table S1-S6

**Additional Supporting Information**

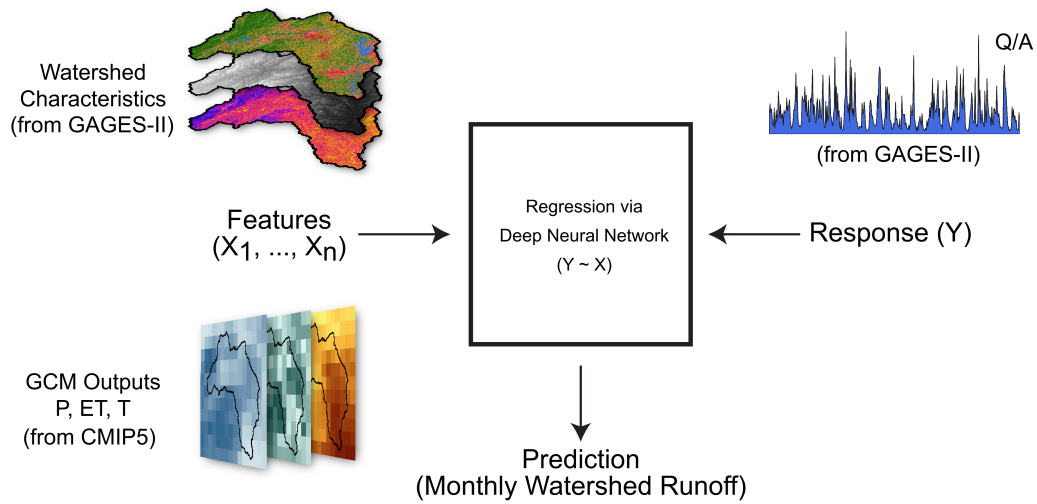
Data and scripts associated with this publication are available on GitHub at [[insert link here upon manuscript acceptance](#)] and Zenodo (DOI: [[insert link here upon manuscript acceptance](#)]).

**Introduction**

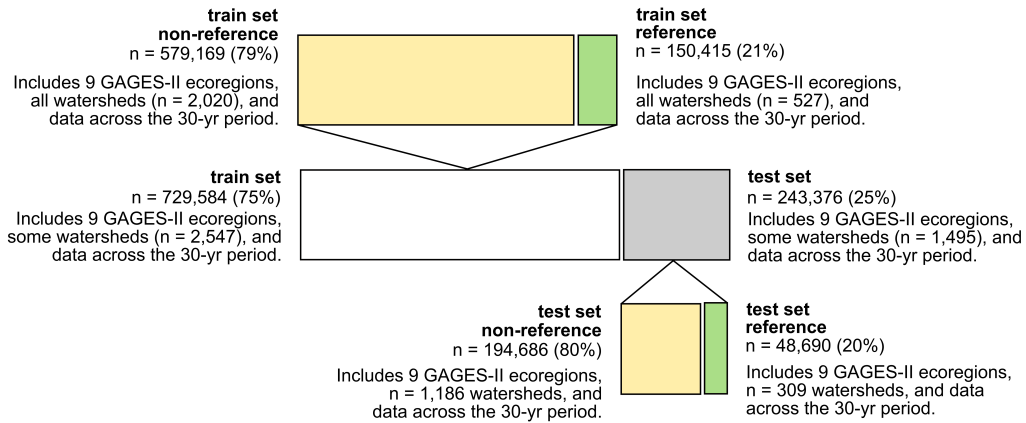
This manuscript supporting information document includes conceptual diagrams showing the architecture of machine learning models used in this study, deep neural network (DNN) model inputs and outputs, and the semi-random training and test set split proportions. We included a figure showing the location and region of watersheds used in this study and several model testing figures. In addition to figures, we included a table describing the DNN input variables and tables with model assessment metrics for non-reference and reference test set results, Q10 and Q90 test set results, and ecoregional results.



**Figure S1.** (a) Architecture of a simple artificial neural network (ANN) with two hidden layers and a limited number of neurons (cyan circles). (b) Architecture of a more complex deep neural network (DNN) with several hidden layers and neurons (blue circles).

