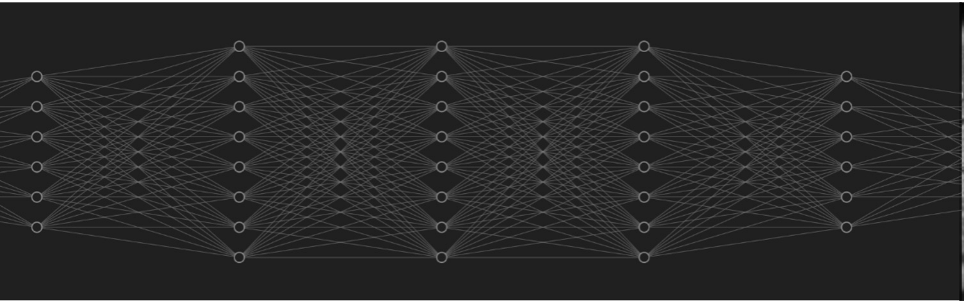
Machine Learning for
Earth System Prediction and Predictability



Maria J. Molina, Assistant Professor
Department of Atmospheric and Oceanic Science
mjmolina@umd.edu; mariajmolina.github.io

Hurricane Andrew (1992)
- Interest in extremes

Florida State University
- Undergraduate studies

Broadcast Meteorology
- New York, NY

Columbia University
- Masters degree

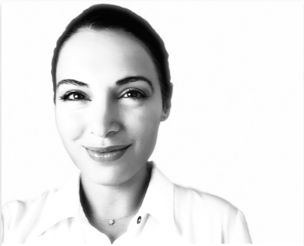
Central Michigan University
- Doctoral studies

National Center for Atmospheric Research
- Postdoctoral Fellowship

University of Maryland
- **Assistant Professor**

OUR TEAM

mariajmolina.github.io



Dr. Maria J. Molina

Assistant Professor

she/her

I am an Assistant Professor within the Department of Atmospheric and Oceanic Science at the University of Maryland and an Affiliate Faculty with the Unive

Jhayron Steven Perez Carrasquilla

AOSC PhD Student

he/him

I'm currently studying subseasonal-to-seasonal (S2S) atmospheric predictability

Emily Faith Wisinski

AOSC PhD Student

Erin Elise Evans

AOSC MS Student (Co-advisor: Dale Allen)

she/her

Cumulus ☁

AOSC Postdog

support animal

Hannah Bao

AOSC Undergraduate (Co-Advisor: Salil Mahajan, Oak Ridge National Laboratory)

she/her

I am a fourth-year Atmospheric and Oceanic

Siddharth Cherukupalli

CS Undergraduate

he/him

I am a second-year Computer Science major at the University of Maryland, College Park. I have previous research experience and also

Bhuvan Jammalamadaka

CS Undergraduate

he/him

Varun Vishnubhotla

CS Undergraduate

he/him

Matthew Chan
CS PhD Student
(Advisor: Metzler)

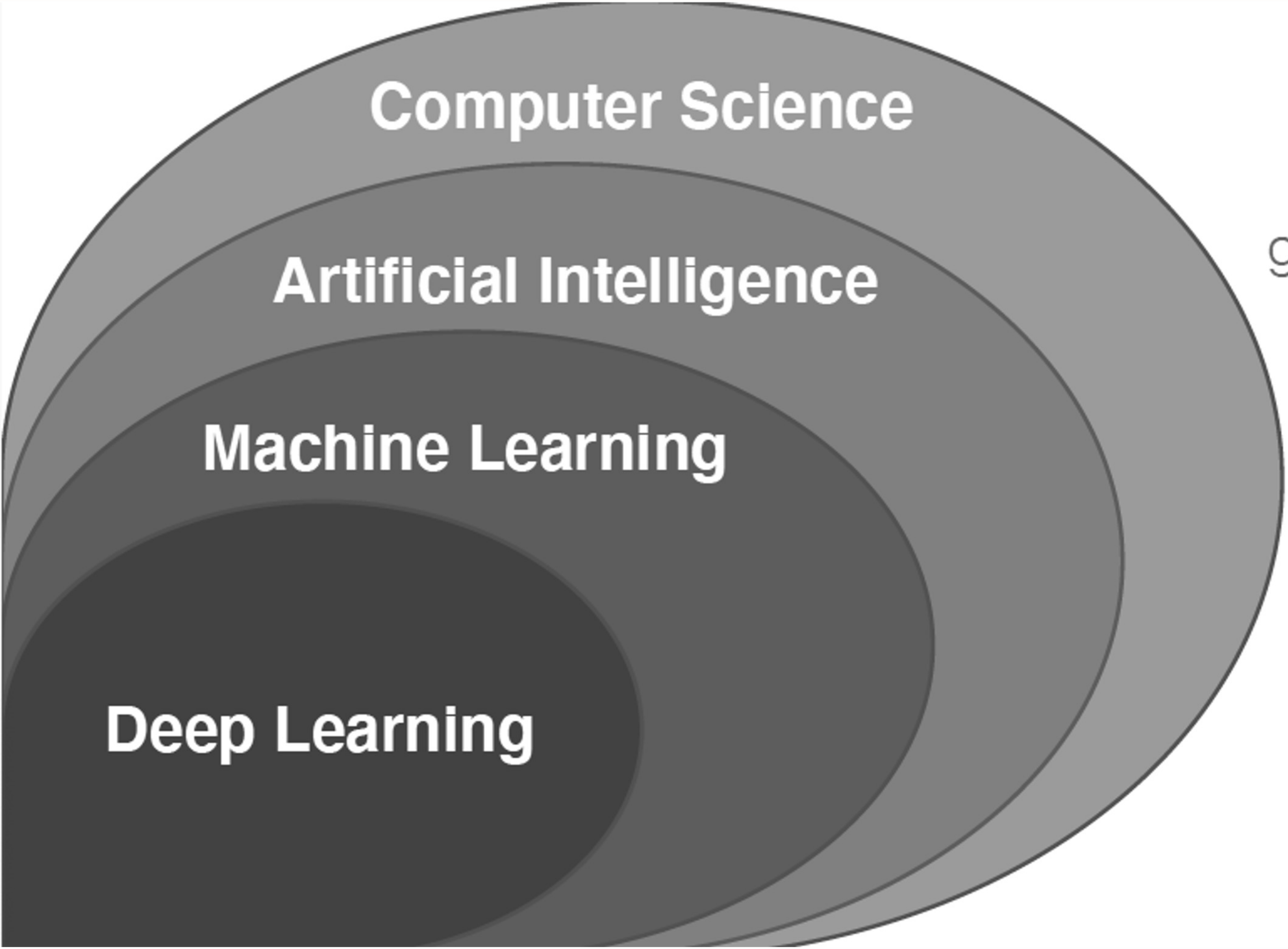
Prediction

…refers to the specific forecasts or outlooks generated for future conditions.

…refers to the inherent limit or potential for accurate predictions (e.g., ability to forecast future conditions given the current state).

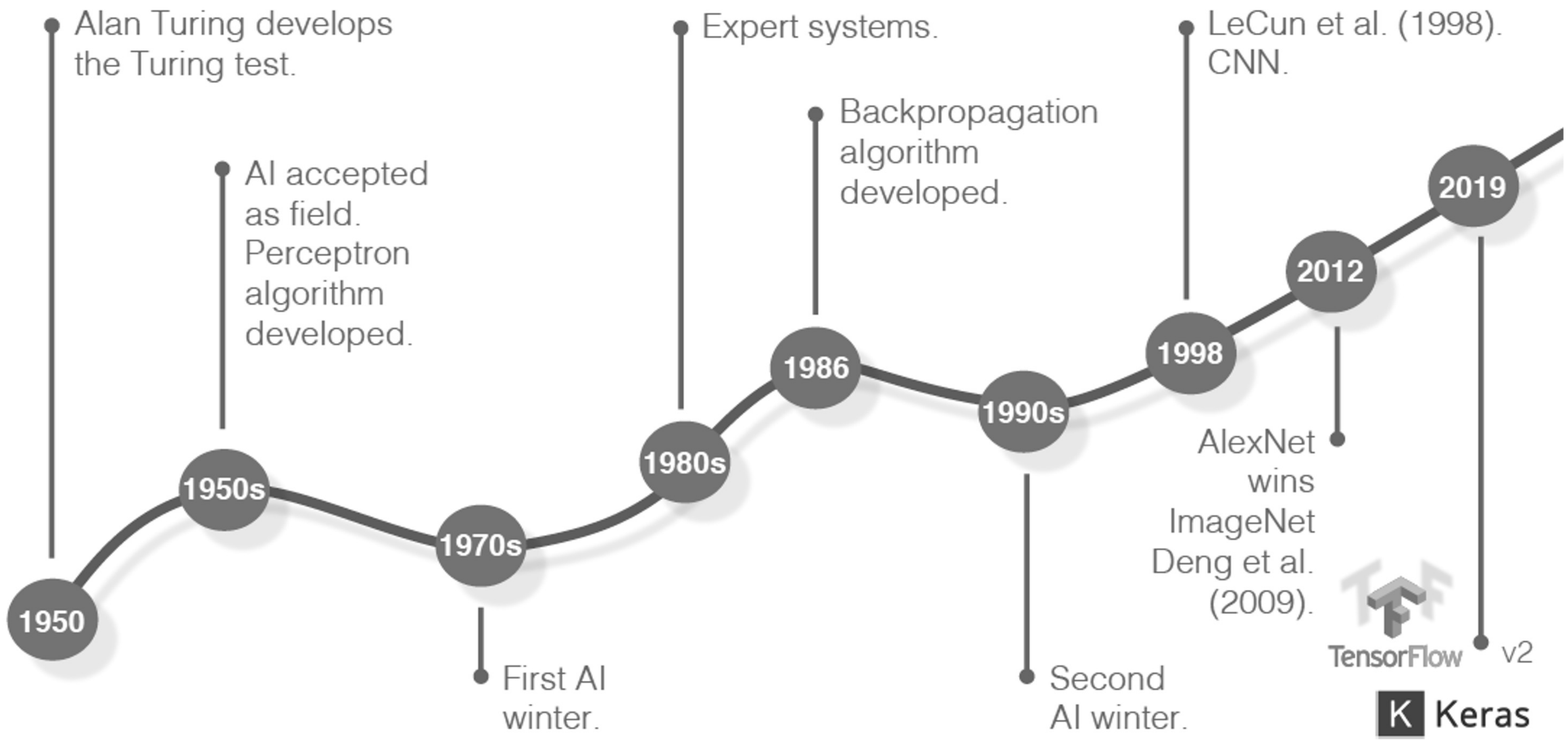
Predictability

Molina, M.J., T.A. O'Brien, G. Anderson, M. Ashfaq, K.E. Bennett, W.D. Collins, K. Dagon, J.M. Restrepo, and P.A. Ullrich (2023). A Review of Recent and Emerging Machine Learning Applications for Climate Variability and Weather Phenomena. Artificial Intelligence for the Earth Systems.



"Field of study that gives computers the ability to learn without being explicitly programmed."

