

FLUX TO FLOW: A CLEARER VIEW OF EARTH'S WATER CYCLE

VIA NEURAL NETWORKS AND SATELLITE DATA

BY

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ABSTRACT

Earth's weather and climate changes dynamically, and humans must monitor the evolution of our environment or fail to plan and adapt. Water is our most valuable resource, and as such it is of the utmost importance to have a continuous view of its movements as water cycles over, in, and under land, in the atmosphere, and in the sea. One way that we observe the water cycle is with satellite measurements. Unfortunately, the resolution of these instruments is typically too coarse to visualize many transient phenomena of interest. If their vision is fine enough, the instrument captures only a small space of Earth at any given time. Furthermore, it is valuable to connect satellite-derived water cycle measurements of large watershed basins with ground truth observations of the rivers flowing through these basins. These connection operations, though, are time and cost prohibitive or limited in performance, with efficient functions veiled behind black box closed-source solutions. Herein, all of the above facts are investigated under the veil of a single name, Flux to Flow (F2F). The name Flux to Flow encapsulates how the work takes several fluxes of geospatial data and transforms them into more coherent flows of knowledge. F2F performs metrologically well in the operation of streamflow forecasting when focused solely on a single or a few hydrological monitoring nodes at a time. Based on the results, future work might entail scaling up of the system to many computing nodes running in tandem, observing more adjacent outputs, or in its application as a standard device in connected municipal systems.

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PREFACE

This thesis follows the manuscript format. Each of the three within carry a similar structure as is typical of the structure one might produce for an academic journal. The three cords form one strand that benefit from being studied together.

Manuscript 1, “Discerning Hydroclimatic Behavior with a Deep Convolutional Residual Regressive Neural Network”, looks at four United States basins and a single streamflow measurement per basin. It also considers just one neural network architecture called Flux to Flow. Upon further consideration, we have realized that the structure itself is more aptly called dcrrnn and pronounced discern. It is called this for two reasons: 1, because of the nature of a trained mind’s ability to learn how to discern the truth from a flurry of information; and 2, because it is an acronym representing the phrase “deep convolutional residual regressive neural network”. The name dcrrnn was accidental and an obfuscation device just to conceal as manuscript 1 was submitted to a double-blind submission. It was undesirable to share the name Flux to Flow because of our ties to the name on the web already. As the work has progressed, dcrrnn is now understood more appropriately as a very specific neural network construction, whereas F2F encompasses the macroscopy of the work. Though there is only a single architecture used in this manuscript, it is both dcrrnn and Flux to Flow. This study considers about seven years of data, considering a daily time scale.

Manuscript 2, “Deep Convolutional Residual Regressive Neural Networks and Sea Surface Temperatures from Aqua and Argo in the 2000s”, focuses in greater detail on a single water-focused essential climate variable (sea surface temperature). The deployed experiments, similar to manuscript 1, features solely the dcrrnn architecture under the name Flux to Flow. The time series studied is relatively short in time, only considering a single year of monthly measurements; however, the size of the geography studied is quite large, considering big pieces of the Atlantic, Pacific, and

Indian oceans.

Manuscript 3, “Holistic Water Cycle Analysis via the Confluence of Climate Model, Satellite, Ground Truth, and Machine Learning Signal Processing Technologies: Two North American Transboundary River Watersheds”, is best understood as the confluence of manuscripts 1 and 2. We fuse measurements of sea surface temperature with measurements of land flow and create images that do not contain nan values, a sometimes frustrating numerical data structure component. We compare the performance of using these fused images against the original technique from manuscript 1 of simply clipping and z-scoring land surface flows and neglecting the ocean. We look at more output targets per moment than manuscript 1, but fewer than manuscript 2. We also use several different neural network constructions to compare the dcrrnn structure against other simpler neural network structures.

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LIST OF ABBREVIATIONS

F2F, Flux to Flow

dcrnn, deep convolutional residual regressive neural network

USGS, United States Geological Survey

NASA, National Aeronautics and Space Administration

AMSR-E Advanced Microwave Scanning Radiometer for EOS

NLDAS, National Land Data Assimilation System

GLDAS, Global Land Data Assimilation System

MODIS, Moderate Resolution Imaging Spectroradiometer

EOS, earth observation system

kg/m², kilograms per square meter

TTS, train test split

NSE, Nash Sutcliffe efficiency

KGE, Kling Gupta efficiency

f³s⁻¹, cubic feet per second

A, actual

M, model

AM, acceptable measurements

σ , standard deviation

KDE, kernel density estimate

.nc, netCDF file

GRACE, Gravity Recovery and Climate Experiment

UTC, Coordinated Universal Time

REMSS, Remote Sensing Systems

PODAAC, Physical Oceanography Distributed Active Archive Center

CMIP, Coupled Model Intercomparison Project

MNIST, Modified National Institute of Standards and Technology

CIFAR, Canadian Institute for Advanced Research
MAE, Mean Average Error
MSE, Mean Squared Error
RMSE, Root Mean Squared Error
GPU, graphics processing unit
K, degrees Kelvin
MW, megawatts
GCD, Grand Coulee Dam
NWIS, National Water Information System
DS, dataset
DOI, digital object identifier
ECV, essential climate variable
L0-L4, levels of NASA data
nan, non-numerical
SST, sea surface temperature
RS, remote sensing
CO₂, carbon dioxide
Q_s, surface flow
Q_{sb}, subsurface flow
m, meters
km, kilometers
nn, neural network
i/o, inputs and outputs
EPA, Environmental Protection Agency
ESI, evaporative stress index
US, United States of America
ETo, reference evapotranspiration

VIIRS, Visible Infrared Imaging Radiometer Suite

GOES, Geostationary Operational Environmental Satellite

nb, *nota bene*

ReLU, rectified linear unit

MDPI, Multidisciplinary Digital Publishing Institute

Δ , difference between two numbers

MANUSCRIPT 1

Discerning Watershed Response to Hydroclimatic Extremes
with a Deep Convolutional Residual Regressive Neural Network

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1.1 Abstract

The impact of climate change continues to manifest itself daily in the form of extreme events and conditions like droughts, floods, heatwaves, and storms. Better forecasting tools are mandatory to calibrate our response to these hazards and help adapt to the planet's dynamic environment. Here, we present a deep convolutional residual regressive neural network (dcrrnn) platform called Flux to Flow (F2F) for discerning the response of watersheds to water cycle fluxes and their extremes. We examine four United States drainage basins of varying acreage from smaller to very large (Bear, Colorado, Connecticut, and Mississippi). F2F combines model and ground observations of water cycle fluxes (precipitation, soil moisture, surface runoff, sub-surface baseflow) to simulate, visualize, and analyze watershed basin response to the varying climates and magnitudes of hydroclimatic fluxes in each river basin. Experiments modulating time lag between remotely sensed and ground truth measurements are performed to assess the metrological limits of forecasting with this platform. The resultant mean Nash Sutcliffe and Kling Gupta efficiency values are both of greater value than 90%. Our results indicate that F2F can be a powerhouse for forecasting watershed response to hydroclimatic extremes in a changing global climate.

1.2 Keywords

water, climate, sustainability, supervised representation learning, societal considerations

1.3 Introduction

Water connects all living things on Earth. It is wielded to power electronic devices, enables plants, food, and animals to grow, serves as the living and recreational space for all creatures, and is nourishment to the human body. It has been both the

subject of, platform for, and weapon of choice in numerous conflicts. Global hydraulic infrastructure is highly variable. Dirty water can be a source of disease and death. It is branded, modified, and sold at differing levels of purity and concentration. The cost of equipment to control the flow of water is high, maintenance is frequent, and changes in demand and supply for water as a resource are constant sources of concern.

Human activities have changed and continue to change Earth's environment. The changes are visible in both short (meteorological) and long (climatological) time scale responses ([58]). As the temperature of Earth increases, the amount of snow and sea ice loses volume over time ([52]; [46]), sea levels rise and swallow up once inhabited land ([59]; [55]), storms intensify ([37]), droughts last longer ([62]), floods become more severe ([45]; [29]), animal populations go extinct ([50]), and the availability of freshwater becomes more unreliable ([21]). Concurrently, manmade Earth observation and control systems continue to improve ([15]; [47]).

Watershed modeling is an important field of research that involves predicting the movement of water through the Earth's system. Earth's system consists of the land, atmosphere, and ocean. Many models have been developed to simulate and predict hydrologic processes, including rainfall, runoff, and evapotranspiration. One popular model is the Soil and Water Assessment Tool (SWAT), which has been used extensively to model hydrology and water quality in watersheds ([1]). Another model, the Variable Infiltration Capacity (VIC) model, has been employed to study changes in streamflow and soil moisture ([6]). General circulation models (GCMs) are an additional important tool in hydrology modeling. GCMs simulate the Earth's climate system, including atmospheric circulation, ocean circulation, and the cryosphere, and provide predictions of future climate conditions ([38]). These models have been used to study the impacts of climate change on water resources and hydrologic processes, such as changes in precipitation patterns and snowmelt runoff ([64]). In addition, GCMs can be coupled with regional ocean modeling systems (ROMS) to study ocean

circulation and its impact on coastal ecosystems ([26]). The Massachusetts Institute of Technology General Circulation Model (MITgcm) is another popular model used to simulate ocean circulation and study the impacts of climate change on marine ecosystems ([43]).

Here, we approach the topic of watershed modeling with a deep neural network. We observe the connections between model output of four United States drainage basins to actual gauged in the river measurements. All basins are larger than a million acres and thus provide ample data to observe how changes in runoff and subsurface flow impacts the quantity of water discharging from the major river within the basin. Given our results, we envision future work applying the same tools to study and consider all of Earth's watersheds at fine fidelity.

1.4 Materials & Methods

1.4.1 Study Areas

Four United States drainage basins with areas of greater than one million acres each were selected as study areas and are shown in Figure 1.1. The Bear River and Connecticut River watersheds are significantly smaller than either the Mississippi River or the Colorado River basins. The satellite imagery used observes approximately 100 square kilometers of area (on the order of 25,000 acres) in each pixel.

1.4.2 Satellite Derived Observations

For each basin there are two input images extracted from raw data obtained through the NASA Goddard Earth Sciences Data and Information Services Center. The raw data is National Land Data Assimilation System (NLDAS) model output. NLDAS is a project run by several United States based institutions and universities. NLDAS takes continental scale meteorological data parameters (e.g., air temperature, wind speed, surface pressure, precipitation, incoming radiation, specific humidity) as

input and deterministically creates water and energy flux layers as outputs. The NLDAS project in its second phase applies several different water and energy balance algorithms to create flux outputs from one common set of meteorological inputs. Here, the Noah water and energy budget algorithm is used. The channels of interest are components of water flux, specifically surface and sub-surface runoff, as they collectively represent the lateral movement of liquid water along and under the surface towards the terminal drainage point at a given point in time ([67]; [41]).

1.4.3 Ground Truth Measurements

Concurrent with the two NLDAS channels is a single gauged in the river streamflow measurement. Daily streamflow measurements from sites near the terminus of each basin are obtained from the United States Geological Survey's National Water Information System. The USGS operates nearly 30,000 daily streamflow data collectors ([17]). Sites were selected based on the availability, proximity to the terminal point of the basin, and relative continuity of data. Gaps in data collection are solved with linear interpolation.

Ground truth streamflow data are critical for hydrologic modeling, as they provide a means of validating and calibrating model results. The USGS National Water Information System (NWIS) is a primary source of ground truth streamflow data in the United States ([54]). The NWIS is a network of over 1.5 million sites that collect measurements of water, some of which are then used to calculate streamflow ([48]). These gauges are operated by the USGS in collaboration with other federal, state, and local agencies, as well as private organizations. The data collected by the NWIS are used for a wide range of applications, including flood forecasting, water management, and environmental assessments ([57]).

The NWIS stream gauges provide a valuable resource for monitoring and managing the nation's water resources. The network covers a broad range of water bodies,

including rivers, streams, lakes, and reservoirs, and the data collected help to support a variety of water-related activities. For example, the streamflow data collected by the NWIS are used to support flood forecasting efforts, which are essential for public safety and property protection. In addition, the data are used to assess water availability for agriculture, industry, and domestic use, and to monitor the health of aquatic ecosystems. Finally, the NWIS streamflow data are used by researchers and policy-makers to develop and refine models of the water cycle, which are critical for understanding the impacts of climate change and human activities on water resources.

The USGS has a long history of collecting and analyzing streamflow data, dating back to the late 19th century when the agency was established ([5]). Since then, the network of stream gauges has expanded and become more sophisticated, incorporating new technologies such as acoustic Doppler current profilers and advanced telemetry systems ([48]). The USGS has also played a key role in developing standardized methods for collecting, processing, and analyzing streamflow data, which have been adopted by other countries around the world ([30]). Today, the USGS continues to operate and maintain the largest network of stream gauges in the United States, providing a valuable resource for hydrologic research and water resources management ([57]). With the growing importance of water resources management and the increasing threat of climate change, the role of the NWIS in monitoring and managing the nation's water resources is more critical than ever.

1.4.4 Data Collection and Preprocessing

For this study, we looked at the time range starting on January 1, 2015, until the most recent output available, March 1, 2022. The NLDAS model output is available in a monthly and hourly product. We combine the hourly data available for surface and subsurface streamflow into a daily product. The raw hourly NLDAS product with all variables is a directory sized 351 gigabytes comprised of 62,805 hourly files.

The summing and extraction of lateral flows shrunk the total file size by a factor of more than 150. Each raw data file consumes 5.8 megabytes of disk space, while each daily surface and subsurface flow extraction 822.7 kilobytes. Filtered data consumes only 2.1 gigabytes and can easily be held on a graphical processing unit when trained with the neural network. File size decreases further when clipped to a particular basin. Images are z-scored relative to themselves, while gauged streamflow data is z-scored relative to the entire time series of seven years. Whitening has been shown to improve the performance of training a neural network ([36]; [13]).

1.4.5 Treatment

For this experiment, we constructed a deep, convolutional, residual, regressive neural network. The images of Earth’s surface and subsurface water flow are passed through this network. Eventually, the transformed images reach a destination where the image shapes have been constrained in size to match that of the target of the input pair; here, the target is one pixel as the daily value for gauged streamflow is a single physical measurement. The problem is one of regression because the prediction of streamflow is continuous and can theoretically be any value greater than zero. We use convolutional neural networks because our input to the network is a sequence of two channel images ([53]). We also use residual learning, which allows us to make the network very deep but control the opacity of the initial structure of the image. This makes training faster ([27]). Rectified linear unit activation functions are applied in all but the last layer of nodes, and batch normalization is used in the residual layers ([2]; [33]). Batch normalization is like the z-score treatment in our preprocessing step. Finally, we selected a variant of stochastic gradient descent for optimization of the neural network nodes ([3]; [39]).

1.5 Results

Hourly NLDAS model outputs of surface and subsurface flow are summed to daily accumulations over the time span of January 1st, 2015, to March 1st, 2022. This time series is 2,617 long comprised of two channel images. Channels are surface and subsurface flow measured in units in kilograms per square meter. Units are analogous to the weight of water in a location. Sample observation output from each basin capturing flow behavior on June 6th, 2021, is displayed in Figure 1.2. The effects of spatial resolution are apparent, as the Bear River and Connecticut River basins have pronounced rectangular edges due to their relatively small size. This pixelation effect is not present in the Mississippi River and Colorado River observations of lateral flow from the basin view at this constrained figure size.

Gauged streamflow measurements of the four target rivers are significantly different in magnitude from one another; therefore, we process each with a z-score treatment to center their mean values around the number zero and standardize each increasing and decreasing integer around intervals of standard deviation. Figure 1.3 shows plots of the gauged streamflow measurements of each basin are plotted in two ways. The four individual strip charts show the change in streamflow over time, and the single overlapping histograms show how often actual measurements in the respective basin occur relative to the average discharge. This is a single dimensional z-scoring system. We also perform a two dimensional treatment to each of the input channels, surface, and subsurface streamflow. Whereas the 1-D treatment uses the entire time series of gauged streamflow measurements for computation, 2-D z-scores are computed based on a single image at a time. Modifiable hyperparameters controls of the network are basin under observation, lag in time between input and output datasets, number of training epochs (forward and backward passes of the neural network) and the ratio of training data to testing data. There is also an override for stopping the model training early when the training data has a Nash Sutcliffe

efficiency (NSE) value of a variable efficiency percentage.

Figure 1.4 shows a sample output from one configuration of the neural network. The topmost graph illustrates the time series of discharge measurements in cubic feet per second of the Bear River. This graph is rotated ninety degrees relative to its sibling hydrograph in Figure 1.3. There is a notable seasonality to this streamflow measurement of Bear. Spring brings melting snowpack in the nearby mountainous terrain and subsequent increases in neighboring river flows. Spring melting snow in 2021 appears more subdued than all other years observed. The Bear River drainage basin is located in between the Great Salt Lake and Yellowstone National Park in the Rocky Mountain region of the United States. The eponymously named river flows in a counterclockwise loop.

The second row plots each modeled observation in the time series against its respective actual measurement. On the left is a study of the model output ordered on the x-axis from low to high flows and corresponding actual measurement on the y-axis. The right plot retains the same axis labels, but instead observes spatial proximity of values. Darker points are more commonly occurring ranges of flow. The left plot also contains two lines of best fit, the ideal or desired line found from the data, and the actual line of fit as exists between the actual gauged streamflow and the neural network model output of streamflow from surface and subsurface flow.

The third and final row shows epochal values during the neural network training process. On the left, the average error between the actual measurements and network output declines as the model goes through its iterations of propagate and backpropagate. Concomitant with error vs. epoch is efficiency vs. epoch. As the error declines towards zero, the NSE measurement increases towards 100%. Here, neural network set to stop at an NSE value of 95%, which occurs in the sixth epoch.