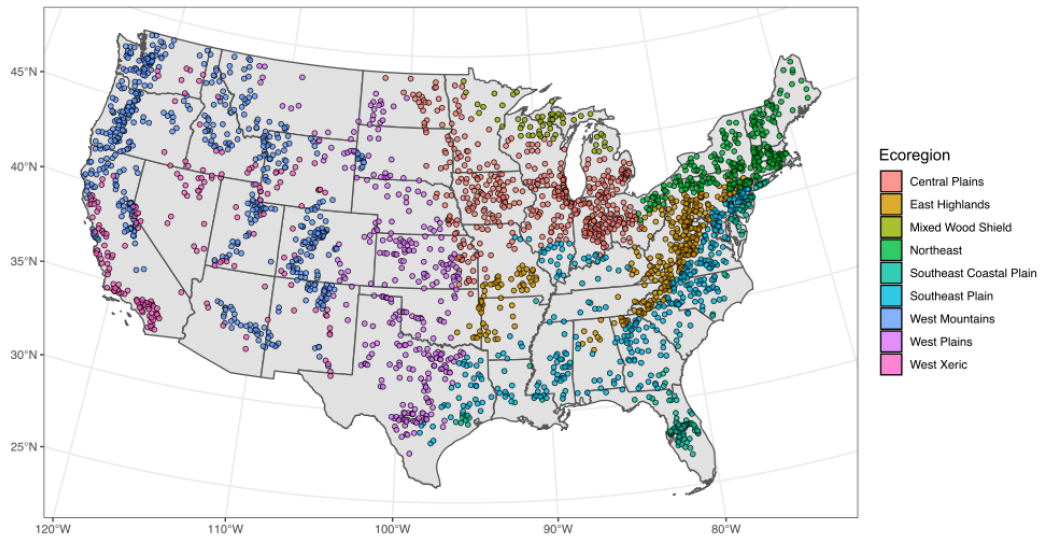


**Figure S2.** Conceptual overview of how we trained a deep neural network (DNN) to predict monthly watershed-scale runoff. The DNN feature variables included watershed characteristics and monthly, gridded, downscaled Coupled Model Intercomparison Project Phase 5 (CMIP5) general circulation model (GCM) precipitation (P), evapotranspiration (ET), and temperature (T). We also used several abiotic and biotic watershed characteristics from the Gages for Evaluating Streamflow version II (GAGES-II) dataset (Falcone et al., 2010). Observed monthly runoff—equal to streamflow at the gauging station (Q) divided by watershed area (A)—was the response variable.

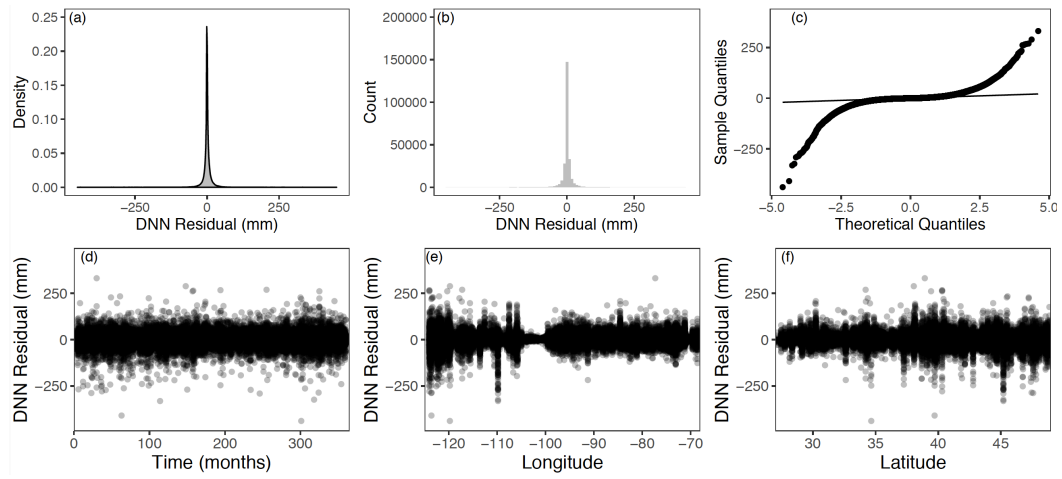


**Figure S3.** Breakdown of observed monthly runoff (i.e., DNN response) data distribution between train and test sets. Yellow represents data from non-reference watersheds and green represents data from reference watersheds. Note that the sum of watersheds does not add to  $n = 2,731$  between the train and test set because of the semi-random sampling grouped by time; some watersheds are represented in both the training and test set but their time points differ. Abbreviations: Geospatial Attributes of Gages for Evaluating Streamflow version II (GAGES-II; Falcone et al., 2010).

