

Deep Learning Time Series Prediction Strategies for Efficiently Emulating Noah Land Surface Model Soil Moisture Dynamics

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Abstract

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This work examines the ability of deep learning time series generative models to accurately and efficiently emulate the hourly temporal dynamics of the Noah Land Surface Model (Noah-LSM) out to a 2 week forecast horizon, given atmospheric forcings and static parameterization provided by the second phase North American Land Data Assimilation System (NLDAS-2) framework. Results from multiple neural network architectures are compared alongside variations in prediction target, loss function characteristics, and model properties. The most performant model types are subsequently evaluated with respect to forecast distance, daily and annual seasonality, and against a variety of regional scenarios, including several extreme event case studies. Ultimately, we present a software system for developing and testing neural networks that use time-varying and static data to estimate temporal dynamics, with the goal of providing a foundation for similar data-driven modeling techniques to be implemented within the upcoming third phase of the NLDAS data record.

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If you wish, you may also thank family or friends. You may conclude your acknowledgments with a dedication rather than using a separate dedication page. Your acknowledgments should be brief and consistent in tone with a formal publication.

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Chapter 1. Introduction

Accurate characterization of the distribution of water content within the soil column by land surface models is critical for governing land-atmosphere interaction in numerical weather prediction (NWP) (Brocca et al., 2010) (Koster et al., 2010), operational decision making preceding and during drought and flood events (Otkin et al., 2016), and for downstream datasets aiding assessment of vegetation health, crop yield prediction, and fire risk characterization (Case et al., 2023). In order to address these needs, the Noah LSM was developed to serve as the land surface component coupled to NWP models including the Weather Research and Forecasting Model (WRF), the Global Forecast System (GFS) (Jin et al., 2010) (Mitchell et al., 2005), and climate models including the NCEP Climate Forecast System (CFSv2) (Saha et al., 2014). Noah LSM also aids National Weather Service forecasts and US Drought Monitor designations within decision support frameworks like the Short-Term Research, Prediction, and Transition high-resolution implementation of the Land Information System (SPoRT-LIS) (Case et al., 2022) (Case and White, 2014), and facilitates research and derived product development by providing soil states for NASA Land Data Assimilation System (LDAS) datasets (Ek et al., 2003).

By applying observational and reanalysis data to Noah and other land surface models, NLDAS has provided the community with consistent and quality-controlled multi-model land surface states and associated forcings in a near real-time capacity since 1999 (Cosgrove et al., 2003), with phase 2 of the project also contributing a retrospective climatology extending back to 1979. The first and second generation data products are calculated on a 1/8 degree geodetic grid spanning land-dominated points in the conterminous United States (CONUS) from 25° to 53° North latitude and 125°-67° West longitude, and are released at an hourly frequency (Mitchell et al., 2004) (Xia et al., 2012b). The third phase of the data assimilation system is currently under development, and aims to implement a wealth of upgrades including new data assimilation techniques and physical parameterizations, an increase in the spatial resolution to 1km², and the expansion of the domain to the full North American continent. As a consequence, the total number of valid land grid cells will increase dramatically from 76,088 in the first two phases to 27,245,580 with NLDAS-3 data products. In addition to the larger domain and updated physical processes used to develop the forcings and land surface states, the NLDAS-3 data suite will feature a variety of derived products. These products are anticipated include gridded climatological anomaly and segmented percentile data, stream routing and discharge estimates, and ensemble mean and spread information using forecast forcings (Kumar et al., 2024).

As the domain size and sophistication of data assimilation systems and land surface models like NLDAS and Noah LSM continues to grow, a niche de-

velops for methods that can generate reasonable estimates of the dynamics of numerical models which require less compute time, simplify the runtime environment of the program, and which can be fitted to observational data and then generalized to broader domains without accruing significant additional complexity to the parameterization scheme. Data-driven modeling techniques like deep learning with artificial neural networks (ANNs) are addressing this need by introducing the ability to approximate the highly nonlinear and conditional relationships between arbitrary predictor and target datasets. This flexibility is accomplished by learning a sequence of transformations which are encoded as a composition of alternating high-dimensional matrix operations and element-wise nonlinear functions, and which serve as a mapping from the vector of predictors to a corresponding target vector (Hornik et al., 1989).

In the context of time series physical modeling, ANNs enable the development of a statistically optimal approximation of the relationship between past states, simultaneous covariate data variables, and unknown current or future states. This general principle has a wealth of use cases. Previous literature shows that ANNs are computationally efficient and reasonably accurate for modeling dynamical systems like Lorenz'95 by formulating the problem as a discrete-time estimator of an ordinary differential equation which isn't explicitly known by the model (Fablet et al., 2018). ANNs can also be structured to have useful properties like the ability to estimate the jacobian of the transfer mapping between inputs and future states, even if the system being emulated isn't differentiable (Nonnenmacher and Greenberg, 2021). The same strategy may be applied to

forecasting the evolution of datasets like ECMWF Reanalysis v5 (ERA5) in a local or global domain, however significant challenges emerge as (Dueben and Bauer, 2018) identify. As they describe, ANNs cannot be constrained by default to conserve quantities like energy and water, and unlike numerical models, their handling of the underlying physical processes as a “black-box” mean that identifying sources of error within the model is difficult and often speculative. Furthermore, Earth system data tend to be highly regionally variable (ex. vegetation types), exhibit nonlinear autocorrelation between multiple variables (ex. temperature, dewpoint, and cloud cover), and are subject to rare but influential outliers (ex. snow and extreme precipitation). As such, although ANNs are adept at handling very nonlinear and conditional problem types, achieving the best performance and interpretability requires the utilization of application-specific knowledge when constructing and evaluating deep learning models.

Within the field of hydrologic modeling, most of the recent literature applying deep learning methods has focused on rainfall-runoff problems, where models forecast the hydrograph of a stream given time-varying atmospheric and land surface states as well as static properties. Inputs are typically considered within a spatial boundary drawn from a watershed outlet where a streamflow station provides the prediction target by directly observing the discharge. To that end, (Kratzert et al., 2018) applies a particular ANN architecture called Long Short-Term Memory (LSTM) networks to modeling discharge from the CAMELS dataset (Addor et al., 2017), which contains daily-resolution streamflow and meteorological forcings alongside parameters describing the topographic, land use, soil,

and geologic properties of 671 catchments. They show that models trained on single basins often outperform models trained using data from multiple basins within a region, and that subsequent “fine-tuning” of a generalized regional model on individual basins slightly improves model efficiency in many cases. Later, (Kratzert et al., 2019) improves on LSTM model performance by modifying the training strategy to optimize an objective function similar to Nash-Sutcliffe Efficiency (Nash and Sutcliffe, 1970), and by introducing a modification to the architecture that allows for static catchment parameters to be separately provided – and their influence separately investigated – from time-varying inputs. These experiments even out-performed several process-based models that were tuned specifically to the individual test basins. In spite of their black-box nature, (Lees et al., 2022) demonstrates that LSTMs used for daily-scale rainfall-runoff prediction maintain information correlated with physical properties of the catchment’s hydrologic state including soil moisture and snow cover, which indicates that they preserve meaningfully interpretable data about their inputs. The general approach of employing LSTMs for discharge forecasting is already being utilized by stakeholders like the United States National Weather Service and River Forecast Center offices in an operational setting with the NASA SPoRT Streamflow-AI product, which uses near real-time Noah LSM soil moisture estimates and outlooks as an input via the SPoRT-LIS data product (White et al., 2025), (Case et al., 2022).

Relatively few publications have applied deep learning techniques to estimate soil dynamics over a consistently spatially gridded domain, akin to the outputs of process-based models like Noah-LSM. In one instance, (Filipović et al.,

2022) applied LSTMs to global daily-scale ERA5 data in order to predict the 3-day evolution of moisture content in an intermediate-depth soil layer. This is conceptually similar to emulating Noah-LSM using NLDAS forcings because ERA5 determines its soil moisture states using the ECMWF Scheme for Surface Exchanges over Land (Balsamo et al., 2009). Additionally, (O. and Orth, 2021) used an LSTM to assist in generalizing in-situ observations at 3 soil depth levels to a regional grid, also using daily ERA5 forcings data as an input, and adjusting predictions to match the pixel-wise gaussian parameters of the ERA5 soil moisture analysis. Both of these approaches use long lead times of 60 days or 1 year, respectively, and make predictions at only a few forecast horizons per execution of the model (3 days and 1 day, respectively).

This work seeks to apply a similar strategy of data-driven modeling for hourly-scale emulation of Noah-LSM over the full NLDAS-2 grid domain, with the goal of generating accurate and computationally reasonable forecasts out to a two-week horizon at three depth levels simultaneously. We will construct a few distinct neural network types suited to this problem structure, compare their results through a variety of bulk statistics and case studies using physical reasoning, discuss lessons learned regarding training methodology, and present a general free and open-source framework for developing time series dynamical estimators using deep learning for gridded physical datasets.

Chapter 2. Background

In this chapter we will elaborate on the history and relevant details of the implementation of NLDAS and Noah-LSM, frame the problem in terms of the difference between numerical modeling and data-driven modeling approaches, and describe the technical properties and pertinent considerations for neural networks intended for time series modeling.

