Explainable AI for Climate Projection, Multi-Year Prediction & **Discovery**

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Ocean Model Development, Data-driven Parameterizations, and Machine Learning in Ocean Models of the Earth System Workshop Sep 09 2024

Do it faster/cheaper

Do it better

Learn something new

ML for post-processing data [e.g. data compression, data analysis]

Predicting the Errors of Forecast Systems

e.g. Chapman et al. (2019), Cahill et al. (in review), Pan et al. (2021), Gregory et al. (2023)

1

ML for post-processing data [e.g. data compression, data analysis]

ML to improve climate models
 E.g. parameterizations E.g. parameterizations Improved Model Parameterizations

e.g. Rasp et al. (2018; PNAS); Schneider et al. (2017; GRL); O'Gorman and Dwyer (2018); Beucler et al. (2020; PRL); Dagon et al. (2020); Brenowitz and Bretherton (2018)

1

ML for post-processing data [e.g. data compression, data analysis]

ML to improve climate models
[e.g. parameterizations]

Combine disparate datastreams to
explore complex systems

ML for post-processing data [e.g. data compression, data analysis]

ML to improve climate models
[e.g. parameterizations]

1

Combine disparate datastreams to explore complex systems

1 Merging observations and model data

ML for post-processing data
1 **1 Exercise Exercise A** [e.g. data compression, data analysis]

ML to improve climate models
[e.g. parameterizations]

Combine disparate datastreams to
explore complex systems

Merging observations and model data

Deep-learning weather + climate
emulators

Experimental: AIFS (ECMWF) ML model: 500 hPa geopotential height and 850 hPa temperature

Base time: Tue 26 Mar 2024 06 UTC Valid time: Sun 31 Mar 2024 00 UTC (+114h) Area : Europe

hysics > Atmospheric and Oceanic Physics

arXiv:2311.07222 (physics)

Submitted on 13 Nov 2023)

Neural General Circulation Models

Dmitrii Kochkov, Janni Yuval, Ian Langmore, Peter Norgaard, Jamie Smith, Griffin Mooers, James Lottes, Stephan Rasp, Peter Düben, Milan Klöwer, Sam Hatfield, Peter Battaglia, Alvaro Sanchez-Gonzalez, Matthew Willson, Michael P. Brenner, Stephan Hover

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General circulation models (GCMs) are the foundation of weather and climate prediction. GCMs are physics-based simulators which combine a numerical solver for large-scale dynamics with tuned representations for small-scale processes such as cloud formation. Recently, machine learning (ML) models trained on reanalysis data achieved comparable or better skill than GCMs for deterministic weather forecasting. However, these models have not demonstrated improved

Physics > Atmospheric and Oceanic Physics arXiv:2310.02074 (physics)

(Submitted on 3 Oct 2023)

ACE: A fast, skillful learned global atmospheric model for climate prediction

Oliver Watt-Meyer, Gideon Dresdner, Jeremy McGibbon, Spencer K. Clark, Brian Henn, James Duncan, Noah D. Brenowitz, Karthik Kashinath, Michael S. Pritchard, Boris Boney, Matthew E. Peters, Chri **Physics > Atmospheric and Oceanic Physics**

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[Submitted on 22 Mar 2024]

An ensemble of data-driven weather prediction models for operational sub-seasonal forecasting

for long-term weather and climate

combines a differentiable solver for d show that it can generate forecasts of

imate on par with the best ML and physics-

recasts ensemble prediction for 1-15 day ure, NeuralGCM can accurately track climate

ML models for 1-10 day forecasts, and with the

ultiple decades, and climate forecasts with 140

Jonathan A. Weyn, Divya Kumar, Jeremy Berman, Najeeb Kazmi, Sylwester Klocek, Pete Luferenko, Kit Thambiratnam

We present an operations-ready multi-model ensemble weather forecasting system which uses hybrid data-driven weather prediction models coupled with the European Centre for Medium-range Weather Forecasts (ECMWF) ocean model to predict global weather at 1-degree resolution for 4 weeks of lead time. For predictions of 2-meter temperature, our ensemble on average outperforms the raw ECMWF extended-range ensemble by 4-17%, depending on the lead time. However, after applying statistical bias corrections, the ECMWF ensemble is about 3% better at 4 weeks. For other surface parameters, our ensemble is also within a few percentage points of ECMWF's ensemble. We demonstrate that it is possible to achieve near-state-of-the-art subseasonal-to-seasonal forecasts using a multimodel ensembling approach with data-driven weather prediction models.