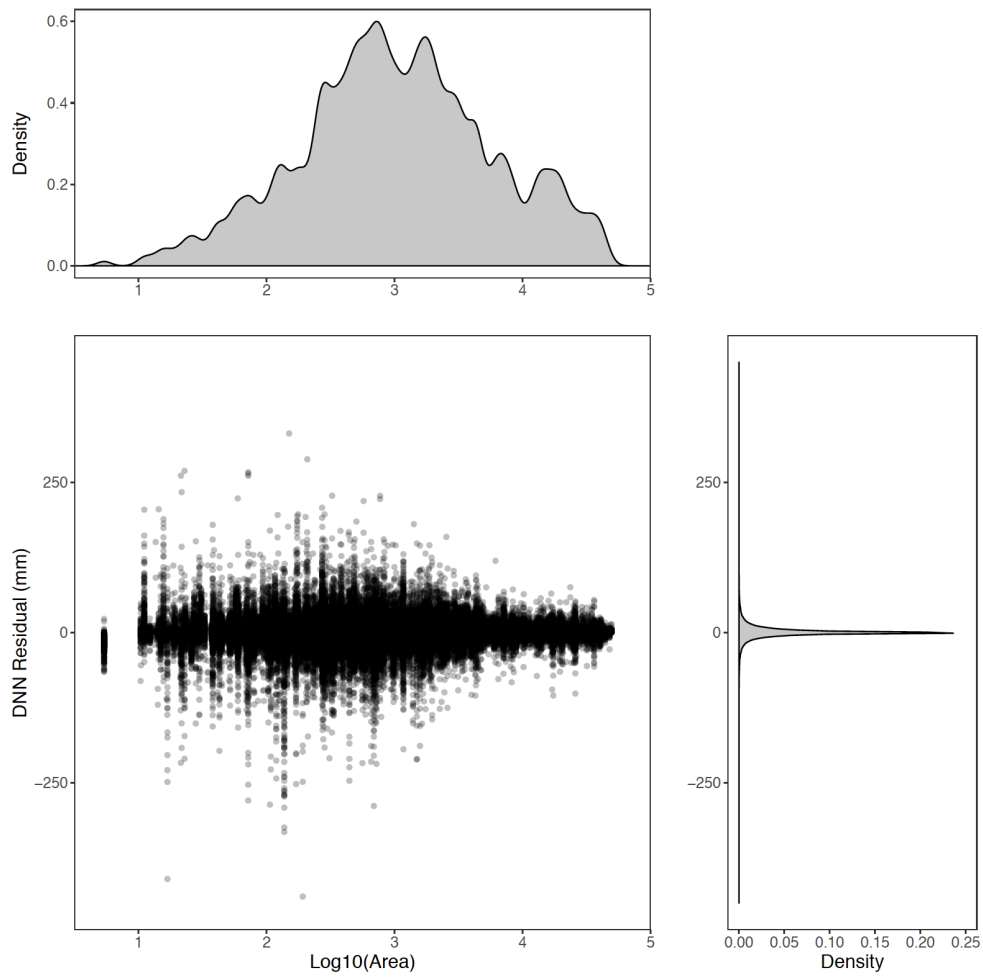




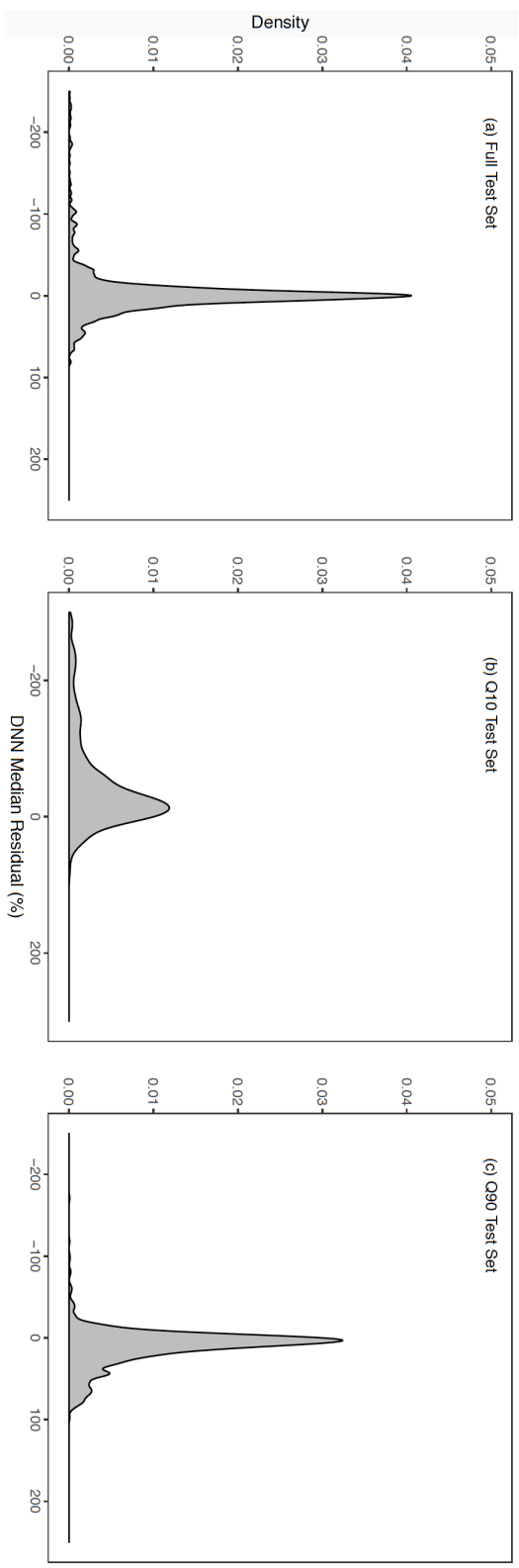
**Figure S4.** Geospatial Attributes of Gages for Evaluating Streamflow version II (GAGES-II; Falcone et al., 2010) watershed ecoregions used in this study.