2.1 NLDAS and Noah-LSM: History and Implementation

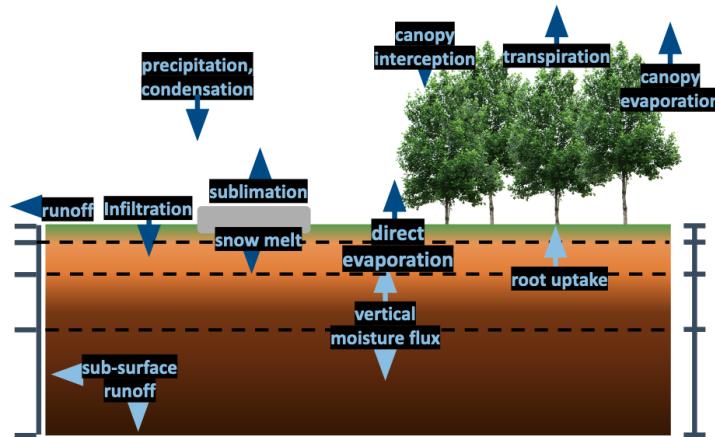


Figure 2.1: Schematic diagram of the feedbacks contributing to the evolution of soil moisture in Noah-LSM

The theoretical framework underpinning Noah-LSM was initially formulated in the 1980s as part of the OSU model, which characterizes boundary layer

moisture and energy fluxes as a 2-layer soil model subject to atmospheric forcings. The model expresses the infiltration and movement of water between the soil layers with the diffusive form of the Richards equation (Mahrt and Pan, 1984), direct evaporation using an analytic approximation of the Penman-Montieth relation in terms of atmospheric stability (Mahrt and Ek, 1984), and basic plant transpiration in terms of vegetation density and soil water content (Pan and Mahrt, 1987). These features form an interdependent system of differential equations that are numerically integrated using a combination of the Crank-Nicholson method and finite-differencing (Chen et al., 1997), which introduces the need for short time steps of 15 or 30 minutes in order for the system to remain numerically stable (Cartwright and Piro, 1992)(Mahrt and Pan, 1984).

The OSU model was later significantly improved, renamed to the first generation of Noah-LSM, and coupled with the NCEP Eta forecast model. Noah-LSM expanded the domain to four soil layers of increasing thicknesses (10cm, 30cm, 60cm, and 100cm), improved runoff dynamics by implementing Philip's equation for infiltration capacity (Schaake et al., 1996), and represented the influence of soil texture on moisture transport by introducing bounds on bare-soil potential evaporation that are determined by the soil composition (Betts et al., 1997) (Mahfouf and Noilhan, 1991). The model also features a significantly enhanced representation of vegetation including a more thorough treatment of canopy resistance via a "Jarvis-type" model of leaf stomatal control (Jarvis et al., 1976) (Jacquemin and Noilhan, 1990), which accounts for the dependence of transpiration on insolation, air temperature and dewpoint, soil moisture content, and vegetation density.

The vegetation effects are scaled by a monthly climatology of normalized difference vegetation index (NDVI) values observed by the NOAA-AVHRR satellite radiometer, which serve as a proxy for green vegetation fraction (GVF) (Gutman and Ignatov, 1998) (Chen et al., 1996), and the depth of root water uptake associated with plant transpiration is determined by a pixel's vegetation class as specified by the Simple Biosphere Model (Dorman and Sellers, 1989). Finally, the model's utility was greatly expanded with the addition of a frozen soil and snow pack parameterization incorporating the thermal and hydraulic properties of fractionally-frozen soil layers, the effects of state changes (Chen et al., 1996) (Koren et al., 1999), radiative feedbacks from partial snowpack coverage, and a snow density scheme (Ek et al., 2003).

Soon after the turn of the millennium, the first generation of NLDAS was under development as part of a multi-institution collaborative effort sponsored by the Global Energy and Water Cycle Experiment (GEWEX) Continental-scale International Projects (GCIP) team. The goal of the project was to incorporate long-term observations of land surface temperature, snow pack depth, and meteorological forcings from multiple sources (in-situ, satellite, radar) into a common framework used to independently evaluate land surface states and energy fluxes with four land surface models including Noah LSM (Mitchell et al., 2004). Over a domain including the full conterminous United States (CONUS) at 0.125° resolution, the models were allowed to spin up over the course of a year, and soil states were recurrently used to initialize subsequent time steps rather than being “nudged” to correct for drift. Land cover and soil texture classification over the

domain was derived by coarsening the University of Maryland and STATSGO datasets, respectively, from their native 1km resolutions (Hansen et al., 2000), surface geometry and elevation is provided by the GTOPO30 dataset (of the Interior, 1997), and the parameter values for soil hydraulic properties were adapted from observations taken at the University of Virginia (Cosby et al., 1984).

Attention remained on Noah-LSM in the following years as it continued to support NLDAS and other data assimilation and forecasting systems, which led to a series of improvements introduced alongside the next phase of the NLDAS project. A seasonal effect was added to vegetation by scaling the leaf area index (LAI) by the GVF within bounds determined by the plant type, and transpiration was scaled by a root uptake efficiency factor determined by the proximity of soil temperature to an optimum growth temperature (298 K). Several parameters were adjusted including the influence of vapor pressure deficit on transpiration rate, the minimum stomatal resistance for several plant species, and hydraulic parameters for some soil textures. The aerodynamic conductance coefficient – an important factor in the strength of moisture and energy fluxes from the surface – was increased during daylight hours, and a basic anisotropy model was introduced by modifying the albedo of some surfaces in terms of the solar zenith angle (Wei et al., 2011). Snowpack physics were also modified to improve surface exchange coefficients, and to gradually diminish the snow albedo over the time since the last snowfall (Livneh et al., 2010) (Liang et al., 1994). These changes introduce new feedbacks and involve sensitive parameters like LAI which have a strong influence on the model’s dynamics (Rosero et al., 2010). The retrospective NLDAS-2 data

Forcing	Unit	Source	Δt	Δx
Precipitation	kg m^{-2}	CPC Gauge observations	24h	14km
		WSR-88D retrievals	1h	4km
Temperature	K	NCEP NARR	3h	32km
Specific Humidity	kg kg^{-1}	NCEP NARR	3h	32km
Surface Pressure	Pa	NCEP NARR	3h	32km
Wind Velocity	m s^{-1}	NCEP NARR	3h	32km
Incident LW Flux	W m^{-2}	NCEP NARR	3h	32km
Incident SW Flux	W m^{-2}	GOES, NARR	3h, 1h	14km
Green Veg Fraction	%	AVHRR NDVI	Monthly	16km
Leaf Area Index	$\text{m}^2 \text{ m}^{-2}$	UMD, AVHRR NDVI	Monthly	16km
Snow Water Equivalent	kg m^{-2}	Noah LSM		14km

Table 2.1: Atmospheric forcings and other time-varying parameters provided by NLDAS-2 at a 1-hourly resolution on the 0.125° CONUS grid. Data are resampled using spatial bilinear interpolation, then temporal disaggregation according to (Cosgrove et al., 2003). NLDAS forcing files also include values for convective available potential energy, the ratio of precipitation from convection, and surface potential evaporation (calculated as in Mahrt and Ek (1984)), but these three values aren't currently used as inputs to the models. Snow water equivalent estimates are an output of Noah LSM by default, but are included as a predictor here under the assumption that they can be provided from a separate model or data assimilation source.

record generated after applying these modifications extends back to 1979, and continues to be updated in a near real-time capacity (Xia et al., 2012b).

The NLDAS-2 time-varying retrospective forcings listed in Table 2.1 will serve as the predictors used by the neural networks to forecast the Noah land surface model soil moisture states. Temperature, humidity, pressure, wind speed and heading, and longwave flux are derived exclusively from the National Centers for Environmental Prediction (NCEP) North American Regional Reanalysis (NARR) data product. As part of the downscaling procedure from their native 32km resolution to the $1/8^\circ$ NLDAS domain, a lapse rate adjustment is applied to the temperature and humidity fields based on the elevation profile. Downward shortwave radiative flux is calculated using a blend of NARR and hourly Geostationary Operational Environmental Satellite (GOES) data, with a ratio-based bias correction based on (Berg et al., 2003) applied to account for a known positive bias in NARR-reported downward shortwave flux, and to mitigate discontinuities arising from the merger the two data sources (Pinker et al., 2003) (Xia et al., 2012a). Precipitation receives a special treatment in order to ensure sufficient spatial resolution and consistency; the Climate Prediction Center (CPC) daily gauge-based product (Chen et al., 2008) serves as the baseline, which is temporally disaggregated to 1 hour resolution using National Weather Service WSR-88D radar retrievals (Fulton et al., 1998). In regions lacking radar coverage, the disaggregation is completed using a weighted combination of the CPC's satellite-derived estimates from morphed passive-microwave and infrared observations (CMORPH) (Joyce et al., 2004), and the CPC Hourly Precipitation

Dataset (HPD), with NARR data as a final fallback (Baldwin and Mitchell, 1997).

Although both the LAI and GVF vegetation parameters are based on multi-year monthly averages, they are disaggregated to an hourly resolution in order to be smoothly variable (Wei et al., 2011), and are thus treated like an atmospheric forcing in this work.

2.2 Distinctions in Modeling Techniques

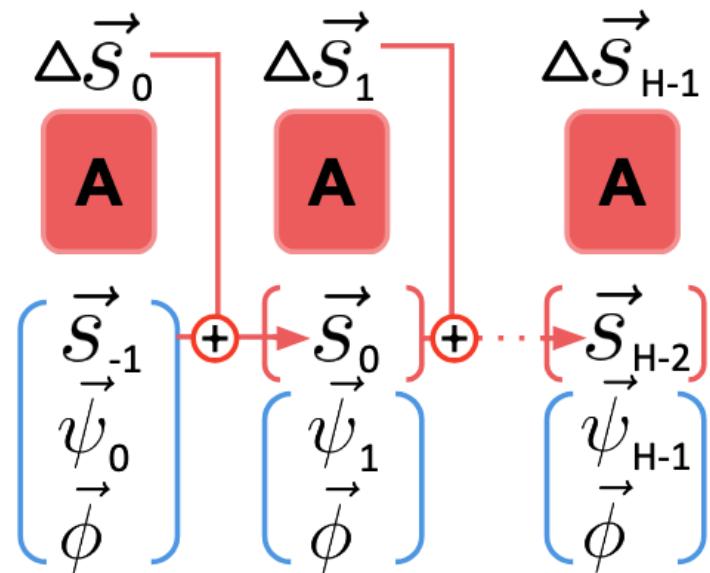


Figure 2.2: Diagram of a self-cycling discrete-time dynamical system with no hidden state. At each time, nonlinear operator \mathbf{A} maps an initial state \vec{s}_{k-1} , exogenous forcing $\vec{\psi}_k$, and time-invariant parameters $\vec{\phi}$ to a new state $\Delta \vec{s}_k$, used to initialize the subsequent time step, and so forth until H predictions have been made.