1959, Arthur Lee Samuel defined ML


Alan Turing develops the Turing test.
1950
AI accepted as field. Perceptron algorithm developed.
1950s
1970s
First AI winter.
Expert systems.
1980s
Backpropagation algorithm developed.
1986
1990s
Second AI winter.
LeCun et al. (1998). CNN.
1998
2012
AlexNet wins ImageNet Deng et al. (2009).
2019
TensorFlow
v2
Keras

Data Availability

Data Rich	Moderate	Data Poor

Neural Networks

PINNs

Symbolic Regression

XGBoost

Gaussian Processes

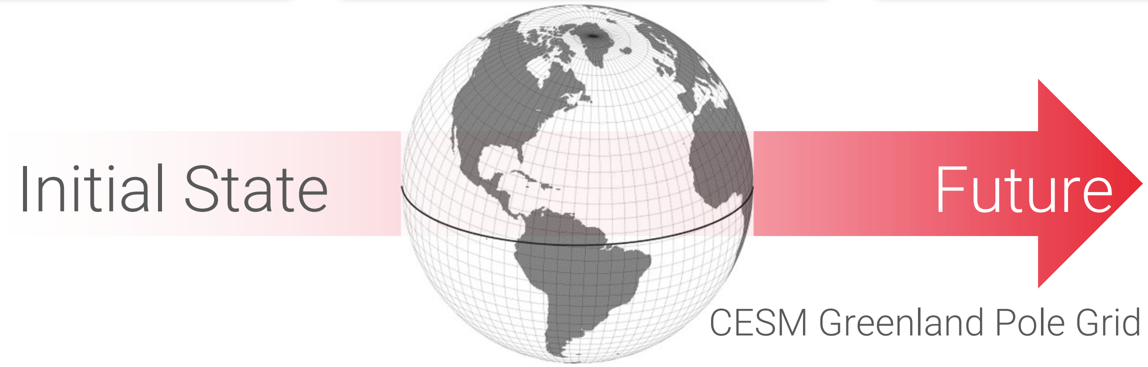
Transfer Learning
Meta-learning

Use of Domain Knowledge

Adapted and Inspired from

“Traditional” numerical weather prediction / climate modeling

Input	Run Model	Output
Observations or Representation of the Initial State	Parameterizations High Performance Computing	Predictions with Certain Lead Time (e.g., S2S)



Molina, M.J., T.A. O'Brien, G. Anderson, M. Ashfaq, K.E. Bennett, W.D. Collins, K. Dagon, J.M. Restrepo, and P.A. Ullrich (2023). A Review of Recent and Emerging Machine Learning Applications for Climate Variability and Weather Phenomena. Artificial Intelligence for the Earth Systems.

ML in traditional physics-based modeling

Initial State

- Data Assimilation
- Parameter Estimation
- Sensor Placement

Run Model

- Physical Parameterizations
- PDE Acceleration
- Emulation
- Online Bias Correction

Output

- Information Extraction
- Offline Bias Correction
- Data fusion
- Downscaling

Molina, M.J., T.A. O'Brien, G. Anderson, M. Ashfaq, K.E. Bennett, W.D. Collins, K. Dagon, J.M. Restrepo, and P.A. Ullrich (2023). A Review of Recent and Emerging Machine Learning Applications for Climate Variability and Weather Phenomena. Artificial Intelligence for the Earth Systems.

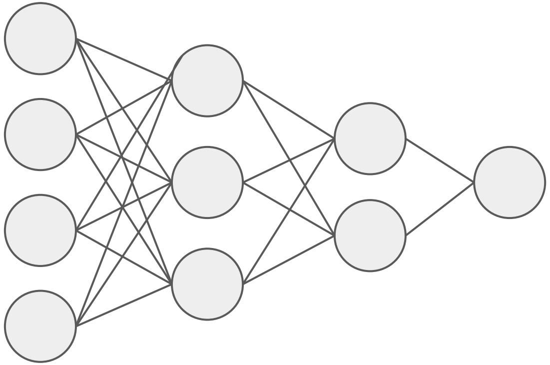
ML-based numerical weather prediction / climate modeling

Input
Observations or Representation of the Initial State

Run Model
Computing

Output
Predictions with Certain Lead Time (e.g., S2S)

Initial State



Future

Molina, M.J., T.A. O'Brien, G. Anderson, M. Ashfaq, K.E. Bennett, W.D. Collins, K. Dagon, J.M. Restrepo, and P.A. Ullrich (2023). A Review of Recent and Emerging Machine Learning Applications for Climate Variability and Weather Phenomena. Artificial Intelligence for the Earth Systems.

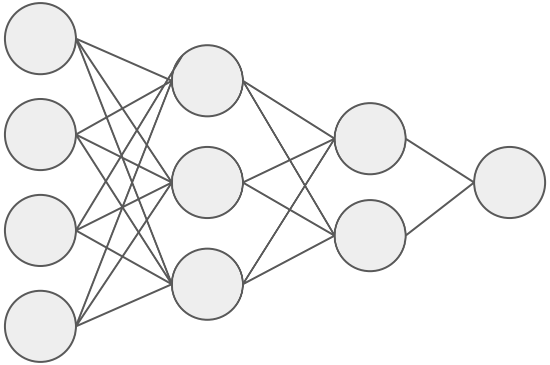
ML-based numerical weather prediction / climate modeling

Input
Observations or Representation of the Initial State

Run Model
Computing

Output
Predictions with Certain Lead Time (e.g., S2S)

Initial State



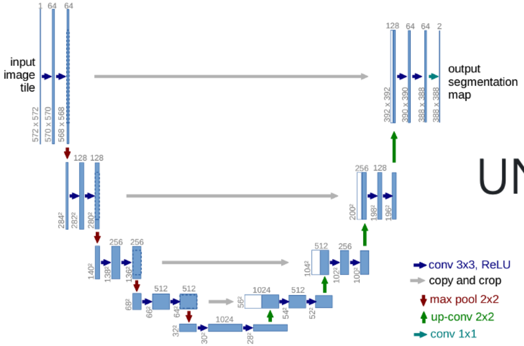
Future

Molina, M.J., T.A. O'Brien, G. Anderson, M. Ashfaq, K.E. Bennett, W.D. Collins, K. Dagon, J.M. Restrepo, and P.A. Ullrich (2023). A Review of Recent and Emerging Machine Learning Applications for Climate Variability and Weather Phenomena. Artificial Intelligence for the Earth Systems.

Detection of Features and Extremes

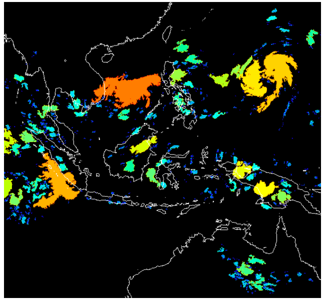
Mary Grace Albright
PhD Candidate, UConn

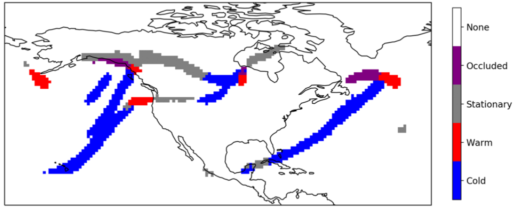
Model Simulations



UNet

Phenomena (MCSs)



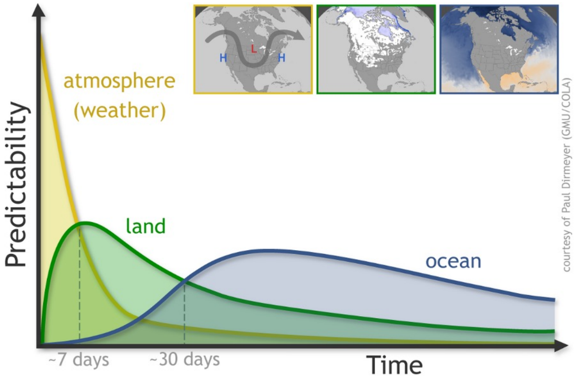


Dagon, K., Truesdale, J. E., Biard, J. C., Kunkel, K. E., Meehl, G. A. and Molina, M. J., 2022. Machine learning-based detection of weather fronts and associated extreme precipitation. JGR: Atmospheres.

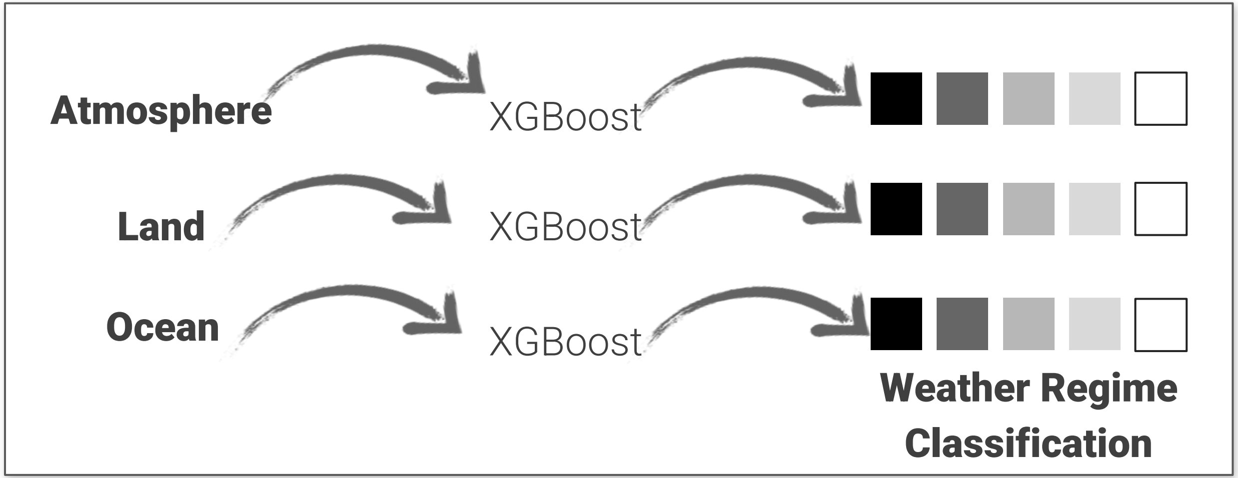
Design experiments to answer questions

Jhayron Steven Perez Carrasquilla

AOSC PhD Student



Richter, J., A. Glanville, T. King et al. Quantifying sources of subseasonal prediction skill; [https://doi.org/10.21203/rs.3.rs-3035271/v1]



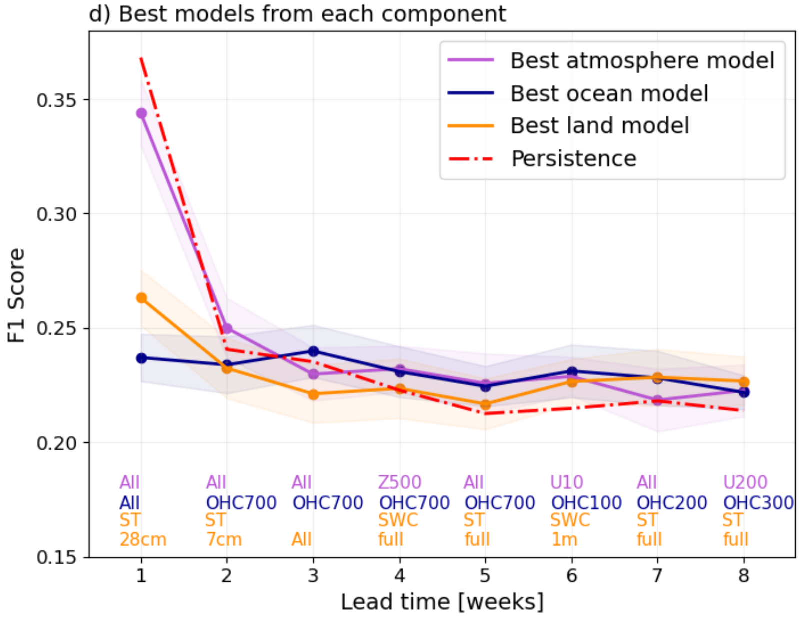
GRAND CHALLENGES GRANTS

Design experiments to answer questions

Jhayron Steven Perez Carrasquilla

AOSC PhD Student

More Skil



Less Skill

Lead time (Weeks 1-8)

Figure by Jhayron S. Perez-Carrasquilla.

GRAND CHALLENGES GRANTS

Design experiments to answer questions

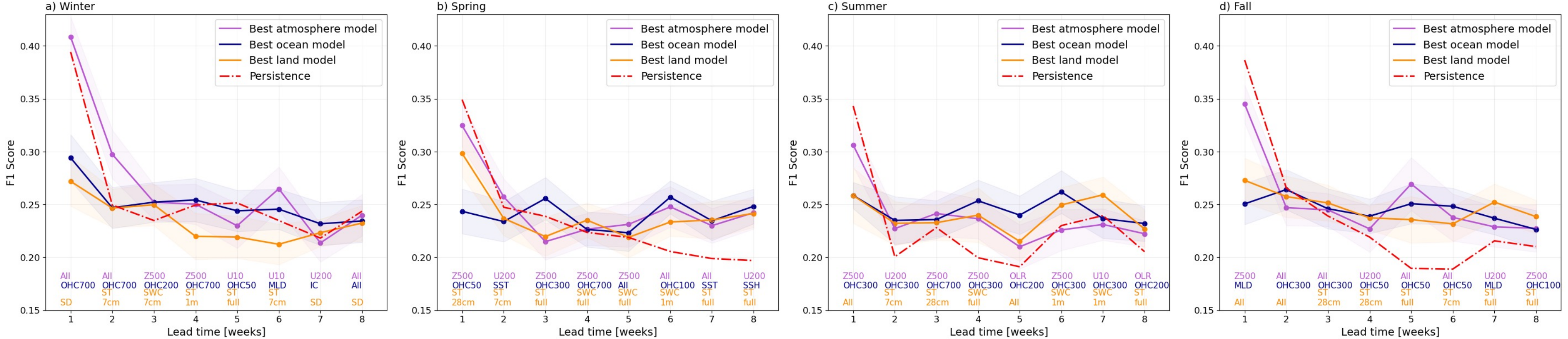


Figure by Jhayron S. Perez-Carrasquilla.