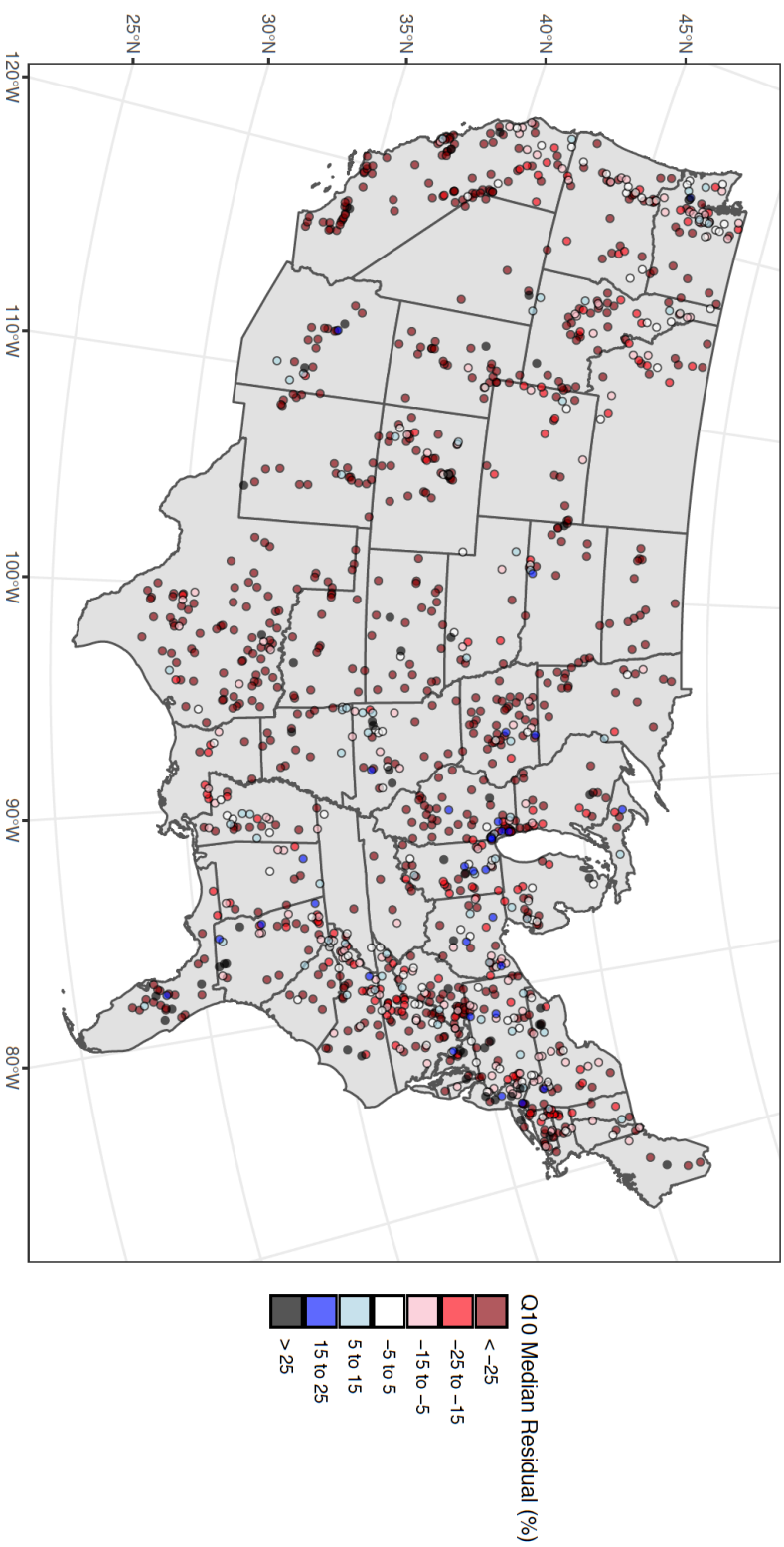
**Figure S5.** Deep neural network (DNN) test set results showing (a) DNN residual density distribution, (b) DNN residual histogram, (c) DNN qq-plot with random normal line-of-best-fit, (d) DNN residuals versus time, (e) DNN residuals versus longitude of the watershed centroid, and (f) DNN residuals versus latitude of the watershed centroid.



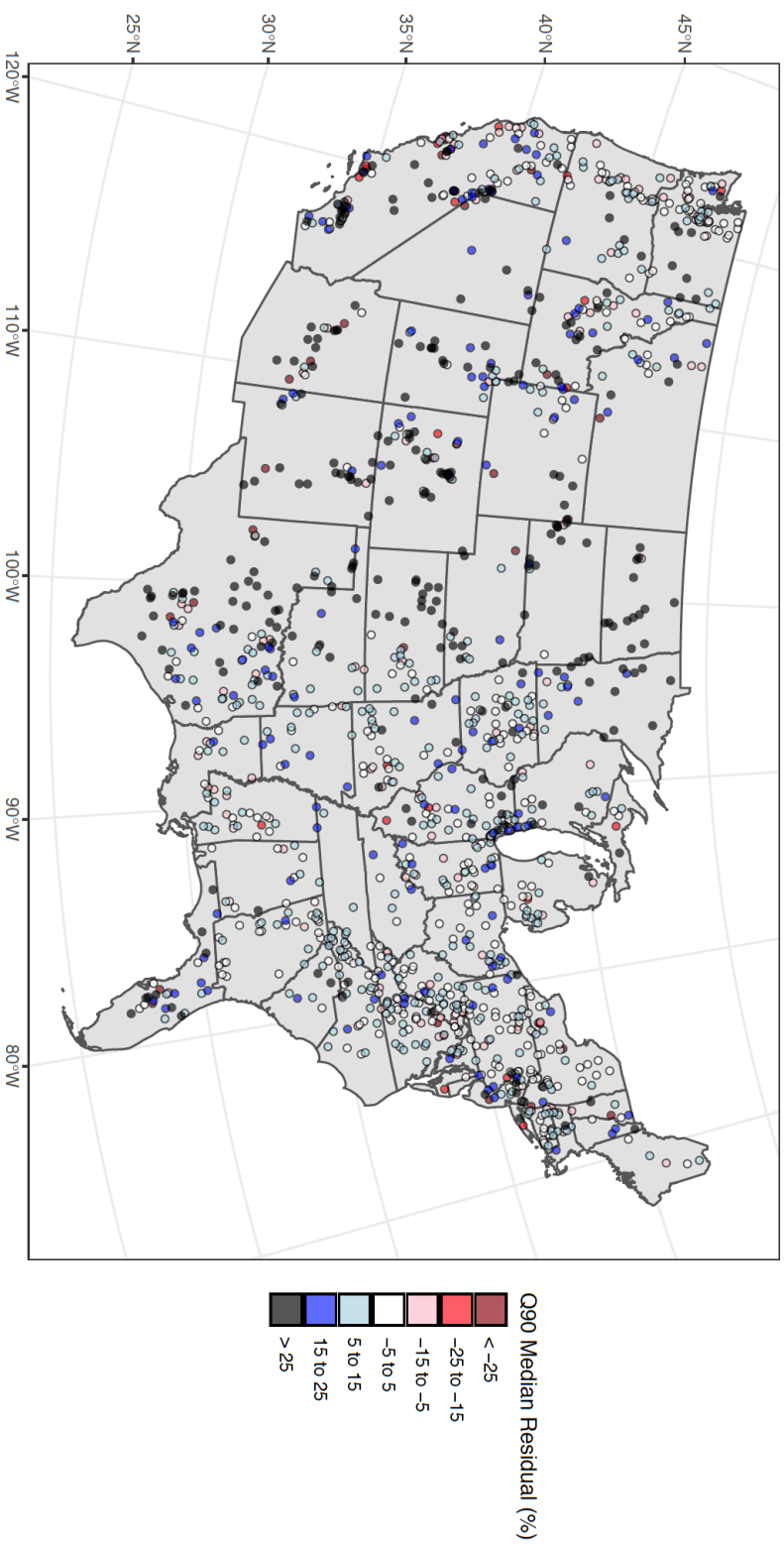
**Figure S6.** Deep neural network (DNN) test set results showing DNN residuals versus logged (base 10) watershed area (center panel). Top panel shows the distribution of logged watershed areas and right-side panel shows the distribution of DNN residuals (i.e., the same as Figure S5a).