2.2.1 Noah-LSM as a Discrete Dynamical System

At its core, Noah-LSM is a collection of coupled differential equations that express the total derivative of land surface states $\frac{d\vec{s}}{dt}$ in terms of the current state \vec{s} , forcing $\vec{\psi}$, and time-invariant properties of each grid cell $\vec{\phi}$. Since the model is implemented as an algorithmic procedure and is not continuously differentiable, we will use the notation $\frac{\Delta\vec{s}_k}{\Delta t} \approx \mathbf{A}(\vec{s}_{k-1}, \vec{\psi}_k, \vec{\phi}_k, \Delta t)$ to refer to the model as a transition function evaluated at a discrete time step Δt , such that the system evolves as a dynamical system described by Equation 2.1.

$$\vec{s}_k = \vec{s}_{k-1} + \mathbf{A}(\vec{s}_{k-1}, \vec{\psi}_k, \vec{\phi}_k, \Delta t) \cdot \Delta t \quad (2.1)$$

Here, \vec{s}_k refers to the model's dynamic state variables like snow pack depth, soil moisture and temperature, and canopy storage, $\vec{\psi}_k$ encodes the covariate atmospheric variables from Table 2.1 (which are derived from weather forecasts or observations), and $\vec{\phi}$ includes time-invariant coefficients of the governing equations like vegetation type/fraction, soil texture, and slope/elevation. As a matter of convention, the time step $k = 0$ refers to the first perturbation of the initial state after applying the model's first increment change estimate, and includes the forcings that informed that perturbation, consistent with the relationships depicted by Figure 2.2.

To generate a time series, Noah-LSM numerically integrates the system of equations using Euler and Crank-Nicholson techniques, which explicitly evaluate the differential equations at several time intervals per computational time step

in order to estimate the nonlinear change in state, which evolves continuously in the real system being modeled. It is crucial that the increment change in time remains small between evaluations of the model (15min for NLDAS-Noah) to mitigate truncation error from the assumption of local linearity (Mitchell et al., 2004) (Cartwright and Piro, 1992). As Figure 2.2 suggests, the model does not retain any “hidden” internal information that is updated between timesteps; at each point, the information available to determine the new change in state is limited to the input domain of the model.

2.2.2 Process-based vs Data-driven Models

The process-based approach of numerical models like Noah-LSM is practically and epistemologically distinct from data-driven techniques like deep learning. In a process-based paradigm, the inductive biases that govern the model’s behaviors can be explicitly understood since they are based on a characterization of the physical system which is derived from theoretical knowledge. Some uncertainty is introduced by the input data, and is shared among all model types; this includes uncertainty from noise and interpolation of forcing observations, discrete treatment of surface types, etc. Aside from that, model error in process-based models arises from sources including inadequacy of the theory for describing the system (that is, phenomena which are neglected or misrepresented, and become a source of unexplained variance), and truncation error accumulated from the approximation techniques used to solve the model’s governing equations. Explicit understanding of the reasons for the model’s behavior has the advantage of be-

ing interpretable, in the sense that particular systems within the model can be independently evaluated and blamed for contributing uncertainty. Additionally, granting the ability to impose absolute constraints within the model structure ensures the outputs fully adhere to some physical requirements, such as conservation of water and energy. Nonetheless, the onus falls entirely on the model developer to adjust many details of the implementation of the processes. The act of tuning a numerical model’s parameters often implies postulating a source of uncertainty, addressing it by manually manipulating coefficients or introducing new systems within the governing equations, and then evaluating the impact of the changes using correlational analysis with a subset of the available data. This can be a laborious process, and typically results in the gradual accumulation of feedbacks and complexity within the model.

In contrast, many data-driven approaches to modeling physical systems – deep learning in particular – sacrifice the explainability and rigorous physicality of their estimates in exchange for developing a statistically optimal approximation of the relationship between the input and output domains by any means available. Although the overall algorithmic structure of the ANN is established by the developer – typically based on broad heuristics from past literature and experimentation – very little control can be asserted over the particular means by which predictions are determined from inputs. Instead, the effectiveness of the ANN’s performance is characterized in terms of a differentiable loss function (also known as the objective or cost function) which may be defined by the developer,

and which is fundamentally (though indirectly) important for determining the solution developed in the training phase.

An ANN’s learnable parameters refer to the real-valued elements of a series of arbitrarily-sized square matrices encoding affine transformations. Each “layer” of the ANN is comprised of one of these affine transformations followed by an element-wise nonlinear operation on its output, and the full ANN typically consists of multiple layers which are combined via composition or any kind of differentiable arithmetic operation. During training, all of the ANN’s learnable parameters are iteratively adjusted by estimating the gradient of the loss function with respect to the parameters (given batched subsets of the predictor/target data pairs) then determining the direction and magnitude by which the parameters in each of the layers should be modified with an algorithm called backpropagation (Rumelhart et al., 1986). The general strategy of determining the sensitivity of the loss landscape to changes in the ANN’s parameters, and tweaking them accordingly, is referred to as gradient descent. Given at least 2 layers (which constitutes the definition of a *deep* ANN), the network is theoretically capable of expressing an arbitrary decision boundary or multivariate function given a sufficient number of parameters (Hornik et al., 1989). This high level of expressivity enables the network to learn complex relationships and generalizations among high-dimensional parameters, given repeated exposure to instances of these relationships during training.

The principle of ANNs using high-dimensional nonlinear correlations rather than explicit processes to model the correspondence between two datasets is pow-

erful because they can approximate a highly nonlinear regression without numerically integrating a complex algorithm, and they can learn their parameterization based on a large volume of data without manual intervention. The quintessential drawback of relying on a black-box approach, though, is that models may perform poorly for no apparent reason, or may perform well for a fraught reason. For example, in one commonly-invoked anecdote described by (Lapuschkin et al., 2019), an image classifier over-performing but failing to generalize at identifying horses in a grassy field was found to actually rely on the presence of the watermark of a particular equestrian photographer whose work was a part of the training data. As such, only regarding bulk statistics and loss performance as indicative of a model’s success is insufficient to consider it trustworthy. In a data-driven paradigm, then, the role of the ANN developer is to facilitate effective and reliable learning through careful training data curation, cognizant loss function and model architecture design, and thorough evaluation of the model’s behavior in local and global scenarios throughout the input domain in order to ensure the effectiveness and consistency of predictions in a variety of inference settings.

Furthermore, it is important to note that in the current scope of this work, it is not possible for the ANNs to leverage their expressivity to out-perform the numerical model. Since the ANNs presented here are merely emulating the processes that are programmed into Noah-LSM, it isn’t reasonable to expect the models to form a more accurate representation of real soil dynamics. Nonetheless, it is conceivable that future work could utilize a similar approach to (O. and Orth, 2021) in order to integrate observational data into the training domain alongside

model data, or to use it as a prediction target. The merger of these two data sources could aid in improving a data-driven model beyond the limitations of a numerical model's structure.

2.3 Deep Learning of Time Series

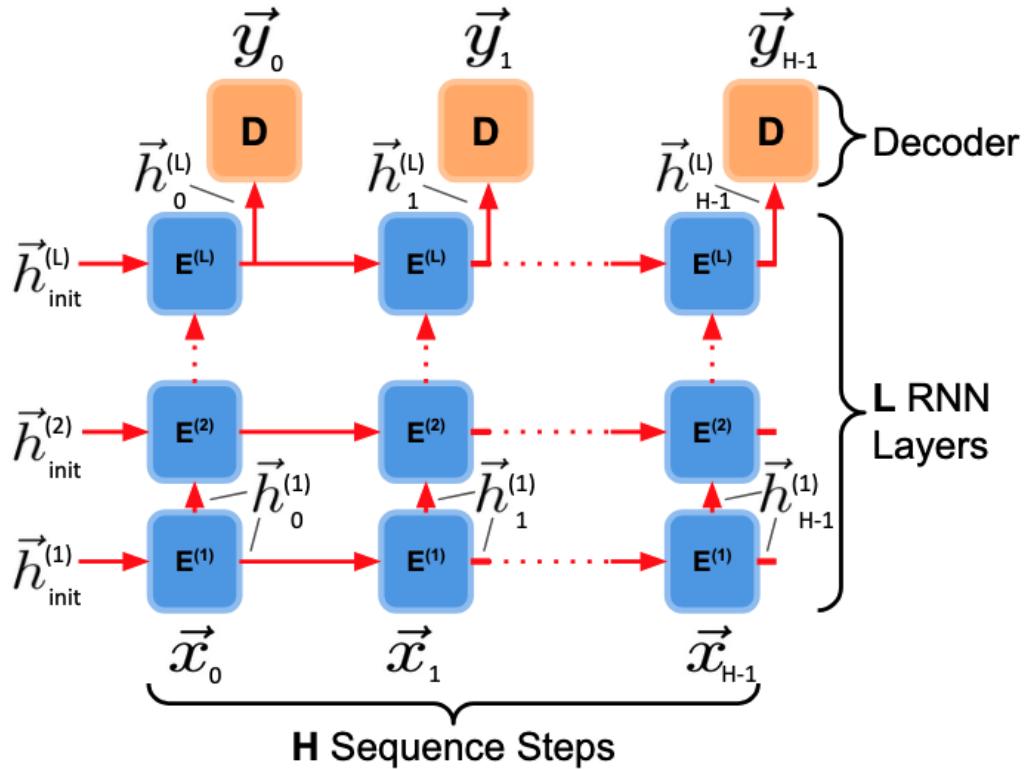


Figure 2.3: Schematic representation of an abstract sequence-to-sequence RNN with multiple layers.

