The World as a Graph
Improving El Niño Forecasts with Graph Neural Networks
Cachay, Erickson, Bucker, Pokropek, Potosnak, Bire, Lütjens (2021).

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We want to forecast ENSO.

Climate networks offer a neat method to represent the world as a graph.

Can we exploit such graph structure for ENSO forecasting?

But how to construct the network?

In the deep learning spirit: let's just learn it.
Why not CNNs?

Convolutional networks achieve SOTA.

Disadvantages of CNNs for seasonal and long range forecasting

- Translational equivariance.
  - But: location is important.
- Spatial locality bias.
  - But: teleconnections are important.
- CNNs use all grid cells.
  - But: sometimes, only oceanic variables suffice.
Why GNNs?

Graph neural networks. [Credits: Geiger, 2021]

Advantages of GNNs

- Scales better than MLPs.
- More flexible than CNNs.
- More efficient than RNNs.
- Can model teleconnections due to non-Euclidean neighborhoods.
- Improves interpretability (structure encoded in graph).
We propose the **first application of GNNs** to long range and seasonal forecasting.

Building upon established previous research we develop and **open-source Graphino**, a flexible graph convolutional network architecture for long range forecasting applications in the climate and earth sciences.

We introduce a novel **graph structure learning module**, which makes our model applicable even **without a predefined connectivity structure**.

We show that our model is competitive to state-of-the-art statistical and dynamical ENSO forecasting systems, and **outperforms** them for forecasts of **up to six months**.

We exploit our model’s **interpretability**, to show how it learns sensible connections that are consistent with existing theories on ENSO dynamics predictability.
Goal: Forecast Oceanic Niño Index (ONI) for a fixed lead time.
Problem Setup

The formalities.

\[ \mathcal{G} = (\mathcal{V}, \mathcal{E}), \] where each \( V_i \in \mathcal{V}, 1 \leq i \leq N, \) is a node of a gridded climate dataset.

For each time \( t = 1..T, \) node feature vector \( V^t_i \in \mathbb{R}^D \) of climatic variable.

Adjacency \( A \in \{0, 1\}^{N \times N} \) with \((i, j) \in \mathcal{E} \Leftrightarrow A_{ij} = 1.\)

Snapshot measurement \( X_t = (V^t_1, .. V^t_n) \in \mathbb{R}^{N \times D} \)

For window size \( w, \) concatenate to obtain \( X = hstack(X_{t1}, .. X_{tw}) \in \mathbb{R}^{N \times wD}. \)

Target \( Y = Y_{tw+h} \in \mathbb{R}, \) ONI index for lead time \( h.\)

Loss \( \mathcal{L}: \) MSE.
GNNs
Graph Neural Networks.

If you haven’t yet, watch it!
GCNs
Graph Convolutional Networks.

• Node embeddings $Z_i^l$ for layer $l$ and node $i$, set $Z^0 = X$.
• Next layer: $Z^l = \sigma \left( AZ^{l-1}W^l \right) \in \mathbb{R}^{N \times D_l}$.
• For continuous $A$, this is a weighted sum inside the sigmoid.
• Aggregate output of last layer $L$ to obtain graph embedding: $g = \text{Aggregate} \left( Z_1^L, ..., Z_N^L \right) \in \mathbb{R}^{D_L}$.
• Finally, use an MLP to forecast ONI: $\hat{Y} = MLP(g)$. 
GCNs are typically shallow, in this case 2 and 3 layers.
Followed by 2 layer MLP.
Batch normalization, no dropout.
Residual connections and jumping knowledge.
Aggregation functions: mean, sum.
To obtain the adjacency $A$, use static node representations $\tilde{X} \in \mathbb{R}^{N \times \tilde{d}_1}$.

\( \tilde{X} \): SST, heat content anomalies, latitude and longitudes.

\[ M_1 = \tanh \left( \alpha_1 \tilde{X} \tilde{W}_1 \right) \in \mathbb{R}^{N \times \tilde{d}_2}, \]  
(1)  
\[ M_2 = \tanh \left( \alpha_1 \tilde{X} \tilde{W}_2 \right) \in \mathbb{R}^{N \times \tilde{d}_2}, \]  
(2)  
\[ A = \text{sigmoid} \left( \alpha_2 M_1 M_2^\top \right) \in \{0, 1\}^{N \times N}. \]  
(3)

$\alpha_1, \alpha_2$ hyperparameters controlling the spread of values and confidence in edges.

Finally, set all but largest $e$ edge weights to 0 to enforce desired sparsity.

Add self-loops to the graph.
Experiments

Data

- Climate model simulations from CMIP5.
  - Augmentation is needed for deep learning.
- Grid resolution 5 degrees, locations in $55^\circ S - 60^\circ N$ and $0 - 360^\circ W$.
- $N = 1345$ nodes after filtering out terrestrial ones.
- Features: SST and heat content anomalies, window $w = 3$ months.
Experiments

Results

- Outperforms state-of-the-art CNN of for up to 6 lead months
- Outperforms the competitive dynamical model SINTEX-F for all lead times.
- Why the decrease in performance for more than six lead months?
- Hypothesis: learning connectivity structure makes the model more prone to overfitting.

Figure: 6 month lead predictions.
The authors employ eigenvector centrality to visualize connectivity.

But: importance $\neq$ centrality.
Interpretability

Most Positive Ollivier Ricci Curvature

- Top: Eigenvector centrality. Bottom: nodes with top 10% positive edges.
Interpretability

Most Negative Ollivier Ricci Curvature

- Top: Eigenvector centrality. Bottom: nodes with top 10% negative edges.
Interpretability

Edges Connected to Node with Highest Negative Unnormalized Ollivier Ricci Curvature
Interpretability

Edges Connected to Node with Highest Eigenvector Centrality