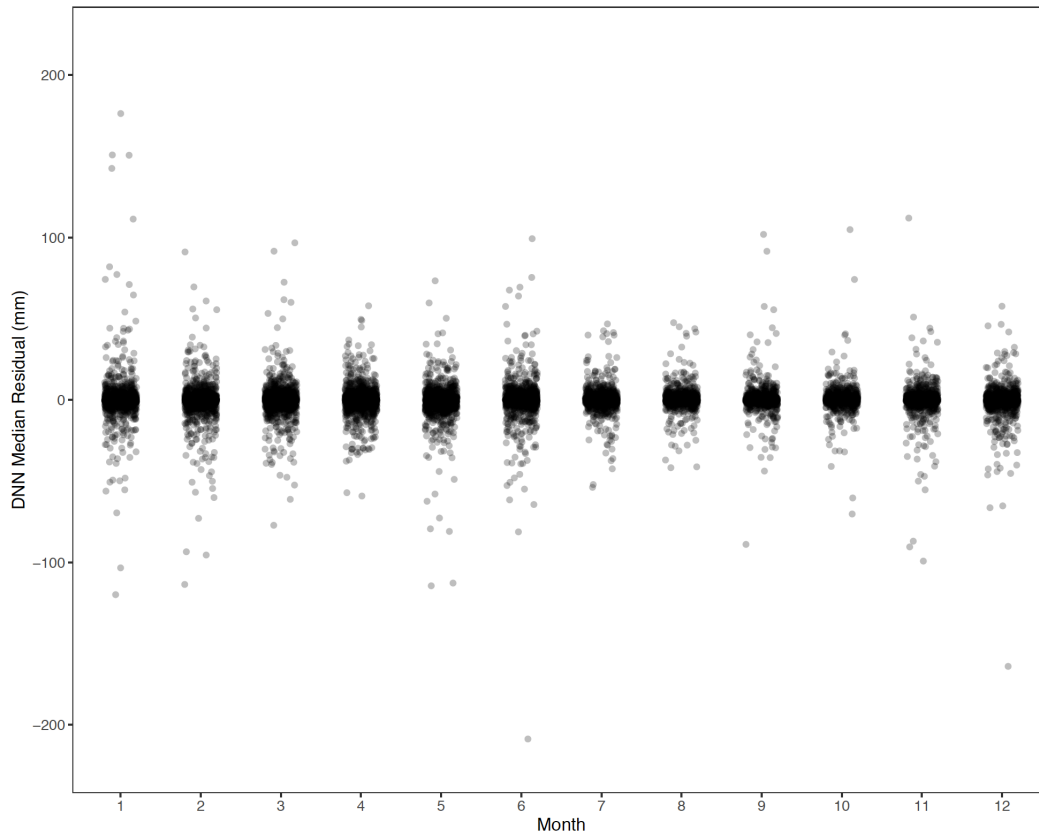
**Figure S7.** Deep neural network watershed median residual density plots for the (a) full test set, (b) Q10 event test set, and (c) Q90 event test set.



**Figure S8.** Deep neural network test set Q10 event median watershed residuals expressed as a percent relative to observations. Point location represents the watershed centroid.



**Figure S9.** Deep neural network test set Q90 event median watershed residuals expressed as a percent relative to observations. Point location represents the watershed centroid.



**Figure S10.** Deep neural network median watershed residuals grouped by month.

January is equivalent to 1 and December is equivalent to 12.