We perform nine iterations of the configuration of 252 experiments. For each of the four basins, there are sixty three experiments per iteration based on nine possible

values of lag and seven possible values of training and test data split, equating to 2,268 individual runs of the same neural network. Each experiment either stops when the measurement of average NSE of the training dataset within an epoch equals 95% (bottom right, Figure 1.4) or the total number of epochs of back and forward propagation of the entire basin dataset reaches 100. Computations are constrained to a single node with two central processing units, a single NVIDIA GeForce RTX 2080 Ti graphical processing unit, and no more than 130 gigabytes of random access memory. Our platform is written in the python programming language and managed with the miniconda package manager. The total run time to compute the experiments within was 83.0 hours.

1.6 Discussion

The results presented indicate relatively favorable performance of the neural network architecture when transforming of surface and subsurface flow into a prediction of basin gauged streamflow; the kernel density estimates (KDE) in Figure 1.5 and Figure 1.6 illustrate this point. We executed a total of more than 2,200 experiments in total using the common architecture. We use two hydrological metrics: Kling Gupta (KGE) and Nash Sutcliffe (NSE) ([49]; [25]; [24]; [40]). For each of these metrics, the peak resultant merit value of the 2,268 experiments is greater than ninety percent with a standard deviation of less than 0.06. The results are tolerant to lagging the data beyond the residence time of water in the atmosphere ([63]; [20]).

Others have observed the changing water quantity of the Mississippi. One study used NLDAS data focused on a subsection of the Mississippi with a higher quantity of streamflow target sites ([51]). Another group considers a different data system altogether for watershed modeling on the upper Mississippi basin ([12]). Some groups suggest that NLDAS is too simplistic and decided to create their own blend. They take a much broader approach than the scope of the problem observed here ([60]).

The same is true for another study, where the study considers several different models and about 1,000 small river basins ([8]). Some use meteorological data as a predictor for electric outages, as seen in a study looking at Connecticut. They, too, use the Nash Sutcliffe efficiency as a figure of merit ([68]) but are approaching the problem with a different lens. Their target is a smaller population and the risk of being without electric power.

This process can be expanded in different ways. Our study relies on the internal programming of NLDAS to compute surface and subsurface flow. There is much uncertainty in these observations based on the natural heterogeneity of the land surface. We do not look at the independent influence of any single forcing variable. Take snow, for example. In large mountain proximal basins such as those near the Rocky Mountains or Himalayan ranges, accumulation of subzero degrees Celsius water in solid form provides a continuous upland buffer tank for the communities with which the river down land serves. As the relative presence of carbon dioxide increases and the land temperature responds in agreement, the duration and scale of snow melt and sea ice responds. It is challenging to equate with exact certainty how much solid water exists. To a degree, interpolating satellite data with gauged data is sufficient, but these apparatuses are challenging to maintain in cold temperatures or in places of very high altitude. One could elect to observe more individual locations as targets, therefore making the relationship no longer image to single value at a given time, but instead image to image. There are studies that consider the impact of slow moving oceanic and atmospheric abnormalities upon the hydrology of the land. Independent variables include the Madden-Julian oscillation ([35]), the El Niño–Southern Oscillation ([31]), and the Atlantic meridional overturning circulation ([34]).

While the NLDAS product used here is of a particular spatial fidelity, the Global Land Data Assimilation System is coarser in its resolution. It is beneficial to the scientific community to have a clearer picture of the meteorological forcing and en-

vironmental responses in the ocean, land, air, and mixed interfaces. One could use this framework to fuse the high resolution NLDAS product with the global GLDAS product and evaluate the result according to one common set of metrics. The software could be packaged and ported to use with an already existent embedded in situ mesh system to provide forecasting information. Instead, one might consider looking at a different time signature, such as seasonally decomposed but over several years. Instead, one might introduce higher resolution localized water quality data into the model. By tracking environmental statistical anomalies relative to other points in time and relative to the global community, municipal decision makers can clue into the trajectory of their land, their structures, and their constituents within. The choice to retreat is not to be approached lightly, but in some instances is becoming the necessary measure ([56]; [28]). This intelligence can also be placed in the hands of consulting engineers to distribute in new and existing infrastructure. Logic is necessary to manage assets of complex hydraulic systems (pumps, motors, chemical feed, aeration, dewatering, gates, valves), and digital twin systems are becoming fashionable.

Water is a vital resource for human societies, and managing water resources is a complex task that requires continuous attention and adaptation. In recent years, the world has witnessed several extreme events that have highlighted the importance of effective water management strategies. Two such events that occurred on opposite ends of the water quantity spectrum were the 2022 Pakistan and Mississippi floods and the 2017 Cape Town South Africa water crisis.

In 2022, Pakistan and the United States were hit by massive floods that caused widespread devastation. In Pakistan, heavy monsoon rains led to flooding across the country, affecting millions of people and causing significant damage to infrastructure and property ([23]). Similarly, in the United States, the Mississippi River experienced severe flooding due to heavy rainfall, causing extensive damage to homes, businesses,

and farmland ([10]). These events demonstrate the devastating impact that extreme water events can have on communities and the urgent need for improved water management strategies.

Strong rotational winds cause the hurricanes and cyclones which carry bulk quantities of water. These catastrophes are notably in their brute strength, and historically have caused the displacement of people, loss of lives, damage to infrastructure, and disruption of social and economic systems. One of the most notable wind driven water-based disasters in recent years was Hurricane Harvey in 2017, which caused catastrophic flooding in Texas and Louisiana ([7]). The storm resulted in over eighty fatalities and more than 125 billion in damages, making it one of the costliest natural disasters in US history. The intensity and frequency of hurricanes are expected to increase due to climate change, resulting in an increased risk of devastating floods and damage to coastal infrastructure ([18]). Another significant event was Cyclone Idai, which hit Mozambique in 2019, causing widespread damage and loss of life. The storm resulted in over 1,000 fatalities and an estimated economic loss of over 2 billion ([32]). Cyclone Idai was one of the worst weather-related disasters to hit the southern hemisphere, highlighting the increasing vulnerability of developing countries to extreme weather events.

On the other end of the water quantity disaster spectrum, the 2017 Cape Town water crisis brought attention to the challenges of managing a sustained lack of renewable water resources over a prolonged period of time. The city of Cape Town, South Africa, faced an unprecedented drought that lasted for several years, leading to a severe water shortage ([4]). The crisis prompted the implementation of strict water rationing measures and increased investment in water conservation and management strategies. This event highlighted the importance of proactive and adaptive water management strategies in the face of changing environmental conditions. Another notable drought event is the recent ten year drought in California, which has led to

significant economic losses with farmers and other industries struggling to cope with reduced water supplies ([11]). Although, California has seen an anomalously large influx of water due to an atmospheric river unleashing massive quantities of snow and rain ([66]; [22]; [14]).

The impact of these water shortages can be devastating, especially in developing countries where water scarcity can lead to malnutrition, disease, and poverty ([61]). The impact of water-based disasters is not limited to the immediate physical damage they cause. These disasters can have long-lasting effects on the environment, including water pollution and ecosystem degradation. For example, the 2011 Fukushima nuclear disaster in Japan led to the release of radioactive materials into the ocean, resulting in significant environmental damage ([42]). The incident had a significant impact on the marine ecosystem, with some species of fish still showing elevated levels of radiation years after the disaster.

Improving water management strategies requires a multi-faceted approach, including better monitoring systems, enhanced cooperation with the environment, and increased public awareness and participation. Effective water management strategies should aim to balance the competing demands of human society and the natural environment while promoting sustainable and equitable use of water resources. The opportunities to improve our monitoring systems are many; however, more people are needed in the conversation to consider how we might better cooperate with the environment.

Effective management and mitigation of water-based disasters require coordinated efforts from multiple stakeholders, including governments, non-governmental organizations, and the private sector. Such efforts include improving early warning systems, developing more resilient infrastructure, and promoting sustainable water management practices. Early warning systems play a crucial role in preparing for and responding to water-based disasters. These systems can provide timely and accurate

information to people in affected areas, enabling them to take necessary precautions and evacuate if necessary ([19]). The development of more resilient infrastructure is also essential in mitigating the impact of water-based disasters. For example, the use of green infrastructure, such as rain gardens and permeable pavement, can help to reduce the impact of flooding by slowing down the rate at which water enters the drainage system ([65]). Additionally, the use of nature-based solutions, such as wetland restoration, can help to improve the overall resilience of ecosystems to climate change and extreme weather events ([9]).

Finally, it is crucial to recognize that the impacts of water-based disasters are not distributed equally. Vulnerable populations, such as those living in poverty or in marginalized communities, are often disproportionately affected by these events ([16]). In addition, climate change is exacerbating the frequency and severity of water-based disasters, particularly in regions with already limited resources and infrastructure ([44]). Therefore, addressing the root causes of vulnerability and promoting equity in disaster management and response must be an integral part of efforts to mitigate the impacts of water-based disasters.

1.7 Conclusion

In this study, we introduce a fresh perspective to studying and understanding the water cycle with a learned representation using modern techniques and data systems. Our results show that a deep convolutional residual regressive neural network (dcrrnn) combined with water flux and gauged streamflow data can exhibit strong forecasting performance according to standard hydrological statistical figures of merit. We used the dcrrnn concept to develop a platform called Flux to Flow (F2F) and examined four major river basins across the United States. F2F can provide strong forecasting performances (Nash Sutcliffe and Kling Gupta efficiency above 90%) in most cases and at various time lags. Through the careful use of visuals and data management,

this approach can provide satisfactory performance for various locations, degrees of fidelity, time scales, and parameters of interest for the water resources and climate science community.

1.8 Code Availability

Scripts are available at <https://github.com/albertlarson/f2f>

1.9 References

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1.10 Appendix

Figure 1.1: Drainage basins under investigation

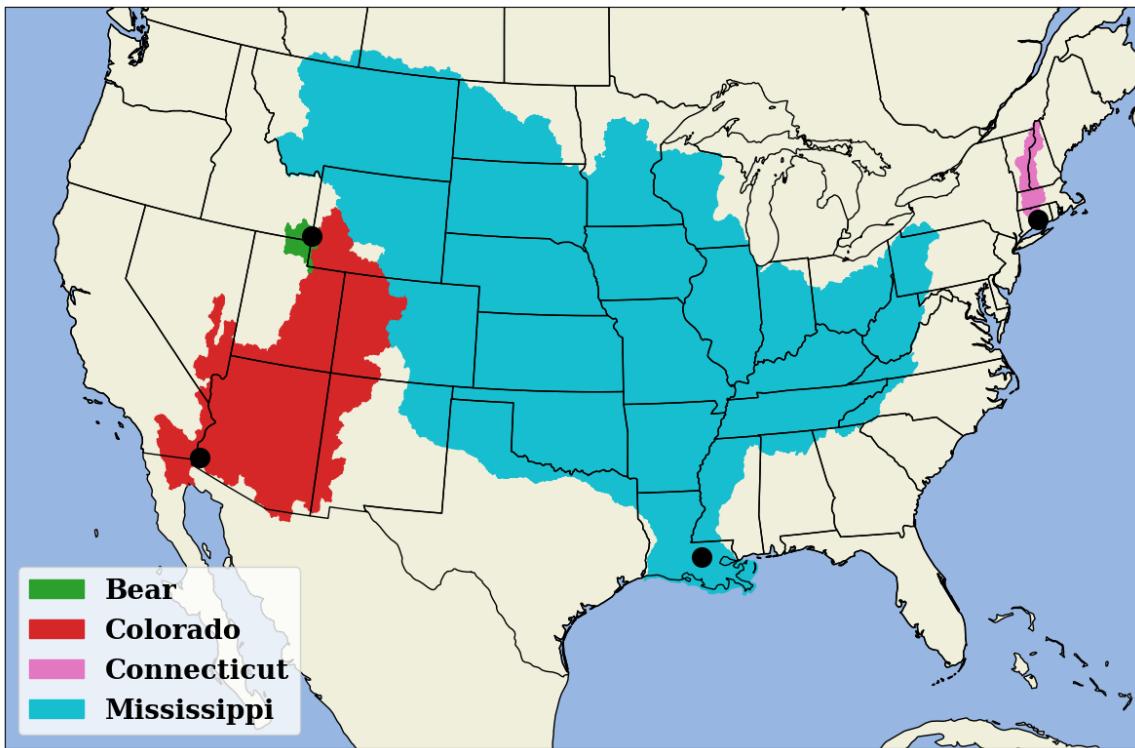


Figure 1.2: NLDAS daily surface and subsurface flows

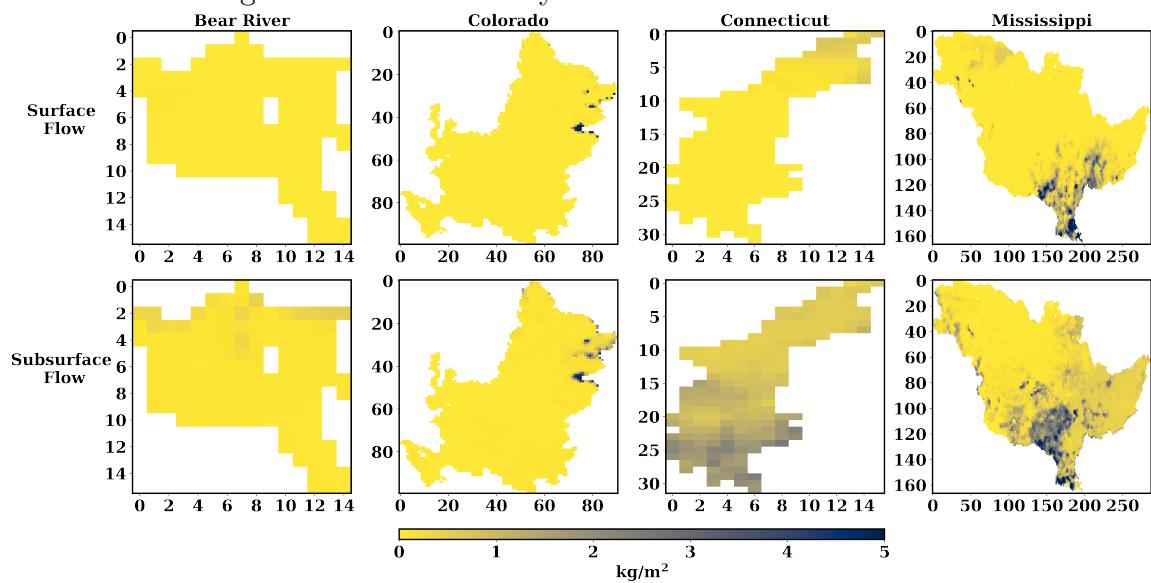


Figure 1.3: Strip chart and histogram plots of z-scored gauged streamflow observations