GRAND CHALLENGES GRANTS

Perez-Carrasquilla, J.S., and M.J. Molina (in prep). An Earth-system-oriented view of the S2S predictability of Weather Regimes. Artificial Intelligence for the Earth Systems. *Presented at the AMS 2024 Annual Meeting.*

NCAR NSF

Ensemble creation

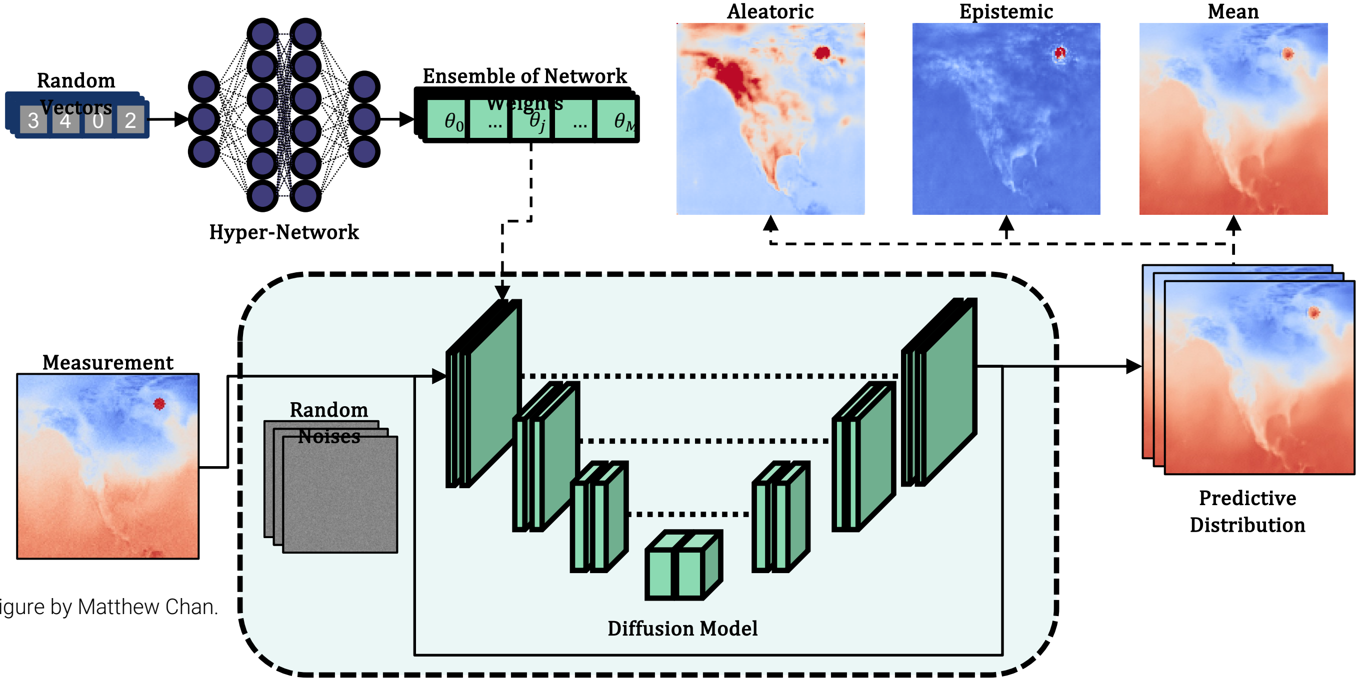
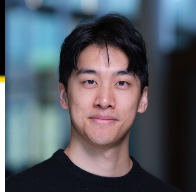
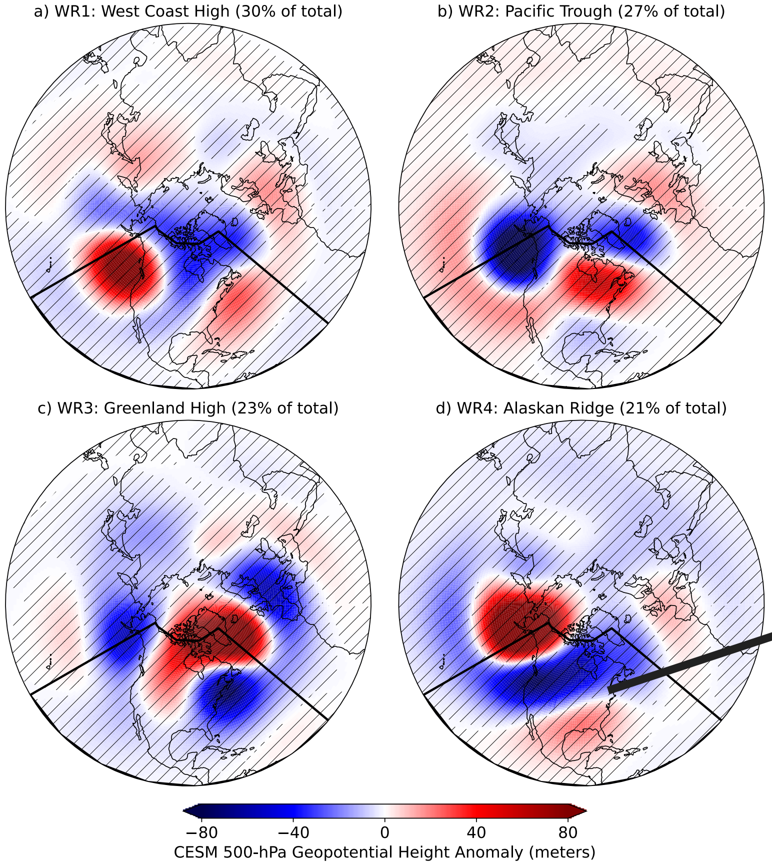


Figure by Matthew Chan.



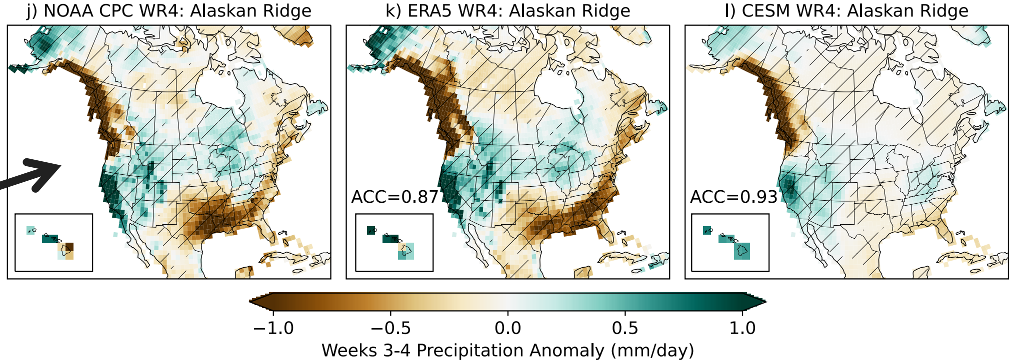
Matthew Chan
CS PhD Student

Chan, M. A., **M. J. Molina,** and C. A. Metzler (Under Review). Hyper-Diffusion: Estimating Epistemic and Aleatoric Uncertainty with a Single Model.