**Table S1.** List of watershed characteristics included as deep neural network input variables (i.e., features). Abbreviations: Coupled Model Intercomparison Project Phase 5 (CMIP5; Maurer et al., 2007; Taylor et al., 2012), United States Geological Survey Geospatial Attributes of Gages for Evaluating Streamflow version II (USGS GAGE-II; Falcone et al., 2010), digital elevation model (DEM), United States Geologic Survey National Elevation Dataset (USGS NED; USGS, 2013).

Number	Variable Name	Description	Units	Data Source
1	LAG0_P	Watershed aretially averaged total monthly precipitation for each month	mm	CMIP5 output
2	LAG1_P	Watershed aretially averaged one month lagged total monthly precipitation for each month	mm	CMIP5 output
3	LAG2_P	Watershed aretially averaged two month lagged total monthly precipitation for each month	mm	CMIP5 output
4	LAG3_P	Watershed aretially averaged three month lagged total monthly precipitation for each month	mm	CMIP5 output
5	LAG0_ET	Watershed aretially averaged total monthly evapotranspiration for each month	mm	CMIP5 output
6	LAG1_ET	Watershed aretially averaged one month lagged total monthly evapotranspiration for each month	mm	CMIP5 output
7	LAG2_ET	Watershed aretially averaged two month lagged total monthly evapotranspiration for each month	mm	CMIP5 output
8	LAG3_ET	Watershed aretially averaged three month lagged total monthly evapotranspiration for each month	mm	CMIP5 output
9	LAG0_T	Watershed aretially averaged mean monthly surface temperature for each month	degrees C	CMIP5 output
10	LAG1_T	Watershed aretially averaged one month lagged mean monthly surface temperature for each month	degrees C	CMIP5 output
11	LAG2_T	Watershed aretially averaged two month lagged mean monthly surface temperature for each month	degrees C	CMIP5 output
12	LAG3_T	Watershed aretially averaged three month lagged mean monthly surface temperature for each month	degrees C	CMIP5 output
13	PPTAVG_BASIN	Average annual precipitation for the watershed from 800m PRISM data for 30-year record (1971-2000)	cm	USGS GAGES-II
14	T_AVG_BASIN	Average annual air temperature for the watershed from 2km PRISM data for 30-year record (1971-2000)	degrees C	USGS GAGES-II
15	WD_BASIN	Watershed mean annual number of days of measurable precipitation from 2km PRISM data from 30-year record (1961-1990)	days	USGS GAGES-II
16	SNOW_PCT_PRECIP	Mean snow percent of total precipitation estimate for period 1901-2000, 1km grid	%	USGS GAGES-II
17	LAT_CENT	Latitude of the watershed geographic centroid	decimal degrees	USGS GAGES-II
18	LONG_CENT	Longitude of the watershed geographic centroid	decimal degrees	USGS GAGES-II
19	ELEV_MEAN_M_BASIN	Mean watershed elevation	m	USGS GAGES-II
20	ELEV_STD_M_BASIN	Standard deviation of watershed elevation	m	USGS GAGES-II
21	RRMEAN	Mean watershed relief ratio, which is equal to the difference between the maximum and minimum watershed elevation over the total length of streams in the watershed	NA	USGS GAGES-II
22	RRMEDIAN	Median watershed relief ratio	N/A	USGS GAGES-II
23	SLOPE_PCT	Mean watershed percent slope	%	USGS GAGES-II
24	SLOPE_SD	Standard deviation of watershed slope	%	USGS GAGES-II
25	UAA_MEAN	Mean watershed upslope accumulation area (UAA) after scaling UAA values from 0 - 1 using maximum scaling	m	USGS GAGES-II
26	UAA_SD	Standard deviation of watershed upslope accumulation area (UAA) after scaling UAA values from 0 - 1 using maximum scaling.	m	USGS GAGES-II
27	BAS_COMPACTNESS	Watershed compactness ratio, which is equal to watershed area divided by the watershed perimeter squared times 100; the higher the compactness ratio, the more compact the watershed shape	N/A	DEM from the USGS NED USGS GAGES-II

Continues on next page.