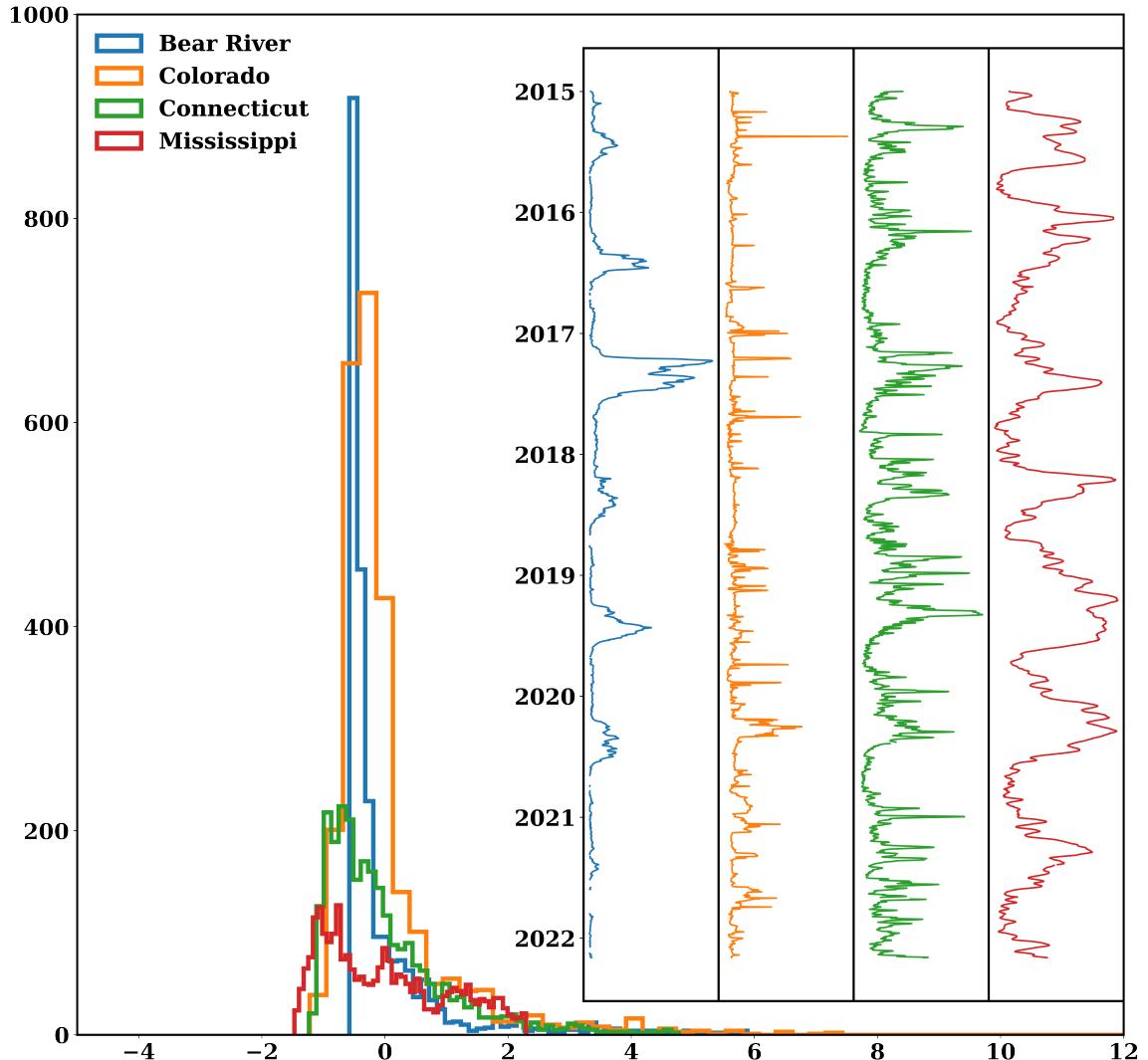


Figure 1.4: Neural network sample output

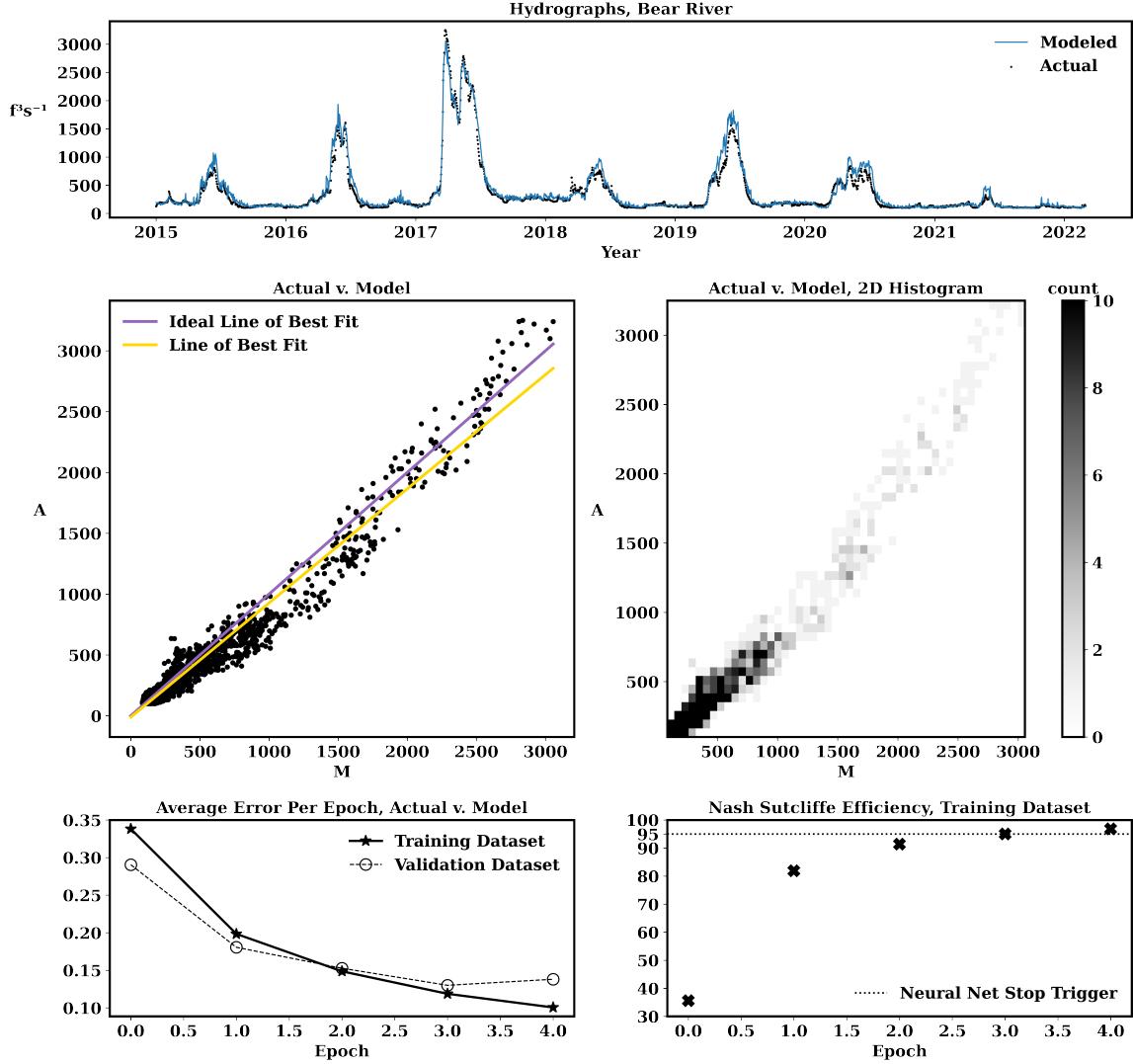


Figure 1.5: Kernel Density Estimates of the 2,268 experiments. Left shows grand NSE and KGE.

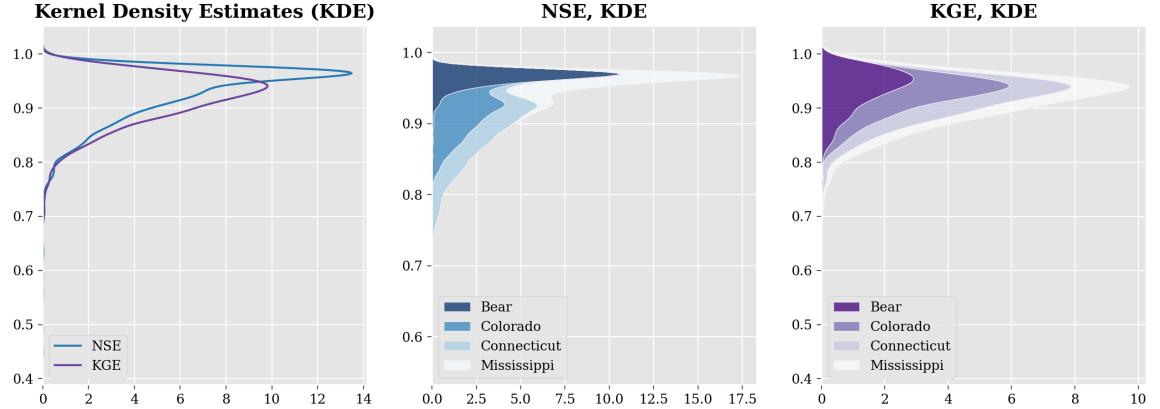
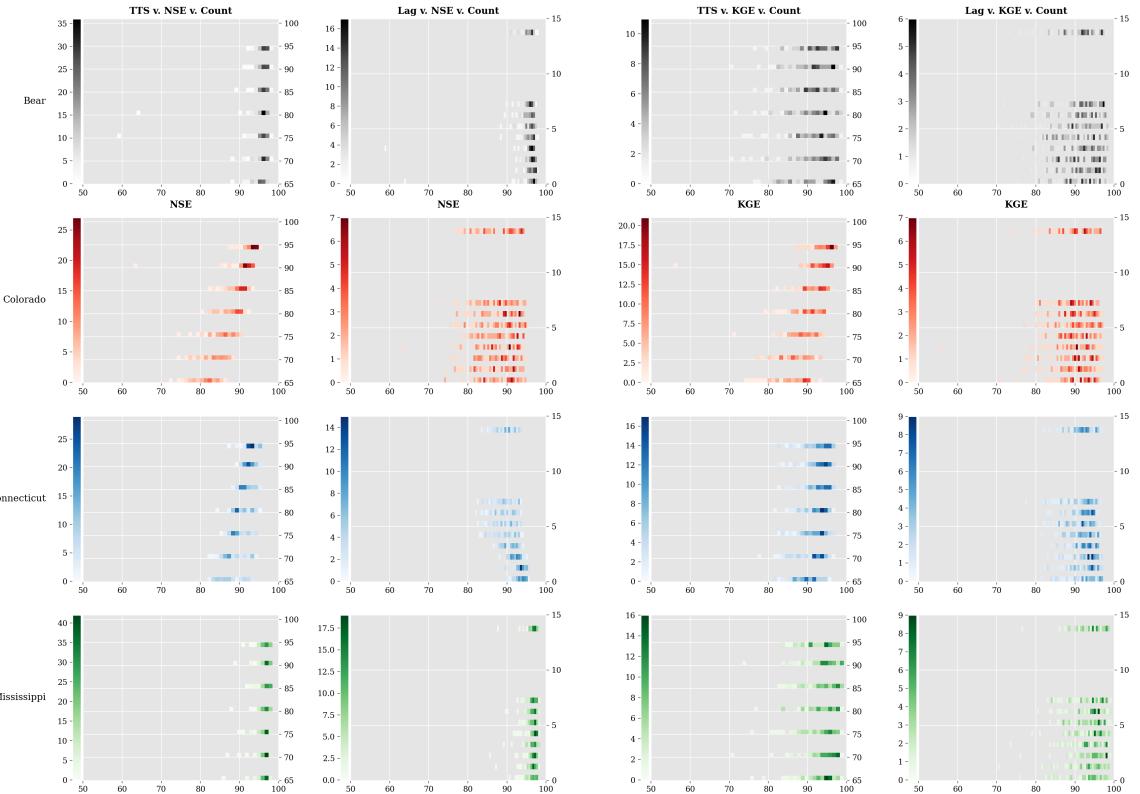


Figure 1.6: 3-D merit plots, basin delineated by color. Intensity of color indicates higher frequency within bin range.



MANUSCRIPT 2

Deep Convolutional Residual Regressive Neural Networks
and Sea Surface Temperatures from Aqua & Argo in the 2000s

Albert Eric Larson and Ali Shafqat Akanda

Submitted to MDPI Remote Sensing

2.1 Abstract

Sea surface temperature (SST) is an essential climate variable that can be measured via ground truth, remote sensing, or hybrid “model” methodologies. Here, we celebrate the progress of high-resolution sea surface temperature via the acknowledgement of a few technological advances from the late 20th and early 21st century. We develop a deep convolutional residual regressive neural network (dcrrnn) platform called Flux to Flow (F2F) and fuse AMSR-E and MODIS into a higher resolution product for capturing gradients and cloud gaps that are otherwise unavailable. Specifically, we utilize three snapshots of twelve monthly SST measurements in 2010 as measured by the passive microwave radiometer AMSR-E, the visible and infrared monitoring MODIS instrument, and the in situ Argo dataset ISAS. The performance of the platform and success of this approach is evaluated using standard figures of merit. Looking forward, we hope to integrate F2F with future satellite data streams such as the ECOSTRESS or Surface Water Ocean Topography (SWOT) datasets to enhance the precision of coastal regions observations of water.

2.2 Introduction

Water is both an essential and abundant resource on Earth, and its availability and quality are critical for sustaining life and ecosystems. Though it is abundant, the majority of Earth’s water, about 97%, is found in the ocean, while the remaining 3% is freshwater found in glaciers, lakes, rivers, and underground aquifers on land. Water is not only crucial for sustaining life, but it also plays a vital role in shaping the Earth’s climate and weather patterns. One significant but understudied climate variable that hydrologists consider is sea surface temperature. SST has a profound impact on the water cycle, specifically evaporation ([18]). Over ocean anomalies like atmospheric rivers can lead to both anomalous and enormous quantities of meteorological water falling on land ([3]). The same is true in the reverse, as the failure of the rains in India

are influenced by the status of the nearby Bay of Bengal and Indian Ocean ([21]). Understanding the relationship between sea surface temperature and the water cycle is critical for predicting and adapting to extreme events, managing water resources, and sustainable the global ecosystem.

Evidence continues to mount that human beings through industrialization have modified and are continuing to significantly modify the climate. However, the modern cause for concern is the rate at which our climate has changed rather than the Boolean of has it or has it not. Measurements of carbon dioxide (CO₂) tell the story: detected values of atmospheric CO₂ have increased by 50% of the starting value at the advent of industrialization ([4]). Invariant to latitude and longitude, the impacts are felt everywhere. Earth's response to our stimuli manifests in the form of heat waves, stronger storms, longer periods of drought, greater impulses of meteorological water accumulation over land, and a general increase in environmental variability. While in wealthy communities, modern civil infrastructure serves as a boundary layer to environment-related catastrophes, the poor and powerless are unequally yoked. One must consider also the importance of the ecology itself. As humanity conquers the environment, in what state are the creatures of the atmosphere, land and oceans? What does the next five, ten, five hundred years look like at the current rate? If deemed unacceptable, what changes can be made to mitigate or adapt to implications of past and present poor actions? What are the global environmental quality standards? How can standards be enforced in unequal nation states?

There are many global environmental observation systems that study the entire Earth from a distance. The sheer volume of effort and observation output can be gleaned by world wide web crawling one example: the details of the Coupled Model Intercomparison Project website. Through this project, expert parties from all over the globe share the effort of simulating Earth by focusing on their separate silos whilst having common tunnels to assemble, communicate, benchmark, and improve.

Remote sensing (RS) instruments have recently (1950 – present) grown in frequency of occurrence, capability, availability, and affordability. Attached to planes, balloons, spacecraft, or other autonomous means, these devices capture images in a controlled fashion over medium to large portions (swaths) of the land, atmosphere, and ocean. The growth of global RS data is pivotal to our ability to continuously view the macroscopic climate system. The output of these RS devices can be studied with a variety of optical techniques, in most cases altered via some logic to provide a more value-added product depending on the data consumer’s needs.

For example, consider the delineation of processing levels provided in the peer-reviewed document coinciding with the deployment of the ECOSTRESS instrument ([6]). A lower value processing level (L0, L1) indicates raw measurements of electromagnetic radiation from the Sun through Earth’s atmosphere off the land / water surface, back up to through the atmosphere to the satellite instrument. In turn, a higher value (L2 – L4) indicates the generation of physical parameters, gridding of swath data, and data assimilation with other parameters. In the instance of ECOSTRESS, the higher levels refer to land surface temperature, emissivity, measures of evapotranspiration, and at Level 4 evaporative stress and water use indices.

Here we investigate the temperature of the ocean’s surface (SST). This target is chosen because of its focus on the behavior of water in the environment, its importance in numerical weather and climate forecasting, and detectability via satellite-mounted RS instrumentation. Also, it has matched continuous ground truth temporospatial measurements that can be investigated for intercomparison of dataset bias, variances, and uncertainties. While it is not practical to grid the entire surface of Earth with sensors, in many situations and places it is extremely valuable to use arrays of dense, spatially linked precise in situ measurements. Satellite observations have a coarse resolution and can miss many interesting small-scale anomalies within the hydrosphere.

We compare the raw satellite observations to the lower resolution but more precise

measurements of sea surface temperature. We apply a treatment to the lower resolution but generally more available satellite instrument (AMSR-E), setting its target output to be the higher resolution MODIS product. Our hypothesis is that fusing the AMSR-E data to MODIS data will create a product that is closer in performance to MODIS than its AMSR-E input.

2.3 Materials & Methods

2.3.1 Sea Surface Temperature (SST)

The origin of SST as a continuously monitored variable began when Benjamin Franklin captured measurements of the ocean as he traversed the Atlantic, acquiring data and synthesizing these observations into information about the Gulf Stream. There is a rich history from that point forward to the present day, and a thorough review available in the literature ([16]).

SST is largely academically segregated into the field of physical oceanography. Nevertheless, the connection between ocean, atmosphere, and land are intimately intertwined. There is a trickling down from global SST anomalies like the El-Niño Southern Oscillation, the Madden Julian Oscillation, the Atlantic meridional overturning circulation, western boundary currents, gyres, and eddies to the availability of food, energy, and clean drinking water. Consequently, better understanding and application of oceanic parameters in consideration of land-based hydrology means improved forecasting and preparation for the future.

2.3.2 Aqua

The Aqua satellite was launched on May 4, 2002 ([19]). Upon it, two instruments sit: AMSR-E and MODIS. Both, among other things, are designed to study the temperature of the ocean. The measurements obtained as the satellite is moving from South Pole towards North always crosses the equator at approximately 1:30 PM

local time nadir (directly below the satellite). In the downward portion of the orbit, the satellite crosses the equator at 1:30 AM local time nadir.

2.3.3 AMSR-E

AMSR-E is a passive microwave radiometer ([13]). The acronym stands for Advanced Microwave Scanning Radiometer for Earth Observing System. There are several products produced on top of the raw radiance data collected by this instrument, and the AMSR-E data is processed by different ground stations depending on the parameter of interest. The produced datasets contain latitude, longitude, several physical parameters (e.g., SST, Albedo, soil moisture) as well as other pertinent metadata. As it pertains to sea surface temperature, AMSR-E is available in Level 2 or Level 3 products, and as part of Level 4 assimilation system output.

To detail a sample, one single Level 2 netCDF (.nc) file containing AMSR-E data was downloaded. The record selected is that of March 3rd, 2004, with a UTC time of 01:07:01. The file contains three coordinates (latitude, longitude, and time) and thirteen data variables.

Each variable is a single matrix comprised of columns and rows of measurements. The important distinction here is that the data structure is stored to reflect the path of the orbit. See Figure 2.1. When the sea surface temperature is plotted as it sits in the matrix, it is difficult to discern what is transpiring. There appears to be some curvature of the measurements, but other than that little is known to an untrained eye beyond the title and colormap.

Inclusion of the latitude and longitude coordinates, as well as a global basemap generates a clearer picture as seen in Figure 2.2. A single Level 2 AMSR-E SST file contains matrices representing one full orbit around the globe. Each file holds partially daytime and partially nighttime observations. Because of diurnal warming, it is desirable to separate the nighttime and daytime passes. Furthermore, many anal-

yses are comprised of an ensemble of satellite observations from different platforms such as this one. A grid makes for more orderly computations at large spatial scales. Certainly, one could elect to grid every observation to the AMSR-E or MODIS native product coordinate system. With our experiments, we choose the path of rectangular gridding. We consider the Level 3 product because of the interest in spatial relationship across large geographic scales and variable time (daily, weekly, seasonally, yearly, generationally).

The Level 3 equidistant rectangular gridded product is accessed via the NASA Jet Propulsion Laboratory’s Physical Oceanography Distributed Active Archive Center (PODAAC) and was produced by Remote Sensing Systems of Santa Rosa, California. This product comes in 25 km resolution and is delineated by daytime and nighttime passes of the satellite. The time series runs from June of 2002 until October of 2011 when the AMSR-E instrument ceased functioning. Figure 2.3 illustrates the point that even without explicitly defining the coordinate system in the visualization, the matrix of SST values is already placed in proper spatial order. Figure 2.4 reinforces the fact that little change occurs with the inclusion of latitude and longitude coordinates when plotted on a rectangular grid.

