Initial Condition Ensemble for GraphCast

CS4681 - Advanced Machine Learning

Research Project Progress Evaluation

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August 2025.

Abstract

The "GraphCast" is a machine learning approach to predict the weather. It used Graph Neural Networks to predict the weather based on 39 years of historical data. The major limitation of this approach is that it produces deterministic forecasts, which can deviate significantly in long-term climate predictions. My approach utilizes the ensembling techniques to overcome this limitation by incorporating the output of the same models, with adding noise to their input. The output of each model instance will be combined and evaluated against the "GraphCast" model.

1. Introduction

GraphCast is a scalable graph-neural-network model that generates deterministic 10-day global weather forecasts in under one minute. Weather conditions are known to be uncertain, as a small change in environmental variables can significantly deviate the outcomes. To make effective decisions considering uncertainties in long-term weather conditions, probabilistic forecasts are required rather than deterministic forecasts.

Traditional numerical weather forecast ensemble techniques address this limitation by tweaking the input and feeding it to multiple instances of models and combining those results to achieve probabilistic forecasting (initial-condition ensemble). But the traditional numerical forecasting models incur a high computational cost.

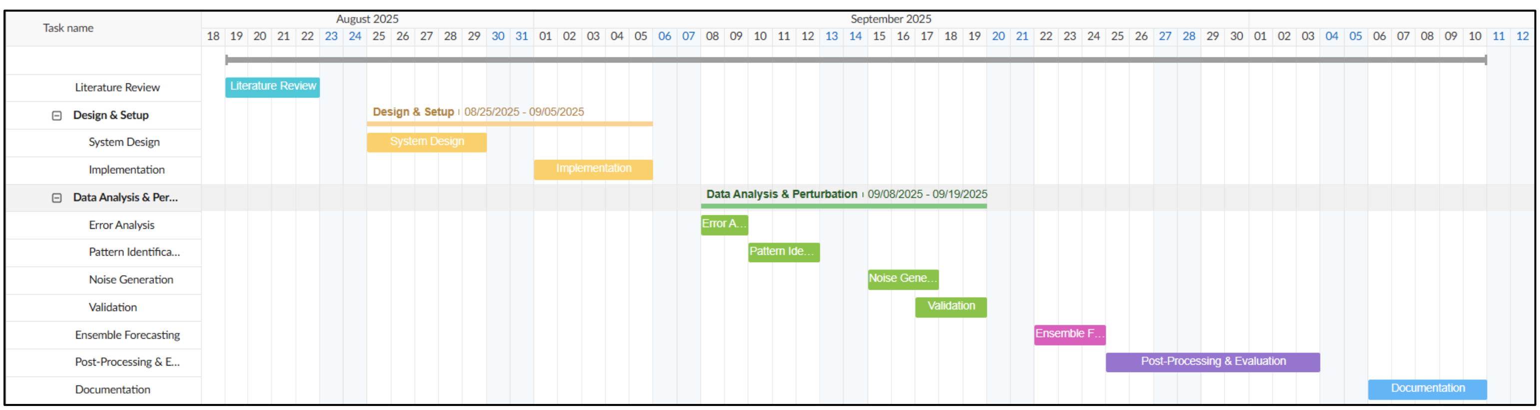
This proposal aims to leverage GraphCast's efficiency to develop a compact initial-condition ensemble to enable probabilistic forecasts with minimal computation. This approach allows for improving the existing "GraphCast" without re-training or fine-tuning the existing model.

2. Methodology Outline

1. Design & Setup (Assignment Objective: Training Strategy Enhancements - ensemble methods)
    - Design and implement an ensemble system (sequential/parallel) using the existing GraphCast model (no re-training/tuning).
2. Data Analysis & Perturbation Generation (Assignment Objective: Data Processing Improvements)
    - Decide how to create the random perturbations (noise).
        - Analyze the difference(error) between the past data and the predicted value.
        - Identify the main patterns in these errors and generate small random noise.
        - Use this noise to tweak the inputs (noise should average to zero-unbiased).
    - Validate perturbations.
3. Ensemble Forecasting
    - Perform inference using tweaked inputs on model instances(may be in parallel).
    - Collect and store results.
4. Post-Processing & Evaluation
    - Compute ensemble mean, spread, and probabilities.
    - Compare ensemble-mean vs deterministic GraphCast forecasts using root mean squared error (RMSE) and anomaly correlation coefficient (ACC) (Comparison b/w SOTA models).
    - Evaluate forecast reliability using reliability diagrams and rank histograms.
    - Tune perturbations for better reliability.
5. Documentation
    - Prepare a paper summarizing this experiment.