The most simple variant of an ANN is referred to as a feed-forward neural network (FNN), which consists of a series of composed layers (see previous section) mapping the input vector directly to the output. Although a FNN is theoretically

capable of simulating Noah-LSM in the manner of Figure 2.2, inductive biases are commonly introduced in model architectures in order to promote efficiency, explainability, stability, and parsimony. For example, most neural networks used for sequence modeling like the recurrent neural networks (RNNs) in Figure 2.3 maintain one or more “hidden” latent parameters \vec{h} with an arbitrary number of dimensions. This vector is modified and passed along by each subsequent iteration, giving the network the ability to make temporal generalizations and propagate information to future predictions. Although \vec{h} is typically difficult to interpret directly, the gradient descent process incentivizes the network to preserve and consolidate information that is needed to accurately generate the full sequence of predictions. Each of the following network architectures ultimately aim to improve the information quality of the latent vector by implementing algebraic structure, introducing statistical uncertainty, and encouraging sparsity.

$$\begin{aligned}\vec{h}_k^{(1)} &= \mathbf{E}^{(1)} \left(\vec{h}_{k-1}^{(1)}, \vec{x}_k \right) \\ \vec{h}_k^{(j)} &= \mathbf{E}^{(j)} \left(\vec{h}_{k-1}^{(j)}, \vec{h}_k^{(j-1)} \right) \\ \vec{y}_k &= \mathbf{D} \left(h_k^{(L)} \right)\end{aligned}\tag{2.2}$$

The RNNs discussed here will follow the general structure described by Equation 2.2, which is consistent with the abstract architecture diagrammed in Figure 2.3, and follows the typical approach for constructing RNNs as outlined in (Russell and Norvig, 2020). The architecture consists of L encoder layers ($\mathbf{E}^{(1)}$ - $\mathbf{E}^{(L)}$) which generate H top-layer latent vectors corresponding to each of

the prediction times, and 1 layer of decoder weights \mathbf{D} which converts each of the top-layer latent vectors to a prediction for the increment change in state $\Delta \vec{s}$ between the current timestep and the next one. Parameters for \mathbf{E} and \mathbf{D} are shared across timesteps, however each of the L layers have distinct parameters. Here, $\vec{h}_k^{(1)}$ is a member of the time series of first-layer latent vectors given the arguments \vec{x}_k and the latent vector from the previous first-layer timestep $\vec{h}_{k-1}^{(1)}$. Moving upward, $\vec{h}_k^{(j)}$ is an intermediate-layer latent vector such that $j \in [2, L]$, and when $k = 0$ (the first horizon timestep), $\vec{h}_{-1}^{(s)} = \vec{h}_{\text{init}}^{(s)}$ for any layer s . In many cases, the initial hidden states $\vec{h}_{\text{init}}^{(s)}$ are randomized or set to zero, however in this project we use a separate spin-up RNN to establish them, as will be discussed in the Methodology section.

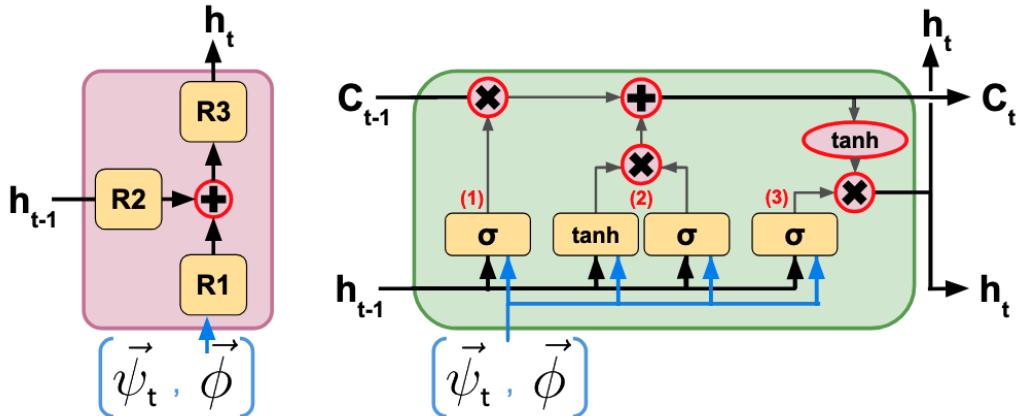


Figure 2.4: Schematic representation of individual RNN cells, the naïve RNN (left), and the LSTM (right)

The term RNN does not refer to a specific neural network architecture, but rather the category of architectures that share their weights across sequence steps. The sub-network unit of weights applied at each timestep (\mathbf{G} or \mathbf{E} in Figure 3.13)

is referred to as a RNN cell, and must contain internal structure for converting inputs from lower layers and the previous timestep into an output. Unlike traditional ANNs which use backpropagation to train on single input-output pairs, each cell must balance the penalty of its loss gradient between contributions from the input at each timestep with contributions from the latent vector of the previous timestep. To accommodate this difference, RNNs are trained using a special type of gradient descent called backpropagation through time, which balances the loss with respect to the two input sources, and accumulates it across all timesteps before updating each cell’s parameters.

The most basic form of the RNN architecture (diagrammed on the left side of Figure 2.4) consists of 3 separate affine operations. As shown in the figure, R_1 and R_2 convert the lower-layer and previous-timestep vectors, respectively, into two uniformly-sized internal latent vectors. The sum of these internal vectors are transformed by a third affine operation, R_3 , into the cell’s output, which is passed along to the higher layer and subsequent steps within the same layer.

This style of naïve RNN is vulnerable to the so-called vanishing or exploding gradient problem, which arises from the fact that the cell output is the direct product of learned matrix operations. Since during training each cell’s weights are updated recurrently based on many sequence steps, the loss gradient with respect to each learned parameter can become incredibly sensitive to changes in each parameter. This can cause weights to become very close to zero, or to diverge to very large numbers, which halts the learning process (Mozer, 1995). Furthermore, since the latent state passed between sequence steps undergoes a

nonlinear transformation at each instance of the cell, it is more tenuous for the network to sustain information over a long context of past observations.

The LSTM architecture addresses these shortcomings by maintaining a separate hidden state \vec{C}_t called the context vector. Rather than being generated by a matrix operation at each step, the context vector is only modified from the previous step’s value using the output of a series of three “gates.” These gates (numbered in Figure 2.4) include (1) the “forget gate”, which uses a FNN to select a vector of values in the range (0,1). The forget vector is multiplied element-wise by \vec{C}_{t-1} in order to selectively emphasize or diminish its activation. The “update gate” (2) transforms the inputs into a new coefficient vector in the range (-1,1), which is added to the context vector in order to retain information from the current time step. Finally, the “output gate” (3) generates a vector of multiplicative coefficients in the range (0,1) used to scale the new context vector \vec{C}_t to the output latent state \vec{h}_t (Hochreiter and Schmidhuber, 1997). The context vector remains stable compared to a hidden vector that is recurrently operated on by the same weight matrix, which facilitates the network to learn over a longer sequence interval.

The Transformer architecture has dominated many sequence modeling tasks in recent literature thanks to the key innovation of multi-head self-attention (MSA), which enables the architecture to learn complicated relationships between individual members of the input sequence regardless of their relative position. Additionally, transformers are efficient to train in parallel, unlike RNN architectures which rely on a chain of sequential operations, which makes them straightforward

to train on a massive scale (Vaswani et al., 2017). The results for natural language processing (NLP) (Devlin et al., 2019) and image classification (Dosovitskiy et al., 2021) tasks are impressive, however there are several key drawbacks that make them less appealing for a time series generation task like this one.

First, the memory cost of a transformer scales quadratically with sequence length since MSA learns parameters relating every possible combination of input steps. This is compounded with the fact that the full input sequence needs to be re-initialized with every step during inference. These properties are a direct trade-off with the Transformer’s ability to train separate sequence steps in parallel. Furthermore, unlike RNNs and CNNs, Transformers don’t have an inherent notion of order. In problems like NLP where sequence position conveys some information, a simple form of locality is introduced by adding a positional embedding vector directly to the inputs. Prior literature shows that transformers equipped with positional embedding still perform no better on basic time series forecasting tasks than a simple 2-layer FNN (Zeng et al., 2022). For these reasons, although MSA is a very powerful tool for many applications, we will be neglecting this very popular architecture in this work.

Chapter 3. Data and Methodology

3.1 Dataset Overview

This section includes a description of the storage of and framework used to interface with the data, insights on the value distributions and spatial variability of the input forcings from NLDAS-2, as well as a look at similar bulk properties of the target soil moisture states and governing processes within Noah LSM. In this work, we define our valid domain to include all points falling within the conterminous United States, excluding those points within the NLDAS-2 domain falling with Canada and Mexico. We also exclude points that are classified as “water,” “bedrock,” or “other” in the STATSGO dataset, since they don’t correspond to meaningful hydraulic properties, and have idle time series. What remains are 50,875 candidate grid cells within a 224x464 pixel domain.

3.1.1 Data Storage System

The data used in this project were acquired from the Goddard Earth Sciences Data and Information Services Center’s Distributed Active Archive Center (GES DISC DAAC) in May of 2024. The DAAC archives the NLDAS-2 forcings and corresponding Noah LSM model outputs as separate hourly files in a GRIB1 format, of which we downloaded the full 12-year time series from January 1, 2012

to December 31, 2023. This subset constitutes 210,384 files with a total size of just over 891.38 GB.

Since this project concerns developing 2-week time series of the forcings on a per-pixel basis, it would be inefficient to extract data from several hundred files for each sequence sample. Furthermore, it is widely recognized in deep learning that input/target pairs from heterogeneous datasets should be globally shuffled during the training process, as outlined by (Nguyen et al., 2022). This is because local subsets may have distribution characteristics that are distinct from the full dataset, so as the model trains on an unshuffled dataset, the loss gradients it experiences may encourage it to converge on a locally-optimal solution that does not generalize well to the overall task. Shuffling is especially salient for geoscience datasets like this one, which are highly spatially and temporally heterogeneous. With this in mind, the overhead from file I/O operations would be prohibitive for sporadically drawing samples from throughout the GRIB dataset during training or inference.

