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

Mitchell T. Dodson

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Approved by:

Dr. Christopher Hain, Research Advisor

Dr. Sundar Christopher, Committee Chair

Dr. Sean Freeman, Committee Member

Dr. Lawrence Carey, Department Chair

Dr. [College Dean Name], College Dean

Dr. Jon Hakkila, Graduate Dean

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., 2012). 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 $1km^2$, 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-

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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

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the evolution 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,

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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, 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 (**?**). 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. 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.

1.1 History of NLDAS and Noah-LSM

Chapter titles should begin with the word chapter and the appropriate number followed by a period. After typing the chapter heading, then type the chapter title. This template automatically formats your chapter titles. Just do not forget to include the chapter heading when you type the chapter name.

All paragraphs throughout your thesis should begin with an $\frac{1}{2}$ inch indentation. It should be double-spaced throughout. Since this is a formal document, do not use contractions. Remember that paragraphs should consist of at least two sentences. Figure 1.1 lists 11 common grammar mistakes. Please avoid these!

1.2 Deep Learning for Time Series Modeling

If your document includes many symbols or acronyms, you may include a List of Symbols, Abbreviations, *etc.* If you want a symbol/abbreviation included in the List of Symbols, be sure to create an entry for it first on the List of Symbols Glossaries.tex file. Once it is created, then you can insert it with a glossaries command. For example, the current temperature outside is 100°s.
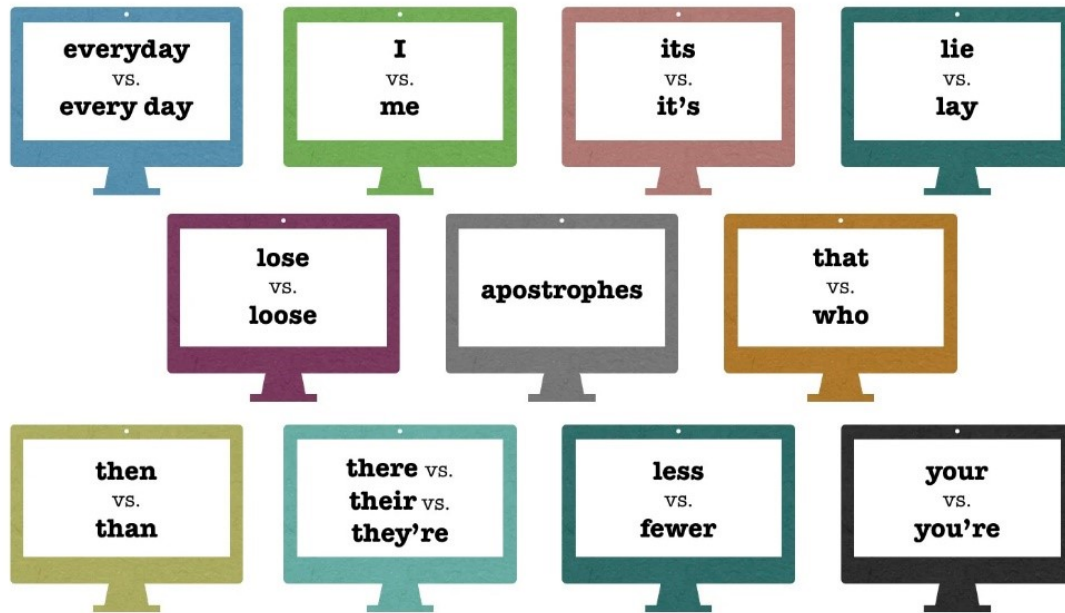
You can capitalize your symbols or make them plural by using different commands included with the glossaries package. However, only those symbols that are actually referenced in the body of your thesis will be present in the List of Symbols. Below are a few more symbol examples.

1D

f

11 Most Common Grammar Mistakes Employees Make

Figure 1.1: 11 Most Common Grammar Mistakes Employees Make. When labeling your figures, single-space if captions extend to two lines

α

r_O

τ_e

Q_{10}

Chapter 2. Adding New Chapter, Creating Sections or Subsections, and Formatting Equations

2.1 Adding New Chapters

You may use the chapter.tex files already contained in this template for chapters 1, 2, and your concluding chapter. However, any additional chapters will need to be created in a separate .tex file and then inserted to your main.tex file with the include command. This template includes examples of how to properly format content, but feel free to delete all the content in these chapter.tex files in order to add your own content.

2.2 Creating Sections or Subsections

When adding sections or subsections, simply use the section or subsection command. LaTeX will format the title of the section and/or subsection correctly automatically. Also, if you use Overleaf as the editor, it automatically has a spelling check with is very convenient.

2.2.1 Formatting Equations

Latex automatically assigns equations numbers based on their location in the document. However, if you want to reference specific equations throughout your work, you will need to manually provide an internal label. Below is an example equation with a created label followed with a reference to this equation.

$$
\begin{aligned}
\nabla \cdot \nabla \psi &= \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \\
&= \frac{1}{r^2 \sin\theta} \left[\sin\theta \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial \psi}{\partial r} \right) + \frac{1}{\sin\theta} \frac{\partial^2 \psi}{\partial \varphi^2} \right]
\end{aligned}
\tag{2.1}
$$

Equation 2.1 will hopefully help you understand how to properly format and reference equations in your document.

2.2.2 Citations

When you make your citations, you will need to first add them to the ref.bib file. Then, use the citation command followed by the name of the citation.**?** LaTeX allows you to control the style of your citations.**?** On the main.tex file, set your bibliography style to the one you prefer.

Chapter 3. Conclusions and Future Work

While organization is flexible, all theses and dissertations, no matter the discipline, share certain scholarly elements. You must provide an introductory statement or overview of your project; identify the significance of your investigation; discuss relevant literature to position your work; describe your methodology; state findings or results and their implications; and present conclusions and, if appropriate, recommendations for future work. Your chapters might be organized by kinds of information (for example, a literature review, methodology, and results), or you may organize conceptually with these elements logically interwoven.

Below is just an example table. Notice that captions for tables are placed above the table while captions for figures are placed beneath the figure. LaTeX automatically formats this correctly

Table 3.1: Frequencies for equal-tempered scale, $A_4 = 440$ Hz. This table shows only the first five notes of a chromatic scale starting on C_0

Note	Frequency (Hz)	Wavelength
C_0	16.35	2109.89
$C_0^{\#}/D_0^b$	17.32	1991.47
D_0	18.35	1879.69
$D_0^{\#}/E_0^b$	19.45	1774.20
E_0	20.60	1674.62

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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.

Figure A.1: Colleges and Universities in Alabama