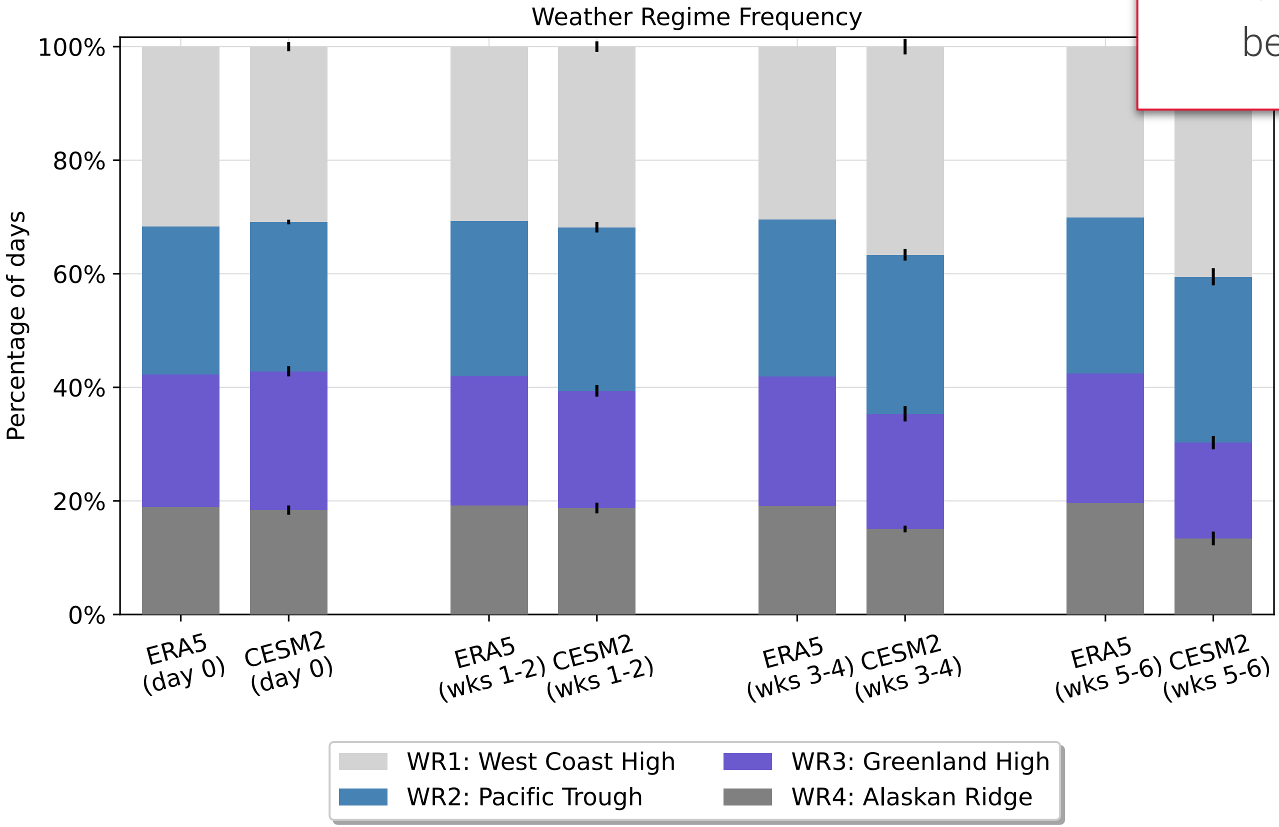
Unsupervised benchmarking

Prediction of precipitation on longer (than weather) timescales is challenging…



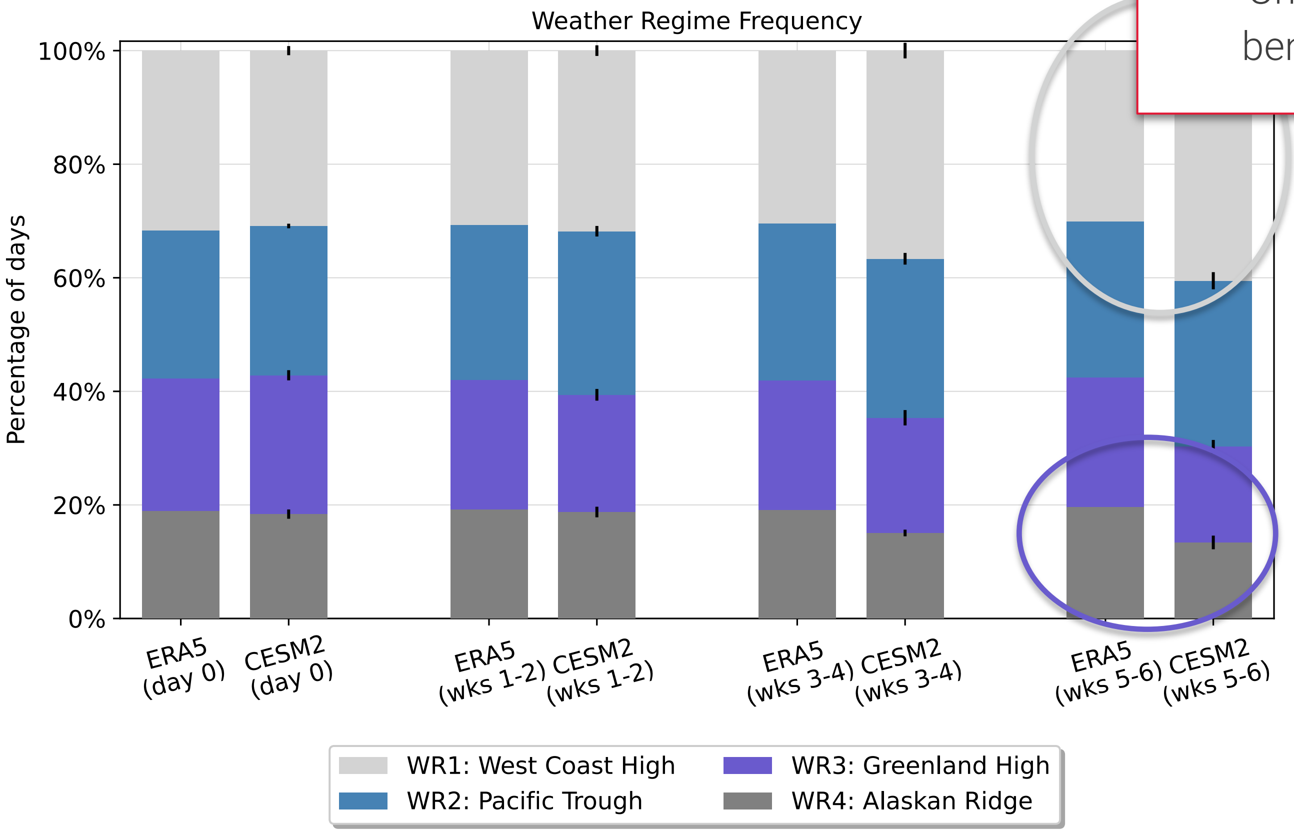
Molina, M. J., Richter, J.H., Glanville, A.A., Dagon, K., Berner, J., Hu A., Meehl, G.A., (2023). Subseasonal Representation and Predictability of North American Weather Regimes using Cluster Analysis. AMS AI for the Earth Systems.

Unsupervised benchmarking



Molina, M. J., Richter, J.H., Glanville, A.A., Dagon, K., Berner, J., Hu A., Meehl, G.A., (2023). Subseasonal Representation and Predictability of North American Weather Regimes using Cluster Analysis. AMS AI for the Earth Systems.

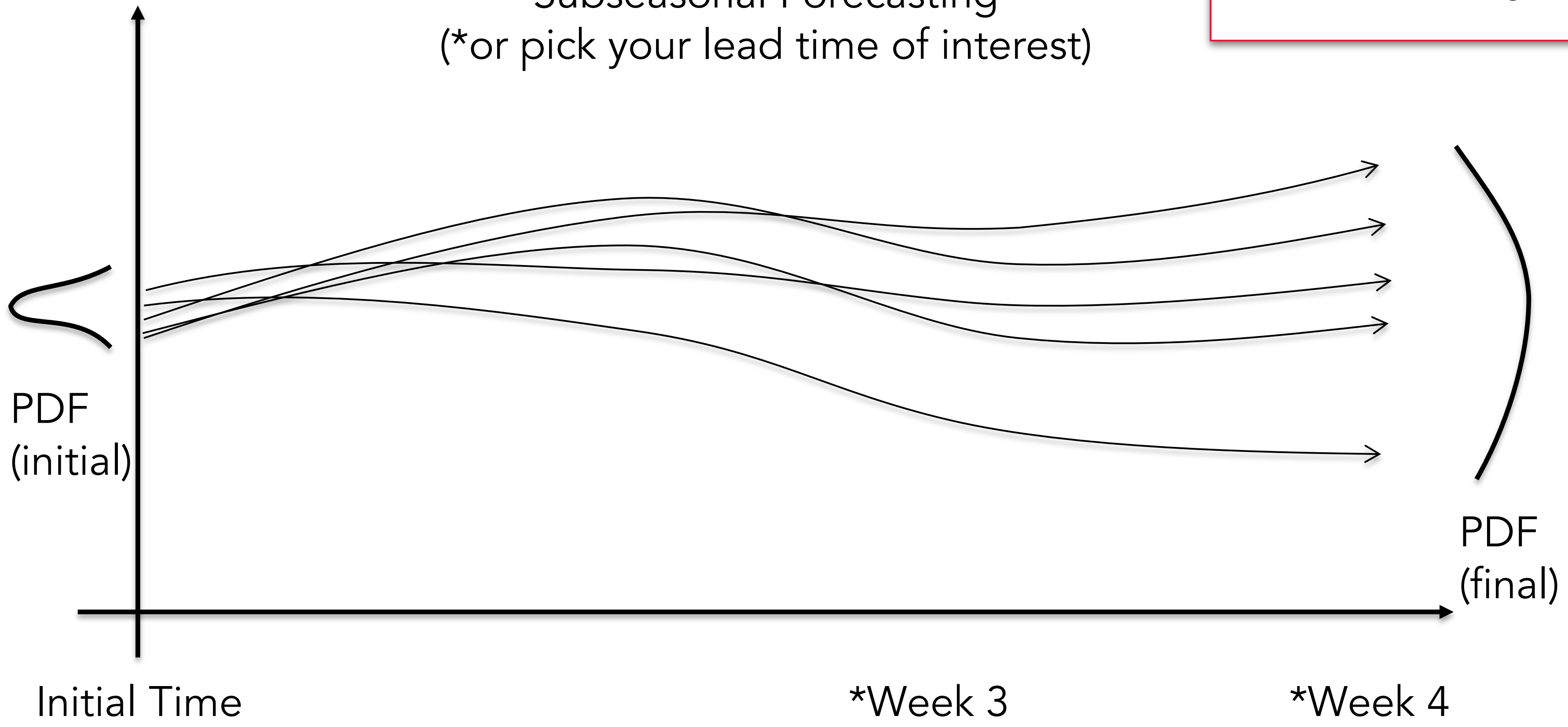
Unsupervised benchmarking



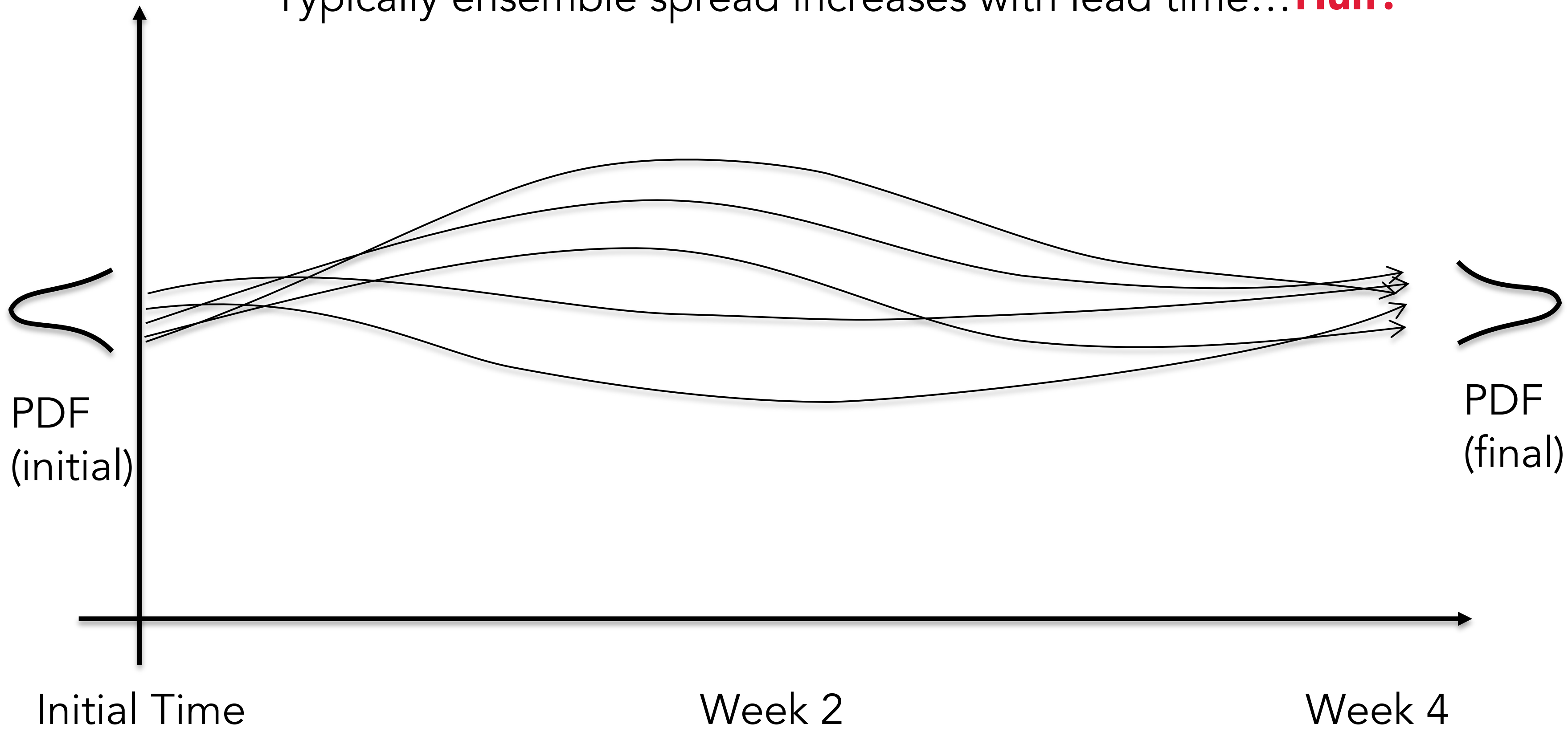
Molina, M. J., Richter, J.H., Glanville, A.A., Dagon, K., Berner, J., Hu A., Meehl, G.A., (2023). Subseasonal Representation and Predictability of North American Weather Regimes using Cluster Analysis. AMS AI for the Earth Systems.

