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Around the World in 36 Nodes: Encoding Spatial Relationships With Graph Neural Networks For Better Earth-System Forecasts

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Introduction

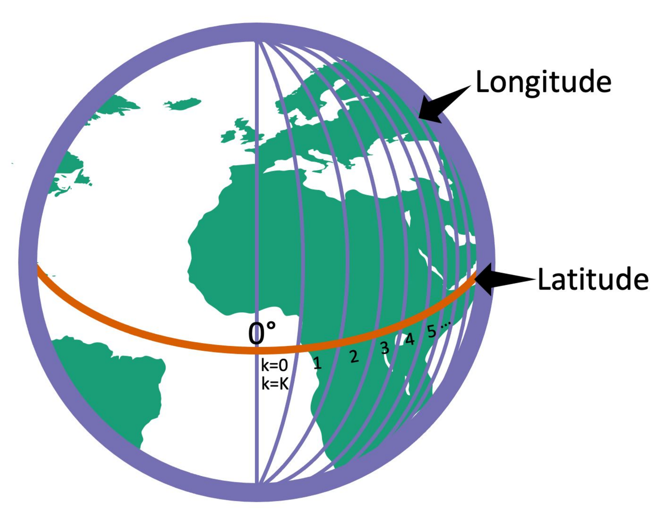
Machine learning is increasingly recognized as a valuable tool in forecasting Earth-system dynamics [1,2,3].

Forecasting the chaotic dynamics of such systems relies on capturing geospatial relationships, yet many machine learning models overlook the incorporation of spatial features into their forecasting approaches.

This research employs graphical neural networks, a machine learning architecture that explicitly encodes geospatial relationships, for forecasting chaotic spatiotemporal data.

Lorenz 96 Model

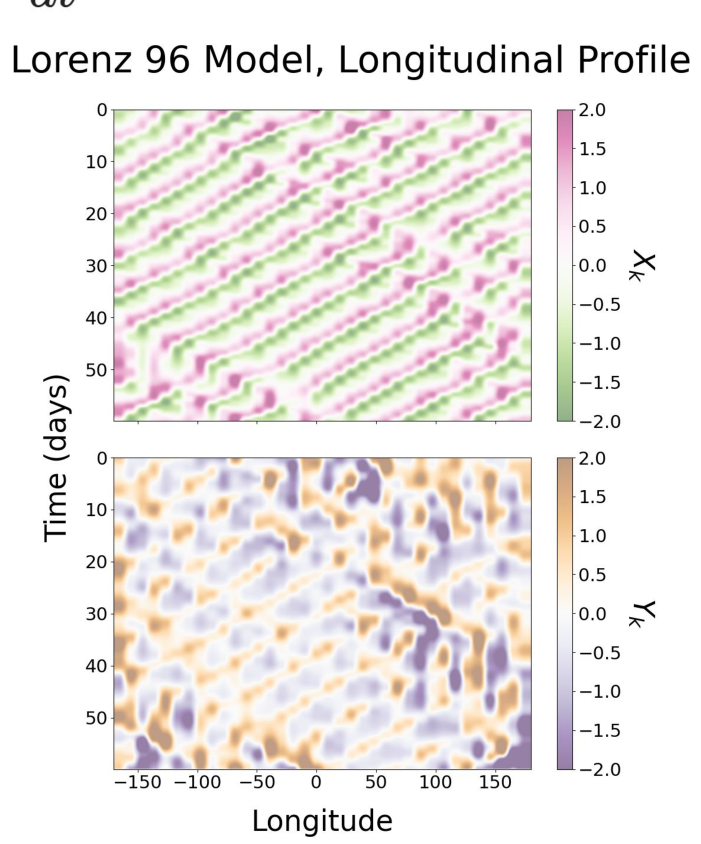
The Lorenz 96 model [4] is a surrogate model of the atmosphere which is **chaotic** yet **simplified**.



