Space Weather with Quantified Uncertainty (SWQU) using machine learning and ensembles

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CIRES / CU Boulder & NOAA Space Weather Prediction Center

<u>Collaborators</u>: G. Wilkie (PPPL), A. Drozdov, J. Bortnik (UCLA), C. Monteleoni, R. Morrison (CU Boulder), T. Berger (Swx-TREC), A. Hu (CIRES-CU), H. Singer (SWPC), G. Toth (U. Michigan)

This work is supported by NASA under grants 80NSSC20K1580 (SWQU), 80NSSC20K1275 (HTMS), 80NSSC21K155 (SWO2R)

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Broader Scientific and Societal context

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SpaceX will lose up to 40 satellites it just launched due to a solar storm

By Jackie Wattles, CNN Business

Updated 7:44 PM ET, Wed February 9, 2022

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Solar geomagnetic storms could threaten more satellites after Elon Musk's Starlink

By Chelsea Gohd published 28 days ago

"That is a drag," NOAA's Bill Murtagh said.

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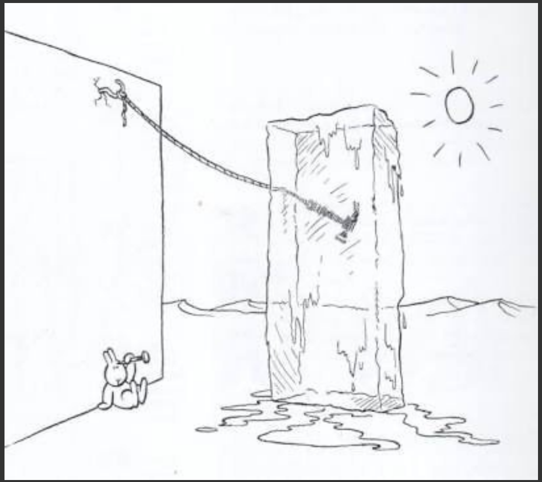
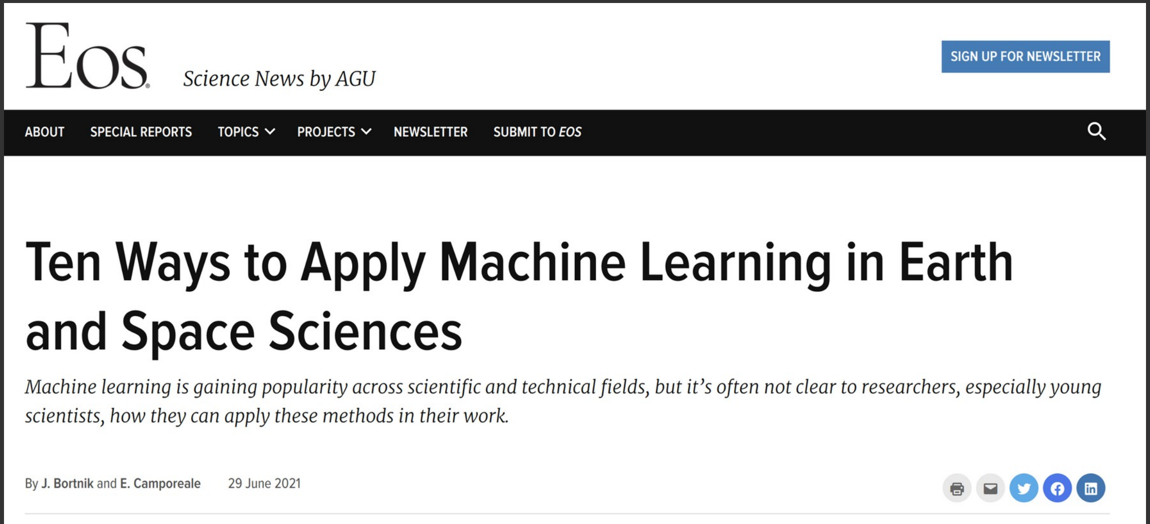


Andy Riley “The book of bunny suicides”

Scientific Question

- Can we estimate the uncertainty associated to model predictions?
  - Can we leverage machine learning tools to do so?

- Can we use machine learning for science discovery?



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Ten Ways to Apply Machine Learning in Earth and Space Sciences

Machine learning is gaining popularity across scientific and technical fields, but it's often not clear to researchers, especially young scientists, how they can apply these methods in their work.

By J. Bortnik and E. Camporeale 29 June 2021

Next Generation Software for Data-driven Models of Space Weather with Quantified Uncertainties (SWQU)

- Joint NSF/NASA pilot program, started in 2020
- The program is expected to directly contribute to the long-term goal of **creating space weather models with quantifiable predictive capability.**
- 6 projects awarded so far

Next Generation Software for Data-driven Models of Space Weather with Quantified Uncertainties (SWQU)

- Forecasting Small-Scale Plasma Structures in the Earth's Ionosphere-Thermosphere System (PI: E. Sutton; CU Boulder [+ Cornell U.])
- Composable Next Generation Software Framework for Space Weather Data Assimilation and Uncertainty Quantification (PI: R. Linares, MIT [+ UCSD, U. Michigan])
- Improving Space Weather Predictions with Data-Driven Models of the Solar Atmosphere and Inner Heliosphere (PI: N. Pogorelov, U. Alabama at Huntsville [+ GSFC, MSFC, LBNL, PSI, SSRC])
- A Flexible Community-based Upper Atmosphere Ensemble Prediction System (PI: A. Ridley, U. Michigan [+ UCAR, GSFC, NRL])
- NextGen Space Weather Modeling Framework Using Data, Physics and Uncertainty Quantification (PI: G. Toth, U. Michigan)

Next Generation Software for Data-driven Models of Space Weather with Quantified Uncertainties (SWQU)

- Ensemble Learning for Accurate and Reliable Uncertainty Quantification (PI: E. Camporeale, CU Boulder [+ UCLA])

Next Generation Software for Data-driven Models of Space Weather with Quantified Uncertainties (SWQU)

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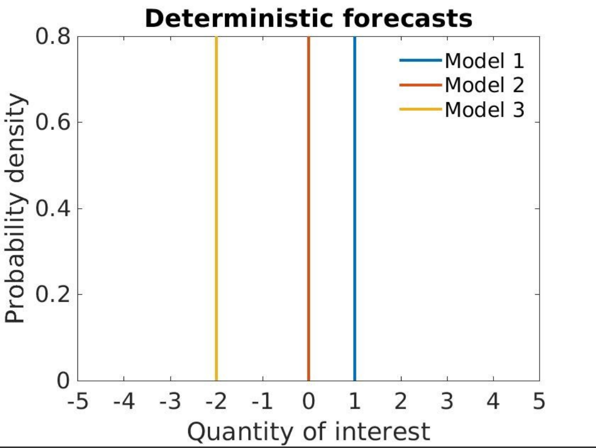