We accumulate the daily daytime and nighttime readings from AMSR-E into monthly products. While a monthly product has already been produced for use with the Climate Model Intercomparison Project, AMSR-E_CMIP5 as available from the does not delineate between daytime and nighttime. Here, we simply compute the monthly average for daytime and nighttime passes on a pixel-wise basis for each month. We finally re-grid the AMSR-E data to the MODIS L3 grid.

2.3.4 MODIS

MODIS, or Moderate Resolution Imaging Spectroradiometer, measures thirty-six different radiance bands in the infrared and visible ranges of the electromagnetic spec-

trum ([5]). Level 3 sea surface skin temperature as obtained from MODIS comes in 4 kilometer and 9 km products, and is derived from a subset of the thirty-six radiance bands. The products are available in daily, average of eight days, and monthly products. They are also delineated by daytime and nighttime passes of the Aqua's polar-orbiting nature. SST products deriving from MODIS are further specified by the length of the waves within the thermal infrared range used to derive the measurement: longer waves (11–12 microns) and middling waves (3–4 microns). The MODIS documentation state that the 3–4 micron wave SST product is less uncertain, but only usable at night because of the daytime sun glint impact on 3–4 micron waves. We use the long wave 11–12 micron infrared measurements to keep constant the source of both daytime and nighttime passes.

The MODIS Aqua Level 3 SST Thermal IR Monthly 4km V2019.0 product comes with latitude and longitude coordinates, SST values and per pixel quality measurements denoting when contamination is likely. The grid is equidistant rectangular, a match with the AMSR-E grid but at a finer original resolution. Of the over thirty million pixels for an entire day of 4 km MODIS pixels, 90% of them in the random sample selected here are deemed contaminated and filtered out (Figure 2.5). This contrasts with the 50% loss of AMSR-E pixels. This great loss in pixels due to quality is attributed to cloud contamination. To compensate, we use the monthly product (Figure 2.6) where a greater amount of time has transpired, allowing for a higher probability of clean global coverage. A randomly sampled MODIS monthly image yields 50% loss, in line with the AMSR-E daily product and much improved upon relative to the daily MODIS observation files.

2.3.5 Ground Truth Measurements

For a source of ground truth data, we selected the “In Situ Analysis System” (ISAS) dataset obtained from the University of California’s Argo repository and pro-

duced by a consortium of French institutions ([8]). An important constraint for this work was to obtain only the surface level measurement of temperature at the highest frequency available during the years of both AMSR-E and MODIS. These products are provided in a gridded format are used to observe temperature measurements at many depth levels. In the publication attached to the ISAS dataset ([8]), the target physical quantity is steric height and ocean heat content; with these as their target output, gridded depth-dependent temperature is stored as a byproduct. The 0.5 degree monthly dataset is presented in a Mercator projection, slightly different than the AMSR-E and MODIS grids. Mercator lines of longitude have a uniform distance in between them; the distance between latitudes from the equator changes. Identical to AMSR-E, we re-grid this data to the MODIS grid and coordinate system.

2.3.6 Treatment

The treatments we apply to the data are several configurations of one common concept: neural networks. Neural networks are not new, but the growth of graphical processing units (hardware) has enabled them to flourish in software. Neural networks are a type of learned representation. A structure is fed connected input and target pairs. Based on the predictive quality of the initial network structure, an error between the neural network output and the target occurs. This error is in turn fed to an optimization algorithm that iteratively and slightly alters each “neuron” of the initial network structure until it reaches a designated optimal state. Via many small calculations and the simultaneous application of statistical mechanics, neural networks are known to provide qualities like that of a brain, such as capturing spatial eccentricities and temporal changes in sets of related images. Neural networks are applied to a range of tasks from the more mundane such as learning a quadratic equation, to the more cutting edge, like extreme event forecasting or cancer detection.

Transfer learning has become commonplace in the field of machine learning ([24]).

Transfer learning places an emphasis on creating reusable treatment structures for others to build on top of without inadvertently causing the audience to get lost in possibly unimportant details. We employ transfer learning to create a complex configuration with a relatively short learning curve. The neural network is characteristically deep, convolutional, residual, and regressive. Our construct is inspired by the work of residual networks ([10]). However, our problem is one of a regressive nature. Sea surface temperature has a continuous temperature range that it exists within. This is a notable difference to some of the more common introductory neural network examples, such as those associated with the MNIST and CIFAR datasets where the number of possible outputs is very small ([25]; [15]). Loss functions associated with regressive problems are constrained to just a couple: mean absolute error (MAE) and mean squared error (MSE). The calculation of the loss function must be differentiable. This is due to the optimization component of neural networks. The literature is rich with publications regarding neural network optimizers, as well as the general mechanics of neural nets ([1]; [14]).

Once neural network architecture and hyperparameters are chosen, training and validation data is loaded into the network. While training the neural network, close observation is made of the reduction in error between training input and output as the neural network begins to optimize or learn. We also monitor the validation dataset at each training iteration. The learning process stops once the training and validation data has been passed through the network a certain number of times, or epochs. When prototyping or pilot-testing the experiment set to be carried out, one should test with a very short number of epochs and a larger sum of epochs to see where good performance meets fast time of computation.

After training, the optimized neural network structure is intentionally frozen. Before the point of freezing, the neurons of the network can be adjusted for optimization, like a student asking a teacher for advice when studying. The frozen state and infer-

ence imposed upon it is like a student being prompted with a pop quiz and no teacher assistance. This test or input data are similar enough to the training that the teacher believes the student will have success in passing the test according to the selected merit (mean squared error, the loss function). After the test, the performance of the model is evaluated and a decision is made regarding next logical steps in the research.

A neural network can become biased to its training inputs. It starts to memorize the training dataset, which does not make for a generally applicable algorithm. Avoidance of biasing comes at the cost of variance ([9]). Applying dropout is one technique to systematically prevent system bias by simply “turning off” a certain percentage of random neurons at each iteration of the algorithm ([11]; [22]). Another approach is the application of early stopping. The loss function of a neural network typically looks like a very steep curve down to a flat bottom. Rather than allow the network to persist in the flat bottom for long and become overfit, simple logic can be employed to stop training early when the network shows evidence that it has reached an optimal state. Percentage of data split between training and testing proportions is another relevant training hyperparameter. A larger proportion of the dataset being part of the training portion could lead to overfitting of the model and lack of generalized predictability. On the other hand, insufficient training data might lead to an inability to adequately characterize the reality of the data pairs.

The image sets subjected to treatment are on the large side computationally. Holding many one million or nine million pixel images within the memory of a single graphical processing unit becomes intolerable to the device. One could elect to use multiple GPUs or a compute node with a great provision of memory. Here, we constrain the experiment to a single GPU and cut the images up into smaller pieces of square data. Our patch size is fixed at 100 x 100, though this is a tunable hyperparameter. Figure 2.7 shows a Pacific Ocean study region, highlighting Hawaii and regions east. While this image is too large to process directly in the neural net-

work, we can solve this problem by creating the eighteen patches of 100 x 100 pixels, representing the 300 x 600 pixel region under observation.

Neural networks do not function when nan values are present in any of the images. We enacted a broad treatment to the AMSR-E and MODIS images, computing the mean of the entire image, excluding the nan values. Then, where the nan values are present, we replace them with the mean value. This has the convenient byproduct of introducing into the neural network many training pairs where the input and output are simply comprised of the average global SST value as obtained via the AMSR-E and MODIS instrument.

2.4 Results

We prepared the SST data for nine different cases all studying the year 2010: the **A**tlantic, **P**acific, and **I**ndian Oceans segmented by monthly **D**ay, **N**ight, and **H**ybrid (nb, hybrid means day and night images averaged together) observations of SST (nb, first letters of the previous are bolded to call attention for their use in Figure 2.8). We train the neural network on the first ten months of the year, validate with the eleventh month, and test with the twelfth month. A training session runs for 100 epochs. Each image in the geographically constrained time series is 300 pixels x 600 pixels in size, divided up into eighteen 100 x 100 pixel segments to incrementally feed the neural net.

In all instances, both training and validation loss functions drop by several orders, indicating successful training without overparameterization as would be indicated by low training error but high validation error. Performance of network as it relates to the test data, December 2010, is seen in the upper plot of Figure 2.8. The goal is for measurements labeled Pred or Optim to bring the RMSE value between AMSR-E and Argo or MODIS down. Pred is the prediction directly from the neural network. The Optim case takes the Pred and performs a band pass on the signal. If there are

any measurements outside three standard deviations of the mean, they are replaced with nan values instead. This is a device meant to combat some of the challenges with coastal artifact.

In every case, the RMSE between the optim and MODIS is higher than the AMSR-E input. In some instances, the test case of December does make an optim output that is closer to Argo than the input AMSR-E. In some cases, though, it makes a worse performing product with regards to Argo than either AMSR-E or MODIS. A bright spot is that the optim output is closer to MODIS than the Argo product. See Figures 2.9 and 2.10 for samples of how the RMSE translates to actual transformation of the images.

2.5 Discussion

While the continual development of a relatively open extract, transform, and load ([2]) system along with creation of the actual destination for the loaded data (namely the neural network treatment and posttest analytics) is certainly a plus, the results of this study request future engagement. In every case of this study, the neural network appears to struggle with coastal regions. This is due to the nature of the land sea boundary layer in all these datasets. At the presence of land, the raw data (as they are downloaded as .nc files) are given a non-number (nan) designation. Neural networks weren't designed optimally for the currently produced segregated RS datasets. The datasets appear to be manufactured with the understanding that one group of people are still more interested in ocean behaviors, another land behavior. For the purpose of training a neural network using the convolutional flavor, images with no nans are needed. As referenced earlier, steps were taken during the training process to circumvent the presence of land by substituting those pixels temporarily with the local mean value. Another option is the application of the substitution of the nan values with the mean as computed by the entire “scene” or day. There is the

potential and a likelihood that the substitution of these values is introducing a source of structured noise. This noise might be leading to the higher than preferable test performance as denoted in Figure 2.8. Furthermore, it is probable that this structured noise is hindering training of the neural network process itself.

As it relates to computer vision tasks such as this set of experiments, the use of mean squared error as a loss function has been called into question as an appropriate target ([23]). Their results certainly warrant some concern, and our experiments have some corroboration with their findings. Our images are single channel inputs and can be considered grayscale pictures. When displaying SST images, we use a colormap based on what we know to be the physical limits of the parameter itself. This is a different approach than typical of image based machine learning techniques. Alternate loss functions to the standards baked into PyTorch are available ([12]). These functions require the inputs to be either between 0 and 1 (grayscale) or 0 and 255 (color images). Another avenue is the pursuit of physics-based loss functions ([20]). While neural networks are a useful tool, they alone are not a silver bullet, especially as it relates to geophysics. However, the neural network community has a keen interest in computational efficiency.

We applied a land mask generated from the MODIS instrument. Aqua has far surpassed its projected useful life span and was designed before the new millennium. The new Surface Water Ocean Topography (SWOT) mission launched in 2023 ([7]; [17]). It will bring many new insights to the hydrology community. Among those insights are a more precise global picture of Earth’s coastal regions.

Only a fraction of the available data was observed in this study. The ISAS Argo dataset was a single file attached to a DOI address of over fifty gigabytes. We extracted simple the surface layer of this dataset. There is great value in consideration of SST depth layers. Furthermore, we studied monthly time series images of all three raw datasets. AMSR-E and MODIS each have near complete global pictures within

two to three days. These datasets are then transformed in different ways and can lose fidelity by various types of decimation such as regridding from swaths to squares, uncertainty in formulas used for conversion from base input to high level (L2 - L4) physical parameter, or by forms of compression.

Cloud cover is a persistent factor at play within the community. The question of “is the measurement (pixel) currently observed impacted in an undetectable way?” can’t fully go away, because even at the hyperlocal “nowcasting” time scale there is missed detection of events. Because of the pervasive challenges, people need to come together. Great global solutions require more cooperation, engagement, and the act of building bridges with one another. Missions like the International Space Station, Artemis, Landsat, and GRACE, and SWOT are only examples of what global cooperation can result in. Here at the microscopic level of single parameter consideration, we need more of the same type of teamwork. Dynamic collaboration amongst many stakeholders raises economic efficiencies. Improvement of just a single ECV requires takes the participation of a deep supply chain. Water is life. It connects the global ecosystem in nearly every facet, from food supplies, health of exotic wild animals, to the manufacturing of semiconductor chips and the treatment of industrial water. A clearer perspective is always welcomed to help sustain life. The missions of Aqua and Argo certainly achieved their planned missions in that way.

2.6 Conclusion

Sea surface temperature is an essential climate variable and crucial to understand the movement of water throughout the hydrosphere. The beginning of the 21st century marked a new frontier in the measurement of SST via the Aqua mission and Argo program. We observed three overlapping datasets focused on measurements of sea surface temperature: AMSR-E microwave measurements, MODIS infrared measurements, and ISAS Argo float in situ measurements. We focus the study on three large

oceanic regions: Indian, Pacific, and Atlantic. We used Flux to Flow, an extract, transform, load, treat, and evaluation framework based around a deep convolutional residual regressive neural network. We attempt to transform the coarser resolution satellite product towards the finer one and intercompare all datasets. While the neural network performs well according to its typical loss functions, we find that the presence of frequent nan values, the limitations of mean squared error as a loss function used in computer vision tasks, and the sheer size of output target quantities compounded with high desired precision results in limited success when applying the neural network transformation. However, we believe that a greater quantity of resources focused on a smaller area per resource with this architecture might allow for better capture of the relationship between AMSR-E and MODIS. More generally, we see the future of this framework including other treatment algorithms, experiments where fewer output target values are considered, or computing resources run in tandem to build a bigger network for a potential better grasp on the transformation process.