Unsupervised benchmarking

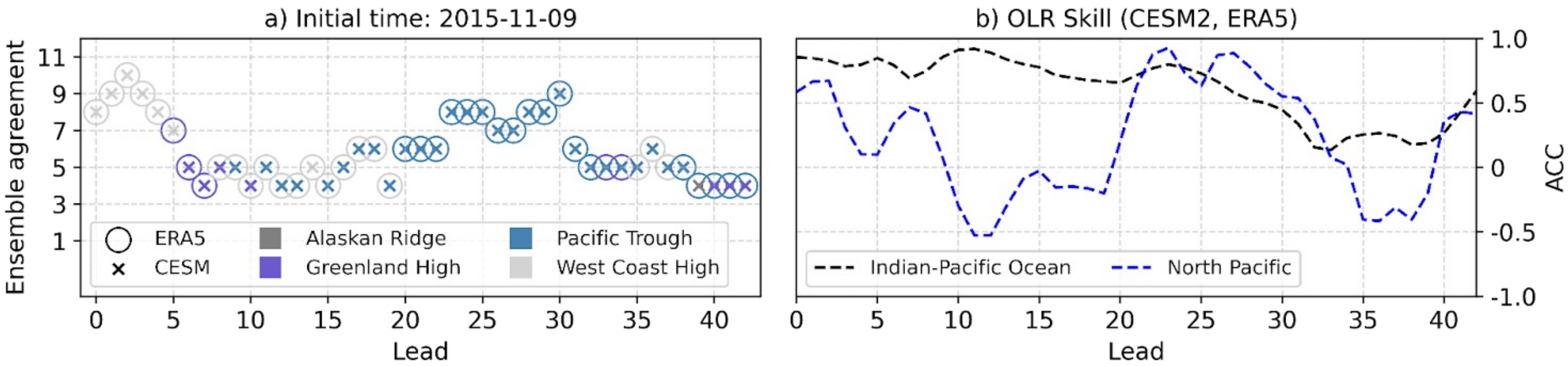
Subseasonal Forecasting
(*or pick your lead time of interest)



Typically ensemble spread increases with lead time…**Huh?**



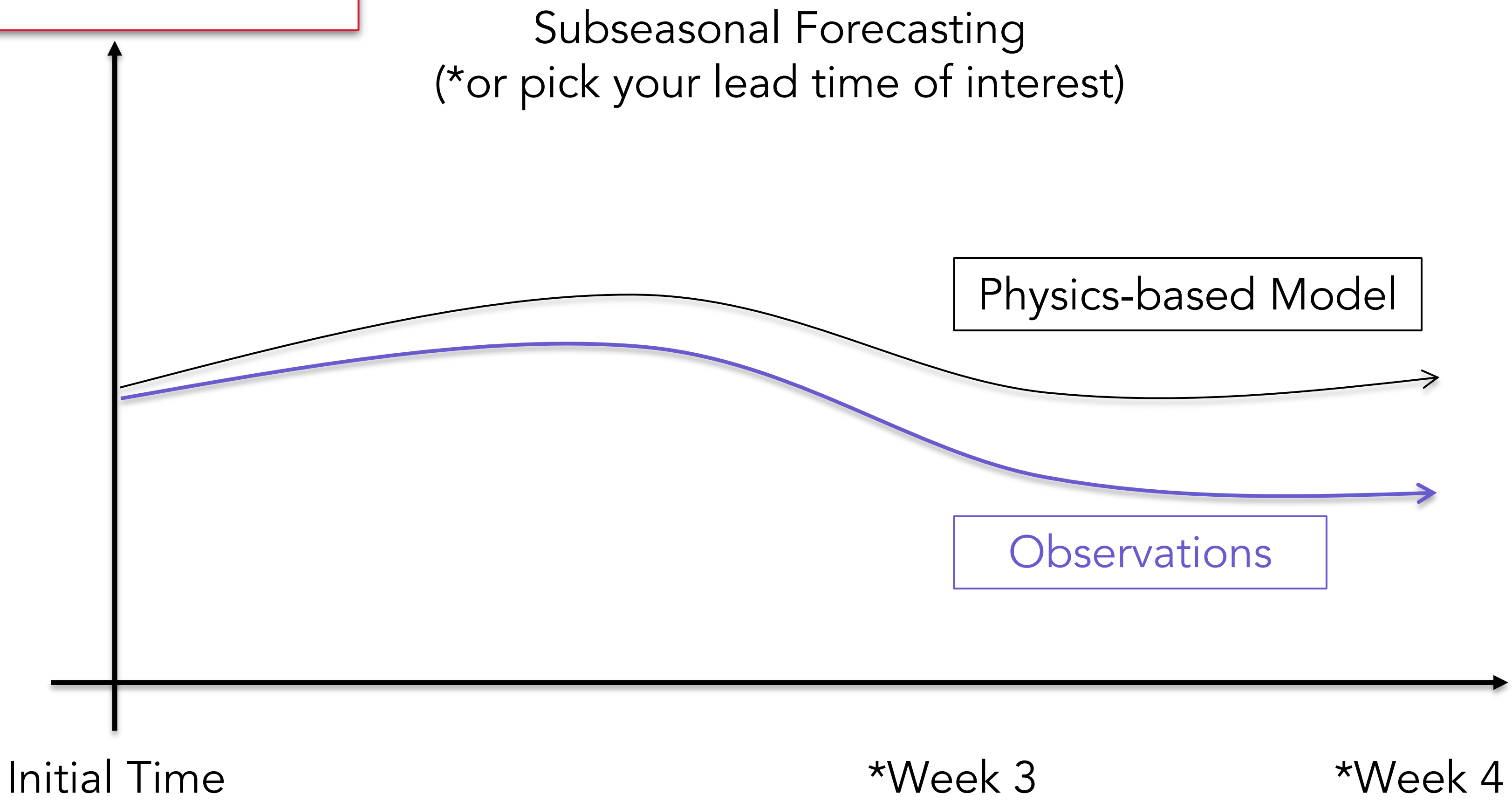
Unsupervised benchmarking



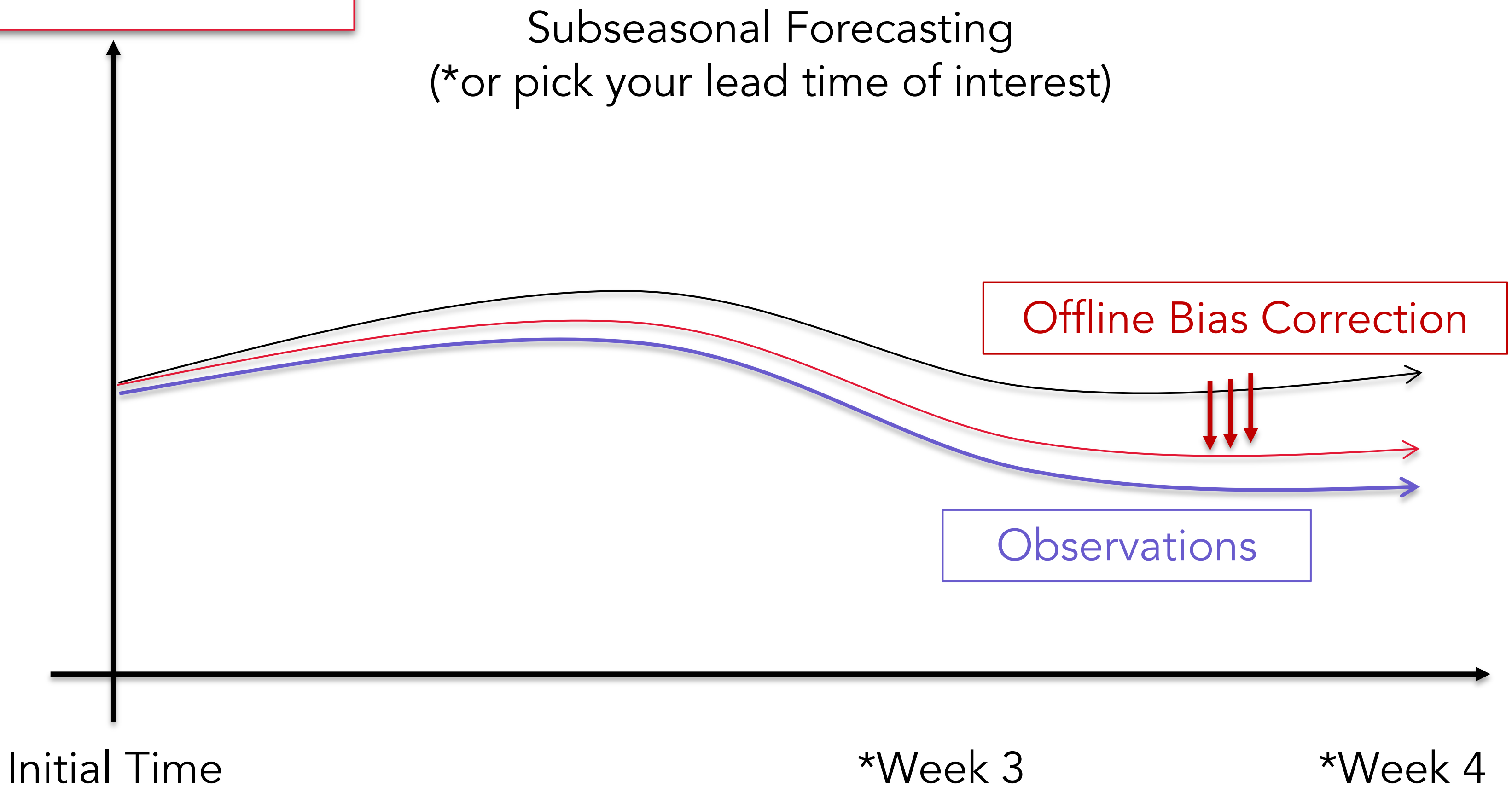
"Ensemble realignment"?

Molina, M. J., Richter, J.H., Glanville, A.A., Dagon, K., Berner, J., Hu A., Meehl, G.A., (2023). Subseasonal Representation and Predictability of North American Weather Regimes using Cluster Analysis. AMS AI for the Earth Systems.