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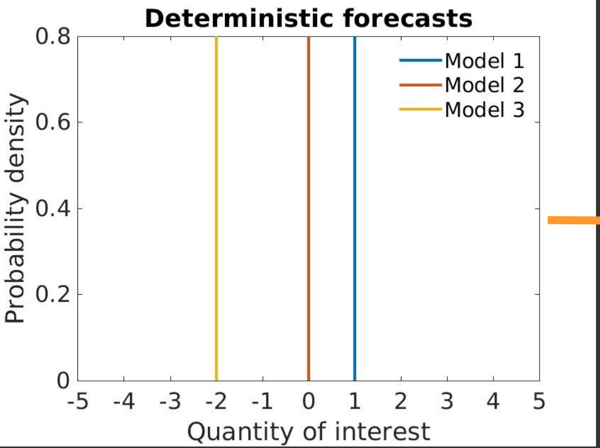

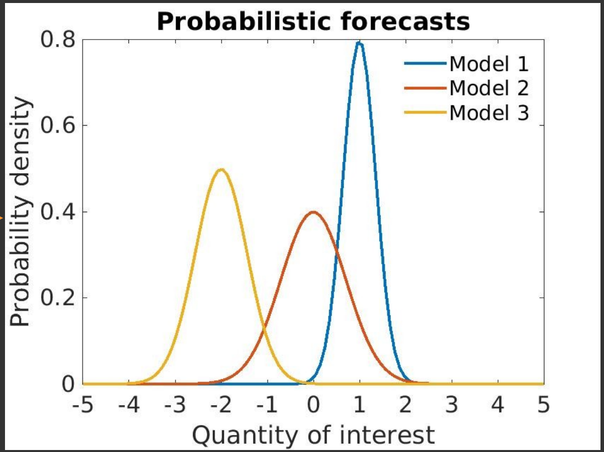

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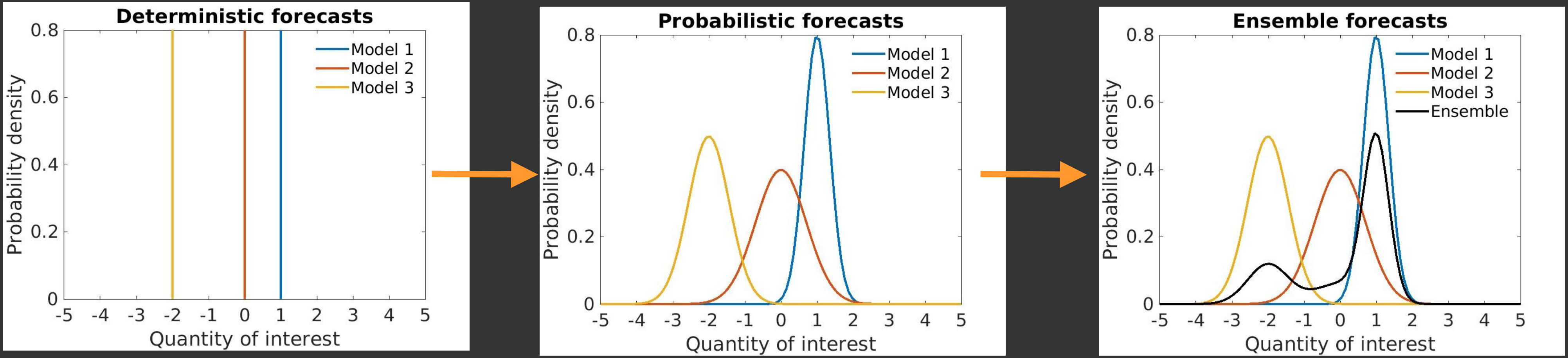


NON ACTIONABLE → ACTIONABLE

ACCRUE: Accurate and Reliable Uncertainty Estimate

Take home message

ACCRUE is a method that:

- Estimates the uncertainties associated with single-point outputs generated by a deterministic model, in terms of Gaussian distributions;
- Ensures the optimal trade-off between accuracy and reliability;
- Does not need to run ensembles. It costs as much as training and executing a neural network
- It is **model agnostic**
- Code available: zenodo.1485608

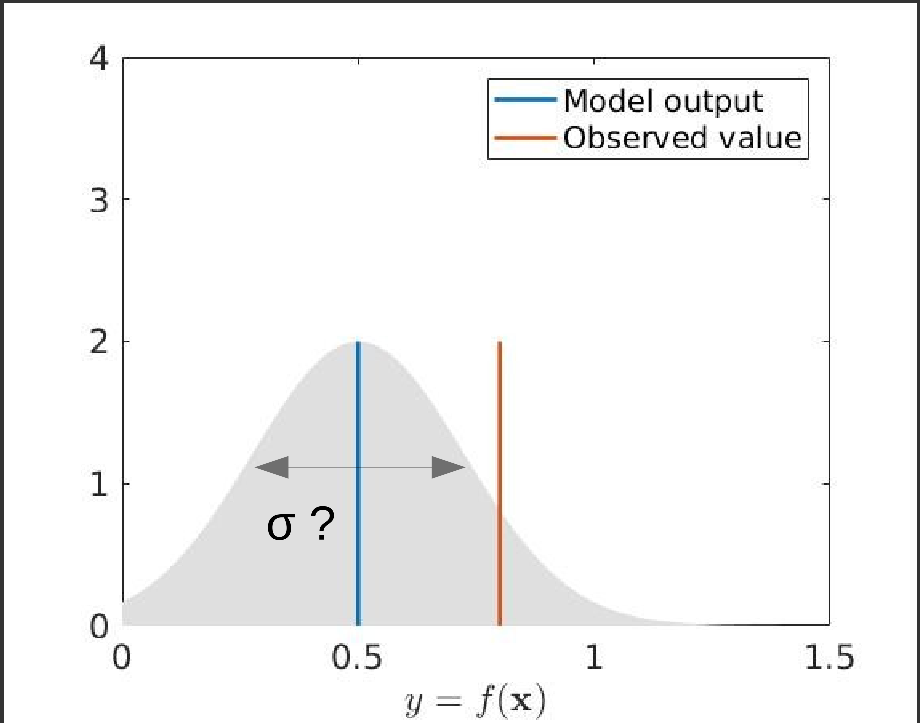
What's under the hood?

Let us assume that for a single (multidimensional) input **x**, our model predicts an output y = f(x).

Blue line → Model output
Red line → Real (observed value)

<u>Working hypothesis:</u>
We want to use the model output as the mean of a Gaussian distribution that is interpreted as a probabilistic forecast.

What is the optimal width of a Gaussian forecast?