2.7 Code Availability

Scripts are available at https://github.com/albertlarson/f2f_sst

2.8 References

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2.9 Appendix

Figure 2.1: L2 AMSR-E SST field, March 3, 2004, no coordinate system

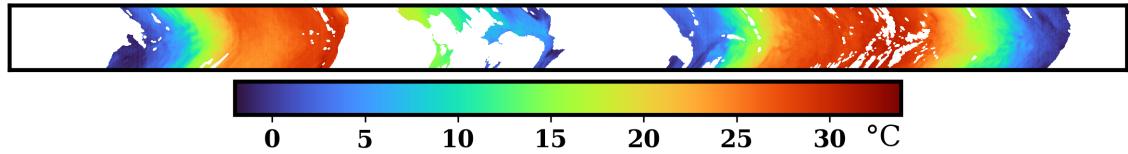


Figure 2.2: L2 AMSR-E SST, plotted with available coordinates and world map

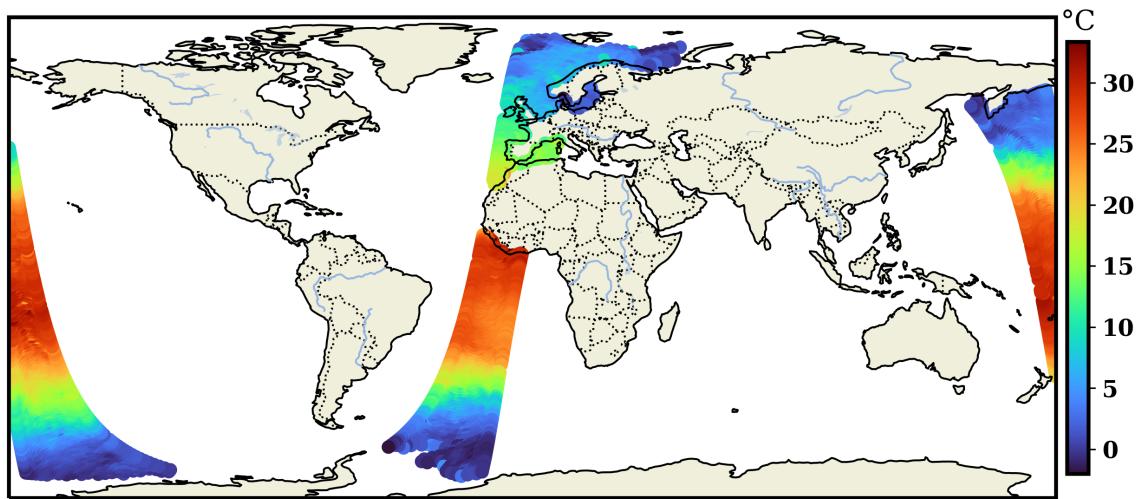


Figure 2.3: L3 AMSR-E file plotted without supplied coordinate system



Figure 2.4: L3 AMSR-E file plotted with available coordinates and world map

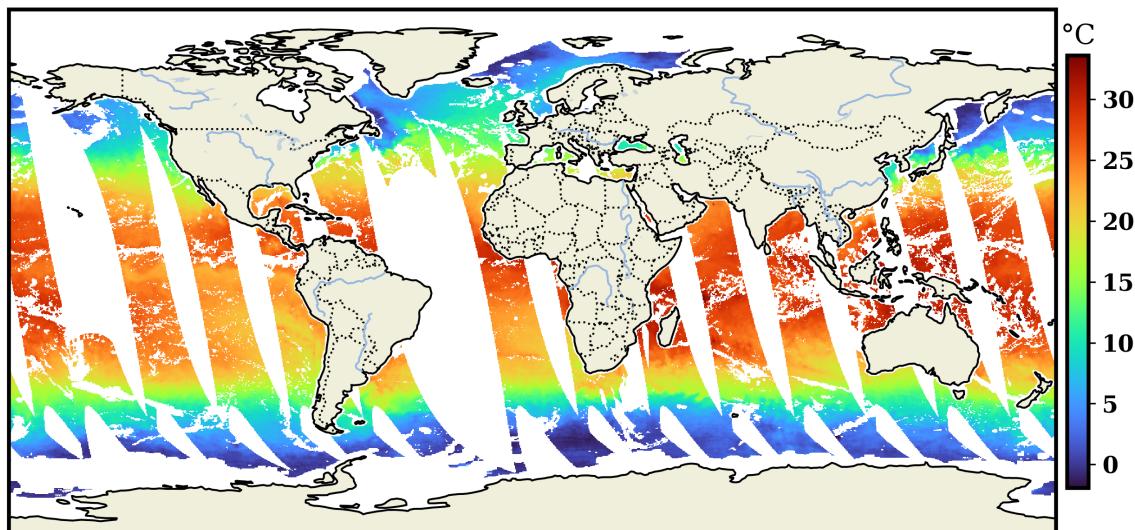


Figure 2.5: L3 daily MODIS file containing only high quality flagged pixels

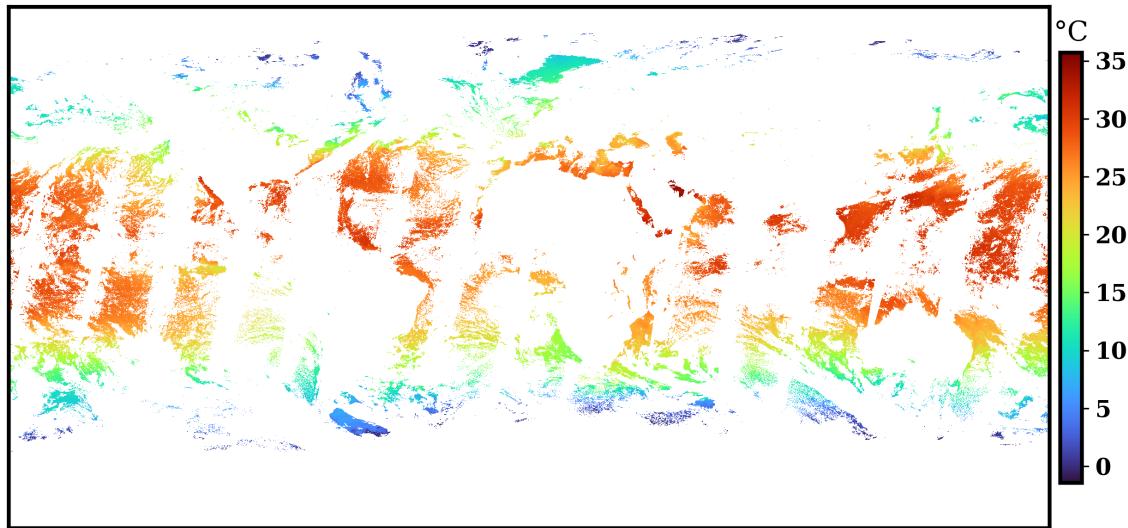


Figure 2.6: Monthly L3 MODIS image containing only high quality observations

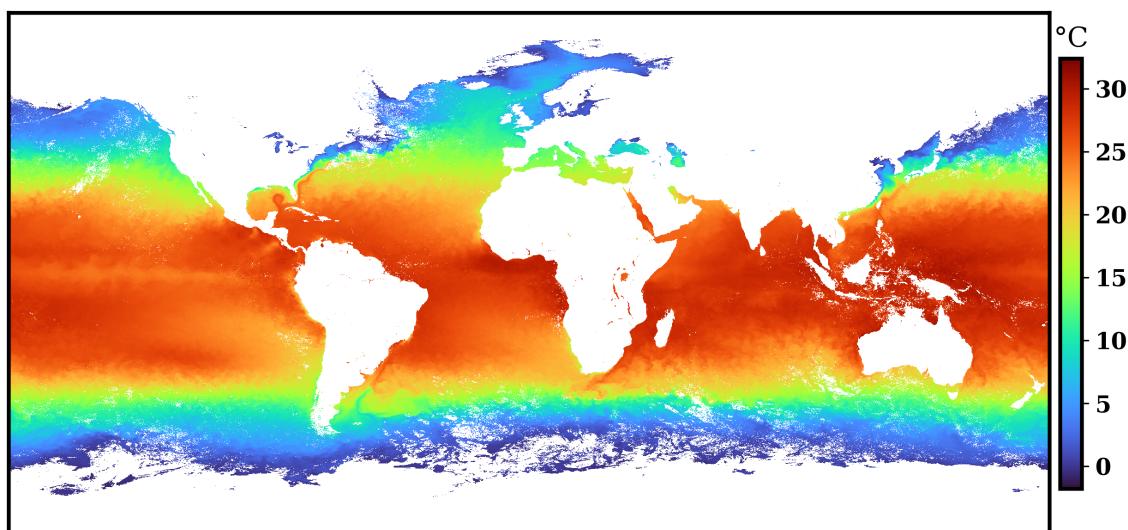


Figure 2.7: Sample training monthly observation; January 2010 MODIS day observation of the Hawaiian Islands; segmented into 100×100 pixel regions.

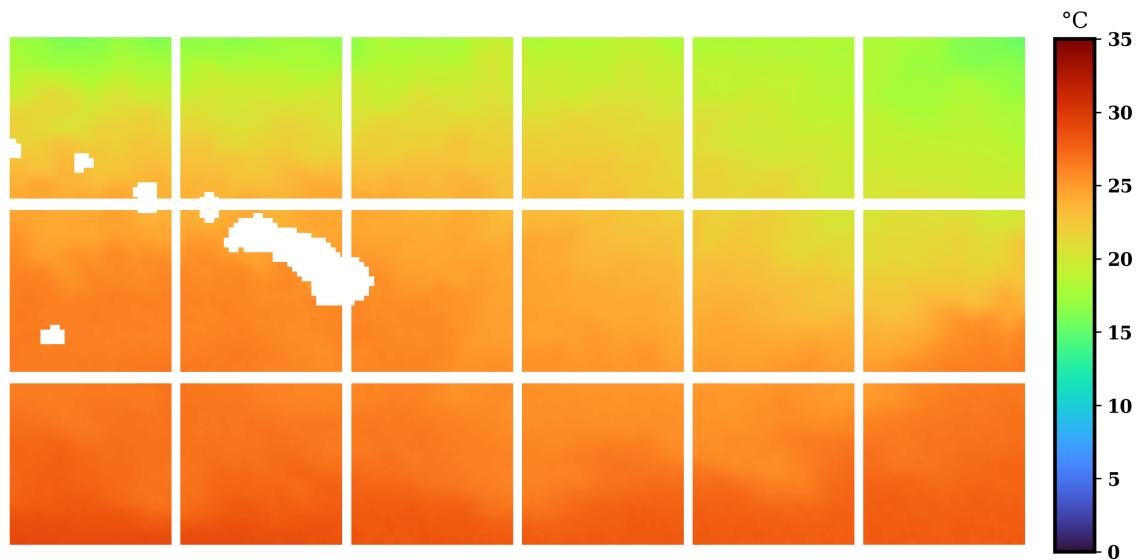


Figure 2.8: December 2010. The top panel shows the distances from Argo and MODIS to predicted, optimized prediction, AMSR-E and each other for all nine experiments. Two bottom panels are plots of training and validation losses during neural network training.

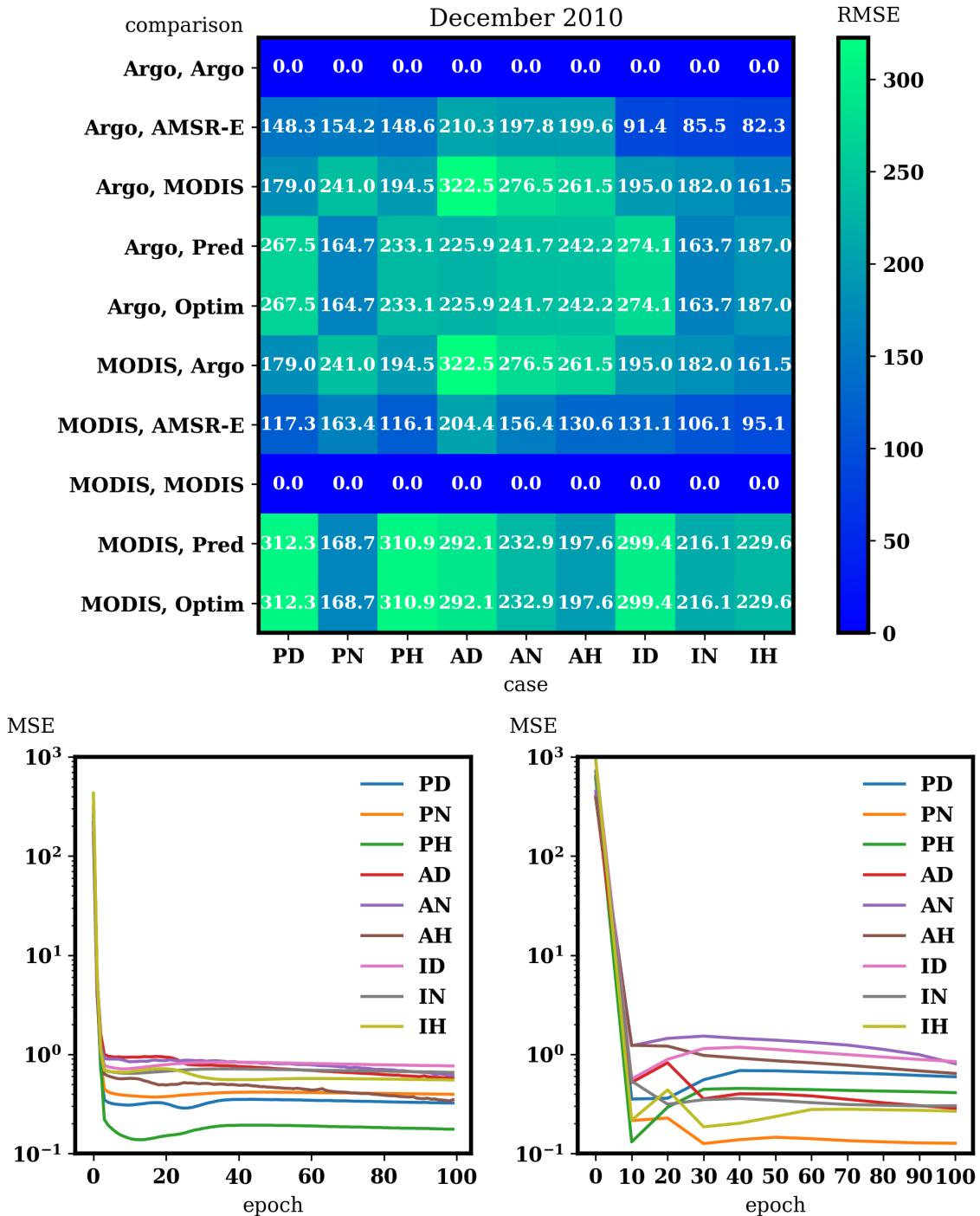


Figure 2.9: Relatively “good” perceptual change, Pacific Night case

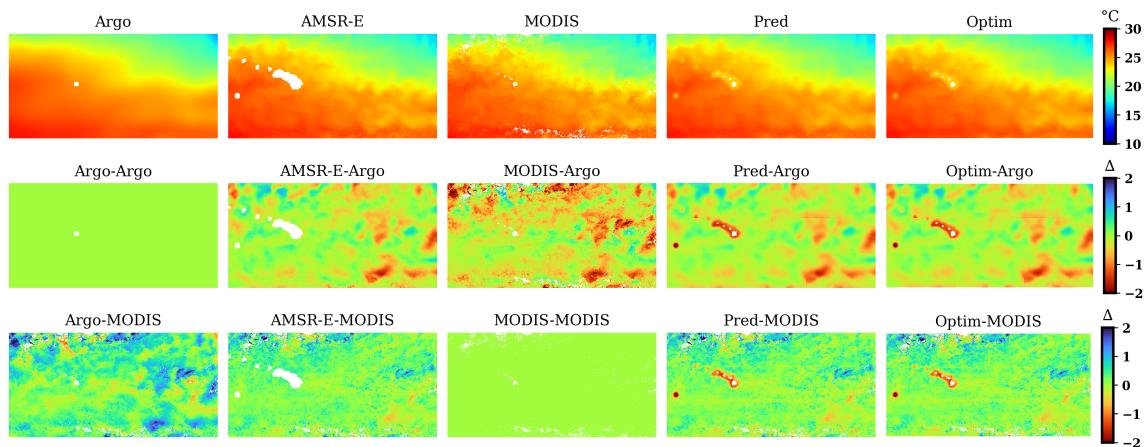
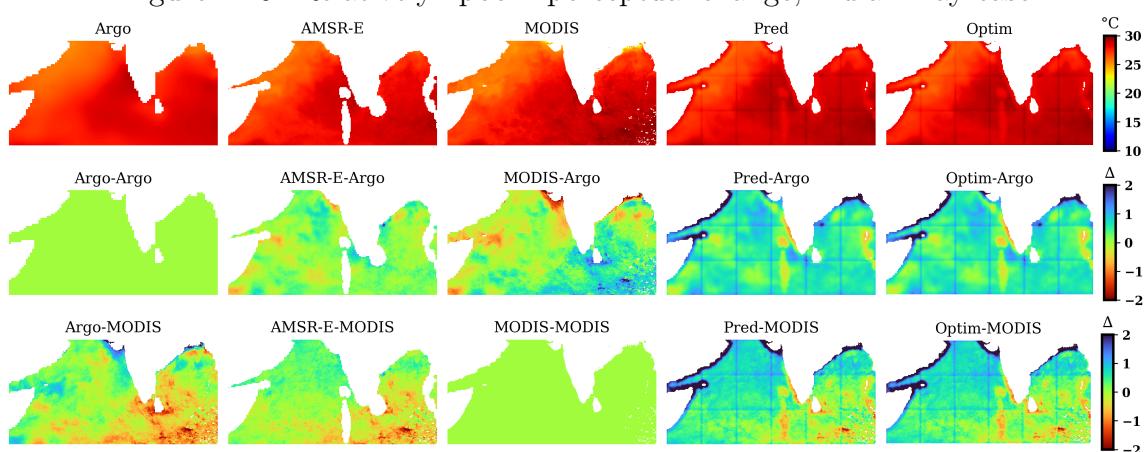


Figure 2.10: Relatively “poor” perceptual change, Indian Day case



MANUSCRIPT 3

Holistic Water Cycle Analysis via the Confluence of Climate Model, Satellite,
Ground Truth, and Machine Learning Signal Processing Technologies: Two
North American Transboundary River Watersheds

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3.1 Abstract

Water continuously cycles throughout the land, ocean, and atmosphere. Accordingly, it is important for hydrological analyses to consider water as it moves throughout the entire hydrosphere, and not just a single facet of the process. We use neural networks as a device to transform geospatial observations of water quantity and quality into forecasts of ground truth streamflow measurements. Two very large transboundary basins, the Columbia River and Yukon River, are subjects of this investigation. We first describe the basins. Then we create two datasets for each basin: one with coupled surface flow, subsurface flow, and sea surface temperature of the basin adjacent oceans; and another with simply the surface and subsurface flow land measurements constrained to the definitive boundaries of the delineated watershed. Finally, we load these datasets into Flux to Flow (F2F), our neural network test platform. Our results indicate that, even with the smallest neural network we try (four neurons only), use of sea surface temperature greatly improves forecasting of monthly streamflow from up to two years lag between the input images and the output gauged streamflow measurements. We see the future use of the F2F pattern having more output targets and likely requiring multiple compute nodes to scale the work. We discuss and identify drought monitoring as a suitable next step. We believe this work has only scratched the surface regarding the integration of land and ocean parameter datasets to fields devoid of non-numerical observations.

3.2 Keywords

water, water quantity, streamflow, sea surface temperature, GLDAS, MODIS, Columbia River, Yukon River, z-score, Nash Sutcliffe efficiency, neural networks

3.3 Introduction

Depending on the location, there are different water related signals that humans can witness and measure. These time variant water signals include but are not limited to parameters such as rainfall, snowfall, cloud cover, fog, ice, soil moisture, streamflow, river height, body of water temperature (lakes, seas, ponds, oceans), tidal timing and intensity, waterbody color, turbidity, and trace chemical concentrations in the water. These variables are commonly cloistered into variables of the land, variables of the atmosphere, and finally but certainly not least important variables of the ocean. Together they form the hydrosphere. We focus on variables of the land and variables of the ocean; however, we affirm the impact of the atmosphere upon land and ocean. Even at long time scales, there are certain parts of the globe that are constantly obscured from viewing with traditional bands of the electromagnetic spectrum due to noise such as clouds, wind, or other interference. This fact places an emphasis on the need for continuation of innovation in satellite measurements, ground sensors, and the spectrum of devices in between. The state of the science is still in many instances ‘flying blind’; Earth’s environment is dynamic and complex and modern solutions need to grow to combat modern problems.

We consider two extra-large basins. As an added complexity, we target trans-boundary watersheds. The motivation behind the use of transboundary watersheds is to simulate differences or nuance when leaving the gates of our national data systems in the acquisition of gauged river discharge measurements. In this instance, our journey is a short one to the northern riparian of the United States: Canada. Our view considers seventeen years of data, spanning years at monthly snapshots as opposed to the shorter end of the time spectrum (seconds, minutes, hours, days, or weeks). The two basins selected herein (Yukon River, Columbia River) are unique because of, among other features, their: 1, far from equatorial latitude; 2, proximity to the integration of land and ocean; 3, great range in quantity of water infrastructure

between the two habitats; 4, large range of elevation change.

We study surface and subsurface flow as computed for one of the GLDAS datasets. Additionally, we couple the two GLDAS datasets to MODIS sea surface temperature, creating a global dataset mostly devoid of non-number pixels. Of interest is the predictability of several gauges at a time when using the clipped version of GLDAS versus our custom ocean-enabled version of GLDAS. Furthermore, we modulate the lever of z-scored datasets versus non-z-scored datasets. We find that combining surface flow with subsurface flow (derived measurements of the changing weight of water in a region) and sea surface temperature has a markedly improved performance in predicting gauged streamflow than the datasets containing only surface and subsurface flow.

