A toy model to investigate stability of AI-based dynamical systems

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Context

Once implemented inside the model, most of current AI-based parameterizations faces numerical instabilities. After a few integrations, the model explodes.

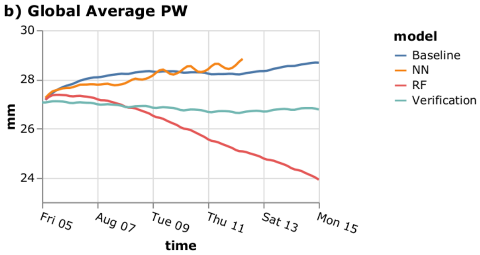


Figure 1: An example of divergence with an AI-based parameterization scheme. Brenowitz et al., 2020 [3]

Objectives

Objective.

Study of the stability of a toy model, after its dynamics has been learnt by a feedforward NN.

References

[1] Rasp, S.: Coupled online learning as a way to tackle instabilities and biases in neural network parameterizations: general algorithms and Lorenz 96 case study (v1.0), Geosci. Model Dev., 13, 2185–2196, https://doi.org/10.5194/gmd-13-2185-2020, 2020.

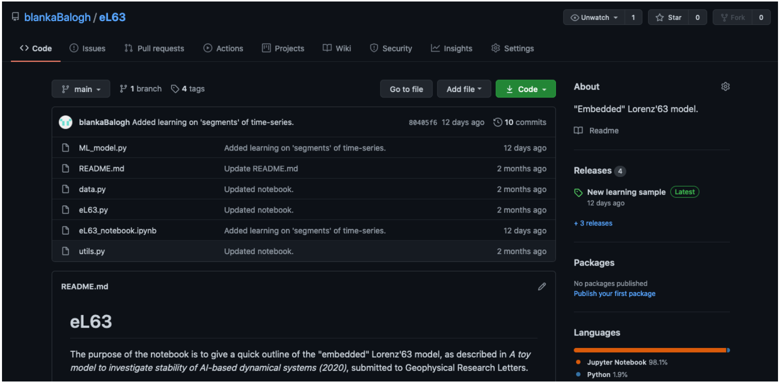
[2] Brenowitz, N. D., Beucler, T., Pritchard, M., Bretherton, C. S. (2020). Interpreting and Stabilizing Machine-Learning Parametrizations of Convection, Journal of the Atmospheric Sciences, 77(12), 4357-4375. Retrieved Feb 24, 2021, from https://journals.ametsoc.org/view/journals/atsc/77/12/jas-d-20-0082.1.xml

[3] Brenowitz, N. D., Henn, B., McGibbon, J., Clark, S. K., Kwa, A., Perkins, W. A., Watt-Meyer, O., Bretherton, C. S. (2020). Machine Learning Climate Model Dynamics: Offline versus Online Performance. https://arxiv.org/abs/2011.03081

[4] Balogh, B., Saint-Martin, D., Ribes, A. (2021). A toy model to investigate stability of AI-based dynamical systems. Geophysical Research Letters, 48, e2020GL092133. https://doi.org/10.1029/2020GL092133

Code & notebook

Code & notebook: https://github.com/blankaBalogh/eL63.



Learning L63 – 1/2

Objective. Learning L63 dynamics with NNs.

$$\begin{aligned}\dot{x}_1 &= \sigma(x_2 - x_1),\\ \dot{x}_2 &= x_1(\rho - x_3) - x_2,\\ \dot{x}_3 &= x_1 x_2 - \beta x_3\end{aligned} \tag{1}$$

With (σ, ρ, β) fixed, the ML problem of learning L63 can be written:

$$\dot{\mathbf{x}} = f(\mathbf{x}) \tag{2}$$

In the following, (σ, ρ, β) values are set to $(10, 28, 8/3)$.

Learning L63 – 2/2

Learning sample. 'orbit' of length 10^4 integrations.

Neural Network setting. 5-layers deep feedforward NN learns to predict L63 time derivatives. $R^2 > 0.999$ over an independent 'test' subset of the learning orbit.

Validation. Generation of a long orbit (2.10^4 integrations) with the NN predicted tendencies.