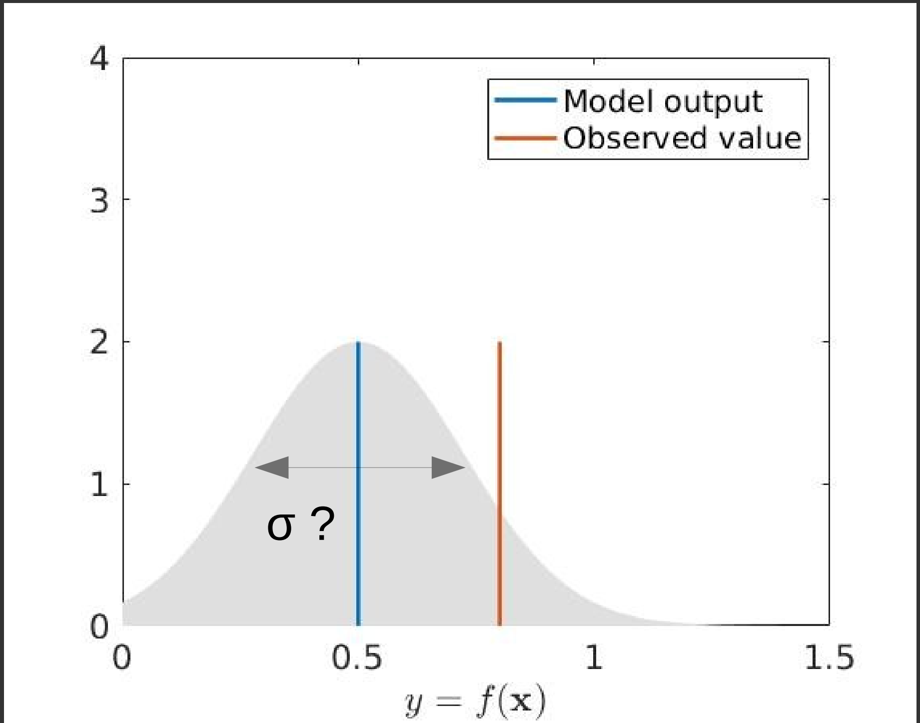


What's under the hood?

What is the optimal width of a Gaussian forecast?

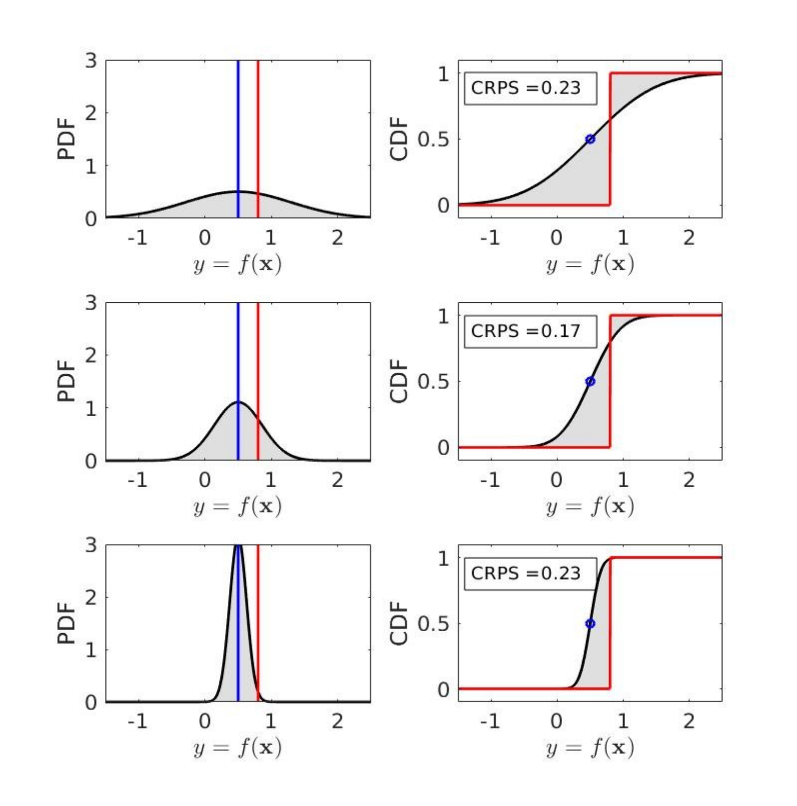
It's the one that gives you the

best accuracy (sharpness)
AND
best reliability (calibration)



Accuracy (Sharpness)

- Different metrics for measuring accuracy of a probabilistic forecast:
  - Negative Log Likelihood (Ignorance Score)
    - Measures the value of the probability density function (pdf) at the observation
  - Continuous Rank Probability Score (CRPS)
    - Measures the 'distance' between the cumulative distribution function (CDF) of the prediction and the CDF of observation
- Bottom line: The optimal width of the Gaussian distribution that represents your uncertainty is the one that **'fits the data the best'**



Blue line → Prediction
Red line → Observation

Reliability (a.k.a. Calibration)
What is a probabilistic forecast anyway?

Risk Analysis, Vol. 25, No. 3, 2005 DOI: 10.1111/j.1539-6924.2005.00608.x

"A 30% Chance of Rain Tomorrow": How Does the Public Understand Probabilistic Weather Forecasts?

Gerd Gigerenzer,[1]* Ralph Hertwig,[2] Eva van den Broek,[1] Barbara Fasolo,[1] and Konstantinos V. Katsikopoulos[1]

TABLE 2. Responses to Q14a, the meaning of the forecast "There is a 60% chance of rain for tomorrow" (N = 1330).

	Percent of respondents
It will rain tomorrow in 60% of the region.	16
It will rain tomorrow for 60% of the time.	10
It will rain on 60% of the days like tomorrow.*	19
60% of weather forecasters believe that it will rain tomorrow.	22
I don't know.	9
Other (please explain).	24

* Technically correct interpretation, according to how PoP forecasts are verified, as interpreted by Gigerenzer et al. (2005).

Communicating Uncertainty in Weather Forecasts: A Survey of the U.S. Public

REBECCA E. MORSS, JULIE L. DEMUTH, AND JEFFREY K. LAZO

National Center for Atmospheric Research, Boulder, Colorado*

Reliability (a.k.a. Calibration)
What is a probabilistic forecast anyway?

If a model is ‘perfectly calibrated’,
“X% chance of rain” means:

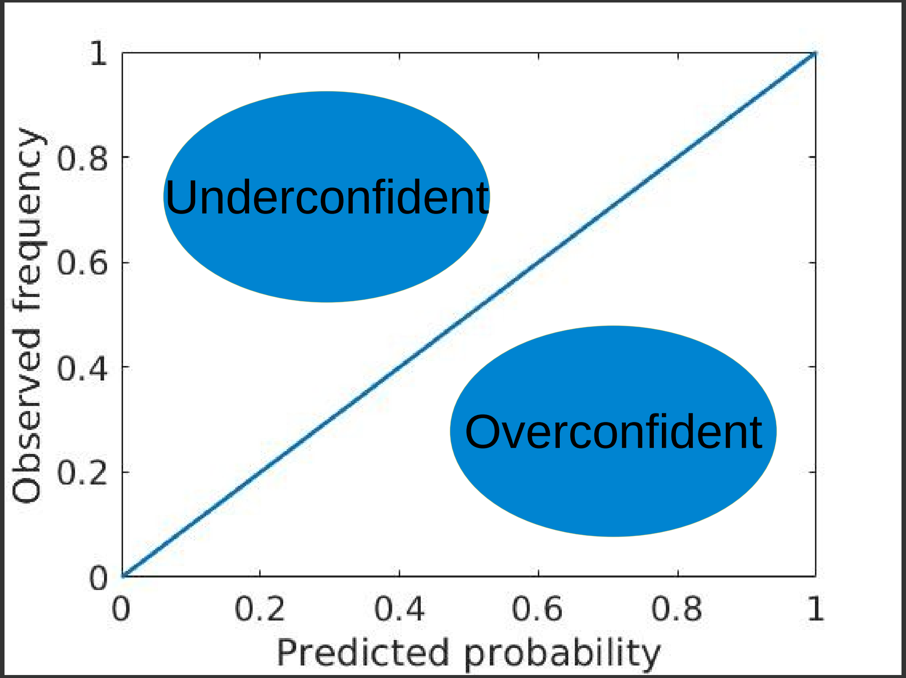
Reliability (a.k.a. Calibration)
What is a probabilistic forecast anyway?