To address this problem while maintaining the spatiotemporal structure of the data, we develop a custom file standard using the HDF5 format – hereafter referred to as the TIMEGRID – and extract the full 12-year NLDAS and Noah LSM record as a collection of them. The HDF5 format offers a system for memory-mapped data chunking in multiple dimensions, which means the data therein can be sparsely buffered and accessed on a per-chunk basis without loading the entire file into memory: a considerable advantage for thoroughly shuffling or accessing subsets of contiguous data within large files. In practice, each timegrid contains

3 years of data covering 1/6 of the spatial domain, and stores the 4-dimensional time-varying data (time, latitude, longitude, data type), 3-dimensional static data (latitude, longitude, data type), and timestamps alongside a string-serialized attribute dictionary. The attributes contain information on abbreviated and full data type names, ordering, units, and sources, which are sufficient to inform a variety of accessor methods with a wealth of downstream use cases.

3.1.2 Spatial Data Characteristics

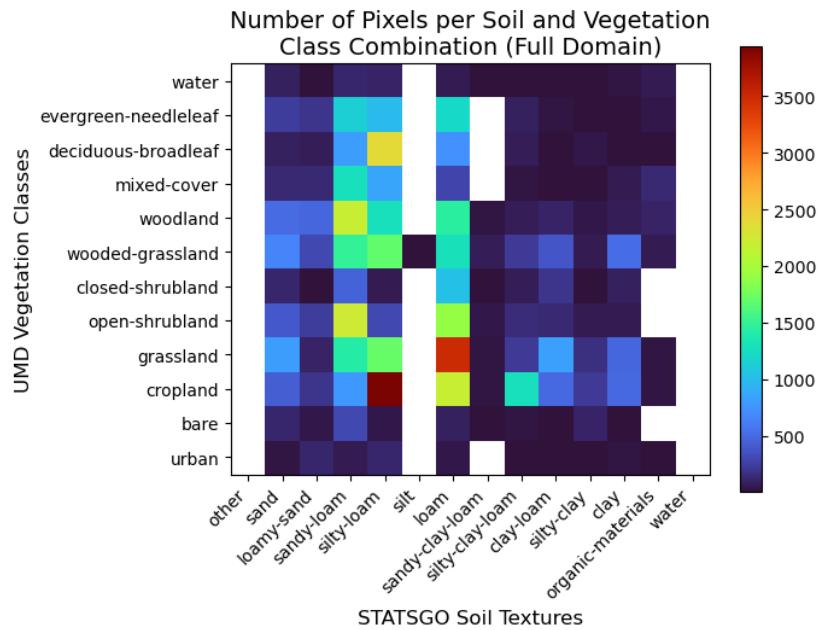


Figure 3.1: Full-domain combination matrix of vegetation and soil classes

One important aspect of the NLDAS-2/Noah-LSM datasets is the relationship between static and dynamic parameters, and the regional variance of both of these input types. Given any particular forcing time series, the subsequent

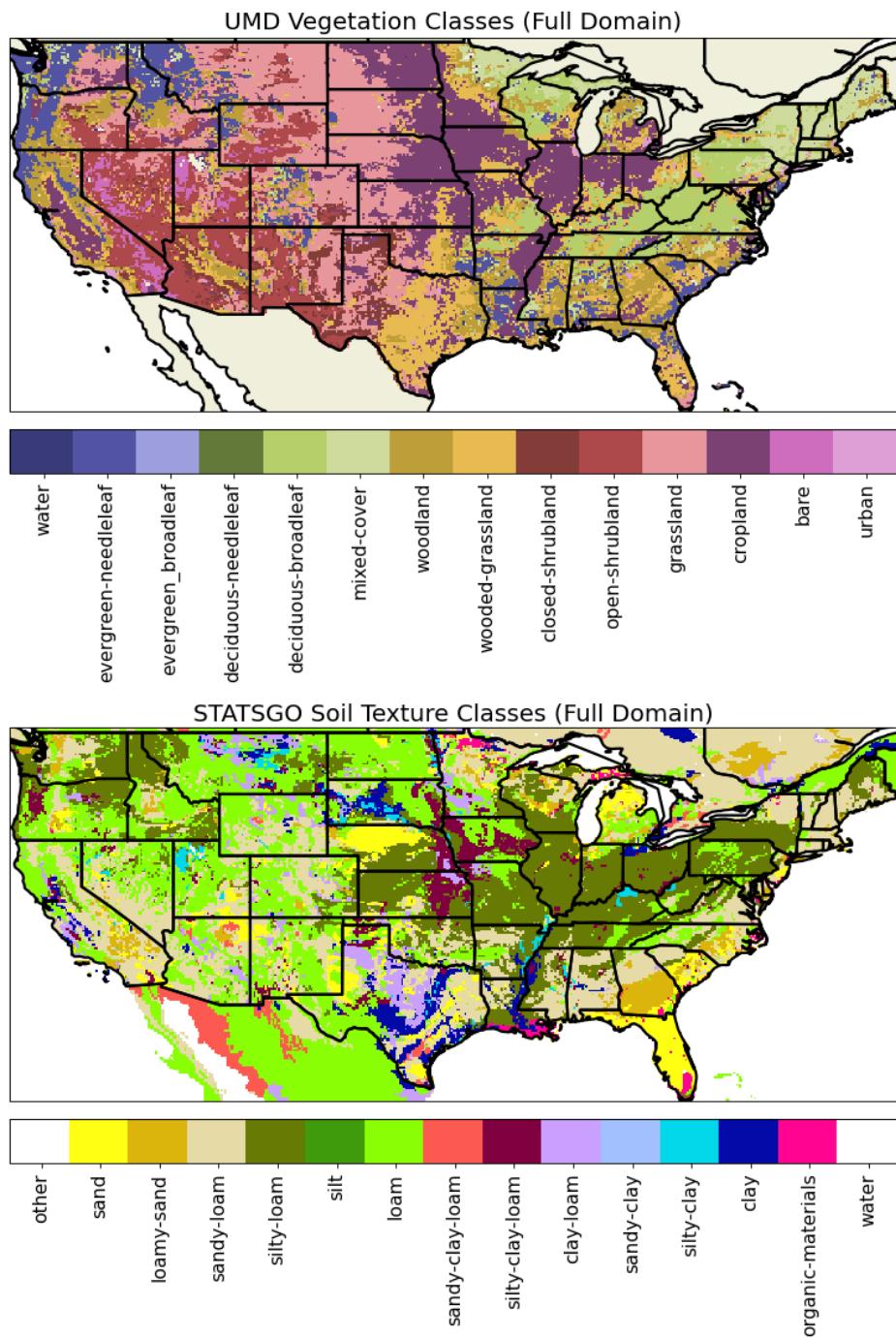


Figure 3.2: Spatial distribution of vegetation and soil classes

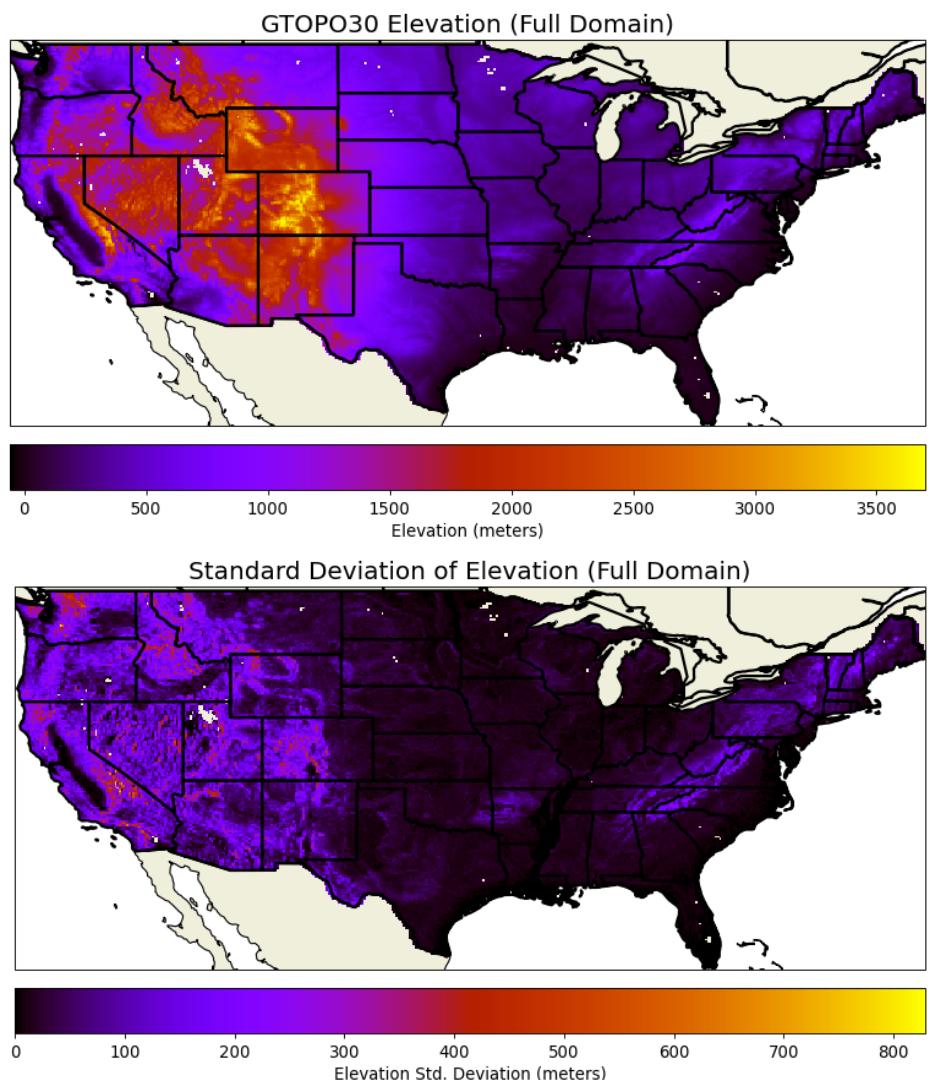


Figure 3.3: Elevation and standard deviation of elevation on the CONUS domain

land surface response is modulated by values for vegetation type, soil texture, elevation, standard deviation of elevation, slope, and slope aspect, which are consistent per-pixel throughout the dataset. In this work, we will only train models informed by the first four. Slope and aspect were left out because within Noah-LSM they are only used within the snowpack parameterization (Barlage et al., 2010), and snow is generally not a target variables for the models presented here. Furthermore, slope correlates strongly with the standard deviation of elevation. In retrospect, however, these inputs may have increased the information available to the models for estimating the transference of water from snow melt to the soil layers, especially in mountainous regions like the Rocky Mountain and Sierra Nevada ranges. An evaluation of the impact of these parameters on model results is left for future work. Elevation is mainly used to perform orographic regressions on pressure, temperature, humidity, and precipitation while resampling forcing data, however it could be useful as a predictor that indicates processes relevant to mountain snowpack dynamics.