Subjects: Atmospheric and Oceanic Physics (physics.ao-ph); Machine Learning (cs.LC) Cite as: arXiv:2403.15598 [physics.ao-ph] (or arXiv:2403.15598v1 [physics.ao-ph] for this version)

long-term stability and physical consistency. We present ACE (AI2 Climate

parameter, autoregressive machine learning emulator of an existing comp resolution global atmospheric model. The formulation of ACE allows evalua such as the conservation of mass and moisture. The emulator is stable for conserves column moisture without explicit constraints and faithfully repro model's climate, outperforming a challenging baseline on over 80% of track requires nearly 100x less wall clock time and is 100x more energy efficient model using typically available resources.

Existing ML-based atmospheric models are not suitable for climate predict

 ϵ ML for post-processing data
1 **1 [e.g. data compression, data analysis]**

ML to improve climate models
[e.g. parameterizations]

Combine disparate datastreams to explore complex systems

Merging observations and model data

Deep-learning weather + climate

Machine Learning: a tool with many uses.

Climate change communication

 \blacksquare ML for post-processing data
 \blacksquare [e.g. data compression, data analysis]

ML to improve climate models
[e.g. parameterizations]

Combine disparate datastreams to
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Merging observations and model data

Deep-learning weather + climate
emulators

Machine Learning: a tool with many uses.

e.g. Zanna & Bolton (2020)

OUR GOAL:

To develop and implement AI tools to leverage imperfect climate models in support of earth system prediction across time and space.

Climate models provide inaccurate, but invaluable "parallel universes" to mine for information

https://futurism.com/parallel-universes-many-worlds-theo

Time Remaining Until Critical Warming Thresholds are Reached

Time Remaining Until Critical Warming Thresholds are Reached

Trained on annual maps from 10 realizations from across multiple climate models

Train neural network to ingest a single annual temperature map and predict the number of years until a warming threshold is reached

Train neural network to ingest a single annual temperature map and predict the number of years until a warming threshold is reached

Observations

Berkeley Earth Surface Temperature

Transfer Learning

Transfer Learning

- Base-CNN Initialized with 2023 Observations
- Transfer-CNN Initialized with 2023 Observations
- Estimated Observed Exceedance Year
- 7 Training Climate Model Ensembles **CMIP6 Spread**

But how did the network update its prediction?

…what if we could learn which regions of the globe were most relevant to improving the prediction with observations?

Opening the Black Box with XAI

In the past few years multiple papers have come out demonstrating the use of AI explainability methods for earth science

JULY 2024

(Manuscript received 25 August 2023, in final form 8 March 2024, acce

BOMMER ET AL.

MARINA M.-C. HOHNE^{a,b,e,f}.g.

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Finding the Right XAI Method-A Guide for the Evaluat

PHILINE LOU BOMMER.^{a,b} MARLENE KRETSCHMER.^{c,d} ANNA HEDSTRÖM

ABSTRACT: Explainable artificial intelligence (XAI) methods shed light on the pred rithms. Several different approaches exist and have already been applied in climate s ground truth explanations complicate their evaluation and comparison, subsequently method. Therefore, in this work, we introduce XAI evaluation in the climate context and tion properties, namely, robustness, faithfulness, randomization, complexity, and localiza ous work as a case study where the decade of annual-mean termeerature maps is predicte perceptron (MLP) and a convolutional neural network (CNN), multiple XAI methods a reference to a random uniform explanation are calculated for each property. Independ XAI methods such as Integrated Gradients, layerwise relevance propagation, and inpu able robustness, faithfulness, and complexity while sacrificing randomization performan SmoothGrad, NoiseGrad, and FusionGrad, match the robustness skill but sacrifice faithf domization skill. We find architecture-dependent performance differences regarding rob tion skills of different XAI methods, highlighting the necessity for research task-specific evaluation. Overall, our work offers an overview of different evaluation properties in the climate science context and shows how to compare and bench mark different explanation methods, assessing their suitability based on strengths and weaknesses, for the specific research problem at hand. By that, we aim to support climate researchers in the selection of a suitable XAI method.

SIGNIFICANCE STATEMENT: Explainable artificial intelligence (XAI) helps to understand the reasoning behind the prediction of a neural network. XAI methods have been applied in climate science to validate networks and provide new insight into physical processes. However, the increasing number of XAI methods can overwhelm practitioners, making it difficult to choose an explanation method. Since XAI methods' results can vary, uninformed choices might cause misleading conclusions about the network decision. In this work, we introduce XAI evaluation to compare and assess the performance of explanation methods based on five desirable properties. We demonstrate that XAI evalual tion reveals the strengths and weaknesses of different XAI methods. Thus, our work provides climate researchers with the tools to compare, analyze, and subsequently choose explanation methods.