It consists of the following differential equations:

$$\frac{dX_k}{dt} = -X_{k-2}X_{k-1} + X_{k-1}X_{k+1} - X_k + \frac{hc}{b}Y_k + F$$

$$\frac{dY_k}{dt} = -cb(Y_{k+1}Y_{k+2} + Y_{k-1}Y_{k+1}) - cY_k + \frac{hc}{b}X_k$$



In our simulation, we use the coupled two-system model:

- K = 36 nodes
- F = 8 forcing
- h = 1 coupling

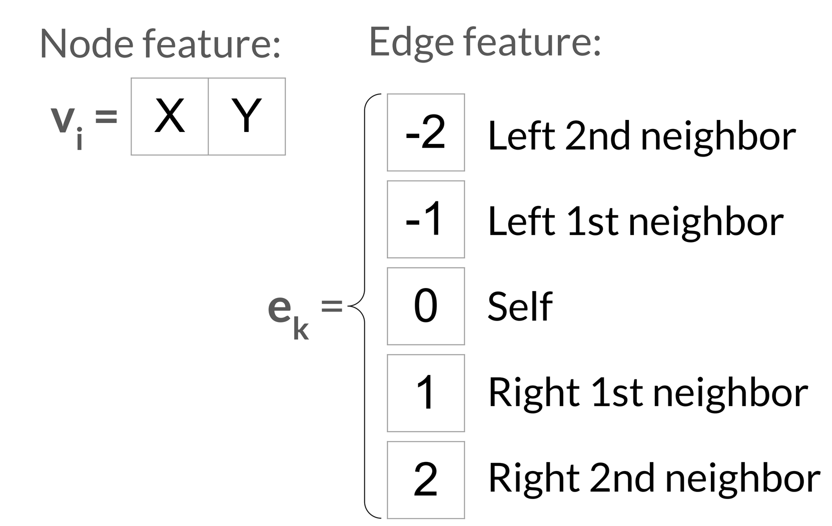
Each unit of time in the simulation equals to roughly 5 days, based on error-doubling rate.

Graph Neural Networks

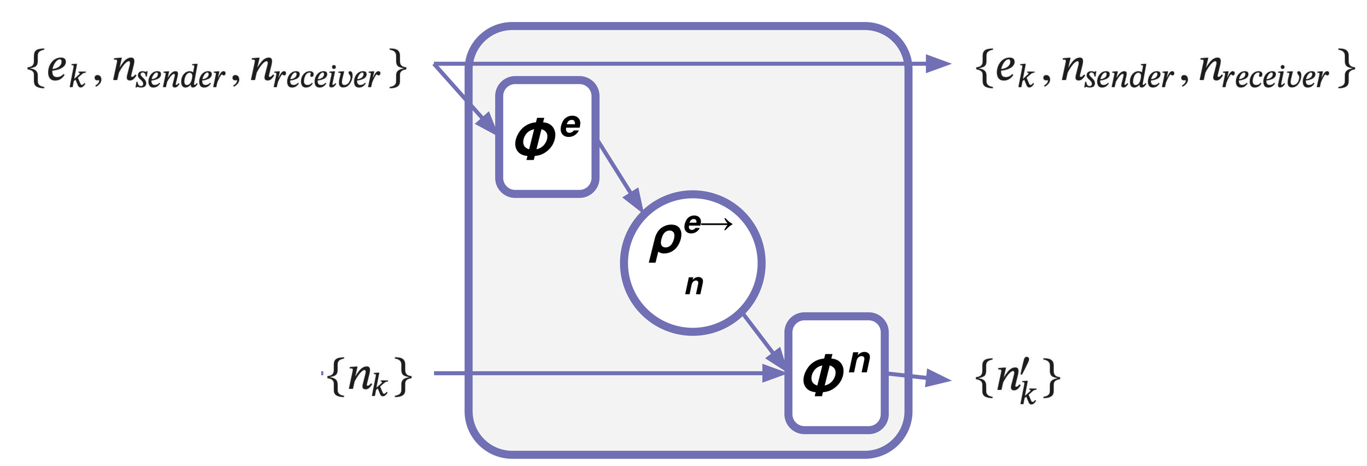
Graph neural networks (GNNs) are a generalization of common convolutional neural networks which can operate over arbitrary graph structures.