If a model is ‘perfectly calibrated’,
“X% chance of rain” means:

It rained X% of the times the model predicted

“X% chance of rain”

(for any value of X)



Two objective optimization problem

- It turns out that reliability and accuracy are competing objectives, that is they cannot be optimized simultaneously!!
- We define the Accuracy-Reliability (AR) cost function:

$$AR = CRPS + \beta * RS$$

Accuracy

Reliability

$$\mathrm{CRPS}(\varepsilon, \sigma) = \sigma\left[\frac{\varepsilon}{\sigma}\operatorname{erf}\left(\frac{\varepsilon}{\sqrt{2}\sigma}\right) + \sqrt{\frac{2}{\pi}}\exp\left(-\frac{\varepsilon^2}{2\sigma^2}\right) - \frac{1}{\sqrt{\pi}}\right].$$

$$\mathrm{RS} = \sum_{i=1}^{N}\left[\frac{\eta_i}{N}(\operatorname{erf}(\eta_i)+1) - \frac{\eta_i}{N^2}(2i-1) + \frac{\exp(-\eta_i^2)}{\sqrt{\pi}N}\right]$$

- We solve this optimization problem with a deep neural network

ACCRUE: Accurate and Reliable Uncertainty Estimate

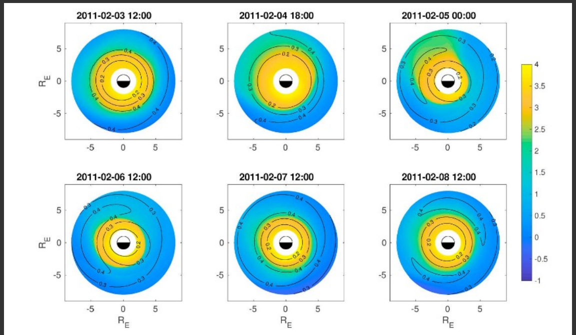
International Journal for Uncertainty Quantification, 11(4):81–94 (2021)

ACCRUE: ACCURATE AND RELIABLE UNCERTAINTY ESTIMATE IN DETERMINISTIC MODELS

Enrico Camporeale[1,] & Algo Carè[2]*

[1]*University of Colorado, Boulder, Colorado, USA*
[2]*University of Brescia, Brescia, Italy*

Method			CRPS	RECAL	KM	ACCRUE
Score				CRPS		
Dataset	Size	Dim.				
Boston Housing	506	13	0.25 ± 0.05	0.25 ± 0.04	0.25 ± 0.03	**0.23 ± 0.04**
Concrete	1030	8	0.22 ± 0.03	0.23 ± 0.13	0.26 ± 0.02	**0.21 ± 0.03**
Energy	768	8	0.059 ± 0.03	0.056 ± 0.03	0.087 ± 0.01	**0.052 ± 0.01**
Kin8nm	8192	8	0.17 ± 0.005	0.16 ± 0.01	0.24 ± 0.005	**0.16 ± 0.005**
Power plant	9568	4	0.13 ± 0.003	0.13 ± 0.05	0.15 ± 0.002	**0.12 ± 0.01**
Protein	45,730	9	0.38 ± 0.02	0.47 ± 0.13	0.40 ± 0.007	**0.37 ± 0.02**
Wine	1599	11	0.48 ± 0.03	0.50 ± 0.29	**0.46 ± 0.02**	0.48 ± 0.06
Yacht	308	6	0.06 ± 0.08	0.06 ± 0.02	0.19 ± 0.02	**0.06 ± 0.02**
Score				Cal. err. (%)		
Dataset	Size	Dim.				
Boston Housing	506	13	26.2 ± 7.9	20.6 ± 5.5	17.5 ± 3.7	**16.7 ± 5.9**
Concrete	1030	8	22.6 ± 5.8	14.4 ± 3.8	22.1 ± 3.0	**11.5 ± 3.9**
Energy	768	8	29.3 ± 8.9	29.2 ± 8.0	28.3 ± 2.8	**13.0 ± 6.5**
Kin8nm	8192	8	15.9 ± 1.28	8.3 ± 1.30	25.5 ± 0.5	**5.8 ± 1.28**
Power plant	9568	4	12.5 ± 1.4	3.4 ± 0.9	16.1 ± 0.8	**2.6 ± 0.8**
Protein	45,730	9	13.1 ± 0.8	**5.0 ± 0.9**	10.6 ± 0.9	5.4 ± 0.88
Wine	1599	11	16.0 ± 3.7	**7.9 ± 2.0**	8.0 ± 2.4	8.3 ± 2.4
Yacht	308	6	26.0 ± 9.4	24.3 ± 13.5	36.6 ± 3.0	**19.5 ± 8.5**



Space Weather

RESEARCH ARTICLE
10.1029/2018SW002026

On the Generation of Probabilistic Forecasts From Deterministic Models

E. Camporeale[1,2], X. Chu[3], O. V. Agapitov[4], and J. Bortnik[5]

[1]Center for Mathematics and Computer Science (CWI), Amsterdam, The Netherlands, [2]Cooperative Institute for Research in Environmental Sciences, University of Colorado, Boulder, CO, USA, [3]Laboratory for Atmospheric and Space Physics, University of Colorado, Boulder, CO, USA, [4]Space Sciences Laboratory, University of California Berkeley, Berkeley, CA, USA, [5]Department of Atmospheric and Oceanic Sciences, University of California, Los Angeles, CA, USA

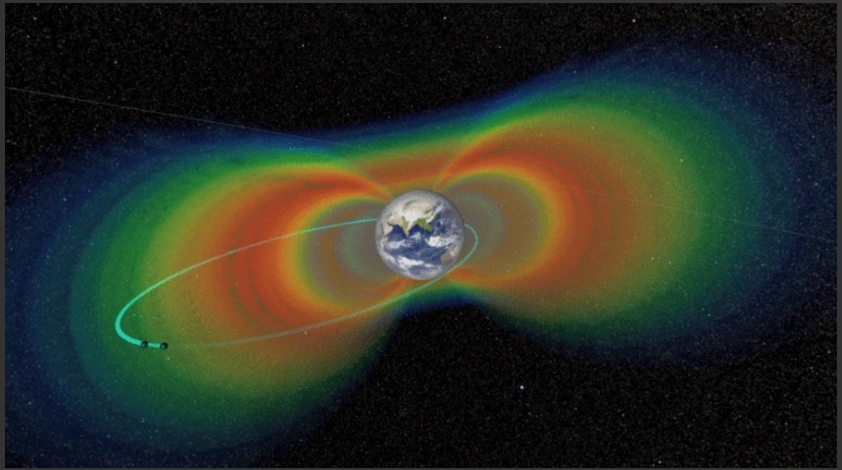
Key Points:
- We introduce a new method to estimate the uncertainties associated with single-point outputs generated by a deterministic model
- The method ensures a trade-off between accuracy and reliability of the generated probabilistic forecasts
- Computationally cheap model:

