

LSTMs for Inferring Planetary Boundary Layer Height (PBLH)

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Abstract

In this paper, we describe new work which is part of a larger study to understand how machine learning could be used to augment existing methods for calculating and estimating the Planetary Boundary Layer Height (PBLH). We describe how a Long Short-Term Memory (LSTM) Network could be used to learn PBLH changes over time for different geographical locations across the United States, used in conjunction with the WRF-Chem model. If the machine learning method could achieve accuracy levels similar to the model-based calculations, then it is feasible for the deep learning model to be used as an embedded method for the WRF-Chem model. The paper shows promising results that warrant more exploration. We describe results for two experiments in particular. The first experiment used 20 geographical locations for a two-month period of hourly WRF-Chem calculated PBLH. In this experiment, we evaluated how well the LSTM could learn PBLH by using limited data across a set of nearby locations. This model achieved RMSE of .11 on predicted PBLH. The second experiment used one year of hourly PBLH calculations from the WRF-Chem model to evaluate the LSTM prediction for a selection of three locations with separate LSTM models, achieving RMSE scores of 0.04, 0.01 and 0.05, respectively. We describe these results and the future plans for this work.

Introduction

The Planetary Boundary Layer (PBL) is known for being the layer above the Earth's surface for which aerosols are present (Stull 1988). Accurate calculations of the top of the PBL can better inform air quality forecasts. Machine learning methods that can improve PBL calculation accuracy and improve computational calculations are of interest to the earth science community. The work described in this paper outlines how a Long Short-Term Memory (LSTM) network could be used to learn how planetary boundary layer heights are changing over time for various geographical locations. LSTM networks enable predicting accurate results from the complex data representation within the appropriate training time and resolving the constraints of RNN (Griff et al. 2017). Recently, the LSTM network-based weather

forecasting has gained great attention in the weather prediction domain. The ability to model the temporal data sequences along with the long-term dependency through the memory blocks makes the LSTM model a superior choice in weather forecasting studies (Gayathiri Kathiresan 2019).

Since WRF-Chem (Peckham 2012) model-based PBLH calculations inherently include features such as wind, temperature, and humidity, the objective of this study is to determine if the LSTM is able to learn to predict PBLH without explicitly using these additional features. By learning patterns of PBLH temporal changes over geographical points across the United States, can it accurately predict future PBLH just by learning these patterns of change? If the network is able to learn to predict future PBLH based on past historical PBLH, the deep learning model could be called upon to predict PBLH for a number of time steps in the future as an embedded method to the WRF-Chem process. Two experiments have been conducted that use WRF-Chem model output. The first focuses on training an LSTM for 20 geographical locations over dates in the months of November through December for the year 2016. This study is part of a larger study of understanding how ceilometer-based backscatter can be used for PBLH estimations to augment model calculations for improved PBLH calculations (Caicedo et al. 2017; Delgado et al. 2018). The second focuses on training LSTMs for specific locations using WRF-Chem data for the year 2018-19.

Background

WRF-Chem (Peckham 2012) is a fully coupled "online" chemistry model, which has the air quality component consistent with the meteorological component (Grell et al. 2005). In this study, the gas-phase chemistry and aerosol module is based on the Carbon Bond Mechanism Z (CBM-Z) (Zaveri and Peters 1999) and Model for Simulating Aerosol Interactions and Chemistry (Zaveri et al. 2008), respectively. While there are several other PBL schemes, YSU scheme (Hong and Pan 1996; Hong and Lim 2006) is selected for the runs reported in this work. An extended discussion of the different model PBL parameterization schemes and their success (or otherwise) in comparison with lidar observed PBL data in this same study region is reported elsewhere (López, Archilla, and Quintana 2020). Model Radiation treatment utilizes the Rapid Radiative Transfer Model

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for General Circulation Models (RRTMG) short-wave and long-wave radiation schemes (Iacono et al. 2008), including the aerosol radiation feedback.

Related Work

LSTM models have been long utilized for air quality and weather prediction problems. In (Karevan and Suykens 2018), authors used a spatio-temporal stacked LSTM model for temperature prediction. They showed improvement in the performance of their prediction model using the stacked LSTM model. Weather prediction has been studied in (Fente and Singh 2018), using LSTM models. In this work, multiple LSTM models were trained for different combinations of weather parameters.

The problem of weather prediction has been studied in (Hewage et al. 2019) and (Zaytar and Amrani 2016) and stacked LSTM architectures have been utilized and been compared to traditional forecasting models. In the former, Hewage et. al. (Hewage et al. 2019) compared the result of weather prediction with (WRF) NWP model and showed accuracy of LSTM model's result. In the latter, Zaytar et. al. (Zaytar and Amrani 2016) showed results of forecasting temperature, humidity and wind speed. In their paper, they showed that LSTM based neural networks can be considered as an alternative model to traditional models for forecasting weather conditions.