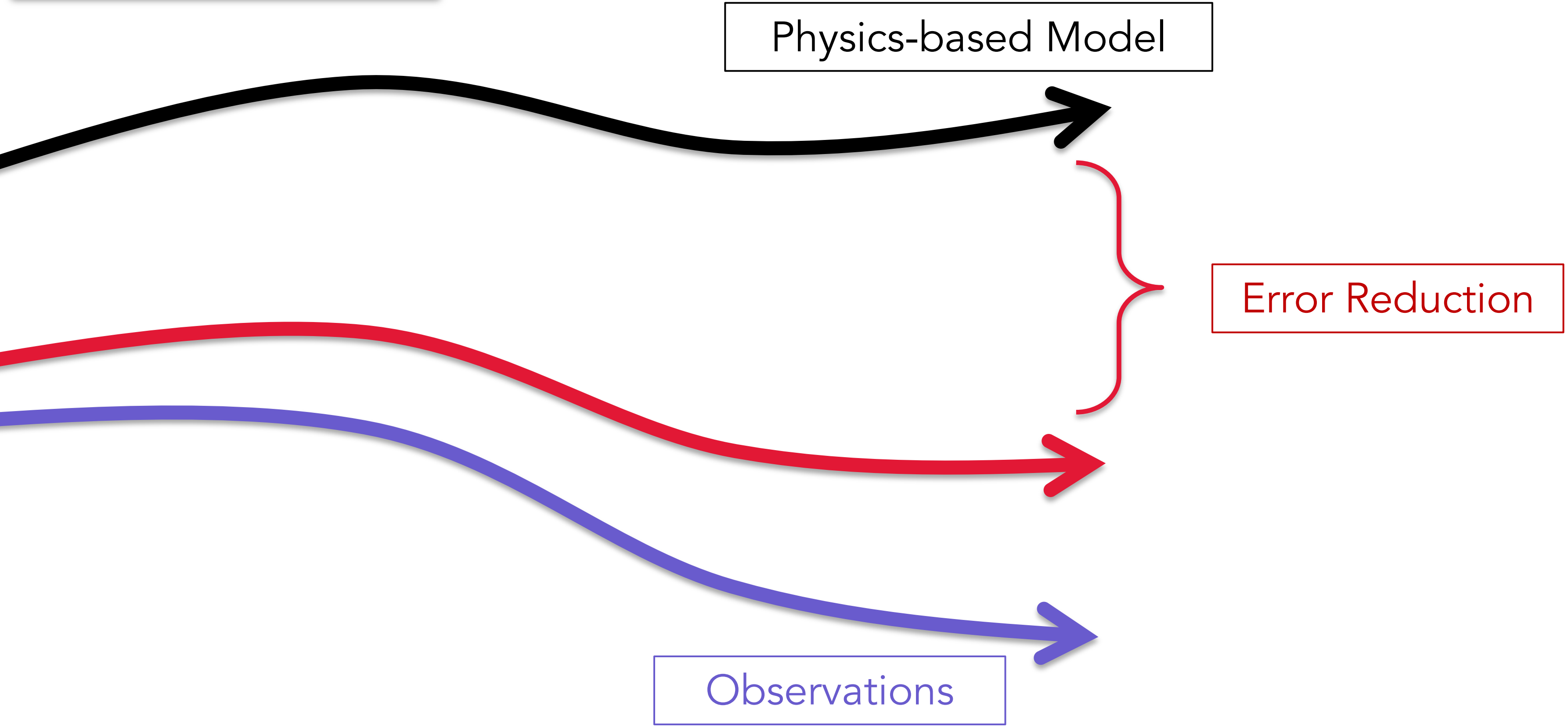
Offline bias correction



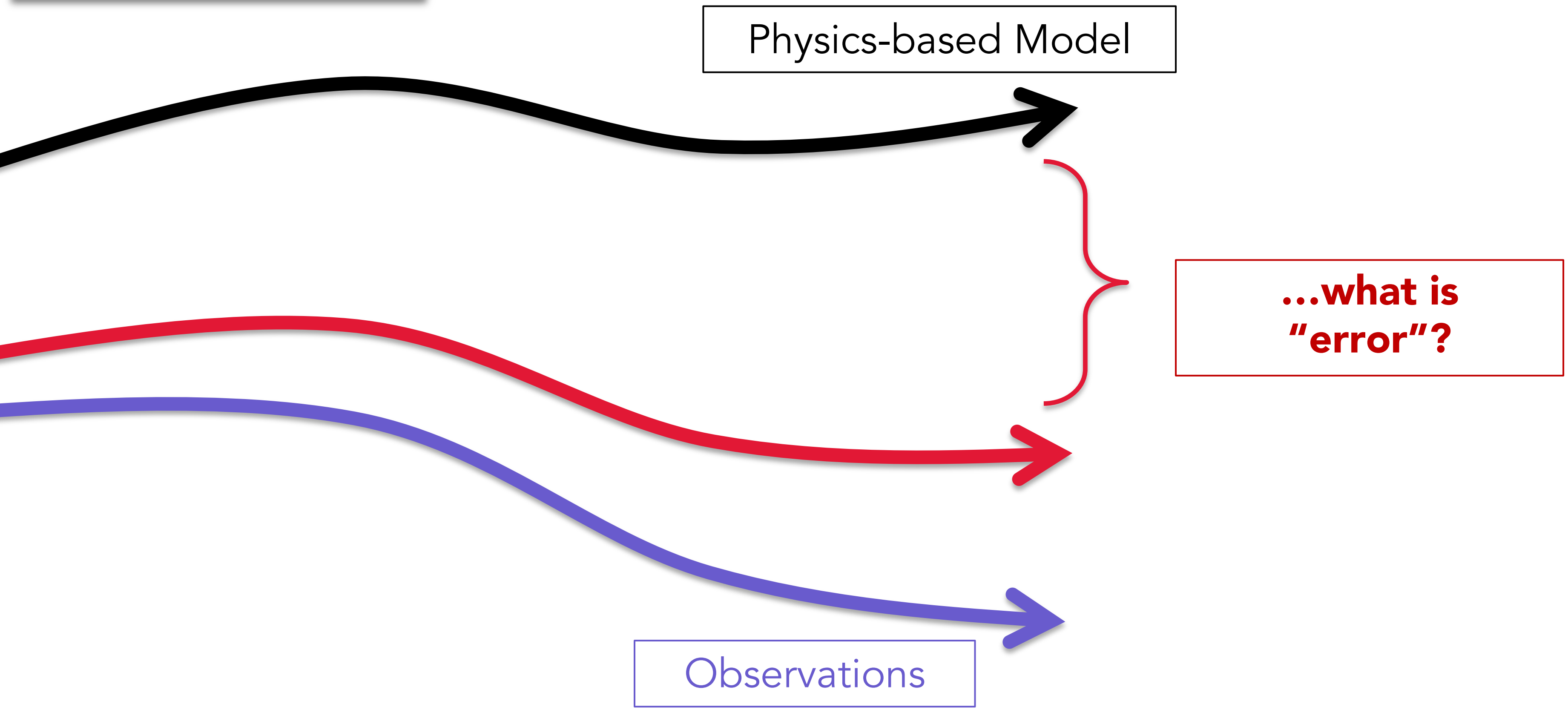
Offline bias correction



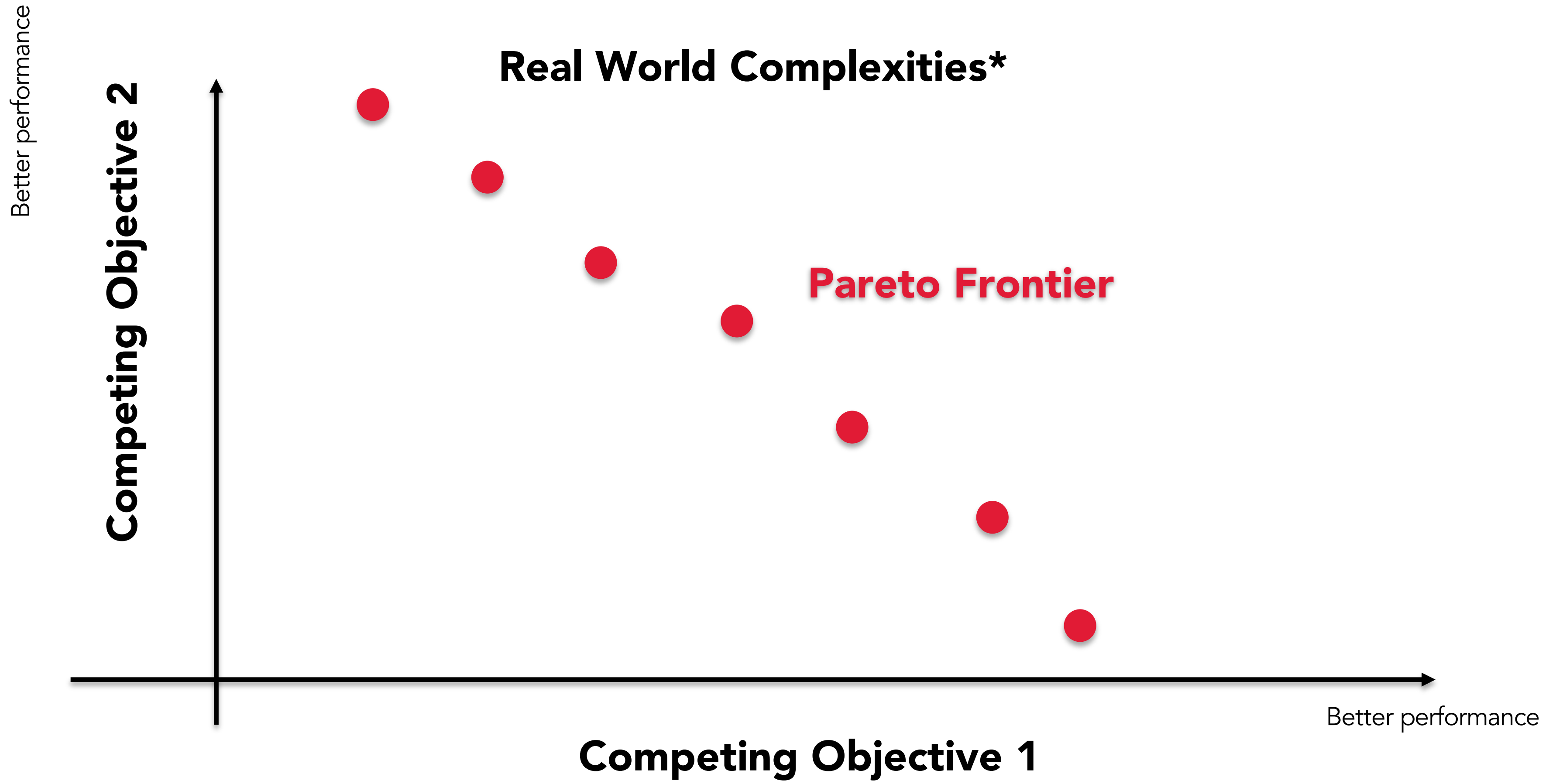
Offline bias correction



Offline bias correction



Real World Complexities*



*this is for illustration purposes (not real data)

Leverage the multiple (competing) goals of end users to generate a large ensemble for offline bias correction.

Molina, M.J., K. Dagon, J. Schreck, J. S. Perez Carrasquilla, K. J. Mayer, N. Sobhani, D. J. Gagne, I. Ebert-Uphoff, C. A. Metzler, J. Richter, and G. A. Meehl. (In Preparation). Macro- and Micro- Large Ensemble Methods along the Pareto Frontier for Bias Correction of Subseasonal Forecasts. JAMES.

The multiple objectives used for bias correction…

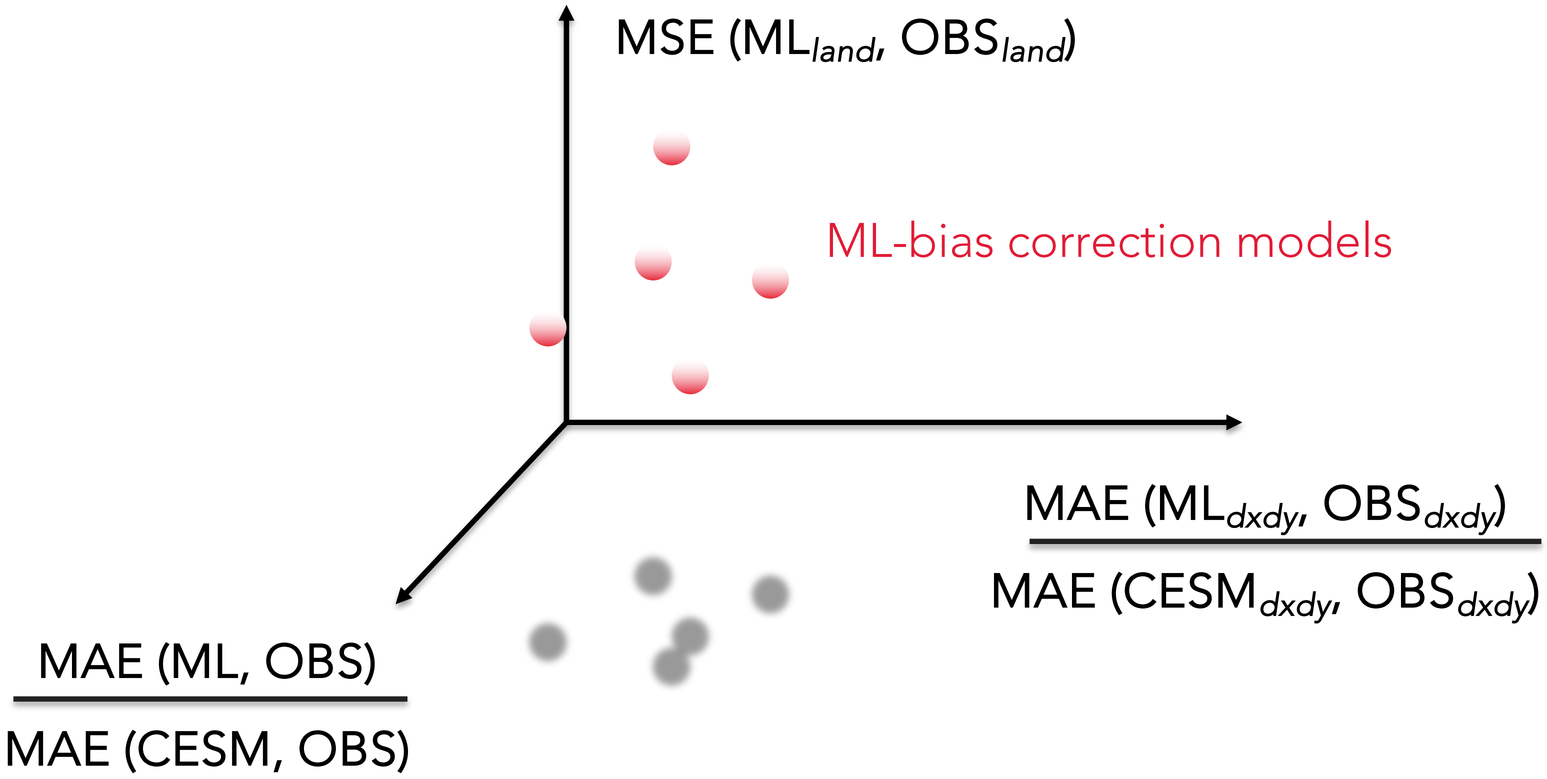
$$\mathrm{MSE}\,(\mathrm{ML}_{land},\ \mathrm{OBS}_{land})$$

$$\frac{\mathrm{MAE}\,(\mathrm{ML},\ \mathrm{OBS})^{*}}{\mathrm{MAE}\,(\mathrm{CESM},\ \mathrm{OBS})}$$

$$\frac{\mathrm{MAE}\,(\mathrm{ML}_{dxdy},\ \mathrm{OBS}_{dxdy})^{*}}{\mathrm{MAE}\,(\mathrm{CESM}_{dxdy},\ \mathrm{OBS}_{dxdy})}$$

*few caveats to note

Molina, M.J., K. Dagon, J. Schreck, J. S. Perez Carrasquilla, K. J. Mayer, N. Sobhani, D. J. Gagne, I. Ebert-Uphoff, C. A. Metzler, J. Richter, and G. A. Meehl. (In Preparation). Macro- and Micro- Large Ensemble Methods along the Pareto Frontier for Bias Correction of Subseasonal Forecasts. JAMES.