As described in the background, the vegetation classes encode the properties of the canopy relevant to precipitation interception and land surface shading, the efficiency of plant transpiration at removing water from the soil, and the number of layers from which water is drawn (that is, the rooting depth). Since the vegetation parameter is discretely categorical within the Noah-LSM algorithm, we employ a special method of introducing them into the model called class embedding, which is elaborated upon in the next subsection. The soil texture class corresponds to a variety of hydraulic properties identified by (Cosby et al., 1984),

which include field capacity, hydraulic conductivity, porosity, wilting point, matric potential, and Skempton's pore water pressure ("B" parameter). These describe physical characteristics of the soil-water system including the rate of downward percolation of water, the efficiency and limits of plant water uptake, the speed of infiltration, and the total amount of water that soil can contain per unit volume. The basic observable feature of soil that determines all of the hydraulic properties is the size distribution of its constituent particles, which is often articulated as the mass fraction of sand, silt, and clay components within the soil. In the interest of providing the models with real-valued inputs having relatively low dimensionality, these three texture components will serve as the representation of soil texture for the ANNs trained here.

The interplay between plant water uptake and soil water dynamics as governed by the static inputs represents a considerable source of complexity within Noah-LSM. Furthermore, as Figure 3.1 demonstrates, the distribution of combinations of soil and vegetation categories is extremely non-uniform, which makes it more difficult for ANNs to learn solutions that are general. Figure 3.2 shows the geographic locations of vegetation and soil classes. The most common class combination is silty-loam soil types juxtaposed with cropland, with 3,945 members found dominantly in the Midwest and lower Mississippi river basin, with some contribution from the Columbia Plateau in Washington and Eastern Nebraska. Next most common are the 3,490 pixels in loamy grasslands, which are distributed widely throughout the West US including the high plains, Western Texas and New Mexico, Utah, and Idaho. The remaining combinations all have fewer than 2,500

members within the domain. Sand and clay dominated soils form the upper and lower extremes of soil particle size, respectively, and thus have rather different soil water characteristics. The sandiest soils are found in Southern Coastal Plains, Michigan, Texas, the Nebraska Sandhills, and the desert Southwest. Clay soils are relatively rare compared to silty and sandy soils, and considerably more spatially heterogeneous. They are mainly found in tight groupings around Central Texas, the Mississippi Alluvial Plain, Eerie Lake Plains, and the Missouri River Basin in South Dakota. Despite their infrequency, clay soils span the full range of surface classes.

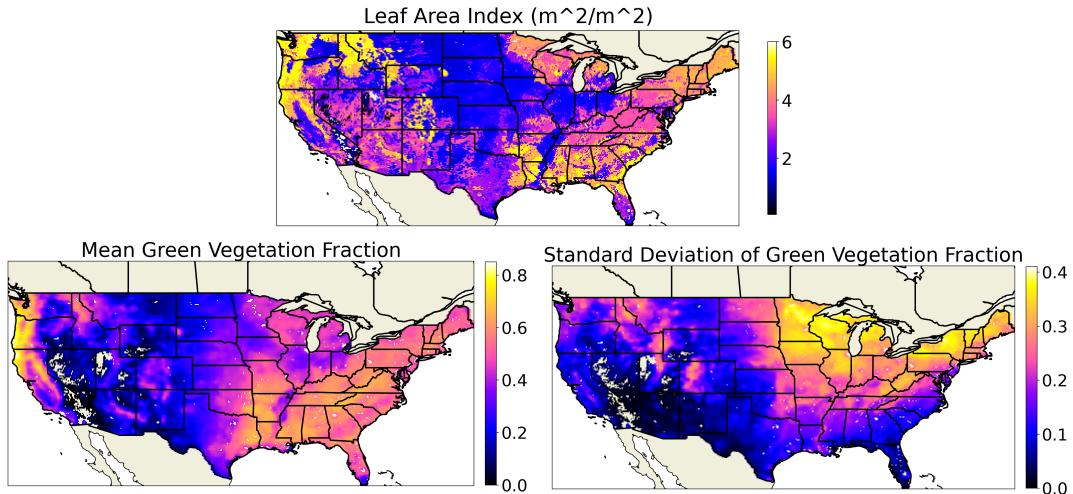


Figure 3.4: Gridded mean and standard deviation of vegetation input parameters (2012-2023)

Although they vary smoothly on an hourly basis, the LAI and GVF parameters are similar to static parameters in that they cycle consistently per-pixel on an annual basis (rather than dynamically changing based on variable atmospheric conditions), and modulate the soil water dynamics via through their effect on the

vegetation parameterization. As Figure 3.4 indicates, the densest annual-averaged canopy cover corresponds to evergreen needleleaf surface types, and there is almost no canopy over croplands and grasslands of the Midwest, California Valley, and the Great Plains. The greenest satellite-derived vegetation covers the West Coast and Sierra ranges, followed by the South and Northeast. The standard deviation of GVF indicates the regions of most significant seasonal variability, which corresponds to deciduous-dominant locales.

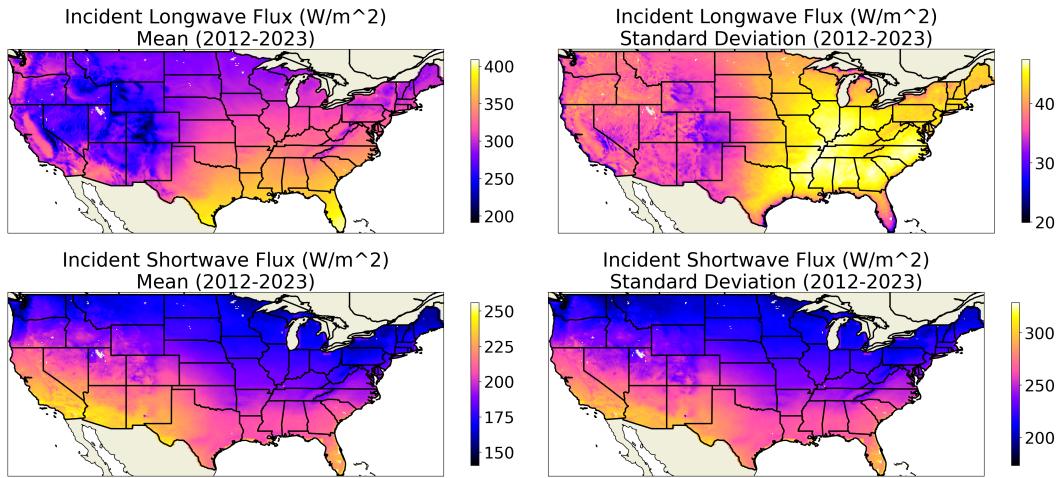


Figure 3.5: Gridded mean and standard deviation of radiative forcings (2012-2023)

In addition to the substantial regional variability of the static parameterization of Noah-LSM, there are considerable regional and seasonal differences in the NLDAS-2 atmospheric forcing time series. Figure 3.5 shows the mean and standard deviation of radiative features over the full spatial and temporal domain, which demonstrates the distribution of annually-averaged downwelling radiation. Feedback from terrestrial emissions mean that longwave radiation is highest in regions that are generally cloudier, have warmer land surface temperatures, and

are lower in elevation. The shortwave flux is highest at lower latitudes due to Earth's axial tilt, and in arid regions where there are fewer clouds.