Rainfall prediction has been a category of weather prediction problems and has been the focus of multiple studies, such as (Poornima and Pushpalatha 2019) and (Samad et al. 2020). Poornima. et. al. (Poornima and Pushpalatha 2019) presented Intensified Long Short-Term Memory (Intensified LSTM) based Recurrent Neural Network (RNN) to predict rainfall. They compared their results with Holt-Winters, Extreme Learning Machine (ELM), Autoregressive Integrated Moving Average (ARIMA), Recurrent Neural Network and Long Short-Term Memory models in order to show the improvement in the ability to predict rainfall. Samad et.al. (Samad et al. 2020) utilized an LSTM based Recurrent Neural Network (RNN) for the prediction of rainfall. They showed accuracy and performance of the model on a standard rainfall dataset.

In this study, to learn PBLH changes over time, the problem is formulated as a time series forecasting model where a stacked LSTM network is built and trained on data from two different WRF-Chem models.

Approach

The overall approach is a stacked LSTM that learns to predict PBLH for given geographical locations by training the LSTM on large data sets generated from WRF-Chem models. These models provide PBLH for various geographical locations, different periods of time across different seasons, however explicitly defined features such as wind, temperature, and humidity are excluded. The current LSTM uses a single uni-variate methodology. In the single uni-variate approach we train the network using two different models to explore two different ideas. In the first method, a stacked LSTM trained on multiple geographical locations,

using two months of WRF-Chem output (specific to the East Coast) was used. This method used output for the period of November 29, 2016, to December 30, 2016, in coordination with related work of applying machine learning methods to ceilometer backscatter profiles for an ad hoc campaign (Sleeman et al. 2020) conducted by the University of Maryland Baltimore County Physics Department. The second method also used a stacked LSTM but was trained on individual geographical locations and was based on data from a year of WRF-Chem output (for most of North America) for the period of January 2018 to January 2019.

The stacked LSTM model used for both approaches is shown in Figure 1 and was constructed by sequencing three LSTM layers with 50 units each taking three arguments viz. no. of units, return sequences and input shape. The input shape was the shape of the input data set. The parameter for return sequences was set to 'True' to stack the three LSTM layers. A dense layer was added specifying an output of one unit after the three stacked LSTM layers. The optimizer used was 'Adam' and the loss function used was set to 'mean squared error'. The next step is to compare this model with a multi-variate LSTM methodology.

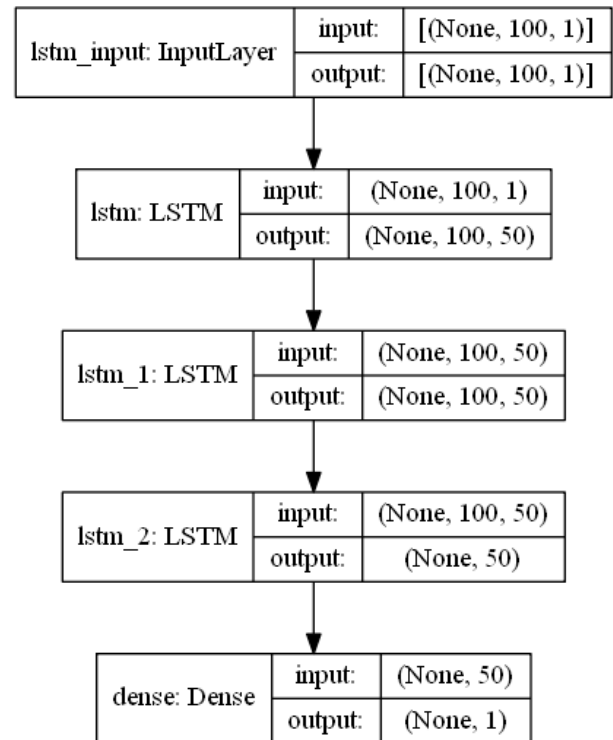


Figure 1: LSTM network

Data Set Description

For each data set, WRF-Chem model data was transformed with each instance having N number of historical PBLH, X_1 and instance $N + 1$ as its respective outcome Y_1 . The 1 to N window then shifts by 1 and the next set of instances, X_2 constitute of 2 to $N + 1$ instances, with instance $N + 2$

as its outcome, Y_2 . This continues until all data is consumed resulting in a data set $X_1, X_2 \dots X_k$ with N features each and respective labels $Y_1, Y_2 \dots Y_k$. The N is set to 100 for the experiments discussed in this paper.

After scaling and reshaping, the data was converted into a 3D array with X train samples, 100 timestamps, and one feature at each step to be fed into the network built above.