The wide lens guiding motivation behind this study is three-fold: 1, to improve the reader's understanding and capability to 'quickly' visualize the pertinent available macroscopic modern water cycle monitoring data sets; 2, to highlight state of the science level data typically used by experts for the generation and interpretation of global policy targeted outputs; and 3, to present a narrative of water (hydrology, limnology, oceanography) as the focal point of study because of its status as a primary building block of life.

3.4 Materials & Methods

3.4.1 Yukon River Watershed

The Yukon River and greater watershed are situated within part of the state of Alaska, and the eponymously named Canadian territory known simply as Yukon (Figure 3.1). A thorough baseline hydrological artefact of the Yukon River exists ([6]). The headwaters of the Yukon River emerge from the constellation of finger style lakes (e.g., Atlin Lake, Marsh Lake, Teslin Lake, Gladys Lake) known customarily as the Southern Lakes region along the northwestern border of the Canadian province of British Columbia. Sampled along the route of the river, one is likely to find bedrock,

confined and unconfined aquifers, a host of unique soil profiles, vegetation, permafrost, and a not to be understated flurry of flora and fauna friendly to subarctic climatology. At a microscopic, chemical level, the frequent boreal forest attributes concurrent with the frigid temperatures are well understood ([40]). Zooming out to a wider view than just the Yukon, evidence continuously mounts regarding the impacts of the changing climate. As goes the rest of the world, the Yukon feels an impulse. Nitrogen and phosphorous pollution are two of the more notorious organic chemical components that when unmanaged can wreak havoc on a watershed, causing eutrophication, loss of biodiversity ([7]). It's a short walk down the primrose path to a river lacking in a once endemic species of fish ([27]).

The Yukon River is famous for its salmon. In the last several years, the Yukon has come under public scrutiny for declining populations of chinook and chum in the Yukon and its neighbor river the Kuskokwim. A combination of bycatch in pollack fisheries, overfishing, marine heatwaves and algae blooms are causing the environment to become potentially less suitable for fish. There are prevalent modern terrors such as “forever chemicals” and the ubiquity of microplastics in the hydrosphere to the degree that many careers are being dedicated to the study as it relates to contamination of our waterways ([45]). It is a wonder at all sometimes that our river ways can sustain any life given the way some humans steward the gift. Humanity has much work to do to repair and improve the current status quo.

Environmental flows, or “e-flows” is “the quantity, timing, and quality of water flows required to sustain freshwater and estuarine ecosystems and the human livelihoods and wellbeing that depend on these ecosystems” ([3]). Considering a perspective filtered through the comprehension of e-flows, the Yukon has natural advantages. It is in a higher latitude, close to the North Pole (there's a town called North Pole in Alaska along the Yukon). Because of the high latitudes, constantly cold (equatorially relative) temperatures, and sometimes very long dark periods of time, there's a

tendency for life forms to shirk away from this environment. As such, the river is less prone to farming, heavy nutrient loading, or industry strain. That is not to say that its observation is in vain or without merit, far from it. Large swaths of previously unoccupied or lightly occupied land are important ones to observe with greater clarity the forcings and results of the natural global Earth phenomena as it is subjected to human intervention.

Physically, the Yukon River and surrounding land has all the features one desires in a naturally occurring surface water: beautiful lakes, high mountain scenery, sinuous meanders, novel woodland creatures. For example, erosion drives the creation of oxbow lakes, small slices of river cut off after anomalous water patterns drive unusual erosion in a suitable soil substrate. The Yukon is home to many cyclically migrating birds, as well as a habitat for many bears ([35]). Bears are attracted to the Yukon's most notorious creatures: the chinook and chum populations traversing the watercourse.

3.4.2 Columbia River Watershed

South of the Yukon Basin, at the southern edge of British Columbia and the boundary between the contiguous US and Canada lies the beginning of the Columbia River (Figure 3.1). The watershed is split into two major parts by the Cascade Mountain range running northerly from Oregon up into British Columbia. Land wise, the basin is primarily east of the Cascades. The western half of the larger Columbia drainage basin as divided by the Cascades finds a large share of water in the flows of the Willamette River. The waters of the Willamette stem from Waldo Lake, and it moves in a northerly direction before merging with the formal Columbia River. The Willamette unfortunately came under great scrutiny for the exhaustion of its goodwill to the point of receiving the designation of one of the United States most polluted waterways ([34]). There are efforts to restore the waterway that have

logged twenty-five active years and are beginning to restore these damaged arteries and veins of water.

The Willamette meets the Columbia in Portland, Oregon, and there is a short portion that flows north and west into the Pacific Ocean, catching a view of Mount Saint Helens to the east as the Columbia traces the boundary between the states of Oregon and Washington. Prior to Portland, the Columbia has a long meandering path through Washington and the Canadian province of British Columbia. Moving against the current, one follows the river in an easterly direction until coming upon the Tri-Cities in Washington. Kennewick, Pasco, and Richland are the three towns at the confluence of the Columbia and the other two of its other major tributaries (Snake River and Yakima River). All proverbial roads of the Columbia move upwards in elevation, and the coherence of a singular river eventually dissipates. Where Yakima for example weaves back into the Cascade Range, there are many finger lakes serving as the upper riparian.

Snake River is the largest tributary of the Columbia, its starting line in Wyoming trekking a westward course just north of Bear River. The Snake River's headwaters are outflows of Yellowstone. The Columbia River and Snake River share a potentially overlooked but crucial feature from their convergence backwards: a vector of hydraulic projects along both of their paths, none more notable than the Grand Coulee Dam (GCD). GCD is a hydroelectric power generating dam, with a power generating capacity of 6,809 megawatts (MW)). GCD is the largest power station (not just hydro, but of any type) in the United States. Though, it is dwarfed in size to the Chinese Three Gorges Dam, which boasts an installed capacity of 22,500 MW.

The eponymous Columbia ultimately has its headwaters in British Columbia where it forms from a series of three finger lakes: the smaller Slocan Lake and the protracted-in-length Upper Arrow Lake and Kootenay Lake. The three direct suppliers of water are amongst the Columbia Range of mountains. Furthering the point,

there is also a Mount Columbia in the range.

3.4.3 Data Sources

This study compiles together several large portions of data from five different institutions. NASA provides the two land variables, surface and subsurface flow. These variables are derived by integrating several meteorological forcings into the Noah water balance algorithm. The Noah land surface model has a rich history dating back to the late 1980s with formal named implementations released in the middle 1990s ([11]). Surface and subsurface flow are produced measurements of unit kilograms per square meter and represent the spatial weight of water at a given time in each location ([52]). Noah factors known soil properties, solar radiation, precipitation, wind, pressure, humidity, and changes in the purses of snowpack (if applicable to the region).

The sea surface temperature product used is one of the monthly outputs from the MODIS instrument on the Aqua satellite. In this instance, the thermal longer wave infrared band observed by MODIS is selected ([37]). Furthermore, we use the data product that only looks at nighttime passes of the MODIS sensor. Daytime passes captured are ignored because of the potential diurnal warming effect that manifest in daytime observations. The skin of the ocean can become surficially inflated. Our preference is to a measurement of the ocean closer to the signature of the depths of the waters rather than the strength of the sun on a given day. Solar radiation is already encompassed in the calculation of land flows, so we attempt to limit its impact.

Gauged streamflow for both basins are obtained through the United States Geological Survey and Canada's bureau of climate and the environment ([47]; [10]). In all instances, we constrained ourselves to near continuous basin measurements over the entirety of the time series. The requirement of continuity (no non-number pixels

and preferably no interpolation between months) plays a part in the quantity of measurements per basin. The study length is 210 single month measurements, beginning with July 2002 (coinciding with the first available monthly measurement of MODIS) and ending with December 2019. Measurements of actual streamflow in cubic feet per second for each basin are provided in the Figure 3.2.

3.4.4 Preprocessing

We run two distinct workflows across the time series for the Columbia and the Yukon basin. Motivated by a desire to understand whether the coupling of monthly SST to the GLDAS measurements of water flux across land impacts the speed and ability of the neural networks to learn algorithms connecting the inputs and outputs (i/o), we create datasets that are comprised just of surface and subsurface flow, and those that combine time aligned SST with the surface and subsurface flow measurements.

The process of combining land and surface measurements is illustrated in Figure 3.3. In the top row, we have one measurement of surface (Q_s) and subsurface (Q_{sb}) flow. In the second row first column, we have added those two measurements together pixelwise. In the second column, second row, the combined Q_s and Q_{sb} are integrated with the corresponding monthly measurement of SST. In row two column two, having the single colormap representing all numbers provided causes a “washed out” effect where the Q_s and Q_{sb} measurements disappear because their physical range here are roughly between 0.0 and 1.0 kilograms per meter squared, as opposed to the wider 0.0 to 20.0°C range. Concurrently, row three captures the dynamic ranges of water flux over land, and the temperature of the ocean’s surface temperature.

In their respective raw formats, the land and ocean variables have different resolutions and different grids for each pixel of data. This fact makes assimilation of the data in its raw state impossible. The fix for this problem is bilinear regridding. We

retain the MODIS grid and resolution of approximately 9 km x 9 km per pixel. To facilitate regridding, we utilize xESMF, a high level python package hooked into the Fortran, C, and C++ based Earth System Modeling Framework ([55]). We input the source image (Qs and Qsb), the destination grid (SST), and the type of regridding (bilinear). The algorithm provides as an output our source image in the destination grid.

We also use a windowing technique to eliminate nan values from the MODIS SST images. The PyTorch software suite has the function to create tiles of uniform smaller images from a large input ([42]). We unfold each MODIS raster into smaller non-overlapping squares. Within each tile, we set the software to find any non-number values and replace them with the average of the available numerical values in the tile. One could simply take the mean of the entire global image and replace non-number values that way; however, this is prone to the creation of unusual bias due to the wide variance of sea surface temperature based on location of observation. By using this tile method, we limit potential bias through the consideration of pixels only that are in relative proximity to each other. After gap filling, we fold the tiles back up into the original image size.

Our control preprocessing in the study follows the same chain found in the first iteration of Flux to Flow. We clip the measurements of Qs and Qsb to the geographical constraints captured in the publicly available shapefiles for each basin. To do this, we involve a few different publicly available software packages. We open the shapefile (a digital vector storage format) with GeoPandas ([26]), convert the vector file to a GeoJSON file with shapely, and clip each measurement of surface and subsurface flow with rasterio ([18]) and xarray ([23]). As opposed to the coupled land and ocean images, we do not add the measurements of surface and subsurface flow together. We fill any non-number values with the mean of the available measurements.

3.4.5 Treatments

To investigate the capabilities and limitations of neural networks as they pertain to the calibration and prediction of streamflow from land and surface measurements of water, we run 1,920 experiments total, 960 for each basin. The 960 experiments are spread amongst five neural network configurations of increasing complexity. Of the 192 configurations per neural net, we run experiments splitting the datasets into training data and test data splits of 70% / 30%, 80% / 20%, 90% / 10%, and 95% / 5%. The more data that is in the training set, the higher likelihood of better performance in the testing regime. We have six different lag profiles (zero lag, one month lag, three month or “one season” lag, six month or “two season” lag, one year lag, and two years lag). We test between z-scoring and not z-scoring the input channels. Lastly, we have an option whether to shuffle or not shuffle the training data. Shuffling data is known empirically to improve statistical learning ([33]).

Four of five neural networks have a single hidden layer. Single hidden layer neural networks, with enough neurons in the hidden layer, are theorized to be capable of universal function approximation ([22]). Concurrently, we evaluate the feasibility of using a single hidden layer of differing sizes (4 neurons, 30 neurons, 200 neurons, and 1,000 neurons) to approximate the transformation algorithm between location specific water flux to flow measurements. To facilitate these networks, we reshape each input raster of shape height times width into a vector of one by (height times width). The vector passes through the hidden layer, receives signal conditioning via rectified linear units (ReLU), and outputs six or seven (based on the basin under observation) predictions for each of the streamflow gauges. Based on the difference between the predictions of streamflow output by the model and the actual measurements of streamflow according to the mean squared error loss function, backpropagation and adjustments of the neurons of the network are made using the Adam optimizer ([30]). Regardless of the neural network architecture, the learning process (forward propaga-

tion, the calculation of loss, backpropagation and updating of weights) is performed 100 times (otherwise known as 100 epochs) across the training dataset. Model testing simply makes a single pass through the unseen testing data (the most recent in time data, quantity dictated by the lag of the test case and the percentage of data devoted to testing).

The fifth and most complex network is a convolutional structure loosely based on a modern image classification architecture ([20]). Each of our input channels are forced into a convolutional space (sometimes referred to as the latent space) where the input images are considered in many dimensions by the machine. This function allows for automatic feature learning by the machine of potentially important structural details or patterns unique to the SST fields. To hedge against the potential for the machine to miss the mark, this latent space learning is containerized, added to the input that was used to feed latent space learning, and then fed into a conventional neural network structure that bottlenecks down the input images to 100 neurons, fifty neurons, twenty neurons, ten neurons, and finally the output size of either six or seven neurons. In contrast to the image classification network, our structure has a regressive target output. A regressive target output simply imputes that the value of streamflow can be any continuous value (within reason) greater than zero.

3.5 Results & Discussion

The 1,920 experiments were split into their respective basins, the Columbia and Yukon. Each set of 960 experiments ran on their own node comprised of at least one NVIDIA GeForce RTX 2080 Ti GPU and 64 GB of CPU RAM. Due to its slightly larger per image pixel size (200 x 800 for the SST enabled, 38 x 143 for Qs and Qsb only), the Yukon test set ran for approximately twenty eight hours while the Columbia basin (200 x 600 for SST enabled, 46 x 57 for Qs and Qsb only) tests lasted only 21.5 hours.

In developing the test set of experiments, we again encountered the implications of the “washed out” effect as seen in the preprocessing portion of this document. Upon feeding the single channel hybrid ocean temperature and land flux images into a standard z-score treatment of our network, we found that regardless of the complexity of the network and with no lag of the data, performance was very poor. A z-score is computed by mean centering the data under observation ($0.0 =$ mean of the data) and dividing by the standard deviation (z-scores between -1.0 and 1.0 are all of those within one standard deviation away from the mean). The values of Q_s and Q_{sb} have a relatively small range to that of SST. Therefore, the dynamics of the Q_s and Q_{sb} were overshadowed by the larger range of measured SST values. One can’t simply mix two physical parameters and then compute a z-score. They have two different dynamic ranges. Dynamic range is the general placement of a collection of values on the number scale, as well as and possibly more importantly the distance between their largest and smallest observed value. Our fix consisted of going back to the preprocessing step, computing the z-scores for SST and $Q_s + Q_{sb}$ individually, and then and only then merging them into a single time series image for each month.

In Figure 3.4 we present aggregate results of the testing data ran through their respective trained models. Ignoring all the other parameters (lag, quantities of training and test data, use or abstention from the use of z-scoring, shuffled or non-shuffled data), there is an evident distinction. The use of SST coupled with Q_s and Q_{sb} changes the performance of neural network streamflow prediction. Nash Sutcliffe efficiency, or NSE, is a metric frequently used to evaluate hydrological modeling efforts ([38]). A negative or near zero value implies a poor model prediction, whereas a value close to 1.0 indicates a strong penchant to accurately predict the actual streamflow. Calculations of NSE herein only consider testing data, not training data. To be clear, let’s consider an imaginary example of a different time scale. A time series of 100 days in a row split into an 80% / 20% train test split means that the model (here the

neural network) learns an algorithm from the first eighty days and then makes inferences about the latter twenty days. Factoring in the training data when computing NSE would give NSE a positive boost, but it wouldn't necessarily be considered fair or unbiased. One can make a very large neural network that simply memorizes the input data, which would give the impression of perfect performance. This is fine if that was the desired task. As a baseline or “mic check” of your system, it is a reasonable device; however, it would likely have little to no practical application beyond getting the metrology for your experiment dialed in. Therefore, we only consider test data.

In Figures 3.5 and 3.6, we disaggregate the results from Figure 3.4 into their respective individual neural network configuration. In the instance of the Columbia, for both non-SST and SST experiments, as the complexity of the neural network increases, the performance of the network with regards to the unseen test data measured by NSE increases. With SST present, performance climbs faster. In column three of Figure 3.5, the single hidden layer network comprised of 200 neurons, the non-SST experiments have a centered NSE value around -1.0, whereas the SST experiments caused a jump to a range between 0.35 and 0.90. The value of SST is even more opaque in the Yukon experiments. In Figure 3.6, the data shows that the simple change from four to thirty neurons combined with the SST-enabled data gives results of model predictability well over 0.0. The non-SST datasets don't see this performance until dcrrnn (pronounced discern and the shorthand name for our fine-tuned deep neural network) enters the proverbial training arena.

In Figures 3.7 and 3.8, we shed the non-SST experiments and smaller single hidden layer configurations; instead, we just focus on experiments with SST and one of two neural net architectures (dcrrnn or the 1,000 neuron single hidden layer neural network). Specifically, we filter and plot two small datasets: 1, a disaggregation of the remaining experiments per basin based on lag between input and output data; and 2,

a disaggregation based on the Boolean variable of z-scored inputs versus non-z-scored inputs.

Both figures indicate the same reality as in the original F2F document. Civil infrastructure creates its own set of nuance and challenges to the modeling realm. The Yukon River is a more continuously wild place. Handling the two different sets of signal chains is like handling the sound profile of a strictly raw acoustic guitar signal versus handling an electric guitar buried underneath a dozen different pedal effects. Though the acoustic player has bends, twists, turns, and hopefully nuance to their playing with time, there is a more finite (yet relatively natural) sonic realm emoting from the acoustic player's hands. The same might be said for the Yukon in its current state, and there is a certain beauty about the natural movements of water and sediment in an unconstrained basin such as the Yukon. It may experience times of drought or flood, but there is not yet any fashioned mass of concrete capable of holding back very high (relative to the baseflow of the river) quantities of the Yukon waters for long periods of time, and consequentially the hydrograph has little artificial complexity.