3. Project Timeline

1. Week 6 (25/08/2025 to 29/05/2025)
    a. Start the design work: mind map to actual design
    b. Refine the design. If this is completed, move to implementation. And start on how to generate perturbations.
2. Week 7 (01/09/2025 to 05/09/2025)
    a. Implement the ensemble pipeline.
3. Weel 8 (08/09/2025 to 12/09/2025)
    a. Analyze the deviation between real and predicted values in the dataset.
4. Week 9 (15/09/2025 to 19/09/2025)
    a. Generate the noise based on the learned patterns.
    b. Validate the noises generated.
5. Week 10 (22/09/2025 to 26/09/2025)
    a. Make forecasting using an ensemble and ensure forecasting is working.
    b. Start processing the output to evaluate the work.
6. Week 11 (29/09/2025 to 03/09/2025)
    a. Process the output of ensembles to get the final output.
    b. Validate the results against the base models.
7. Week 12 (06/09/2025 to 10/09/2025)
    a. Research paper compilation



4. Literature Review

Weather forecasting is one of the significant applications of machine learning (ML) that leverages past weather data to predict future weather conditions. The usage of ML is increasing in weather forecasting, as the newly introduced ML models often outperform the traditional numerical weather prediction (NWP) methods. The limitation of these ML models is, they provide deterministic forecasts and fail to address the uncertainty in the future weather prediction results. This limitation affects its usability in reliable decision-making.

Machine Learning-Based Weather Prediction Models

Machine learning based weather prediction is an alternative approach to forecasting the weather other than the traditional numerical weather prediction (NWP). ML approaches leverage the past weather data and learn patterns, and forecast the weather using the patterns. This field is important as the prediction of weather may help many sectors, such as farming, transport, and disaster management.

"GraphCast" is a significant improvement in using a machine learning approach in weather forecasting. It uses graph neural networks (GNN) to model and predict global atmospheric dynamics 10 days ahead with a fine resolution of (0.25°)[1]. The main goal of this work is to make quick and accurate weather forecasting with high resolution.

"GraphCast" is based on the encode-process-decode framework combined with a multi-mesh icosahedral grid, which allows it to communicate the information across long distances on the Earth's surface efficiently. Initially, the model encodes the inputs by mapping them from a regular grid to a multi-mesh. The inputs include two recent climate states together with other environmental information. Then 16 layers of message passing are applied to process the data, which allows communicating the information from the local as well as distant connections in the mesh. At last, processed features on the mesh points are again decoded onto the initial grid structure. This model was trained on ERA5 reanalysis data from 1979 to 2017 using hour intervals. The model's predictions were compared against HRES forecasts with respect to RMSE and anomaly correlation coefficient (ACC). The test data spans from 2018-2021.

"GraphCast" performed better than HRES for over 90% of the forecast targets. It also showed better anomaly correlation scores at all lead times. "GraphCast" predicted tropical cyclone tracks more accurately than HRES up to five days ahead. "GraphCast" on more recent years of data improved its skill slightly, suggesting that updating the model over time can boost performance.

The major limitation in the "Graph Cast", it only gives a single deterministic forecast, which makes it hard to represent the uncertainty in weather conditions in nature.

In my study, I am looking to address this limitation by ensembling techniques by tweaking the input slightly. I plan to arrange the existing models to address the limitation instead of re-training/tuning them.

Ensemble and Perturbation Methods for Weather Forecasting

Ensemble forecasting converts a single deterministic forecast into a probabilistic forecast by running multiple models with perturbed inputs or various configurations and aggregating the distribution of outcomes. This paradigm addresses the impact of small errors in the atmosphere and provides both an estimate of expected value (ensemble mean) and an estimate of forecast uncertainty (ensemble spread), which is essential for risk-aware decision making.

By using realistic input perturbations, ensembles can be created without re-training/tuning the existing models [2]. But the generated noise should comply with spatial and temporal covariances and project onto physically meaningful modes. Low-cost approaches often focus on the historical forecast analysis errors to generate this noise. Keeping the ensemble mean to zero can help to avoid systematic bias. These strategies help to adapt the probabilistic forecast of traditional NWP without retraining the existing models.

In my approach, I am using perturbation to vary the inputs realistically for the models in the ensemble.

5. References

[1] R. Lam et al., “GraphCast: Learning skillful medium-range global weather forecasting,” arXiv.org, Aug. 04, 2023. https://arxiv.org/abs/2212.12794?mc_cid=2622455cb4&mc_eid=51768751d5

[2] M. Leutbecher and T. N. Palmer, “Ensemble forecasting,” Journal of Computational Physics, vol. 227, no. 7, pp. 3515–3539, Mar. 2008, doi: https://doi.org/10.1016/j.jcp.2007.02.014.