Number	Variable Name	Description	Units	Data Source
28	TOPWET	Watershed topographic wetness index, which is equal to $\ln(UAA/S)$ ; where "ln" is the natural log, "a" is UAA at a given point and "S" is the slope at that point	N/A	USGS GAGES-II
29	MAINSTEM_SINUOSITY	Sinuosity of mainstem stream line, from GAGES-II delineation of mainstem stream lines. Equal to the curvilinear length of the mainstem stream line divided by the straight-line distance between the end points of the line	N/A	USGS GAGES-II
30	STREAMS_KM_SQ_KM	Watershed stream density, relative to watershed area	km per sq km	USGS GAGES-II
31	ROADS_KM_SQ_KM	Watershed road density, relative to watershed area	km per sq km	USGS GAGES-II
32	CLAYAVE	Watershed average percent of clay content in soils	%	USGS GAGES-II
33	SANDAVE	Watershed average percent of sand content in soils	%	USGS GAGES-II
34	SILTAVE	Watershed average percent of silt content in soils	%	USGS GAGES-II
35	ROCKDEPAVE	Watershed average percent of total soil thickness	in	USGS GAGES-II
36	DEVNLCDD6	Watershed percent "developed" from the 2006 NLCD. Sum of classes 21, 22, 23, and 24	%	USGS GAGES-II
37	FORESTNLCDD6	Watershed percent "forest" from the 2006 NLCD. Sum of classes 41, 42, and 43	%	USGS GAGES-II
38	PLANTNLCDD6	Watershed percent "planted/cultivated" from the 2006 NLCD. Sum of classes 81 and 82	%	USGS GAGES-II
39	GRASSNLCDD6	Watershed percent "grassland" from the 2006 NLCD. Includes class 71	%	USGS GAGES-II
40	WOODYWETNLCDD6	Watershed percent Woody Wetlands (class 90) from 2006 NLCD	%	USGS GAGES-II
41	EMERGWEINLCDD6	Watershed percent Emergent Wetlands (class 96) from 2006 NLCD	%	USGS GAGES-II
42	RIP100_DEV	Riparian 100 m buffer "developed" from the 2006 NLCD. Sum of classes 21, 22, 23, and 24. Buffer area spans 100 m on each side of stream centerline for all streams in watershed	%	USGS GAGES-II
43	RIP100_FOREST	Riparian 100 m buffer "forest", 2006 era NLCD. Sum of classes 41, 42, and 43. Buffer area spans 100 m on each side of stream centerline for all streams in watershed	%	USGS GAGES-II
44	RIP100_PLANT	Riparian 100 m buffer "planted/cultivated" from the 2006 NLCD. Sum of classes 81 and 82. Buffer area spans 100 m on each side of stream centerline for all streams in watershed	%	USGS GAGES-II
45	RIP100_71	Riparian 100 m buffer "grassland" from the 2006 NLCD. Includes class 71, buffer area spans 100 m on each side of stream centerline for all streams in watershed	%	USGS GAGES-II
46	RIP100_90	Watershed percent Woody Wetlands in 100m riparian 100m buffer from 2006 NLCD	%	USGS GAGES-II
47	RIP100_95	Watershed percent Emergent Wetlands in 100m riparian 100m buffer from 2006 NLCD	%	USGS GAGES-II
48	BFI_AVG	Watershed average base flow index (BFI), equal to the ratio of base flow to total streamflow, ranges from 0% to 100%	%	USGS GAGES-II
49	CONTACT	Subsurface flow contact time index, which estimates the number of days that infiltrated water resides in the saturated subsurface zone of the basin before discharging into the stream	days	USGS GAGES-II
50	MITDEPAVE	Watershed mean depth to seasonally high water table	ft	USGS GAGES-II
51	CAL_MONTH_1	Calendar month (0 for non-January month, 1 for January)	N/A	This study
52	CAL_MONTH_2	Calendar month (0 for non-February month, 1 for February)	N/A	This study
53	CAL_MONTH_3	Calendar month (0 for non-March month, 1 for March)	N/A	This study
54	CAL_MONTH_4	Calendar month (0 for non-April month, 1 for April)	N/A	This study
55	CAL_MONTH_5	Calendar month (0 for non-May month, 1 for May)	N/A	This study
56	CAL_MONTH_6	Calendar month (0 for non-June month, 1 for June)	N/A	This study
57	CAL_MONTH_7	Calendar month (0 for non-July month, 1 for July)	N/A	This study
58	CAL_MONTH_8	Calendar month (0 for non-August month, 1 for August)	N/A	This study
59	CAL_MONTH_9	Calendar month (0 for non-September month, 1 for September)	N/A	This study
60	CAL_MONTH_10	Calendar month (0 for non-October month, 1 for October)	N/A	This study
61	CAL_MONTH_11	Calendar month (0 for non-November month, 1 for November)	N/A	This study
62	CAL_MONTH_12	Calendar month (0 for non-December month, 1 for December)	N/A	This study

**Table S2.** Model performance comparisons for monthly Q10 and Q90 events in the test set. Abbreviations: Generalized Circulation Model (GCM), median absolute error (MAE), Pearson’s correlation coefficient (PCC), support vector machine (SVM), extreme gradient boosting (XGBoost), artificial neural network (ANN), and deep neural network (DNN). MAE and PCC are reported with the lower and upper 95% confidence intervals in parentheses.

Method	Q10 Test Set				Q90 Test Set			
	Bias (mm)	Slope	MAE (%)	PCC	Bias (mm)	Slope	MAE (%)	PCC
GCM Runoff	1.80	0.43	149.05 (144.55, 153.99)	0.506 (0.479, 0.534)	35.34	0.82	35.36 (34.93, 35.97)	0.767 (0.757, 0.779)
Monthly Normal Runoff	-1.11	0.41	293.91 (286.79, 301.05)	0.792 (0.780, 0.803)	26.82	1.41	48.45 (48.02, 48.86)	0.871 (0.865, 0.877)
Linear Ridge Regression	7.83	8.29E-15	>1000	0.159 (0.152, 0.167)	125.36	8.81E+00	>1000	0.188 (0.178, 0.198)
SVM	-1.30	0.29	736 (718.27, 755.52)	0.555 (0.536, 0.573)	-15.63	1.93	42.67 (42.29, 43.02)	0.824 (0.816, 0.832)
XGBoost	0.85	0.56	125.58 (121.67, 129.42)	0.797 (0.785, 0.811)	13.62	1.06	25.63 (25.26, 25.97)	0.934 (0.930, 0.937)
ANN	0.91	0.63	82.44 (80.38, 84.81)	0.703 (0.681, 0.724)	10.02	1.29	32.00 (31.61, 32.39)	0.908 (0.904, 0.912)
DNN	0.52	0.73	50.87 (49.49, 52.26)	0.880 (0.869, 0.892)	12.94	0.94	15.96 (15.66, 16.27)	0.956 (0.953, 0.958)

**Table S3.** Model performance comparisons for non-reference and reference watersheds in the test set. Abbreviations: Generalized Circulation Model (GCM), Pearson’s correlation coefficient (PCC), support vector machine (SVM), extreme gradient boosting (XGBoost), artificial neural network (ANN), and deep neural network (DNN). PCC is reported with the lower and upper 95% confidence intervals in parentheses.