For the first experiment, the data set used was based on the numeric values of PBLH generated from the WRF-Chem model from approximately 15,000 locations across the latitude, longitude bounds of [36.63,-79.24707] to [40.79,-73.92] respectively recorded at various time stamps from Nov 29, 2016 20:00 hours, to Jan 01, 2017 00:00 hours, as shown in Figure 2 and Figure 3. Figure 2 shows numeric representation of data with columns: date, time, latitude, longitude and the respective recorded planetary boundary height. Figure 3 shows the spread of the data in terms of geographical location on the United States map. The WRF-Chem model consisted of two region, an outer region with 9 KM resolution from 25N to 50N and -70W to -90W. And an inner region consisting of 35N to 45N and -73W to -80W. The prognostic variables of the outer region are specified by every 3 hours obtained from a reanalysis from the NCEP reanalysis. Every hour prognostic variables are specified for the inner region from a reanalysis. The outer region is integrated with a one minute time step and the inner is integrated with a 20 second time step.

date	time	lat	lon	pblh
11/29/2016	200000	36.62983	-75.1622	741.9507
11/29/2016	230000	36.62983	-75.1622	534.1741
12/1/2016	70000	36.62983	-75.1622	1287.512
12/2/2016	0	36.62983	-75.1622	950.3918
12/2/2016	130000	36.62983	-75.1622	1214.292
12/2/2016	180000	36.62983	-75.1622	936.7284
12/3/2016	50000	36.62983	-75.1622	940.426

Figure 2: Example Data from the Model



Figure 3: Geographical Representation of Raw Data

For the second experiment, the data used was for individual sites recorded hourly from Jan, 2018 to Jan 2019, high-

lighted in this paper are sites: site1[44.2062, -63.14245], site2[35.3382, -90.31128], and site3[35.3382,-90.31128]. The WRF-Chem model consisted of the year 2018 and region was most of North America at 2.5 degree resolution from 0 degrees north to 80 degrees north and -60 west to -135 west. Prognostic variables were specified every 6 hours at all grid points and integrated every 6 hours with 3 minute time steps.

Experimentation

There were two main experiments conducted in this study. The first used a 2-month WRF-Chem model focused on the East Coast. The goal of this experiment was to explore how well the LSTM network could approximate PBLH for locations near each other. The second experiment used a 1-year WRF-Chem model focused on most of North America. The goal of this experiment was to explore how well a LSTM network could predict PBLH for specific locations trained on data spanning multiple seasons, without explicitly including features such as temperature.

Multi-Location Experiment

This experiment consisted of 20 locations and data from the model experiment. The 20 nearby locations formed a small patch as shown in Figure 4.



Figure 4: Geographical Representation WRF-Chem Model Locations

The LSTM model was trained on data for 100 epochs with a batch size of 64 and tested on train and test data to evaluate the overall performance of the LSTM model. The training data had 817 examples and the test data included 441 samples. After the model has been trained it was evaluated using the test data.

Single Location Experiment

The second experiment consisted of three sites with 8834 rows of data each. The LSTM model was trained on data for 100 epochs with a batch size of 64. The training data had 5742 samples and the test data included 3092 samples.

Results

Both experiments yielded encouraging results. RMSE was measured for the held-out test set in each experiment. In the 1-year experiment, a comparison with a linear regression method was performed. In addition, a sensitivity study was also performed.

Multi-Location Results

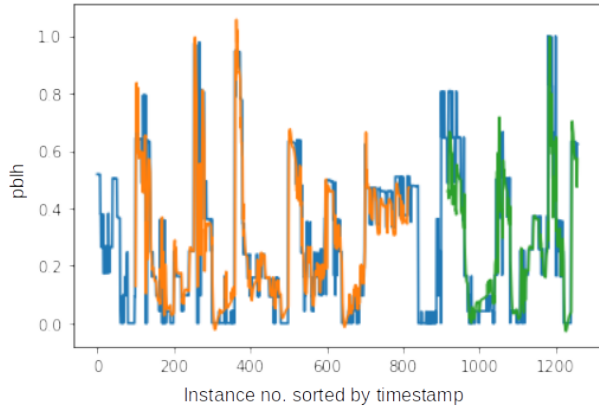


Figure 5: Predicted PBLH for 20 locations- train(orange) and test(green)

A RMSE of 0.11 was achieved for the test data. The results are plotted showing a comparison of predicted data vs original data as shown in Figure 5. The blue line shows the original data. The orange line shows the predicted PBLH for train data and the green line shows the predicted PBLH for test data. Upon close observation, the naked blue line can be seen right before orange and green lines representing the initial 100 instances used to start the prediction for train and test data.