Validation of NN-based L63

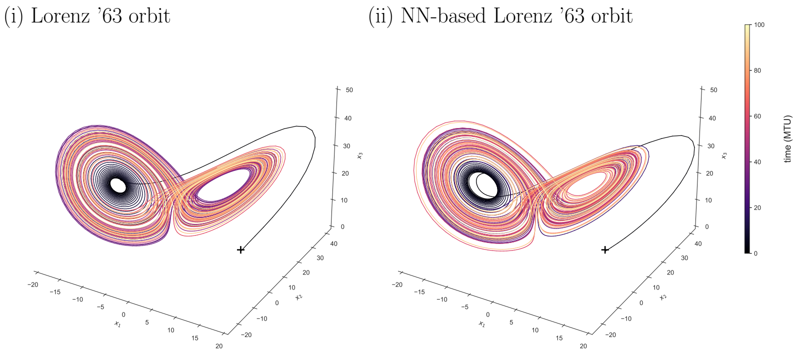


Figure 2: Validation orbits resulting from the integration of: (i) L63 equations and (ii) of the NN model that learnt eq. (2). Only the first 100 MTUs are represented.

Conclusion – Learning L63

Fit to learning sample is great (see validation R2 score), but the resulting NN model does not allow the study of instabilities.

Need of a more complex toy model to study instabilities encountered when developing NN-based parameterizations.
How to conceive a higher dimension ($d > 3$) version of L63 ?

'embedded' Lorenz'63 model (eL63) – 1/2

Objective. Extend L63 to dimension $d > 3$ to create a toy model replicating numerical instabilities.

1. $\mathbf{z} \in \mathcal{B}_z$: dynamics are easy to express explicitly.

$$\begin{aligned} \dot{z}_1 &= \sigma(z_2 - z_1), \\ \dot{z}_2 &= z_1(\rho - z_3) - z_2, \\ \dot{z}_3 &= z_1 z_2 - \beta z_3, \\ \dot{z}_j &= -\kappa z_j, \quad \forall j > 3. \end{aligned} \tag{3}$$

   For sake of simplicity, $\kappa = 1$ hereafter.

2. $\mathbf{x} \in \mathcal{B}_x$ ('learning' space) after random rotation P

$$\mathbf{x} = P\mathbf{z} \tag{4}$$

'embedded' Lorenz'63 model (eL63) – 2/2

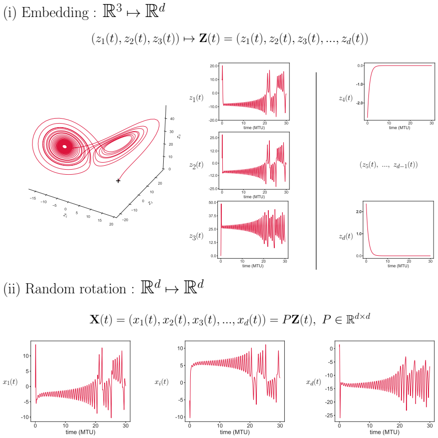


Figure 3: 'embedding' of L63 model. The NN will only see variables from $\mathcal{B}_x$, after applying 'hidden constraint' P.

Evaluation of the NN model – 1/2

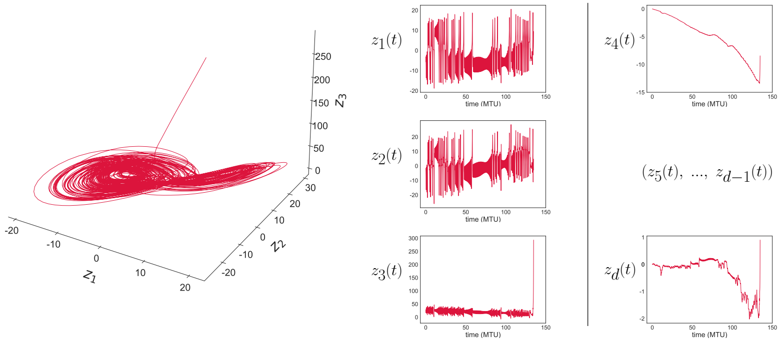


Figure 4: Example of a diverging validation orbit, generated by integration of tendencies from $\widehat{f}_{orb}$. The subsequent NN model of eL63 will be assessed in $\mathcal{B}_z$, facilitating comparison without the random rotation P.