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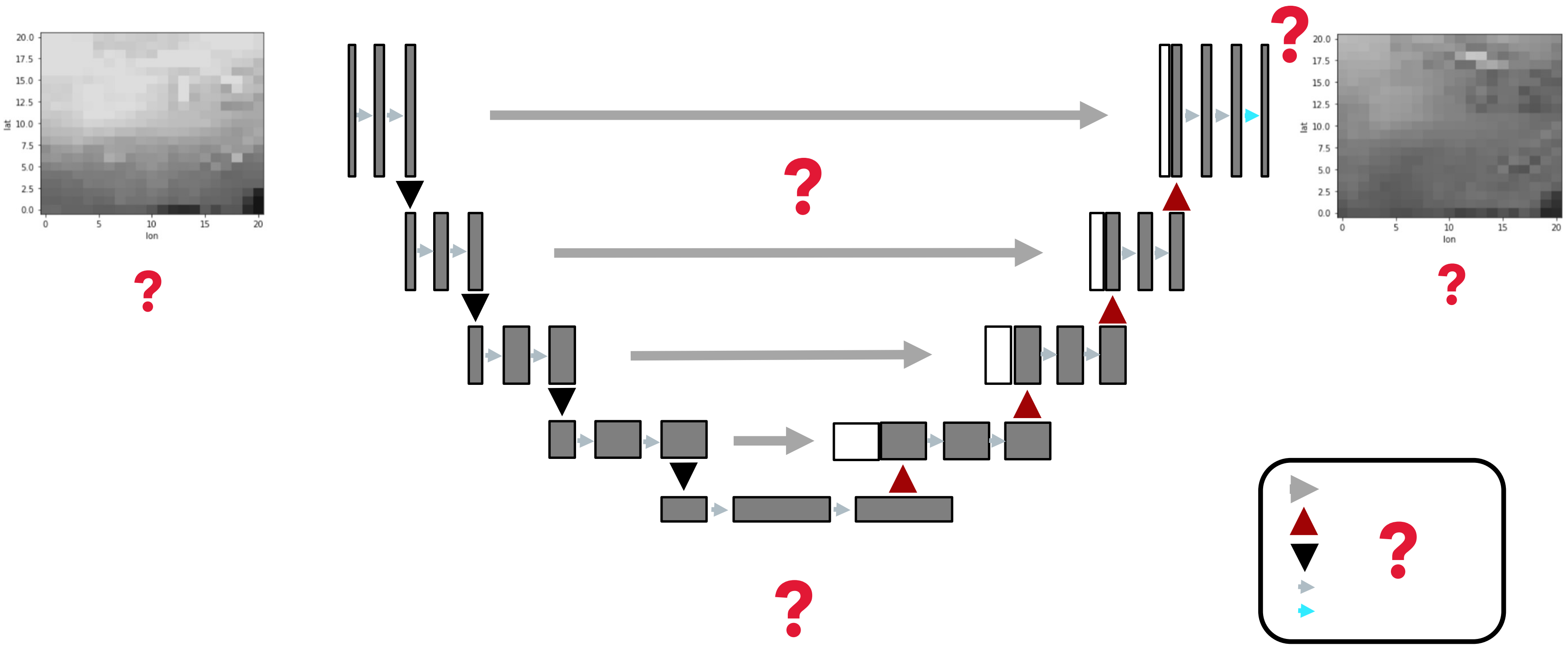
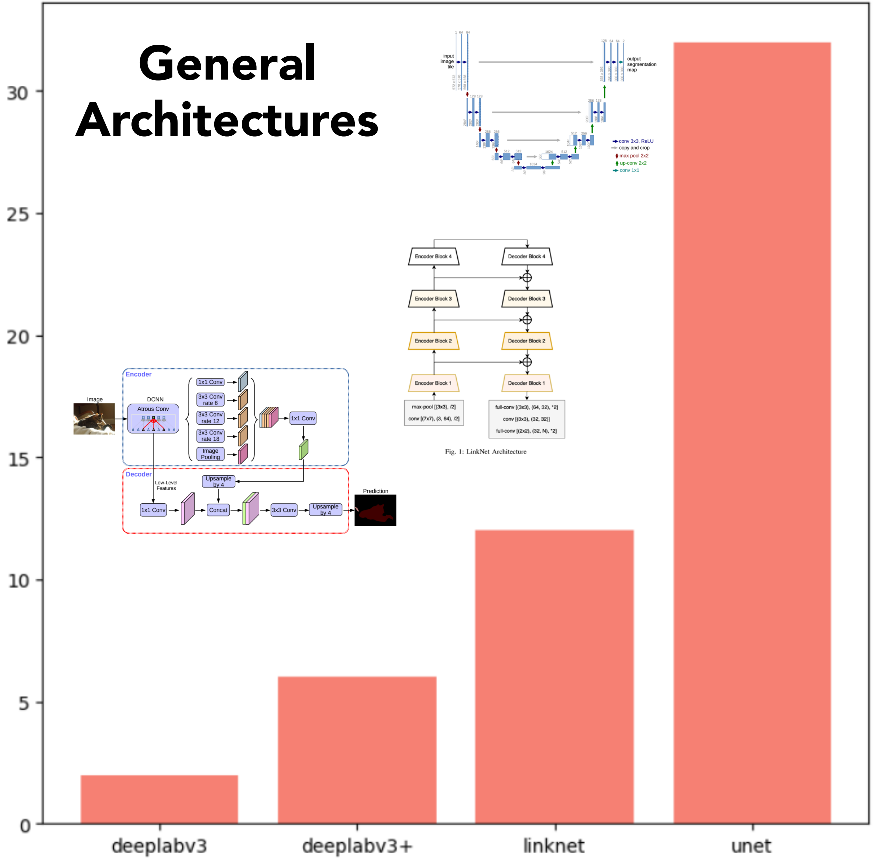
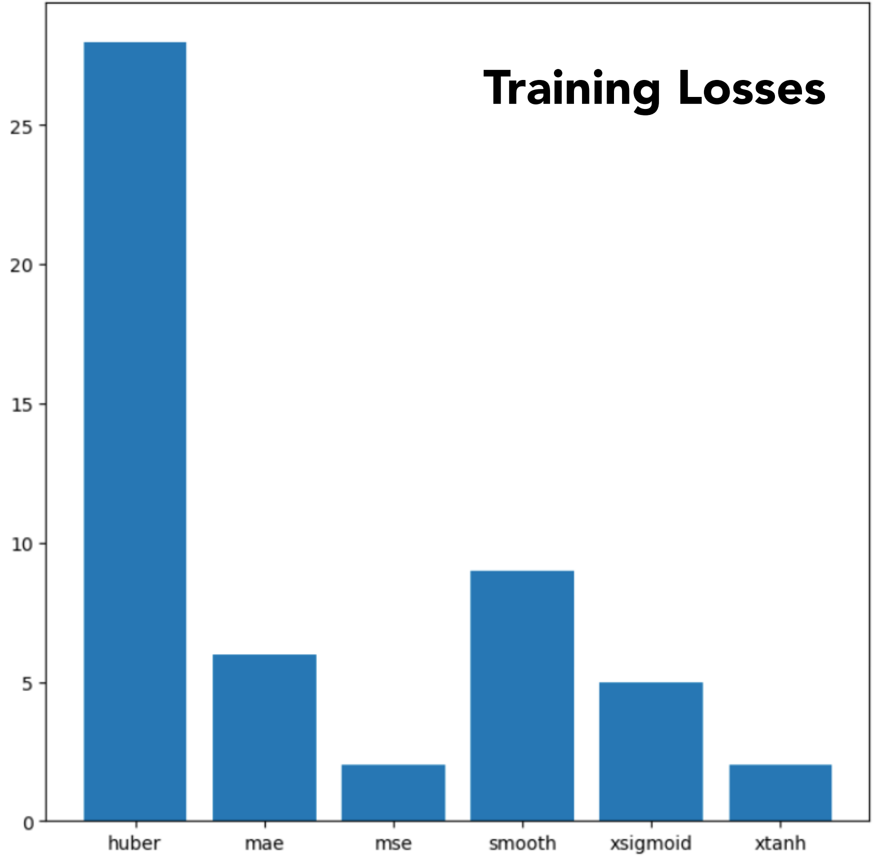
Using an Image-to-Image ML Architecture



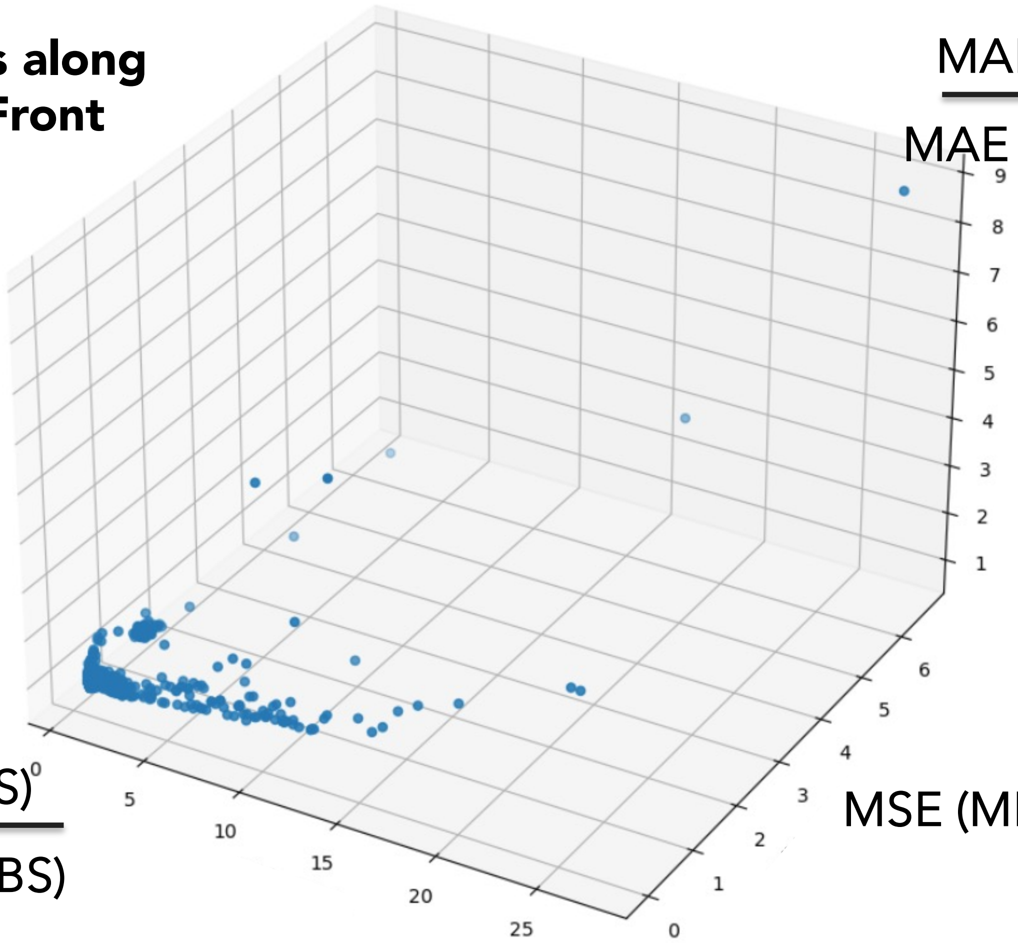
```
INFO:echo.src.reporting:Summary statistics for the current study:
INFO:echo.src.reporting:        Total number of trials in the study: 1015
INFO:echo.src.reporting:        Trials with state COMPLETE: 1015
INFO:echo.src.reporting:        Requested number of trials: 1000
INFO:echo.src.reporting:        ...
INFO:echo.src.reporting:        Total study simulation run time: 111.7938 hrs
INFO:echo.src.reporting:        Average trial simulation run time: 0.1101 hrs
INFO:echo.src.reporting:        The longest trial took 0.7443 hrs
INFO:root:Number of trials on the pareto front: 53
```

53 simulations along the Pareto Front





53 simulations along the Pareto Front



$$\frac{\text{MAE}(\text{ML}_{dxdy}, \text{OBS}_{dxdy})}{\text{MAE}(\text{CESM}_{dxdy}, \text{OBS}_{dxdy})}$$

$$\frac{\text{MAE (ML, OBS)}}{\text{MAE (CESM, OBS)}}$$

$\text{MSE}(\text{ML}_{land}, \text{OBS}_{land})$

Summary

- Machine learning methods can be used for assessing model skill or improving predictability.
- Different processes in the Earth system can enhance predictability at timescales longer than weather.
- How we define error can greatly impact machine learning tuning and predictability.