Single Location Results

The single location experiment was performed for three (randomly chosen) locations (44.2062,-63.1424),(2.41753,-119.82883), and (35.3382,-90.31128) with RMSE values of 0.04, 0.01, and 0.05 achieved. To properly evaluate the LSTM method for the single location experiment, the result of the LSTM prediction for (35.3382,-90.31128) was compared with the prediction using a linear regression model for (35.3382,-90.31128). The results of the linear regression model and the LSTM model are shown in Figure 6b and 6c. In Figure 6c, the blue trend is almost unidentifiable for both train prediction and test prediction, as can be seen by the green trend (predicted test) which overlaps the blue trend (actual data). This implies the prediction is strongly matched to the expected PBLH. The linear regression model resulted in a RMSE of 0.05 in comparison with the LSTM result of 0.05.

To evaluate the predictions further, a correlation study was performed on the test data from the WRF-Chem and predicted data from the LSTM. The mean of the WRF-Chem model-generated test data was subtracted from the test data

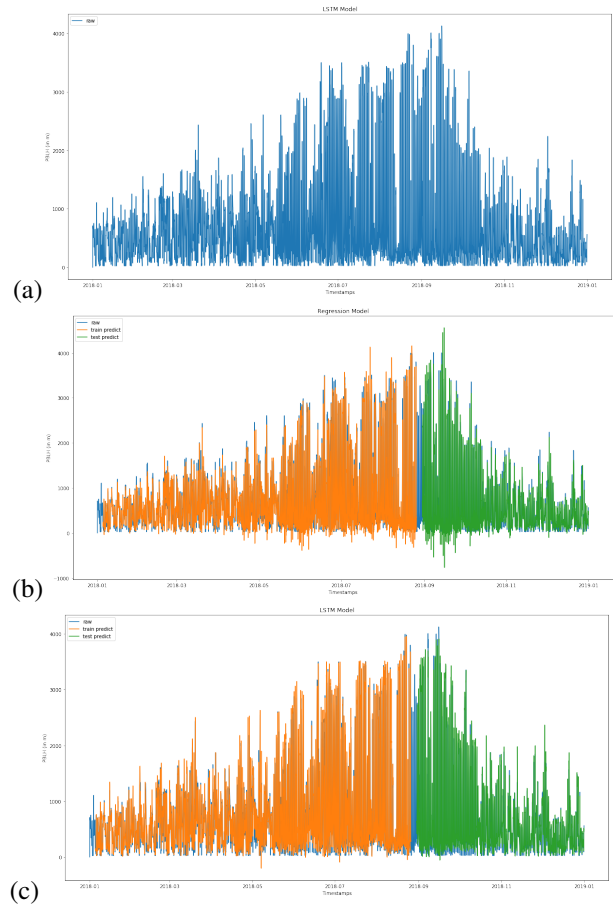


Figure 6: (a) Hourly WRF-Chem PBLH for Single Location (35.3382,-90.31128) (b) Linear Regression for Single Location (35.3382,-90.31128) Hourly Predicted PBLH (c) LSTM for Single Location (35.3382,-90.31128) Hourly Predicted PBLH

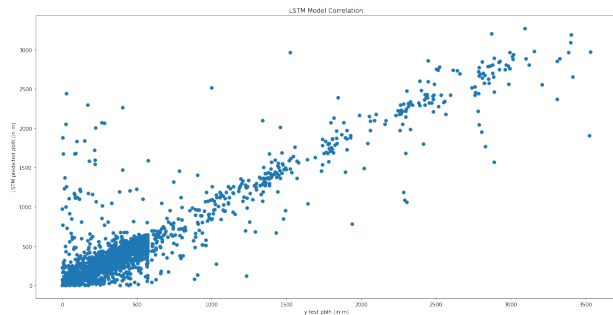


Figure 7: Correlation Study - Mean-Subtracted Results Comparing the WRF-Chem Model PBLH with the LSTM Predicted PBLH for Location (35.3382,-90.31128).

and the mean of the LSTM model predicted data was subtracted from the predicted data. The results were then plotted in Figure 7. The results from this correlation study show strong correlation between the true PBLH of the test data

and the predicted PBLH from the LSTM model.

Conclusions and Future Work

In this study, we present a stacked LSTM model as a prediction tool for tracking planetary boundary layer heights (PBLH) temporal changes. We trained the LSTM model for two data sets generated from the WRF-Chem model for a selection of locations. We showed the performance of inferring the model on a test subset of data and provided a visualization of the results. In this work we show the promise of using LSTM networks for spatio-temporal time series PBLH forecasting. In our future work, we aim to design multivariate LSTM network to perform simultaneous PBLH forecasting for multiple locations with a single network.

Acknowledgments

This work has been funded by the following grants: NASA grant NNH16ZDA001-AIST16-0091 and NSF CARTA grant 17747724.

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