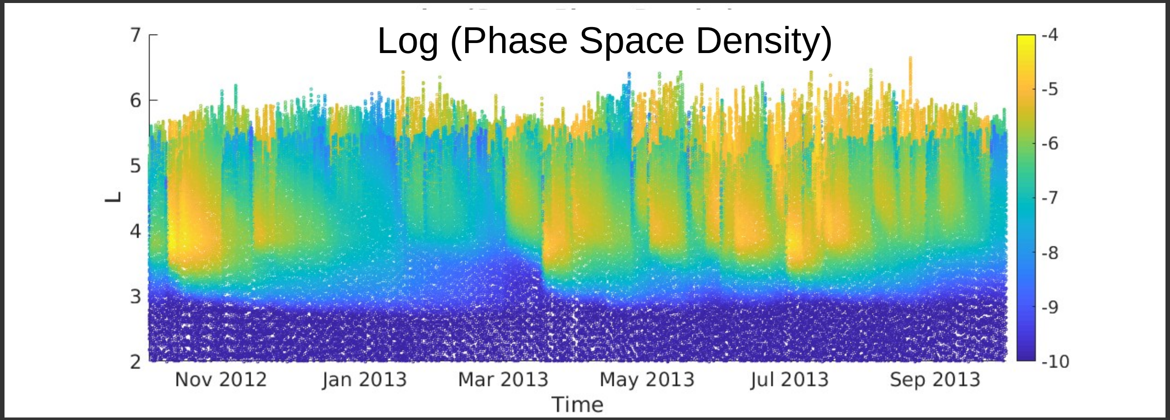
Scientific Question

- Can we use machine learning for science discovery?
  - Inverse problems

Radial diffusion in Earth’s radiation belt (Quasi-linear theory)

$$\frac{\partial f}{\partial t} = L^{*2} \frac{\partial}{\partial L^*}\bigg|_{\mu,J} \left(D_{L*L*} L^{*-2} \frac{\partial f}{\partial L^*}\bigg|_{\mu,J} \right)$$





Inverse problem statement

$$\frac{\partial f(L,t)}{\partial t} = L^2 \frac{\partial}{\partial L}\left(\frac{D_{LL}}{L^2}\frac{\partial f(L,t)}{\partial L}\right) - \frac{f(L,t)}{\tau}$$

- What is the optimal choice of parameters (D_{LL} and τ) that makes the result of the diffusion equation most consistent with data?
- This is an INVERSE PROBLEM (we know the result, and want to infer the inputs), which is much harder than the “forward” model.
- It is completely ill-posed!! (You can find a valid τ for any given choice of D_{LL})
- Instead of pure-diffusion (QL assumption) we use a more general FP equation:

$$\frac{\partial f(L,t)}{\partial t} = L^2 \frac{\partial}{\partial L}\left(\frac{D_{LL}}{L^2}\frac{\partial f(L,t)}{\partial L}\right) - \frac{\partial C f(L,t)}{\partial L},$$

The Physics-Informed Neural Network (PINN) approach to parameter estimation

[HTML] **Physics-informed neural networks**: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations

M Raissi, P Perdikaris, GE Karniadakis - Journal of Computational **physics**, 2019 - Elsevier

… We introduce **physics-informed neural networks** – **neural networks** that are trained to solve supervised learning tasks while respecting any given laws of **physics** described by general …

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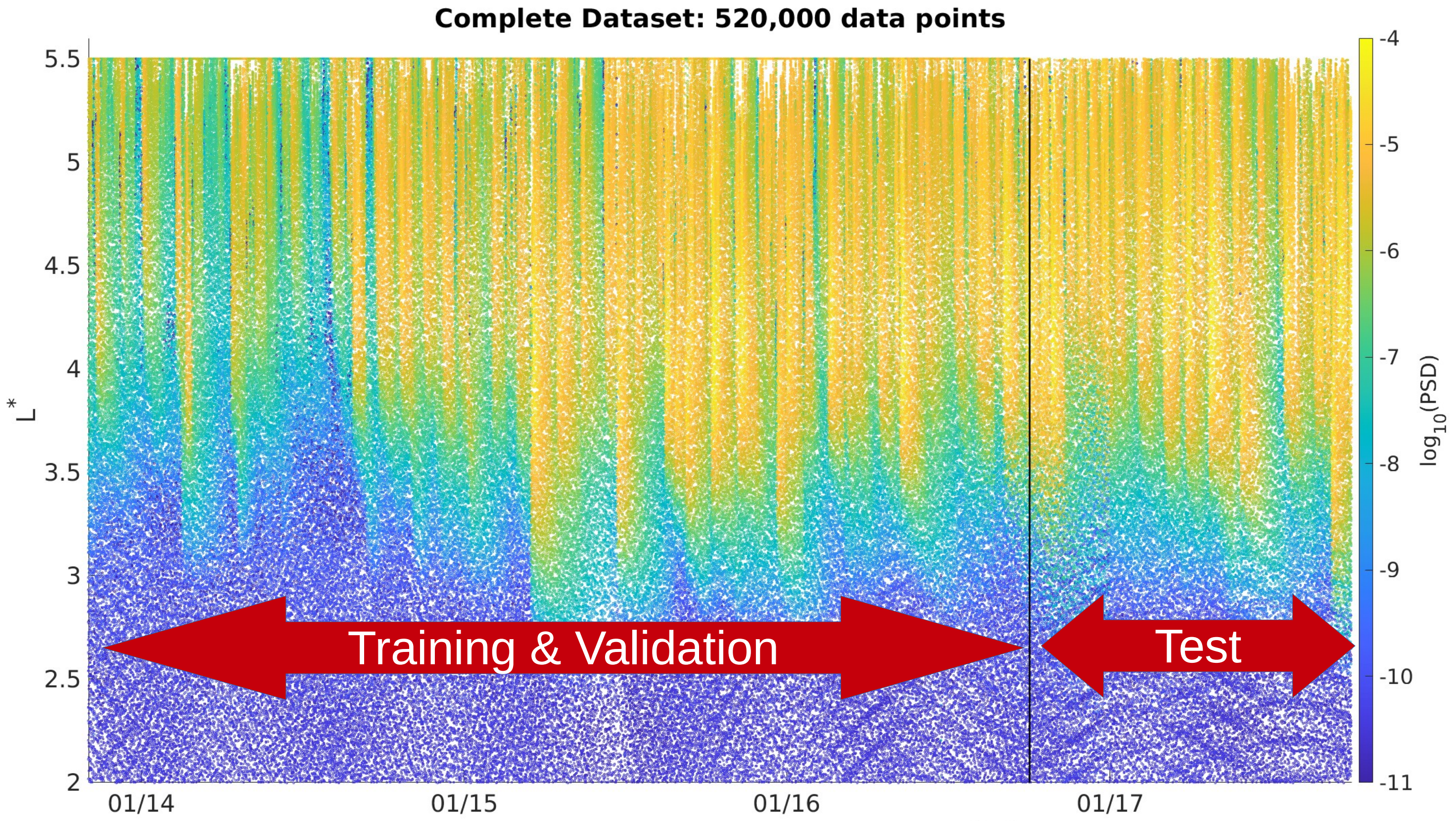
PINN (Physics-Informed Neural Network) in a nuthsell