The same cannot be said for the Columbia River. Since greater control of Columbia's flows sit with single-point sources, and these are manmade devices, optimized performance of F2F in a basin such as the Columbia River basin would benefit from much more data at the inlet and outlet of each point source. A next step might be just considering a single basin (or single State) and accumulating all available hydraulic data. The EPA has its Enforcement and Compliance History Online (ECHO) data available as a representational state transfer (REST) software architecture. In another run of the land data assimilation system (i.e., a hypothetical NLDAS 3 or GLDAS 3), it would be of value to see the impacts of programmatically including a few hundred or thousand continuous point-source or ground truth measurement sources. Certainly, calibration of this many outputs would require either: 1, much

compute time on a single graphics processing unit; or 2, and probably more likely, the use of many GPUs in tandem.

Reference is made in the Materials & Methods to a preference of input images of the ocean associated with the deeper depths of the waters rather than the strength of the Sun on a given day. Our study certainly is self-limited in the depth field. The ocean at places is very, very deep. Soil has geospatial delicacies; the vadose zone is where science is witnessing the fallout from humanity’s continued mishandling of chemicals. These facets beget their own studies, which is outside the scope of this investigation. We acknowledge that although this study shows promising results regarding the use of advanced neural network technology in the forecasting of monthly streamflow out to a lag of two years, true temper of the devices will only come through testing other datasets, time scales, and locations.

Another water-focused avenue we see F2F moving towards is drought propagation. Historically, humanity’s records of drought monitoring are very good, due in part to various backwards looking methodologies. For example, a gridded, spatially interpolated dataset observing the standardized precipitation index (SPI) dating back to 1895 is available ([50]). The U.S. drought monitor time series dates to 2000 ([48]). There is even one digital product measuring the Palmer modified drought index at a 0.5 / 5x5 (degree / square kilometers) resolution dating back to the beginning of the common era, 0 CE, over 2000 years ago ([17]). Future work might take a backwards looking glance through the lens of Flux to Flow. There is potential wisdom to be gleaned from the assimilation of prior discharge information for the sake of better initialization of prediction. This work can take advantage of the ability to break up datasets into smaller pieces and load them onto concurrent graphical processing units. Should one consider the cost and deem it a suitable operational tool, the simplification within Flux to Flow in folding and unfolding of geospatial tensors will serve as a potential balm to data handling challenges.

Drought is intimately linked to water scarcity, and this topic has never been more relevant. Water scarcity represents one of three things: 1 – the condition where no drinking water infrastructure exists; 2 – the condition where the drinking water infrastructure is inhumane; and 3 – the condition where available water resources are used unsustainably over a long period of time. In the modern scientific community, drought is science based, whereas water scarcity is rooted in policy, management, and justice as it relates to the global state of water infrastructure ([49]). These differences notwithstanding, drought and water scarcity are symbiotic in their nature. The destruction of natural ecosystems catalyzes further drought conditions ([16]). As the dynamics of the global climate change Earth’s structure at the air, land, and oceanic interfaces, the occurrence and severity of drought conditions are becoming in some cases greatly exacerbated ([29]; [39]). Therefore, it is necessary to understand the propagation of drought in time as it starts in its most benign state, and how it can take a turn for the worse and become an extreme event.

There are more than fifty different indices related to drought. The National Drought Mitigation Center (NDMC) highlights five digitally, and six in the original software system companion paper ([48]). In all of them, keeping everything else equal, a decline in value equilibrates to a worsening drought condition. A simple model given these eight channels of data could be constructed by averaging the outputs at a given location and time, followed by a whitening technique such as z-scoring and segmentation of the result into bins yielding a single image representation. The timescale of the ‘percent of normal’ statistic changes in response to certain drought condition steps (e.g., from extreme to exceptional drought, the consideration of the condition switches from degree of specialness over a six month period to specialness over a twelve month period). Consideration of prior observations with thoughtful control of influence decay of said observation over time falls under the umbrella of drought propagation concerns. There are other open source software repositories

that have already replicated many of the formal algorithms. One such algorithm of note is the Penman-Monteith equation of reference evapotranspiration (ETo). This algorithm was standardized by the American Society of Civil Engineers after benchmarking against a panel of twenty indices for reference evapotranspiration ([1]; [44]).

Drought propagation studies look at the teleconnections between meteorological, agricultural, hydrological, and socioeconomic drought. Many studies are classified under the drought propagation umbrella, such as those of historical nature that monitor oceanic phenomena like the El Niño Southern Oscillation ([43]; [4]), or the use of global greening strategies as a mitigation effort ([41]; [14]). Studies of drought propagation cover the entire globe, from China ([19]; [24]; [54]) to South America ([4]; [5]; [9]), Central Asia ([21]), Africa ([12]; [51]; [15]) and the United States ([2]).

Figure 3.9 presents a sample output from the National Drought Mitigation Center. Their output has six seven different color based classification codes available to diagnose a region. Attempting the application of Flux to Flow to generate these images using the hybrid fields would only be a slight departure from the current body of experiments. Having such a finite quantity of outputs means that the loss function needn't be of the regressive variety but could take advantage of one of the many classification-based loss functions ([25]), or potentially of the burgeoning transformer-based modeling domain ([28]).

This experiment has several components that distinguish itself: 1, use of optimized computing performance and efficiency; 2, knowledge and selectivity amongst the richness of the geospatial data landscape; 3, consideration at several orders of magnitude of neural network complexity; 4, the openness of the technology; 5, consideration of many experiment samples to root out bias; and 7, use primarily of a collaborative green computing facility. The driving research questions behind this set of experiments were: 1, what impact does the application of sea surface temperature have upon the prediction of streamflow of large watershed basins; 2, how many overlap-

ping, continuous, monthly measurements of gauged streamflow in two transboundary basins can we easily obtain, and what are the characteristics of these measurements; 3, how does Flux to Flow perform when using monthly datasets and greater than one but less than ten output targets? We find that sea surface temperature does have a positive impact upon neural network model predictability of streamflow. Each of these large basins was limited to less than ten. The measurements of discharge vary, indicating a wide dynamic range in the study of these basins. This is expected, as a backyard with a brook is never far away, and wisely planned cities are commonly built around plentiful coiffeurs of surface water resources.

In the future, we may consider different ground truth data sources, particularly the EPA ECHO repository. We also see modern and future satellite missions on the horizon. Of note is the ECOSTRESS satellite and its signature evaporative stress index (ESI) product ([8]; [13]). Following on the success of NASA’s ECOSTRESS is a planned joint initiative between the Indian Space Research Organization and the French Space Agency, known as Thermal infraRed Imaging Satellite for High-resolution Natural resource Assessment or ‘TRISHNA’, and the Copernicus Land Surface Temperature Monitoring (LSTM) mission ([32]; [31]). Both are targeting the latter half of the 2020s for mission launch and will improve the temporospatial coverage of a similar product to ECOSTRESS, which has a resolution of seventy meters by 70 m x 70 m per pixel. This is more than 10,000 times finer resolution than the monthly MODIS product used within that has a pixel resolution of 9 km x 9 km per pixel. However, MODIS has a much more frequent revisit time, seeing the same location multiple times before ECOSTRESS does. This fact is part of the motivation behind such follow on missions. In order to study changes of the planet during the day at very fine resolutions from satellites that are orbiting around Earth, we will need multiples. This practice of redundancy has been already put to work in several satellite missions, such as the two MODIS instruments on the Aqua and

Terra satellite platforms, the multiple GOES, Sentinel, Landsat, GRACE, and VIIRS missions.

We lastly see the potential for the integration of equations such as those used in the companion papers to NLDAS’s streamflow, the Saint-Venant equations ([53]; [46]). Physics-based machine learning is a field of its own. While we are pleased with the use of the convolutional, image focused networks, we see the benefits of more closely knitting historical hydrological advances into the bones of the neural network and think it could help move all experiments to the highest echelon of performance according to NSE ([36]).

3.6 Conclusion

Herein, we investigated the use of neural network architectures and how they can be applied to river flow forecasting of two transboundary watersheds. Our inputs to the networks were derived fields of meteorologically forced surface and subsurface flow, and gauged streamflow data obtained from United States and Canadian bureaus associated with hydrological monitoring. Flow fields only show observations for the land, which can create issues and cause limitations to the quality of neural net model generation and performance outcomes. In response, we also fused time-concomitant sea surface temperature fields to the GLDAS observations of flow, finding a marked difference in the prediction of streamflow. To bolster this study, we considered two different basins of vastly different human imprints and found a clear watermark when the basin is sufficiently artificially modified. We see a continuation of this work by locals to other nations using their continuous gauged streamflow data, the fusion of higher resolution datasets, translation for use as a drought monitoring prediction system, or potential scaling of the system to consider many more streamflow sensors. This study is focused on basins that are relatively high in latitude, and there is certainly nuance in other locations that our modeling did not capture here. Selecting

an equatorial location might produce different nuance. One potential suitor is Hawaii, which would be an opportunity to use requisite higher resolution datasets because of its relatively small size. Hawaii is unique because of the different climates like those on the leeward and windward side of Oahu. It is also favorable because of the relative ease with which continuous data can be secured. This future study might also mark partnerships with an equatorial international institution to obtain continuous streamflow measurements from their waters as a way to formally pollinate this work.

3.7 Code Availability

Scripts are available at https://github.com/albertlarson/f2f_holistic

3.8 References

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3.9 Appendix

Figure 3.1: Extents of the Yukon and Columbia River watersheds and gauge locations.

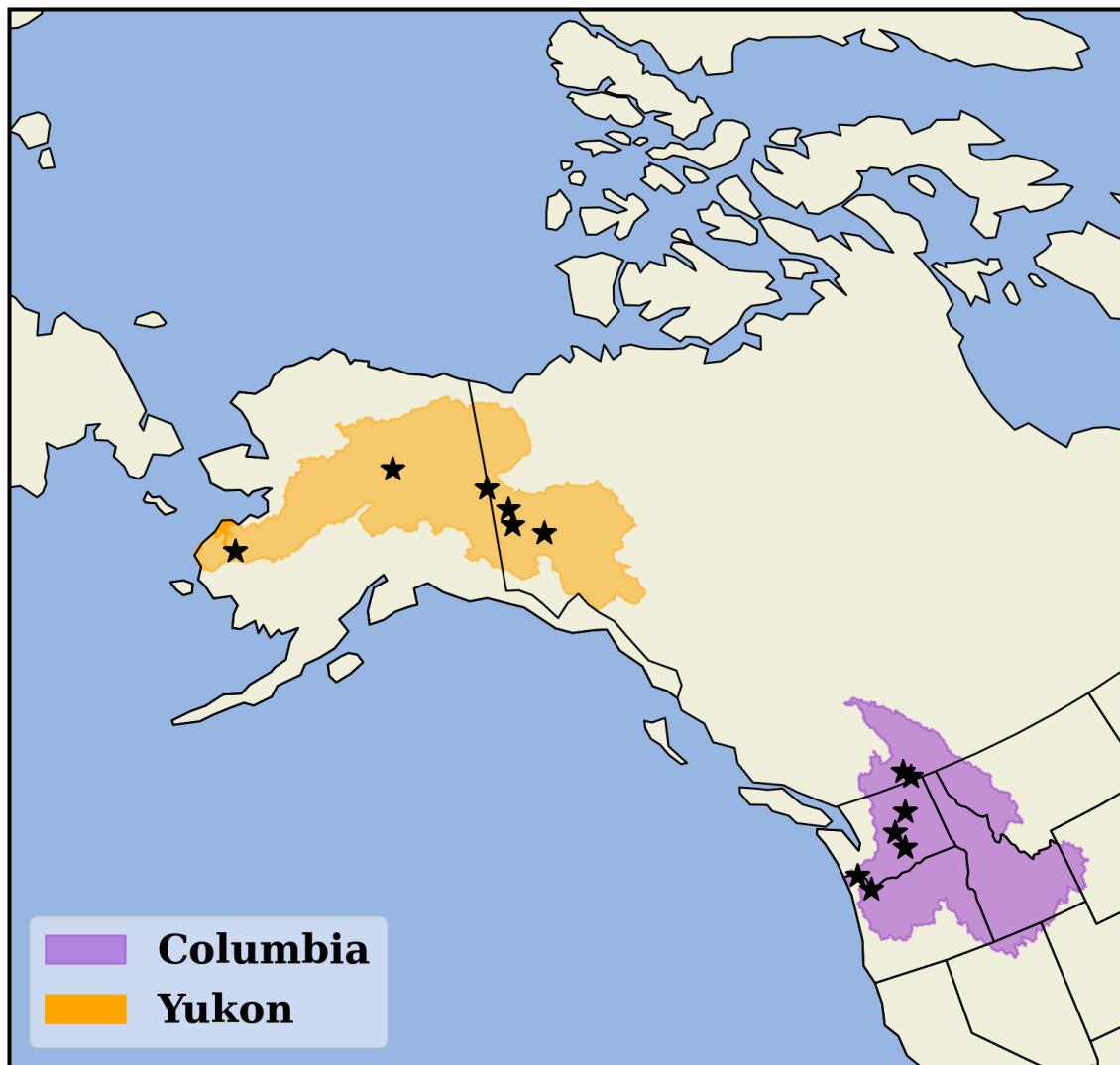


Figure 3.2: Hydrographs of all gauged streamflow data. Second and fourth plots are zoomed in versions of the same colors in the first and third plots. Both have low discharges whose details are lost amongst the larger portions of the river.

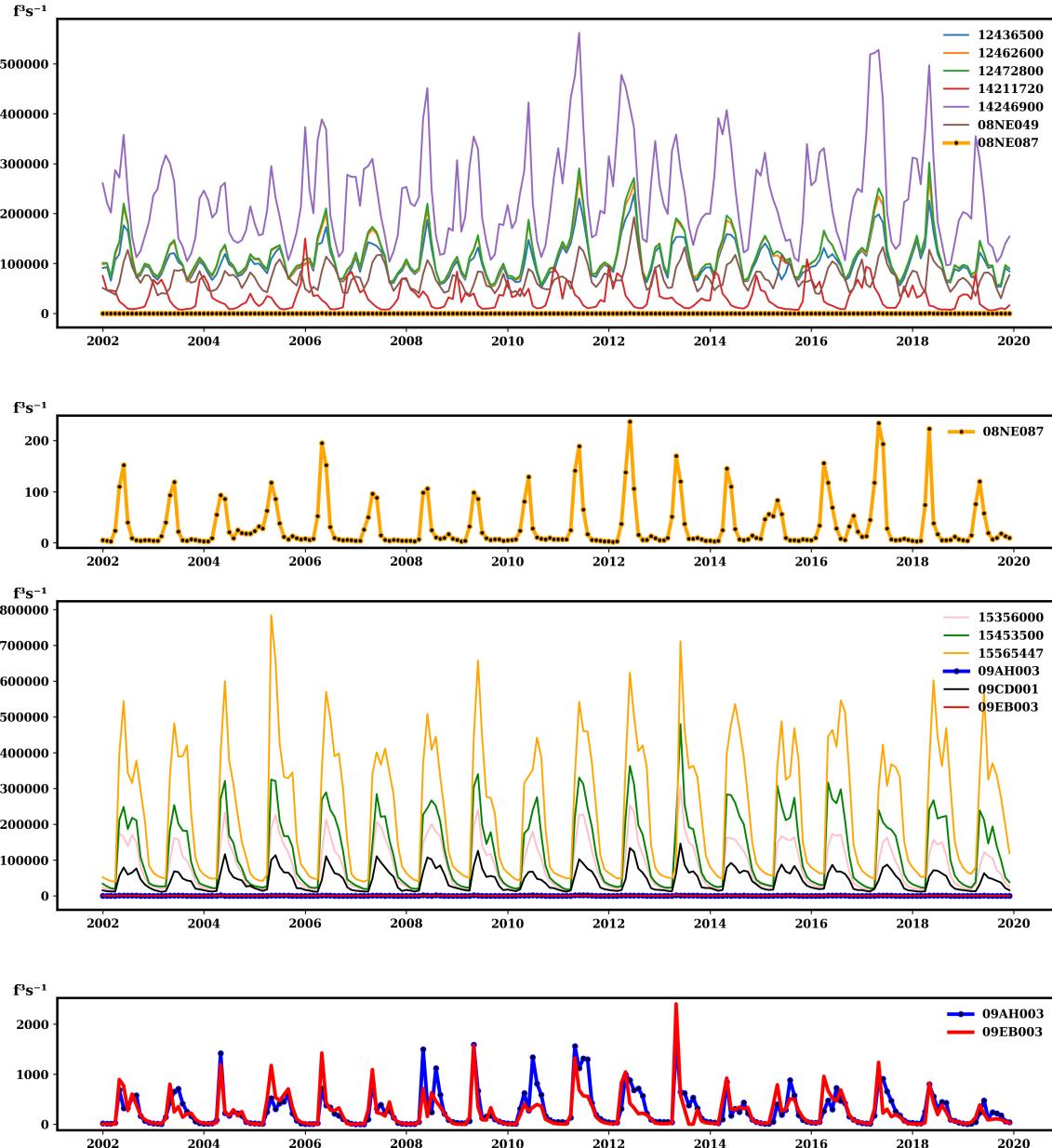


Figure 3.3: Sample observation of surface flow (Q_s), subsurface or groundwater flow (Q_{sb}), $Q_s + Q_{sb}$, flows merged with SST but represented with a single colormap, and flows merged with SST represented with two colormaps highlighting each physical parameter's unique dynamic range.