the attribution is lacking for most of these datasets, making the assessment of XAI in many cases subjective. Also, benchmark datasets specifically designed for problems in geosciences are rare. Here, we provide a framework, based on the use of additively separable functions, to generate attribution benchmark datasets for regression problems for which the ground truth of the attribution is known a priori. We generate a large benchmark dataset and train a fully connected network to learn the underlying function that was used for simulation. We then compare estimated heatmaps from different XAI methods to the ground truth in order to identify examples where specific XAI methods perform well or poorly. We believe that attribution benchmarks as the ones introduced herein are of great importance for further application of neural networks in the geosciences, and for more objective assessment and accurate implementation of XAI methods, which will increase model trust and assist in discovering new science.

received much attention in the meteorological community, such as the concept of receptive fields, underutilized meteorological performance measures, and methods for neural network interpretation, such as synthetic experiments and layer-wise relevance propagation. We also consider the process of neural network interpretation as a whole, recognizing it as an iterative meteorologist-driven discovery process that builds on experimental design and hypothesis generation and testing. Finally, while most work on neural network interpretation in meteorology has so far focused on networks for image classification tasks, we expand the focus to also include networks for image-to-image

translatice

forward pass input \rightarrow output XAI Attribution \rightarrow x_f Prediction \mathbf{r} $Pr(cat)=.8$ Methods of 1 sample ∍⊇ ${x_p}$

Attribution heatmaps are largely consistent with how many climate scientists pose questions

e.g. Montavon et al. (2017), Pattern Recognition; Montavon et al. (2018), Digital Signal Processing

Why businesses need explainable AIand how to deliver it dember 29, 2022 | Article

H.R.6093 - Weather Act Reauthorization Act of 2023 118th Congress (2023-2024) | Get alerts

"(c) ARTIFICIAL INTELLIGENCE INVESTMENTS.—The Under Secretary shall leverage artificial intelligence and machine learning technologies to facilitate, optimize, and further leverage advanced computing to accomplish critical missions of the National Oceanic and Atmospheric Administration by enhancing existing and forthcoming high-performance and cloud computing infrastructure or systems.

"(d) CENTERS OF EXCELLENCE.—The Under Secretary may expand, and where applicable establish, centers of excellence to aid the adoption of next-generation artificial intelligence and machine learning enabled advanced computing capabilities. Each such center may carry out activities that include the following:

Executive Order on the Safe, Secure, and Trustworthy Development and Use of Artificial Intelligence

OCTOBER 30, 2023

Sec. 8. Protecting Consumers, Patients, Passengers, and Students. (a) Independent regulatory agencies are encouraged, as they deem appropriate. to consider using their full range of authorities to protect American consumers from fraud, discrimination, and threats to privacy and to address other risks that may arise from the use of AI, including risks to financial stability, and to consider rulemaking, as well as emphasizing or clarifying where existing regulations and guidance apply to AI, including clarifying the responsibility of regulated entities to conduct due diligence on and monitor any third-party AI services they use, and emphasizing or clarifying requirements and expectations related to the transparency of AI models and regulated entities' ability to explain their use of AI models.

The EU AIA mandates that high-risk AI systems must provide clear and comprehensible information about their capabilities and limitations, and that their decision-making process should be transparent and traceable. Jun 7, 2023

Explainable AI (XAI) will be essential.

Regional transfer learning provides new insights

Surface temperature over Chicago, IL MPI-ESM Large Ensemble; historical + RCP8.5

Surface temperature over Chicago, IL MPI-ESM Large Ensemble; historical + RCP8.5

Surface temperature over Chicago, IL

MPI-ESM Large Ensemble; historical + RCP8.5

Surface temperature over Chicago, IL

MPI-ESM Large Ensemble; historical + RCP8.5

Surface temperature over Chicago, IL

MPI-ESM Large Ensemble; historical + RCP8.5

Predict ocean temperatures 5 years later

CLIMATE MODEL DATA

Overall Accuracy

Trained on climate model MPI-ESM-1-2-LR [3,630 years of data] Evaluated on climate model MPI-ESM-1-2-LR

Focusing on when the AI is most confident leads to skillful predictions

CLIMATE MODEL DATA

Trained on climate model MPI-ESM-1-2-LR [3,630 years of data] Evaluated on climate model MPI-ESM-1-2-LR

Focusing on when the AI is most confident leads to skillful predictions

CLIMATE MODEL DATA

Trained on climate model MPI-ESM-1-2-LR [3,630 years of data] Evaluated on climate model MPI-ESM-1-2-LR

Focusing on when the AI is most confident leads to skillful predictions

OBSERVATIONS

Trained on climate model MPI-ESM-1-2-LR [3,630 years of data] Evaluated on **observations [ERSSTv5; 169 years of data]**