- PINN idea: to include the Partial Differential Equation (PDE) we want to solve in the cost function!

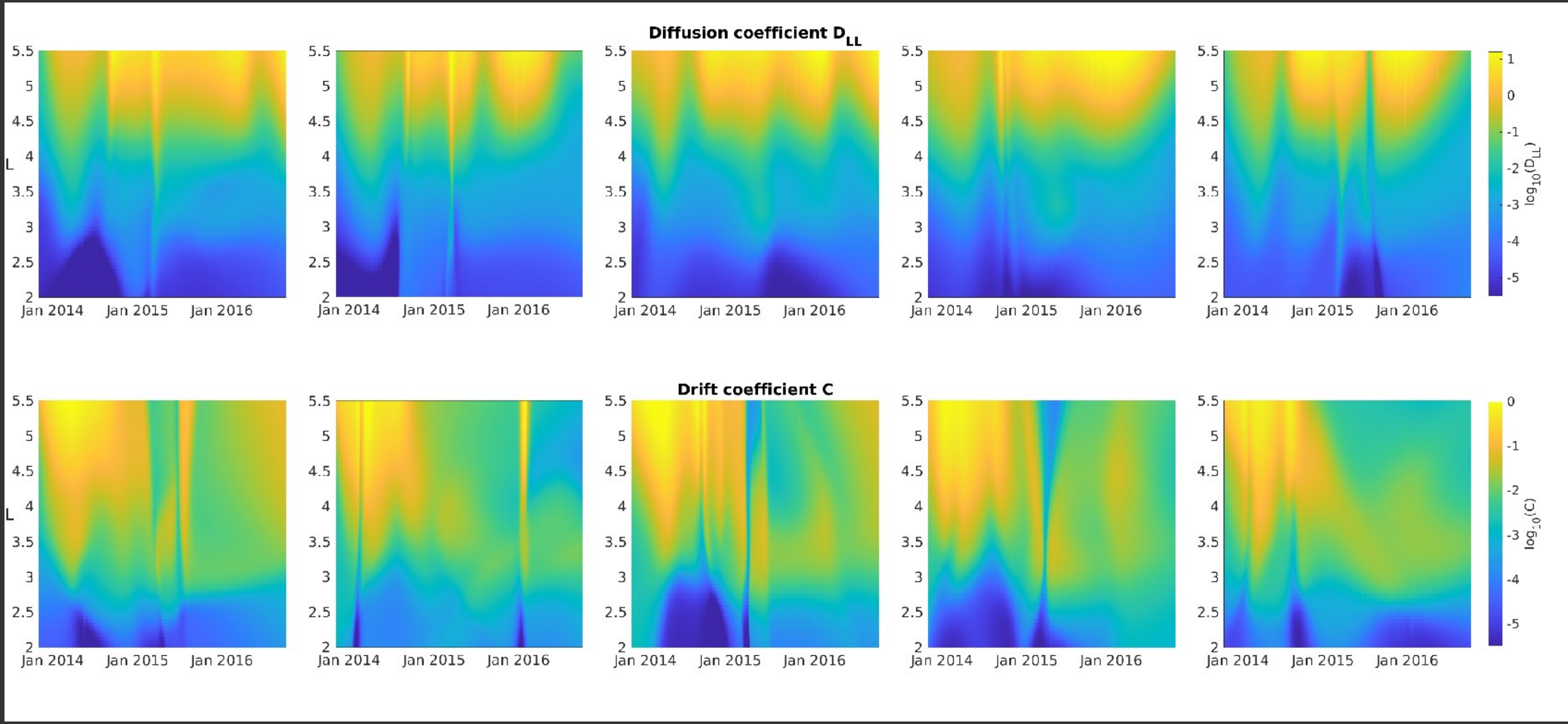
$$\mathcal{C}[f, D_{LL}, \tau] = \left[\frac{\partial f}{\partial t} - L^2 \frac{\partial}{\partial L}\left(\frac{D_{LL}}{L^2}\frac{\partial f}{\partial L}\right) + \frac{f}{\tau}\right]^2 + \left(f - f_{obs}\right)^2$$

- A Neural Net outputs an analytical and differentiable solution.
- The trick under the hood: autodiff (automatic differentiation). All derivatives are computed exactly (using chain rule) !
- This is both:
  - a grid-less method to solve a PDE on a set of points (forward)
  - a way of estimating the coefficients of a PDE (inverse problem)