Data structure

The Lorenz 96 graph structure is preserved using edge and node features. Each data point is a graph with 36 nodes and 180 edges.



Model architecture



Update Functions

$$e'_k = \phi^e(e_k, n_s, n_r)$$
$$n'_i = \phi^n(\bar{e}'_i, n_i)$$

Aggregation Function

$$\bar{e}'_i = \rho^{e\to n}(E'_i)$$

Our GNN is a variation of the GraphNet architecture [5], consisting of two updating steps: one for edge features and one for node features.

Edge update:

Edge features are passed through the edge update function, an MLP, and aggregated by summation.

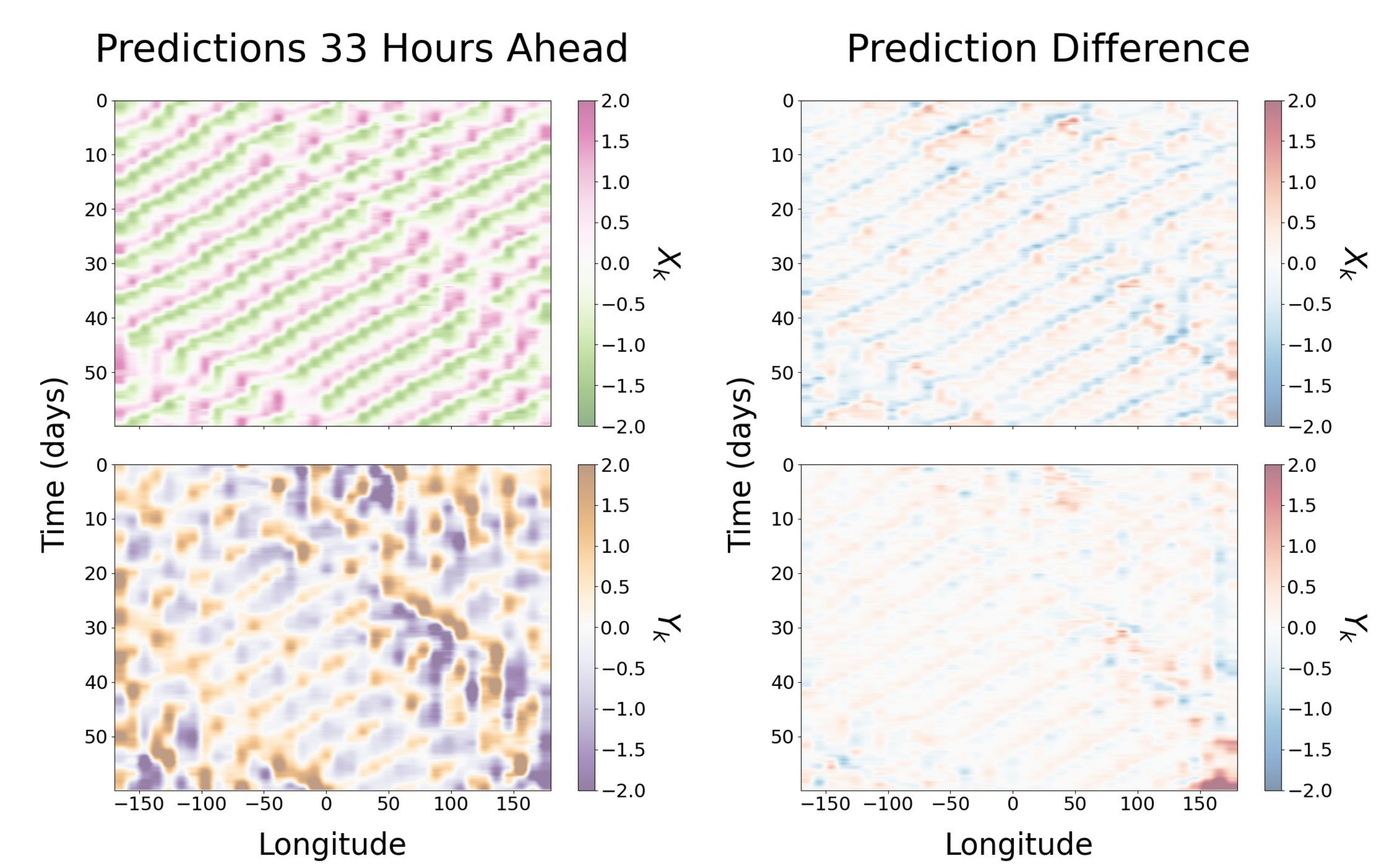
Node update

Node features and aggregated edge features are passed through the node update function, an MLP.

Results

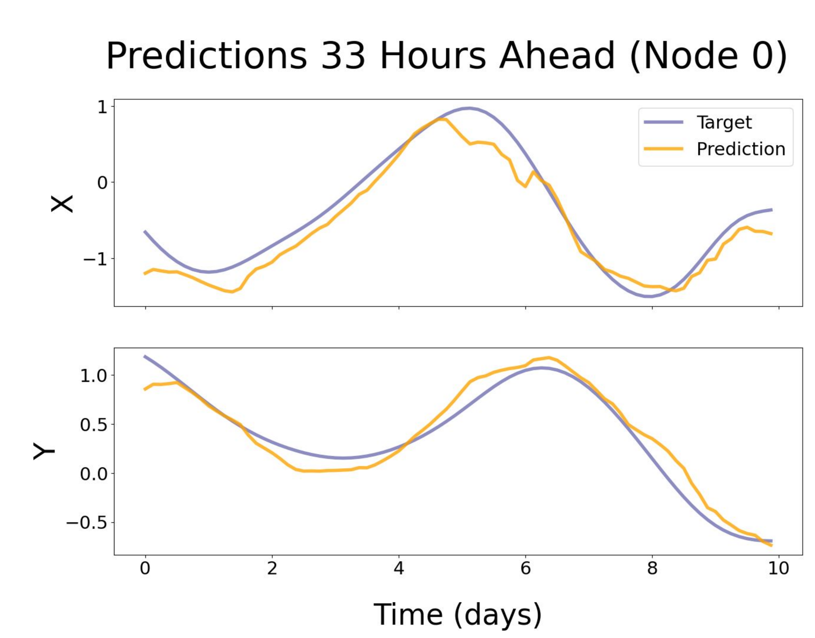
Preliminary predictions

Predictions are made autoregressively from a single data point in time. The predictions occur over four steps of 3 hours each, starting 24 hours into the future and rolling out to 33 hours into the future.



The longitudinal plots of the predictions, 33 hours into the future, suggest the graph neural network is able to capture the chaotic dynamics of the Lorenz 96 model.

The prediction difference from the Lorenz 96 data reveals the presence of some systematic errors rather than purely random noise.



Error Metrics	
Mean Squared Error	0.101
Mean Bias	-0.029
Mean Error	0.221
RMSE	0.305
Centered RMSE	0.301
Correlation Coefficient (R)	0.954
Index Of Agreement	0.934

Next Steps

To better evaluate the potential contributions of GNN, a number of additions can be made, including:

- replacing MLP layers in the GNN with recurrent cells to make results more comparable to common existing time series forecasting approaches
- Conducting more hyperparameter tuning with multiple chained GraphNet Blocks and trained on longer rollouts

References

[1] Chattopadhyay et al., 2021.
[2] Pfaff et al., 2021.
[3] Weyn et al., 2021.
[4] Lorenz, 1996.
[5] Battaglia et al., 2018.

Acknowledgements

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