Thanks to our UMD team

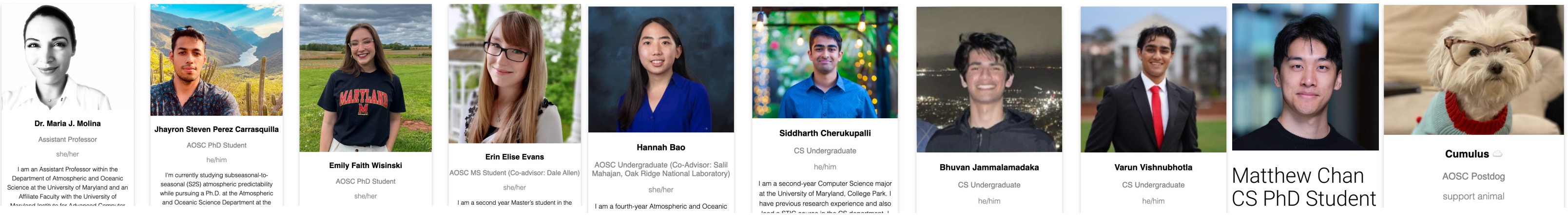
Effective & **equitable weather forecasting** in a changing climate (w/Metzler, CS).

Lightning parameterization for the NASA GEOS Model (w/Allen, AOSC); Erin Evans.

Improved **climate variability and teleconnection** characterization (w/incoming PhD student).

Uncovering of sources of predictability for **subseasonal prediction**; Jhayron Steven Perez Carrasquilla.

Identifying reasons for **El Niño forecast failures** during the springtime predictability barrier; Emily Wisinski.



Email: mjmolina@umd.edu; Website: mariajmolina.github.io

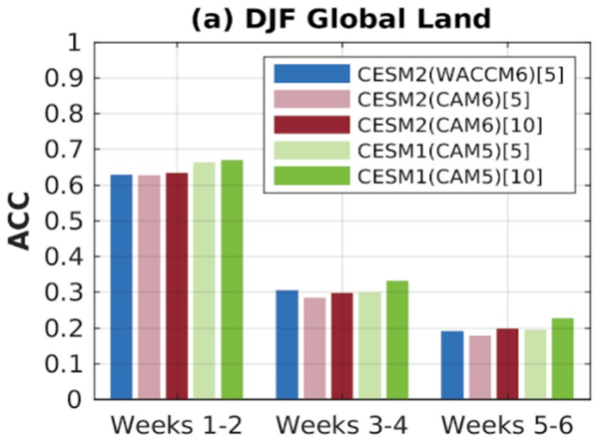
ML for TCs... Ideas?

- Once we define "seeds," can we detect/predict them using machine learning and create a climatological database (with uncertainty)?
- What are the environmental conditions and seed properties that affect transition probabilities of seeds into TCs?
- How generalizable are ML methods to background/changing climate and model/data settings (horizontal resolution)?

Using the CESM2 Initialized Subseasonal Prediction System

- Using a CESM2 20-year hindcast set.
- 15 years used for training and 5 years testing.
- Bias correction of weeks 3 and 4 temperature and precipitation.
- Using ERA5 as labels (weeks 3-4); formal evaluation with NOAA CPC gridded products.

Temperature skill



Richter, J. H., Glanville, A. A., Edwards, J., Kauffman, B., Davis, N. A., Jaye, A., ... & Oleson, K. W. (2022). Subseasonal Earth system prediction with CESM2. Weather and Forecasting, 37(6), 797-815.

Pros and Cons of an Ensemble Based on Multiple Objectives

[Pro] Leverages the pareto front among various stakeholder needs

[Pro] More expansive ML hyperparameter grid search

[Pro] More flexibility to define what error reduction

[Con] Computationally expensive (lots of GPU time needed)

[Con] Generalization is still an issue

[Con] How do we communicate multi-objective spread?

Still more work to do!

Recently refined how to compute "sharpness" in our application.

An Investigation of Metrics to Evaluate the Sharpness in AI-Generated Meteorological Imagery (Draft version - Jan 26, 2024)

Imme Ebert-Uphoff [1,2], Lander Ver Hoef [1], John S. Schreck [3], Jason Stock [4], Maria J. Molina [5,3], Amy McGovern [6], Michael Yu [6], Bill Petzke [3], Kyle Hilburn [1], David M. Hall [7], David J. Gagne [3], Sam Scheuerman [8]

[1]Cooperative Institute for Research in the Atmosphere (CIRA), Colorado State University, Fort Collins, CO, USA.
[2]Electrical and Computer Engineering, Colorado State University, Fort Collins, CO, USA.
[3]National Center for Atmospheric Research (NCAR), Boulder, CO, USA.
[4]Computer Science, Colorado State University, Fort Collins, CO, USA.
[5]Department of Atmospheric and Oceanic Science, University of Maryland, College Park, MD, USA.
[6]School of Computer Science and School of Meteorology, University of Oklahoma, Norman, OK, USA.
[7]NVIDIA, Santa Clara, CA
[8]Mathematics, Colorado State University, Fort Collins, CO, USA

Still more work to do!

Recently refined how to compute "sharpness" in our application.

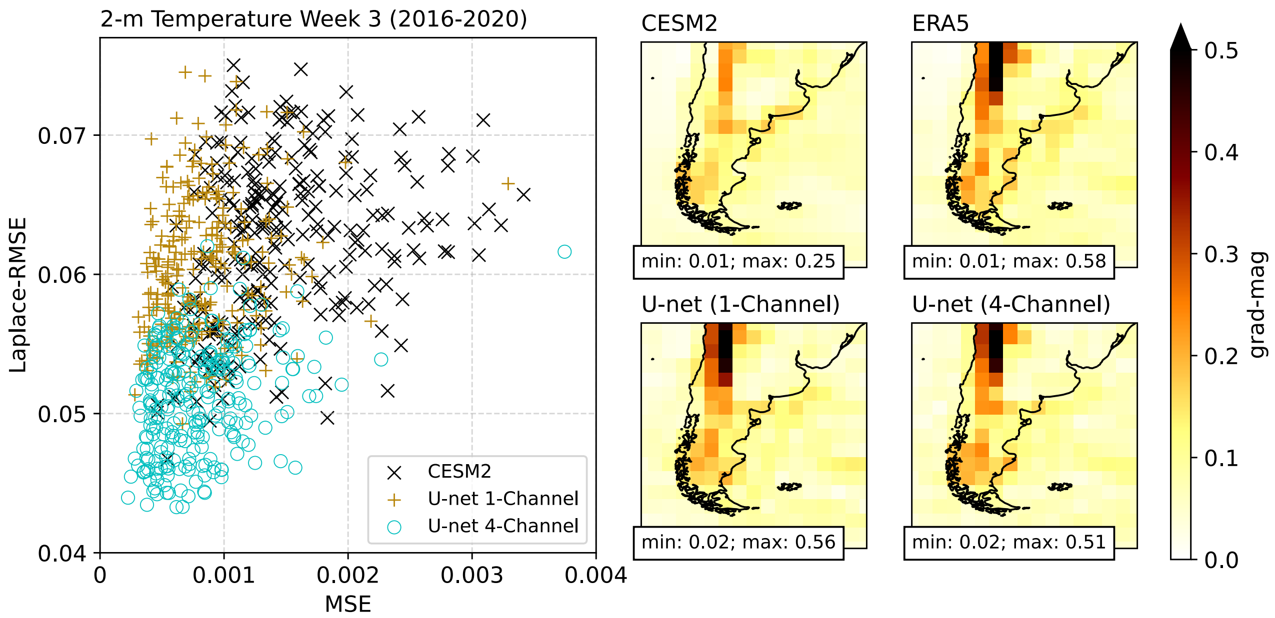
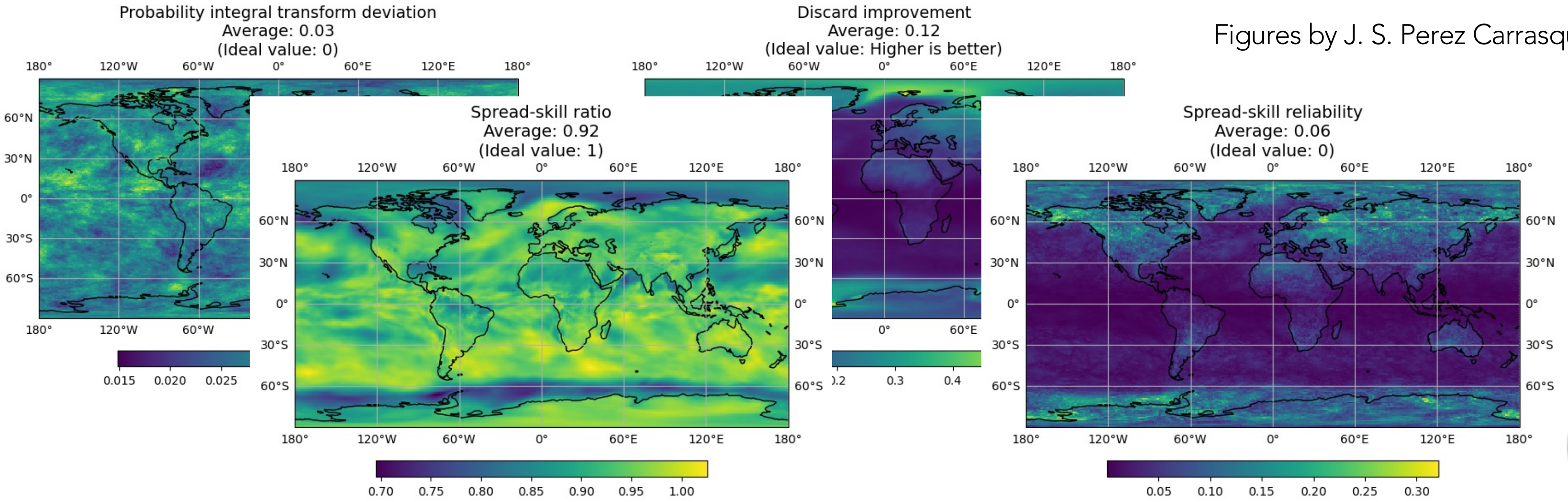


Figure from: Ebert-Uphoff, I., L. Ver Hoef, J. S. Schreck, J. Stock, M. J. Molina, A. McGovern, M. Yu, B. Petzke, K. Hilburn, D. Hall, D. J. Gagne, and S. Scheuerman. An Investigation of Metrics to Evaluate the Sharpness in AI-Generated Meteorological Imagery. (preprint)

Still more work to do!

How does our pareto front ensemble spread compare to ensemble spread based on initial state?

Figures by J. S. Perez Carrasquilla



Haynes, K., Lagerquist, R., McGraw, M., Musgrave, K. and Ebert-Uphoff, I., 2023. Creating and evaluating uncertainty estimates with neural networks for environmental-science applications. Artificial Intelligence for the Earth Systems, 2(2), p.220061.