Van Allen Probes data

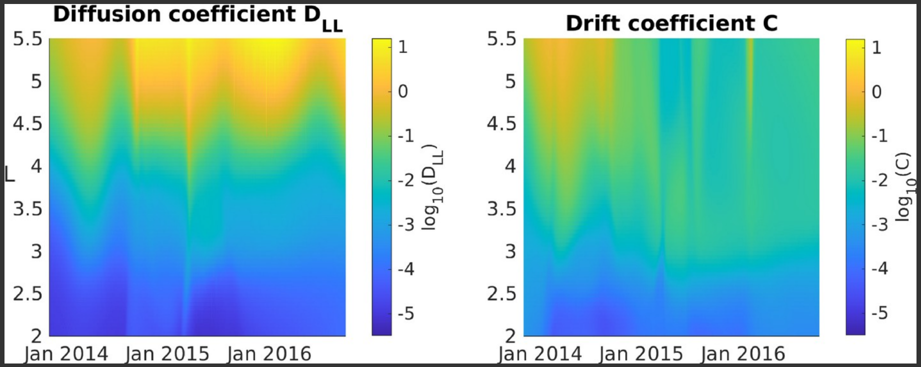


$\mu = 700$ MeV/G $\quad K = 0.1\, R_E\, G^{0.5}$



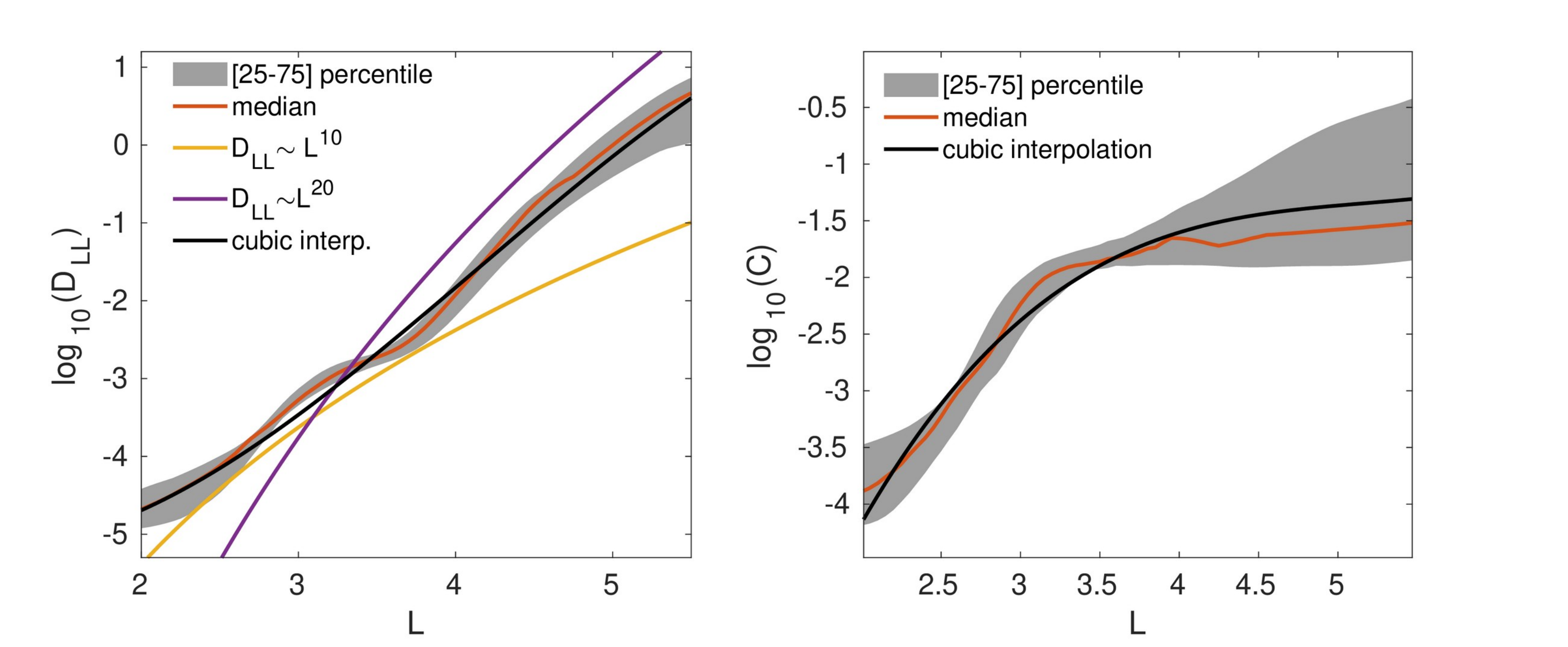
“Best” 5 solutions in an ensemble of 20

This is something you do not get with any other method:
<u>A spatio-temporal characterization of your drift and diffusion coefficients</u>



Average of the best 5 solutions

Statistical analysis of coefficients
(and closing the circle: a simple parameterization)

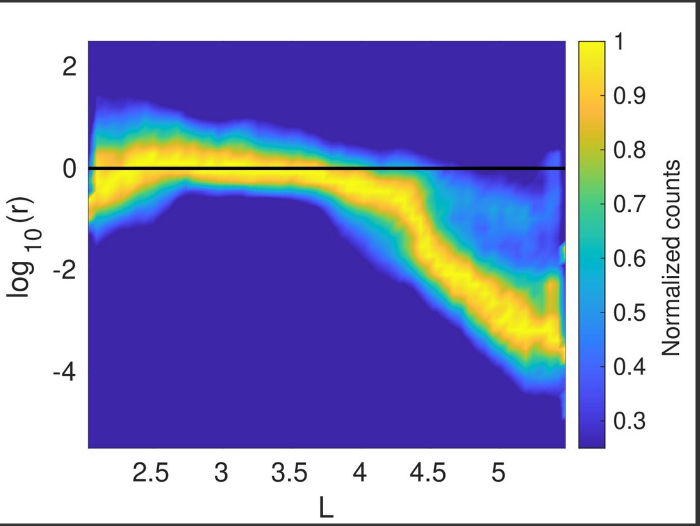


$$\log_{10} D_{LL} = -0.0593L^3 + 0.7368L^2 - 1.33L - 4.505$$

$$\log_{10} C = 0.0777L^3 - 1.2022L^2 + 6.3177L - 12.6115$$

This parameterization outperforms (on a test set) everything that has been done in the literature in the past 20 years!

Discovering new physics:
Relative importance between drift and diffusion



$$r = \left| \frac{1}{L^2} \left(\frac{\partial C f}{\partial L} \right) \Big/ \left[\frac{\partial}{\partial L} \left(\frac{D_{LL}}{L^2} \frac{\partial f}{\partial L} \right) \right] \right|$$

r = Drift term over diffusion term

Drift and diffusion
are comparable for L<4

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Data-driven discovery of Fokker-Planck equation for the Earth's radiation belts electrons using Physics-Informed Neural Networks

Authors

Enrico Camporeale, George J Wilkie, Alexander Yurievich Drozdov, Jacob Bortnik

Published Online: Fri, 25 Feb 2022 | https://doi.org/10.1002/essoar.10510599.1

ML-Helio 2022

https://ml-helio.github.io/

Contact: Enrico.camporeale@noaa.gov

Currently: 180 participants (120 virtual + 60 in person)
NSF funding still available for early-careers!

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The PRAISE initiative:
Promoting Research in AI for the Space Economy

- Space Economy:
  - Space Weather
  - Space Traffic Management
- Realization that AI will become integrated in the decision making process
- AI challenges:
  - Adversarial attacks
  - Out-of-distribution generalization
  - Uncertainty-aware ML
- Bottom-up and inclusive approach to form a strong team and organize ideas around this topic
- Considering proposing a NSF AI Institute for the Space Economy

