Review of gmd-2021-415: AIEADA 1.0: Efficient high-dimensional variational data assimilation with machine-learned reduced-order models

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Verdict: Major Revision

In this manuscript the authors create a machine-learning based emulator of a dynamical model and then integrate it into a standard 4D-Var data assimilation algorithm. They employ a long short-term memory (LSTM) neural network as the emulator, and demonstrate its advantages for 4D-Var, thanks to its easy differentiability. The emulator is demonstrated on a data set produced from WRF simulations, which is impressive given that many of these first studies only consider toy models. The individual components of this system have been tested before by others, but as far as I am aware, the combination shown here is novel.

The paper is mostly well written, and the authors are to be commended especially for the introduction which presents an excellent overview not only of data assimilation algorithms but also the latest results from machine-learning/data assimilation hybrid studies. I would be very happy to see this paper published. However, I did find certain aspects of the description of the techniques and experiments to be lacking. In particular, I did not find the explanation of the LSTM system to be sufficient for me, as a non-expert, and it left me with many unanswered questions. I would advise the authors to go back and rethink this part from the perspective of a data assimilation person. My detailed advice is given below, but in summary: try to explain in plain language what it is that an LSTM neural network is aiming to do, how it compares with the traditional numerical models that it is intended to replace here (from an "external interface" perspective — can an LSTM be a drop-in replacement for a numerical model?), and how it is integrated into a traditional data assimilation system. I have also provided some minor comments which may improve the readability of the paper.

I look forward to the authors' revision.

Major Comments

Section 2.2: As someone who does not use LSTMs, I did not understand any of this section I'm afraid (except for the final five lines). After reading many times, I am still not sure what problem the LSTM is designed to solve. If the authors would like this paper to be read and understood by a broader audience, I think it would be wise for the authors to revise this section substantially. The following tips may be considered. They may seem pedantic, but when we are precise we eliminate confusion.

- The LSTM is introduced as a forecasting technique, in which case I would expect to see an equation like x_t+1 (future state) = M(x_t) (operator applied to initial condition). Yet I cannot discern any such expression from those given. How does one take the Equations 4 and 5 and actually get a future state from an initial state?
- There are many undefined terms and variables, including r, t, T, input sequence, input window, functional prediction, cell and output window.
- The term "observation" on line 157 is ambiguous. I would suggest another term in case the reader thinks of actual meteorological observations.
- What is h? Is it a vector? If so, what dimensions does it have? What does the t subscript mean, and why are all h's in Equation 5 the same?
- What about h? On line 160 it says that this is the output of the function approximated by the LSTM — does that mean h is the LSTM itself?

Minor Comments

- Lines 24, 66: Slight typo uncertainties.
- Line 113: Two "with"s.
- Line 139: I know it's the title of the section, but could the authors define the POD acronym here anyway?
- Line 146: For the benefit of readers (including myself) who have not encountered SVD for a while, could the authors define all of the terms, U, Σ and V here, including their dimensions? E.g., please mention that the columns of U and V are the left- and right-singular vectors, respectively, and that the diagonal of Σ contains the singular values. Additionally, this may be my misunderstanding, but please could the authors double check the stated dimensionality of U? My understanding was that the U and V matrices are square.
- Line 188: Typo references.
- Line 195: Please specify Figure 2, just in case the reader looks to Section 2.
- Lines 216-217: This caused me confusion for a long time because I didn't notice the lack of italics in \$\hat{\text{x}}_i\$. I thought that \$\hat{\text{x}}_i\$ and \$\hat{x}_0\$ were in the same vector space, when in fact \$\hat{\text{x}}_i\$ is in \$\mathbb{R}^N\$ and \$\hat{x}_0\$ is in \$\mathbb{R}^N\$. Could the authors clarify the notation to make Equations 9 and 10 easier to comprehend? For example, perhaps all hat'ed variables can be in the reduced-space?
- Line 236: Did the authors mean to say regional *numerical* weather prediction system?
- Line 242: Typo *temperature*.
- Line 253: Typo calculate.
- Line 254: What does it mean to "coarsen the data by five strides"? Are the coarsened fields obtained by averaging, or simply by subsetting the high-resolution fields?
- Line 264: Z500 is around 5,000 m, so if the identity is chosen as the observation error covariance matrix, that must mean that the simulated errors are on the order of 1 m, which is negligible. Is it definitely the identity, or did the authors mean that it is the identity multiplied by a constant observation error (perhaps 50 m or something)?

- Line 264: Also, please explain for the uninitiated the significance of using the identity matrix as the observation error covariance matrix: i.e., this means that the observation errors are uncorrelated.
- Line 275: Typo achieved.
- Line 285: Are the results presented here (and in Figure 3) averaged across all of the forecasts performed? Or are we looking at one specific case, as representative of all of the cases?
- Line 286: "For all forecasts in the test region" the test data set covers the year 1991, but how are the forecast periods constructed? If the "output window" is 20 days (meaning the forecast is performed out to 20 days), are the forecasts performed back-to-back, meaning there are only 365/20 ≈ 18 forecasts in total? Or do the forecast intervals overlap, so there are 365 forecasts one for each day?
- Line 286: Should this be "test data set" rather than "test region"? "Region" implies some kind of spatial meaning.