Evaluation of the NN model – 2/2

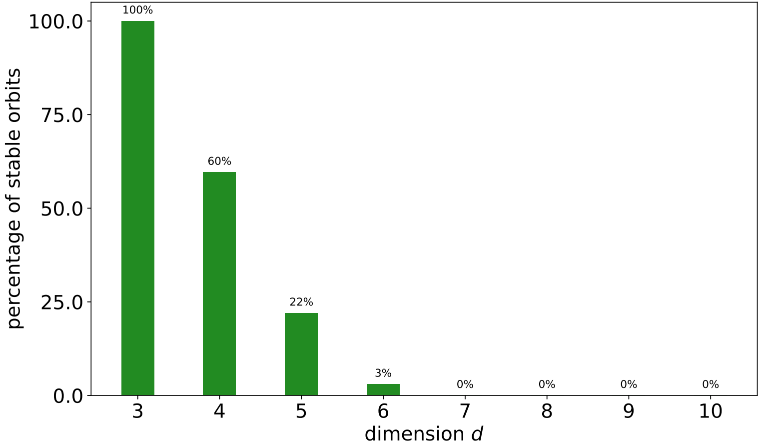


Figure 5: Percentage of stable validation orbits as a function of the embedding dimension d. Stability is computed over 3000 orbits for each value of d.

Conclusions – 'Embedded' L63 model

1. Even with minimal embedding (e.g., $d = 4$), 40% of NN-generated eL63 validation orbits are unstable (or exploding).
2. Stability decays quickly when d increases.
3. With $d > 6$, none of the validation orbits are stable.

eL63 is an extended version of L63, which allows the replication of numerical instabilities when learned by (feedforward) NNs upon a single orbit.

How to make NN models of eL63 stable ?

A new learning sample ?

The new learning sample is built with Latin Hypercube Sampling (LHS). The five-layers deep, feedforward NN is fitted to this new learning sample, $[\mathbf{x}]_{LHS}$.

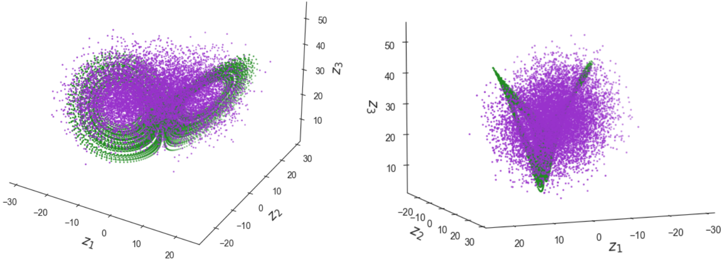


Figure 6: The first 3 components of the state variable **z** from the 'orbital' learning sample (green) and the 'LHS' learning sample (purple). Both samples contains 10^4 individuals.

Validation

Validation. 100 $\widehat{f}_{\mathrm{LHS}}$, 30 random initial conditions.

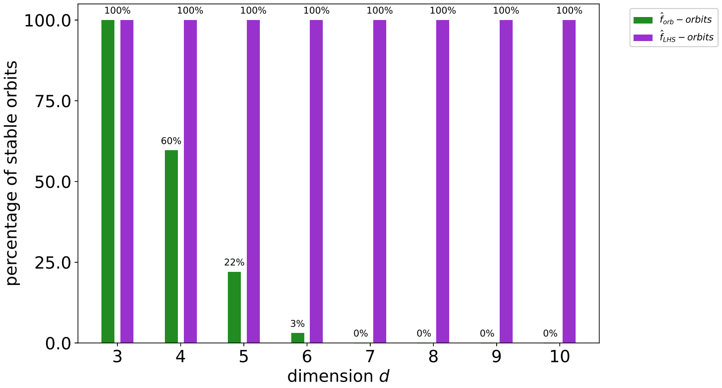


Figure 7: Percentage of stable validation orbits, generated with $\widehat{f}_{orb}$ (green) and $\widehat{f}_{\mathrm{LHS}}$ (purple). NN model is stabilized when fitted to the LHS learning sample (regarding the stability criterion described above).

Conclusion

- L63 model is not complex enough to manifest numerical instabilities when its dynamics is learnt with NNs.
- 'embedded' L63 model, an extended version of L63 to $d > 3$ succeeds in replicating numerical instability issues, when the NN model is fitted to a learning sample consisting in a single orbit.
- The NN model is stabilised (with $d < 11$ at least) when fitted to a specifically designed learning sample. This learning sample was built with LHS.

An LHS sampling is difficult to perform in the case of climate models. This study underlines how much the learning sample is important to grant stability to NN models.