Reach out if interested: enrico.camporeale@noaa.gov

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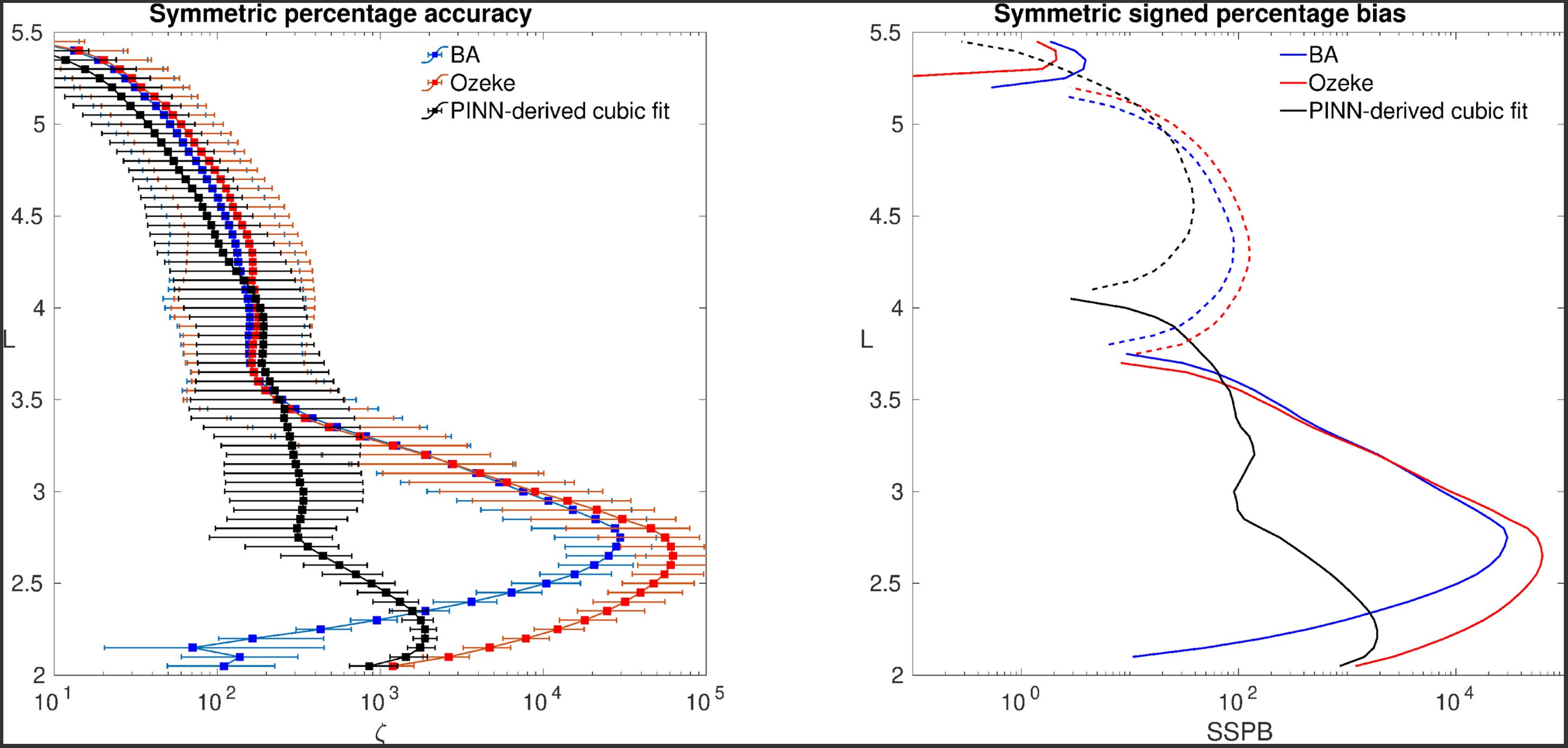
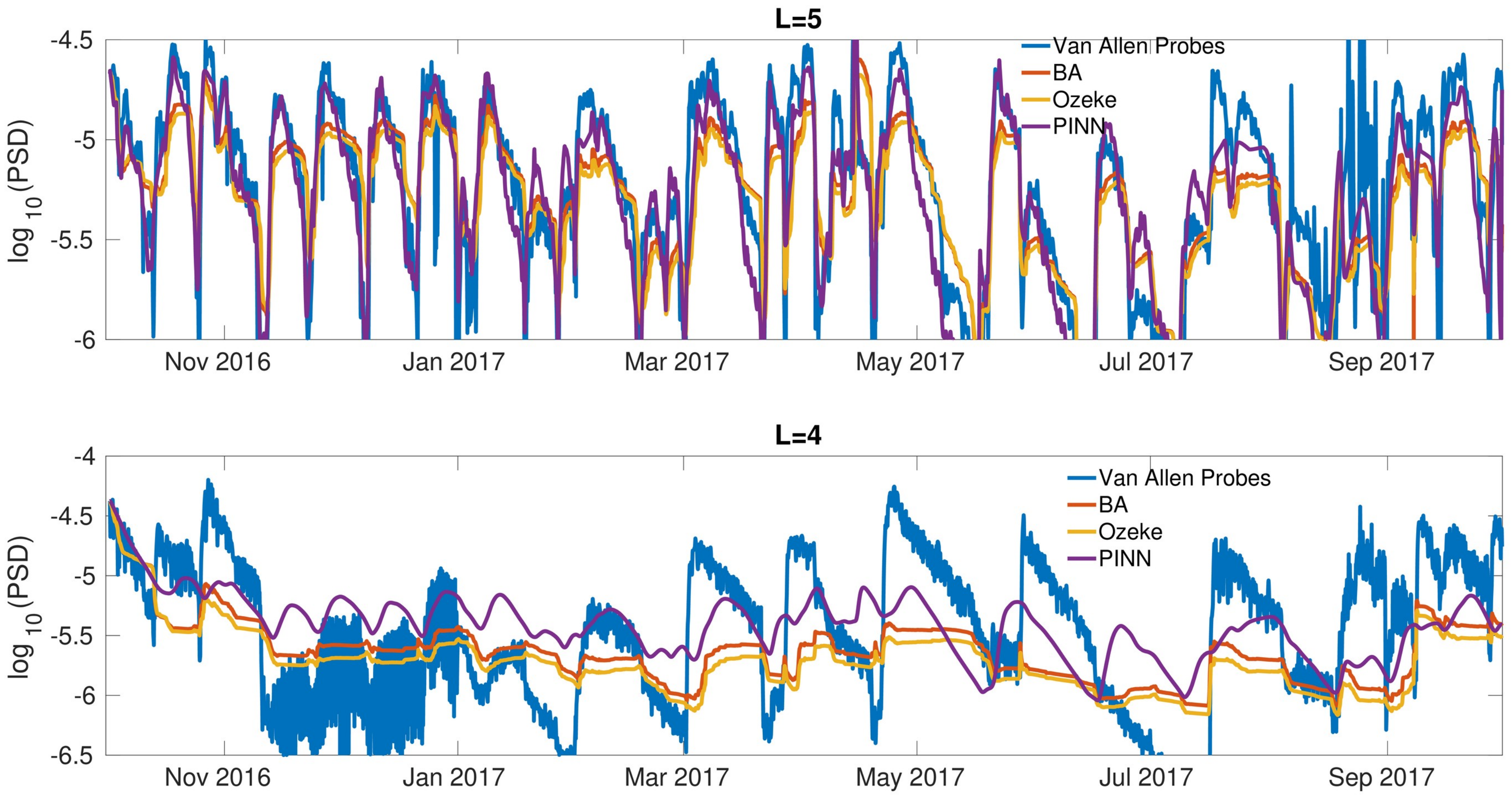
Back-up slides

Results on test set when using PINN-learned coefficients (cubic interpolation)




L=5
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log 10(PSD)
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Nov 2016
Jan 2017
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May 2017
Jul 2017
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Nov 2016
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