Leveraging climate model data provides skillful predictions of the real world

Windows of Opportunity tested on ERSSTv5 observations

Accuracy of 20% most confident predictions of year 1-5 sea surface temperature anomaly

Compare climate model-based network skill

Windows of Opportunity tested on ERSSTv5 observations

Accuracy of 20% most confident predictions of year 1-5 sea surface temperature anomaly

Compare climate model-based network skill

0.50

GCM accuracy

0.75

k) S. Ocean

 0.8

Predicting 5-year average surface temperature at each grid point Applied to 1200 years of CESM2 control simulation

XAI reveals sources of predictability that vary in time and space

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Predicting 5-year average surface temperature at each grid point Applied to 1200 years of CESM2 control simulation

XAI reveals sources of predictability that vary in time and space

nature,
machine intelligence

Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead

Cynthia Rudin[®]

Rudin (2019)

Interpretable AI

Explainable AI tells us where, but not how. Interpretable AI explicitly incorporates the decision-making process into its structure. Models are interpretable by design.

Our Current Goal:

work toward building AI models that mimic scientific human reasoning to improve intrinsic interpretability

Interpretable AI

Explainable AI tells us where, but not how. Interpretable AI explicitly incorporates the decision-making process into its structure. Models are interpretable by design.

$Climate Model$
Atmospheric Predictability as Revealed by Naturally Oscurring Analogues

EDWARD N. LORENZ

Dept. of Meteorology, Massachusetts Institute of Technology, Cambridge, Mass.¹ (Manuscript received 2 April 1969)

ABSTRACT

Two states of the atmosphere which are observed to resemble one another are termed analogues. Either state of a pair of analogues may be regarded as equal to the other state plus a small superposed "error." From the behavior of the atmosphere following each state, the growth rate of the error may be determined.

Five years of twice-daily height values of the 200-, 500-, and 850-mb surfaces at a grid of 1003 points over the Northern Hemisphere are procured. A weighted root-mean-square height difference is used as a measure of the difference between two states, or the error. For each pair of states occurring within one month of the same time of year, but in different years, the error is computed.

There are numerous mediocre analogues but no truly good ones. The smallest errors have an average doubling time of about 8 days. Larger errors grow less rapidly. Extrapolation with the aid of a quadratic hypothesis indicates that truly small errors would double in about 2.5 days. These rates may be compared with a 5-day doubling time previously deduced from dynamical considerations.

The possibility that the computed growth rate is spurious, and results only from having superposed the smaller errors on those particular states where errors grow most rapidly, is considered and rejected. The likelihood of encountering any truly good analogues by processing all existing upper-level data appears to be small.

Method of Analogs

Barnes et al. (2022) Rader and Barnes (2024) Gordillo and Barnes (under review) Fernandez and Barnes (in prep)

our state of interest (a map of the current climate)

Analogs for seasonal-to-decadal prediction

Analogs for seasonal-to-decadal prediction

our state of interest (a map of the current climate)

Analogs for seasonal-to-decadal prediction

* a perfect model application using the MPI Grand Ensemble

Analog Forecasts for North Atlantic Sea Surface Temperature

Traditionally, if two states **"look similar"** it means they have the smallest difference over the entire globe, or a predefined region.

This assumes that every region is equally important for determining how the climate system will evolve. We can do better.

Use AI to learn regions most relevant for a "good analog"

mask

Take this mask and use it to determine the "best analogs" in the standard, non-AI, way.

Use AI to learn regions most relevant for a "good analog"

Weighted Mask

Use AI to learn regions most relevant for a "good analog"

Identify the analogs with the weighted mask

Identify the analogs with the weighted mask

Identify the analogs with the weighted mask

Maps look similar in the precursor regions

Identify the analogs

CLIMATE MODEL RESULTS

Forecasts are skillful

These optimized analogs rival the skill of dynamical models

This approach is interpretable AI!

While one could train a massive black-box AI model to make these predictions, the benefit of analogs is that they are easily understood.

AI is merely used to learn the optimal mask for choosing the analogs. The masks are the "XAI".

Not a new Idea, but renewed interest! e.g. Lorenz (1969), Menary et al. (2021), Lou et al. (2023), Mahmood et al. (2021), Befort et al. (2020), Ding et al. (2018, 2019), Toride et al. (2024) \sim Rader and Barnes (2024)

Learned ENSO Prediction Mask

Analogs can help constrain projections \rightarrow initialized predictions

Analogs can help constrain projections \rightarrow initialized predictions

Yrs 5-7 Surface Temperature Anomalies Western U.S.

Analogs can help constrain projections \rightarrow initialized predictions

Climate change influence the performance of AI models

These are exciting times! XAI will be key to advancing science.

Thank you.

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