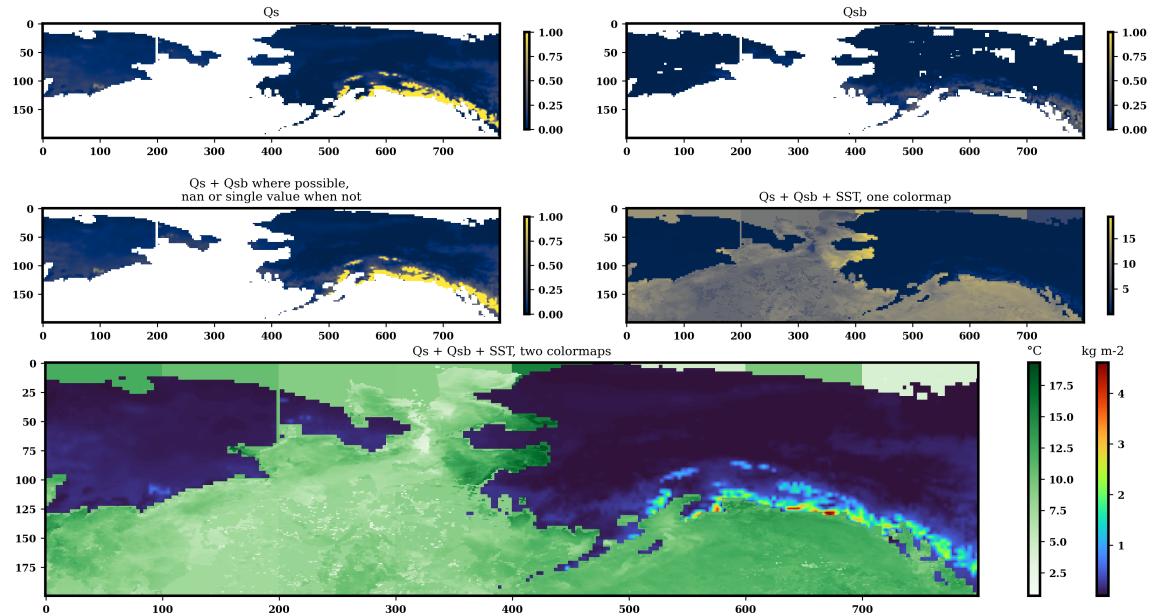


Figure 3.4: Histograms of model predictability across all experiments delineated by whether SST is included as part of the input or not.

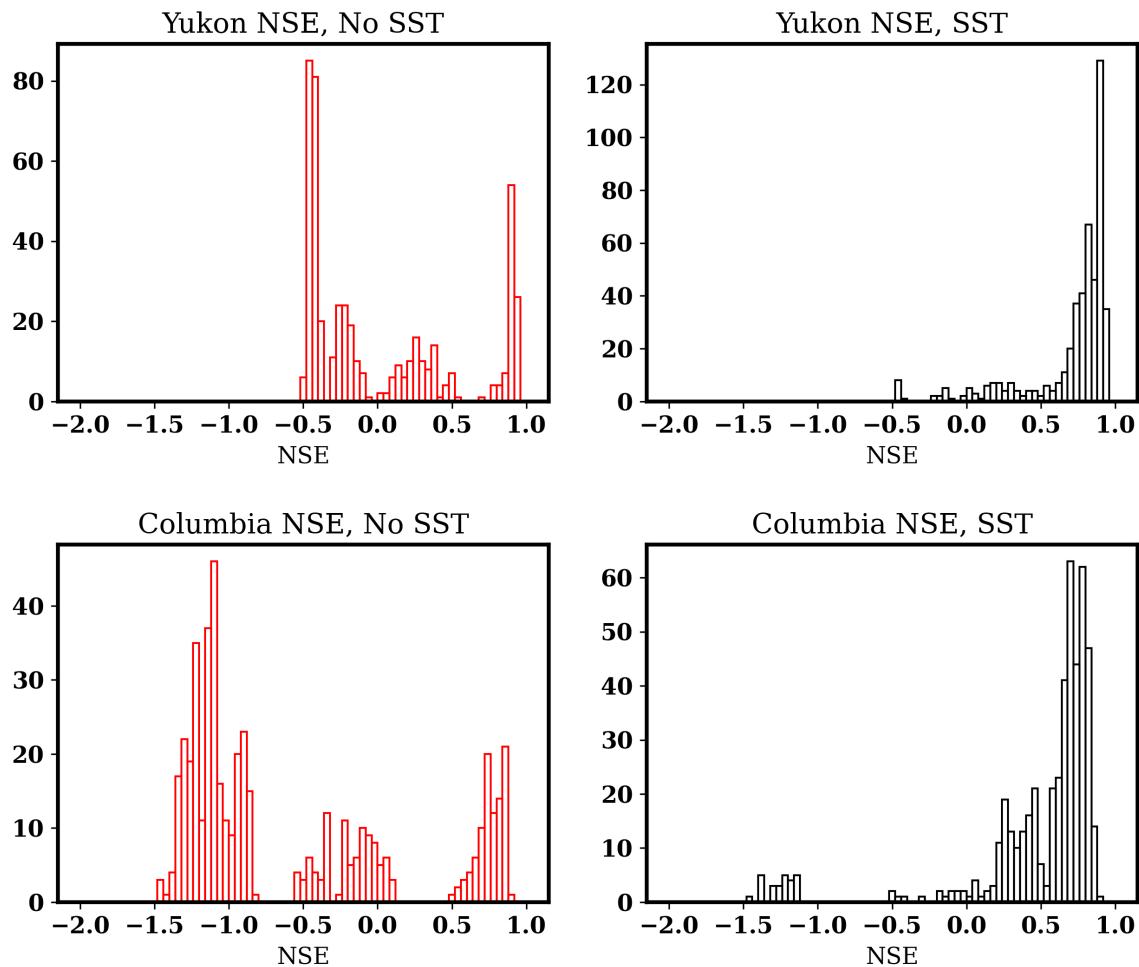


Figure 3.5: Histograms of test results for Columbia experiments deconstructed by neural network architecture at the time of training.

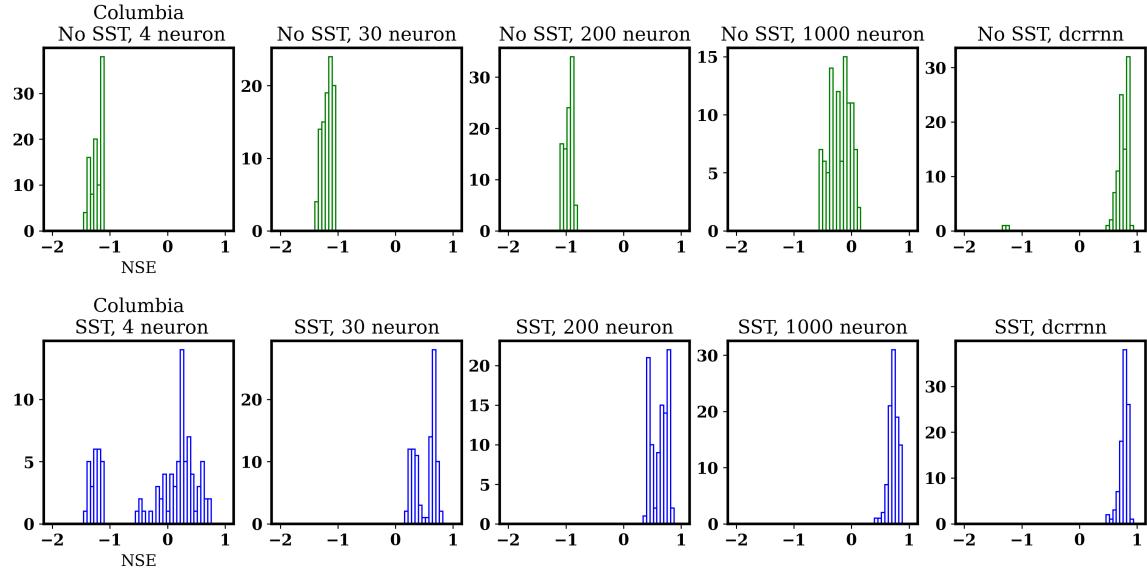


Figure 3.6: Histograms of test results for Yukon experiments deconstructed by neural network architecture at the time of training.

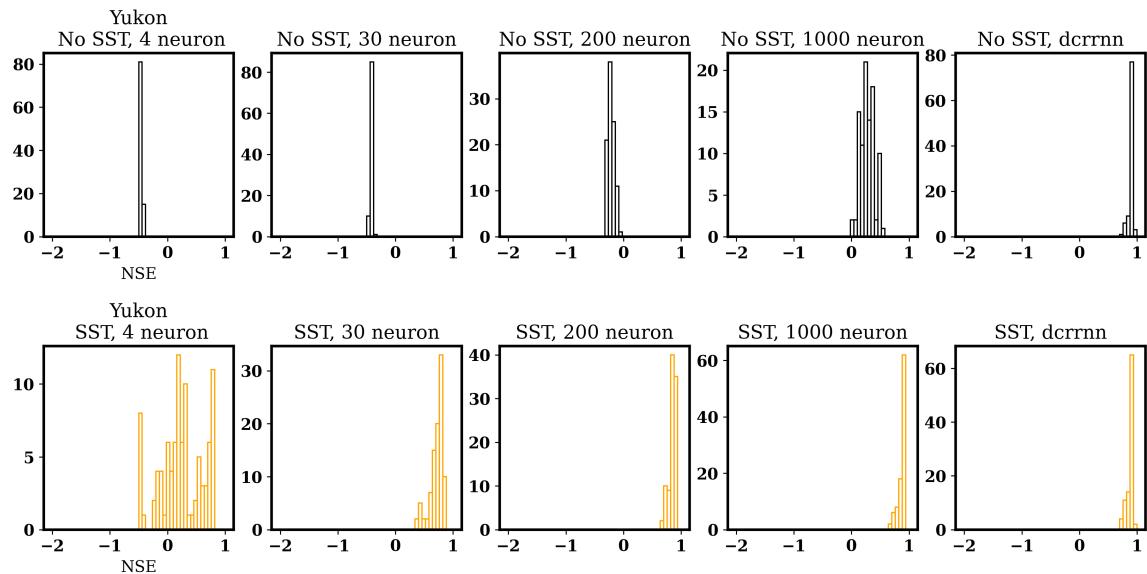


Figure 3.7: Columbia & Yukon experiments using dcrrnn and the 1,000 neuron single hidden layer neural networks, disaggregated by lag.

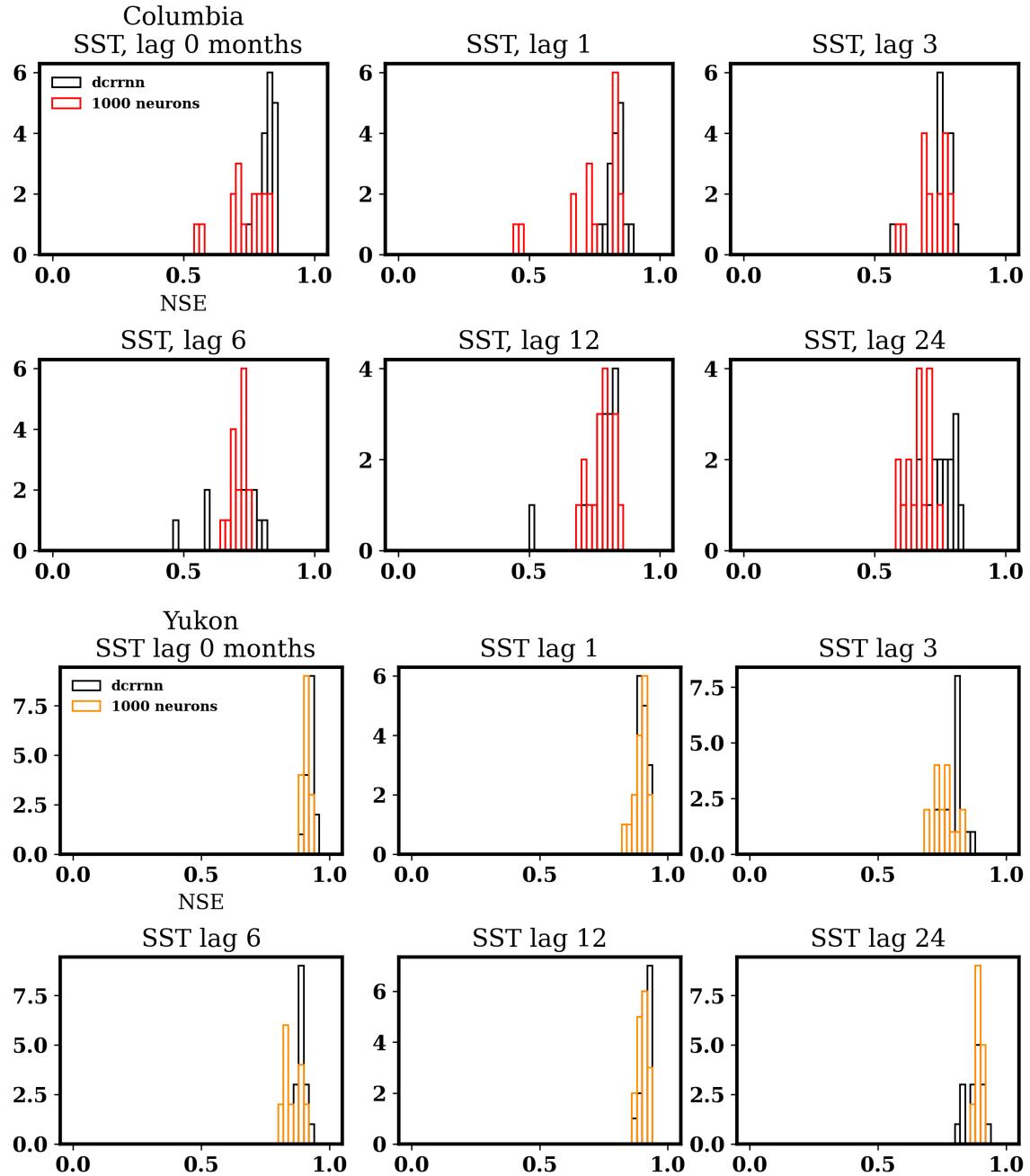


Figure 3.8: Columbia & Yukon experiments using dcrrnn and the 1,000 neuron single hidden layer neural networks, disaggregated by z-scored vs. non-z-scored.

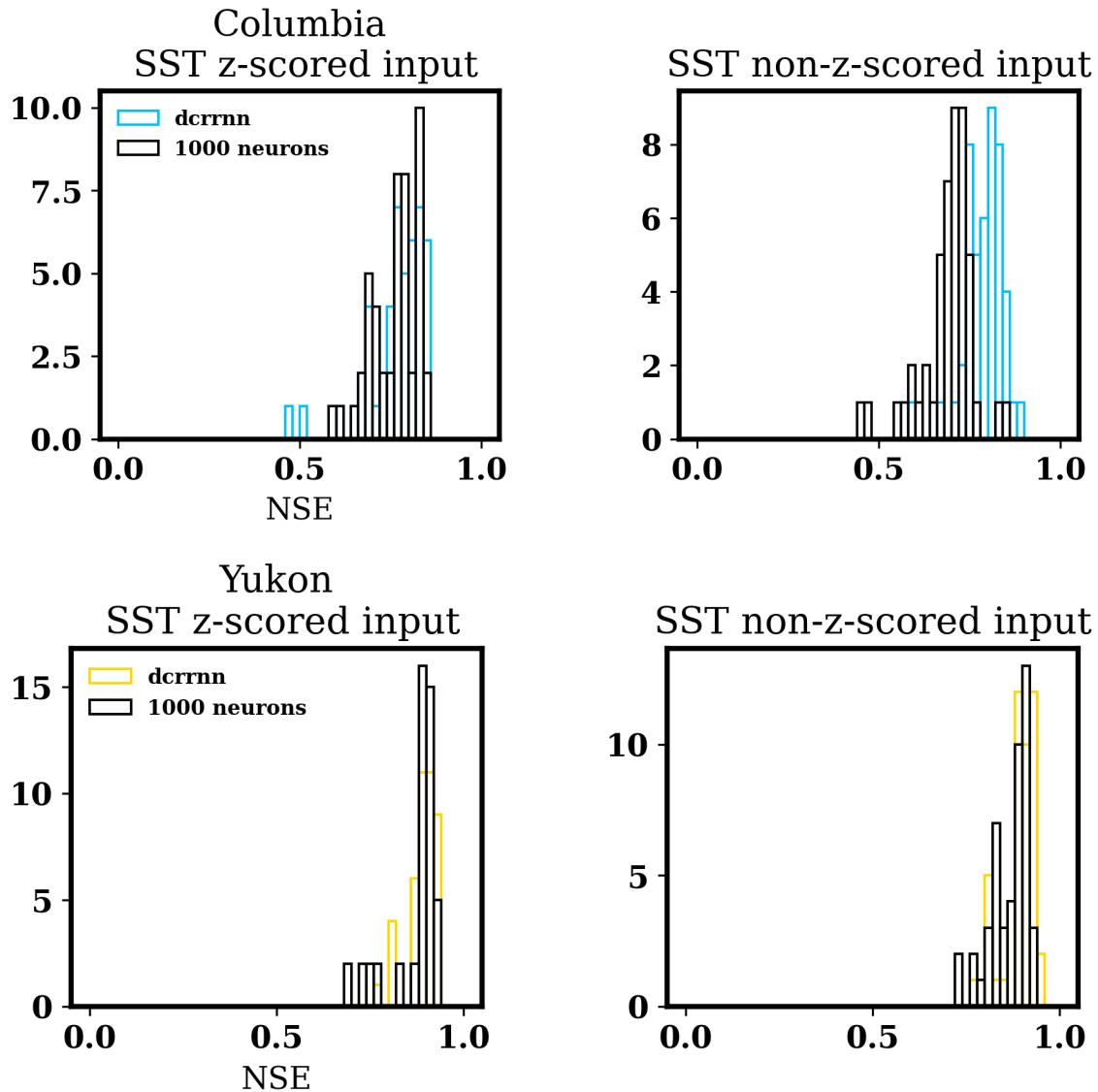


Figure 3.9: National Drought Mitigation Center Weekly Output, March 2, 2023, Drought Monitor Output.