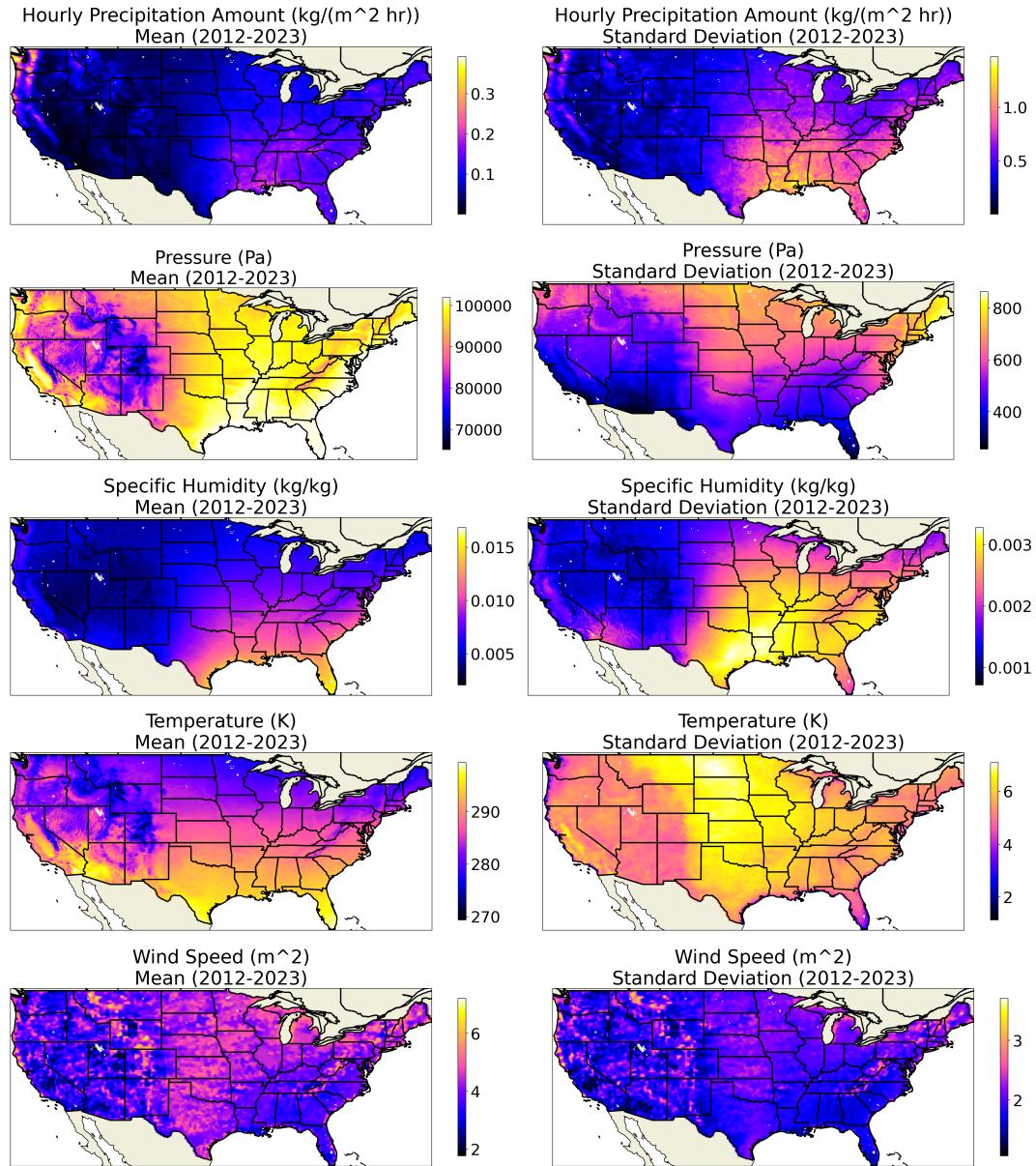


Figure 3.6: Gridded mean and standard deviation of input forcings (2012-2023)

Figure 3.6 displays the same statistics for each of the other input forcings. The precipitation dataset includes liquid rain and snow, and reflects that the highest average values fell in the Pacific Coastal, Cascade, and Sierra Nevada, followed by more moderate values in the broad expanse of the Southeast, with the deep south of Louisiana and Mississippi seeing the strongest variability in precipitation throughout the year. Pressure mainly correlates with altitude, and higher latitudes tend to see the most variance, likely due to the prolonged influence of Rossby waves. Humidity and temperature also strongly correlate with temperature and proximity to the warm gulf, where the highest humidity variance is in the southern states thanks to seasonal intrusions of warm, moist air. The highest

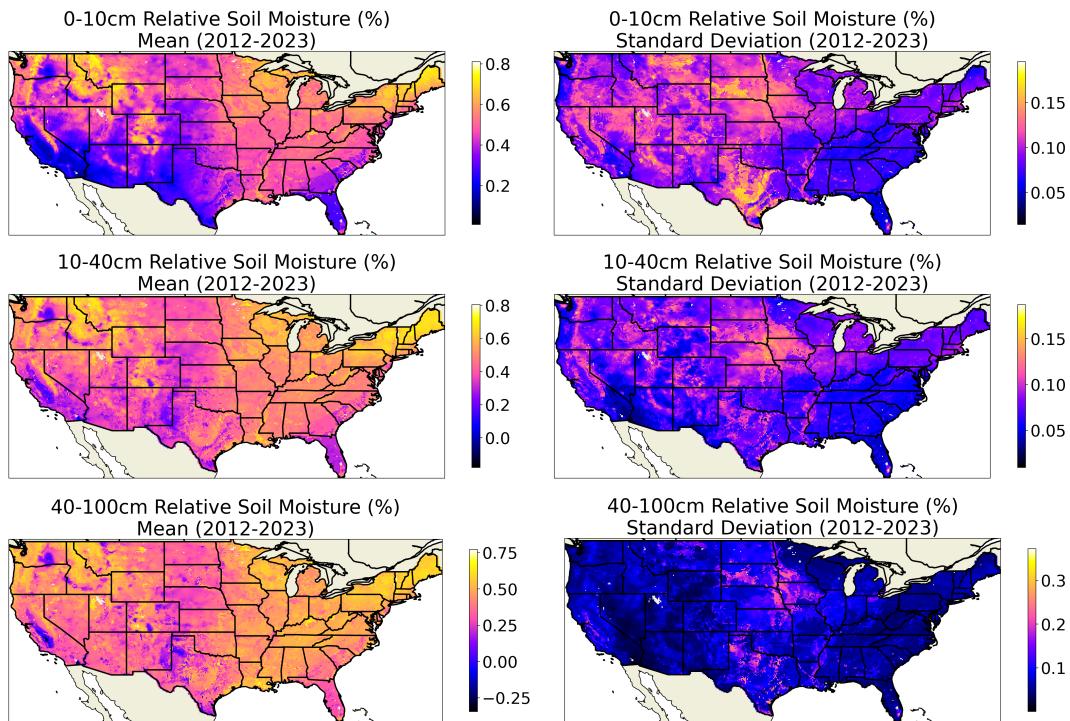


Figure 3.7: Gridded mean and standard deviation of RSM (2012-2023)

temperature variance is found in the high plains where there are considerable intrusions of arctic air in the winter, and solar heating combined with warm air advection from the terrain-driven low level jet in the summer. The wind is locally strongest where there is channeling from mountain slopes, with a broad region of relatively high wind speeds in the plains due to the open terrain.

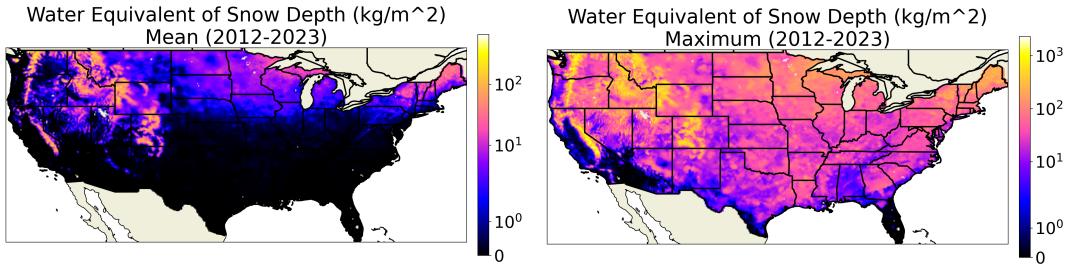


Figure 3.8: Mean and maximum accumulated snow amounts on a log scale (2012-2023)

3.1.3 Data Value Distributions

3.2 Model Architectures

The models that we tested fall into 3 broad architectural categories, as outlined in the background: fully-connected neural networks (FNNs), naïve RNNs, and LSTMs. In this subsection, we will elaborate on the particular implementation of these

The spin-up window layers prior to the first timestep ($\mathbf{G}^{(s)}$ in Figure 3.13) have their own sets of weights since the first-layer arguments include the known past soil states. Only the hidden states corresponding to the final timestep are captured from each layer of the spin-up window, and are exclusively used to

provide historical information to the initial timesteps of the corresponding layers in the prediction horizon sequence. The accumulation step for calculating the

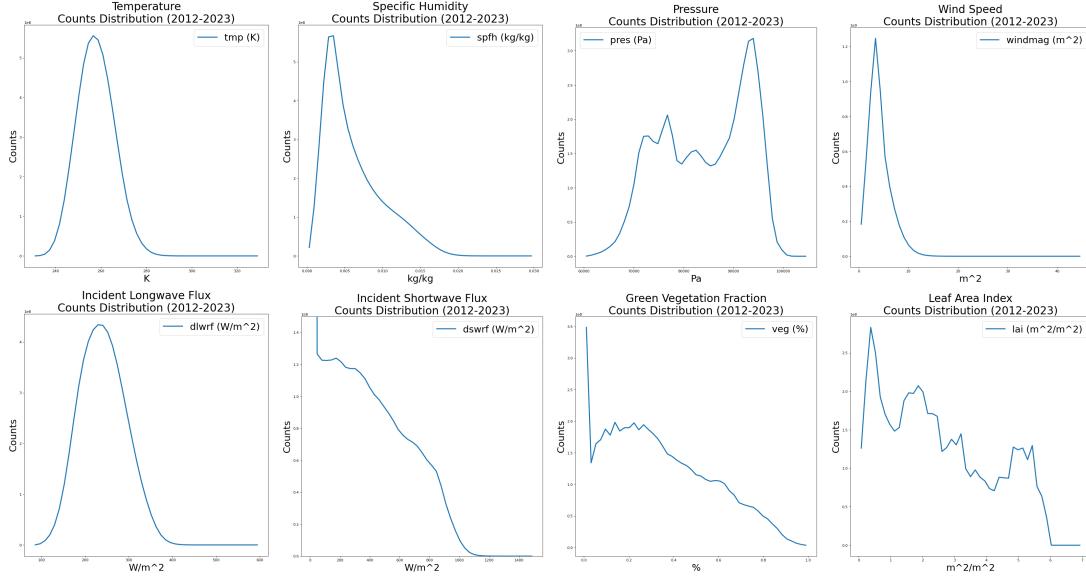


Figure 3.9: Overall distributions of dynamic model inputs (2012-2023)

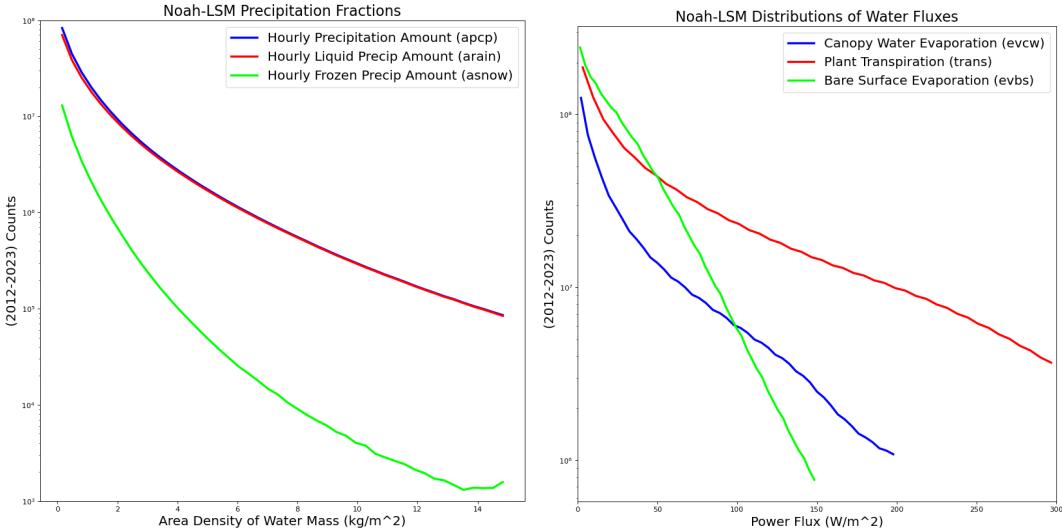


Figure 3.10: Overall distributions of precipitation types (left) and fluxes removing water from the surface system (right), both on a logarithmic axis (2012-2023).

new state \vec{s}_{k+1} with the decoded prediction of increment change in state also emphasizes another property of ANN-based models: unlike numerical models akin to the dynamical system described by Equation 2.1, the ANNs abstract away the concept of a variable increment time between prediction steps. Instead, the ANNs are trained to make predictions at a fixed timestep that cannot be changed during inference.