Method	Non-reference Test Set			Reference Test Set		
	Bias (mm)	Slope	PCC	Bias (mm)	Slope	PCC
GCM Runoff	7.06	0.81	0.787 (0.781, 0.793)	9.02	0.93	0.841 (0.835, 0.848)
Monthly Normal Runoff	0.08	1.01	0.795 (0.791, 0.799)	0.20	0.99	0.829 (0.823, 0.834)
Linear Ridge Regression	38.53	3.42E-14	0.164 (0.160, 0.168)	57.85	6.18E-14	0.126 (0.118, 0.133)
SVM	16.12	1.23	0.755 (0.750, 0.759)	23.46	1.45	0.792 (0.785, 0.797)
XGBoost	-0.08	1.01	0.920 (0.917, 0.922)	-0.34	1.02	0.948 (0.945, 0.950)
ANN	0.308	1.16	0.900 (0.897, 0.902)	-1.19	1.23	0.935 (0.932, 0.937)
DNN	2.36	0.94	0.954 (0.953, 0.957)	2.60	0.95	0.971 (0.969, 0.973)

**Table S4.** Modeled versus observed runoff bias comparisons by ecoregion for the test set. Abbreviations: Generalized Circulation Model (GCM), support vector machine (SVM), extreme gradient boosting (XGBoost), artificial neural network (ANN), and deep neural network (DNN).

Model	Central Plains	East Highlands	Mixed Wood Shield	Northeast	Southeast Coastal Plain	Southeast Plain	West Mountains	West Plains	West Xeric
GCM Runoff	1.96	7.98	13.55	8.07	3.23	2.79	13.56	0.55	2.63
Monthly Normal Runoff	-0.03	-0.03	0.04	-0.05	-0.30	-0.15	-0.08	-0.01	-0.10
Linear Ridge Regression	21.22	41.26	55.34	54.61	29.21	39.21	120.11	11.64	14.43
SVM	-20.46	-48.82	-11.48	-66.89	-14.97	-35.59	-18.87	-3.63	0.01
XGBoost	-0.62	-2.12	-0.24	-3.19	2.46	0.59	-0.41	-0.22	0.74
ANN	0.38	-1.24	5.28	-2.44	4.88	-0.25	1.31	0.69	1.33
DNN	1.46	1.85	1.98	0.83	7.31	1.82	2.49	0.84	1.97

**Table S5.** Modeled versus observed runoff slope comparisons by ecoregion for the test set. Abbreviations: Generalized Circulation Model (GCM), support vector machine (SVM), extreme gradient boosting (XGBoost), artificial neural network (ANN), and deep neural network (DNN).

Model	Central Plains	East Highlands	Mixed Wood Shield	Northeast	Southeast Coastal Plain	Southeast Plain	West Mountains	West Plains	West Xeric
GCM Runoff	1.07	0.95	1.01	1.02	0.76	0.96	0.81	0.76	0.56
Monthly Normal Runoff	1.01	1.00	1.00	1.00	1.01	1.01	0.99	0.99	1.03
Linear Ridge Regression	-5.01E-15	-4.82E-14	2.56E-13	5.41E-14	-7.75E-15	3.99E-14	1.88E-13	2.23E-14	1.37E-14
SVM	1.29	1.79	1.30	2.20	1.05	1.55	1.37	0.65	0.77
XGBoost	1.03	10.50	1.10	1.07	0.96	1.00	1.01	1.00	0.90
ANN	1.11	1.16	1.14	1.14	1.08	1.14	1.22	1.19	1.24
DNN	0.96	0.97	1.08	0.98	0.87	0.98	0.93	0.96	0.89

**Table S6.** Modeled runoff versus observed runoff Pearson’s correlation coefficient comparisons by ecoregion for the test set. Abbreviations: Generalized Circulation Model (GCM), support vector machine (SVM), extreme gradient boosting (XGBoost), artificial neural network (ANN), and deep neural network (DNN).

Model	Central Plains	East Highlands	Mixed Wood Shield	Northeast	Southeast Coastal Plain	Southeast Plain	West Mountains	West Plains	West Xeric
GCM Runoff	0.81	0.83	0.58	0.81	0.68	0.86	0.80	0.74	0.73
Monthly Normal Runoff	0.56	0.66	0.84	0.70	0.61	0.60	0.86	0.60	0.66
Linear Ridge Regression	-0.06	-0.07	0.41	0.06	-0.07	0.08	0.42	0.17	0.07
SVM	0.73	0.78	0.53	0.69	0.56	0.77	0.78	0.58	0.59
XGBoost	0.88	0.91	0.85	0.88	0.77	0.90	0.95	0.84	0.84
ANN	0.88	0.91	0.72	0.88	0.79	0.90	0.92	0.78	0.80
DNN	0.94	0.96	0.83	0.94	0.80	0.95	0.97	0.91	0.90