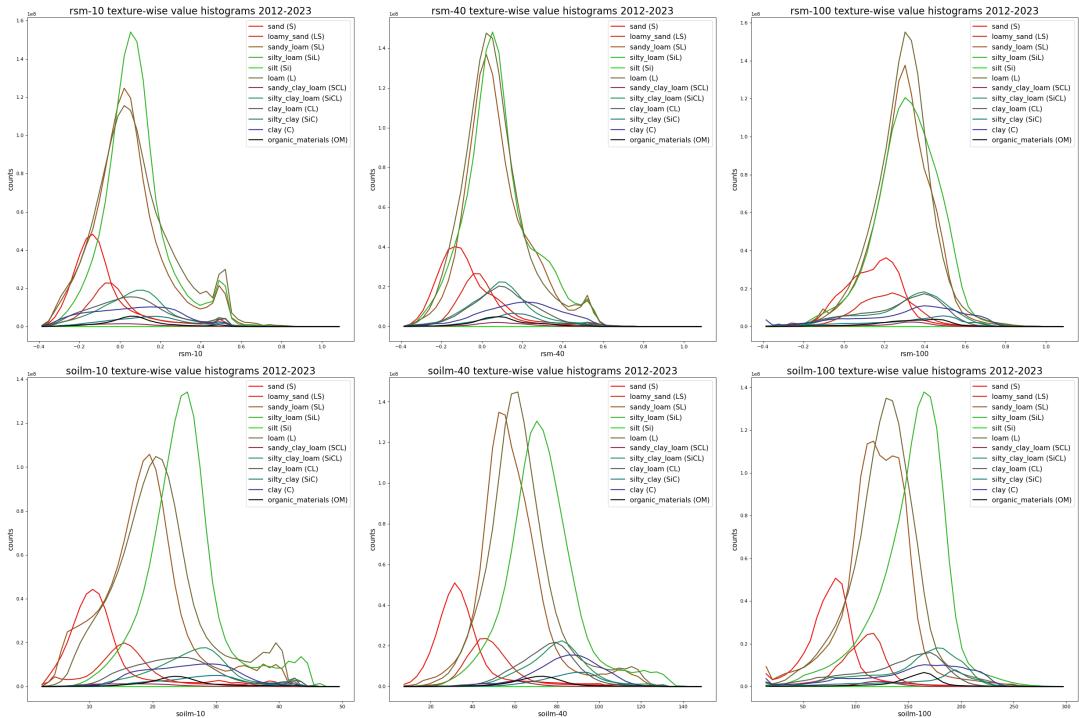


Figure 3.11: Distributions of relative soil moisture (top) compared to those of soil moisture area density (bottom) at the first three depth levels, separated by soil texture category.

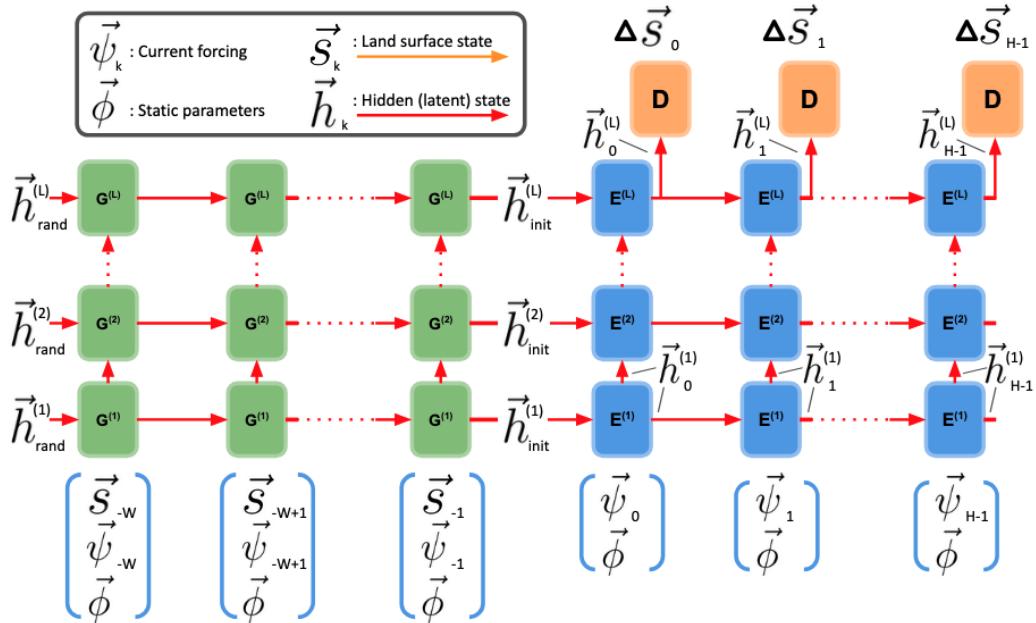


Figure 3.12: Sequence-to-sequence RNN architecture with spin-up window cells \mathbf{G} for initializing first-step weights, and fully-connected decoder \mathbf{D} .

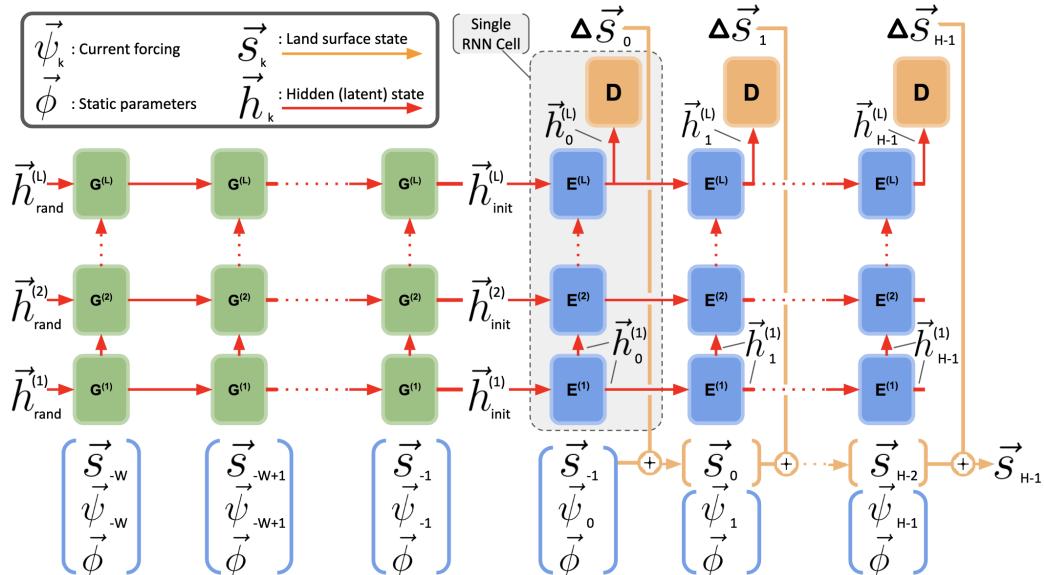


Figure 3.13: Sequence-to-sequence RNN with explicit output state accumulation.

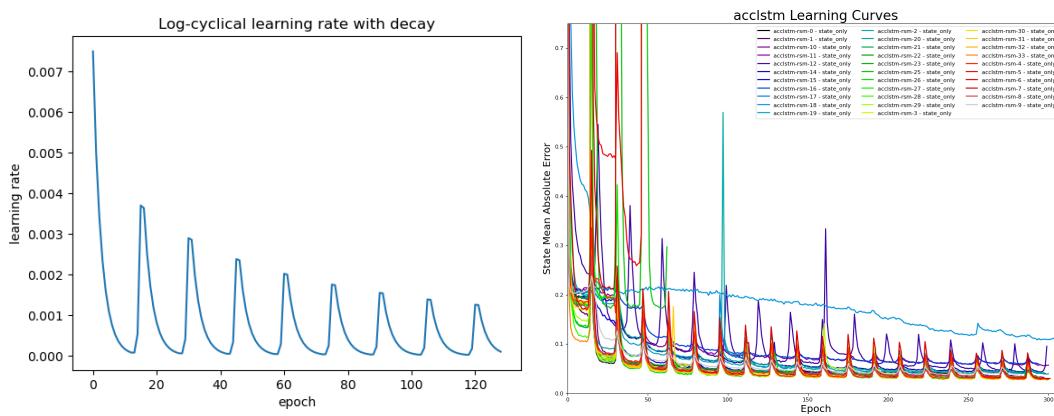


Figure 3.14: Sequence-to-sequence RNN with explicit output state accumulation.

3.3 Training Paradigm

3.4 Evaluation System

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Appendix A: An Example Appendix

Appendices should appear at the very end of your thesis. Make sure to label each Appendix with a letter starting with "A". Any tables and/or figures located in the appendix should be labeled accordingly. For example, below is figure A.1 because it is the first figure that appears in Appendix A.