Quantifying uncertainty via machine learning models in aquatic remote sensing

Advances in foundational and future optics
NASA Ocean Biology & Biogeochemistry
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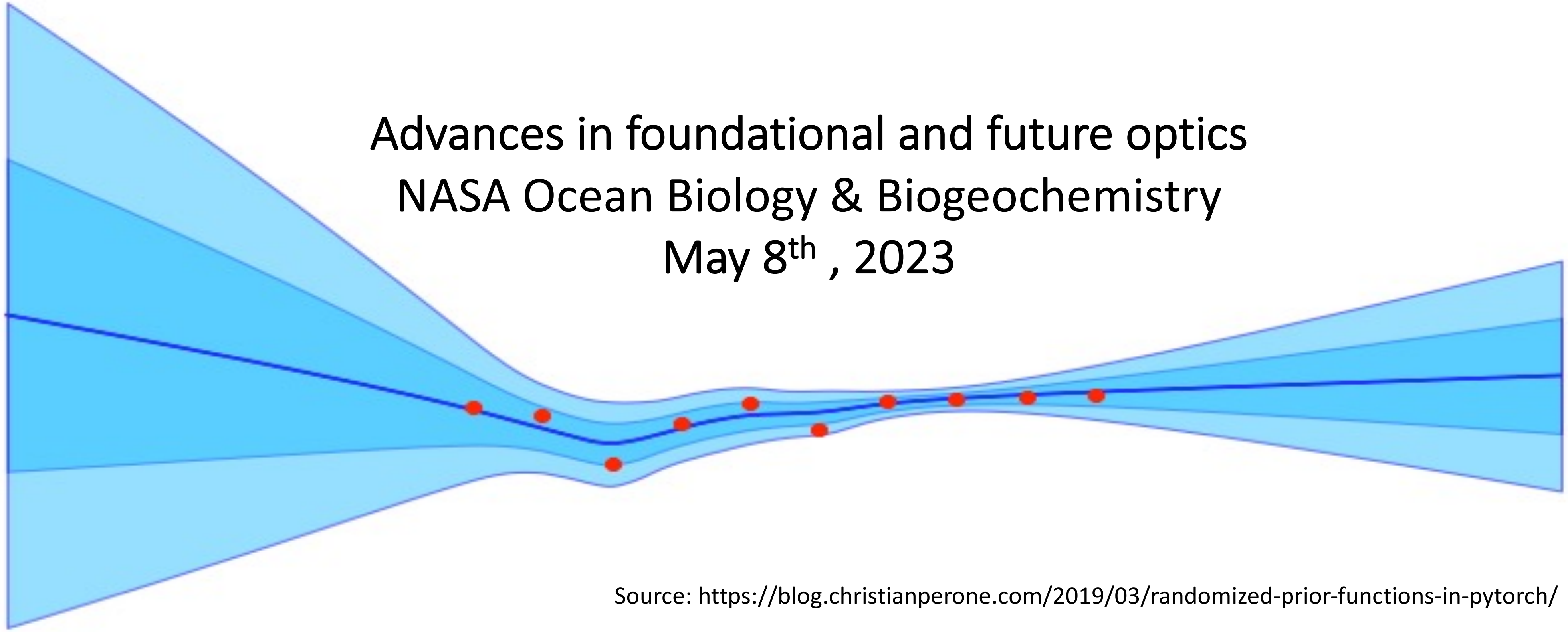

Source: https://blog.christianperone.com/2019/03/randomized-prior-functions-in-pytorch/

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Outline

1. Why do we use Machine Learning (ML) for aquatic remote sensing?

2. Why is the uncertainty estimation important in ML?

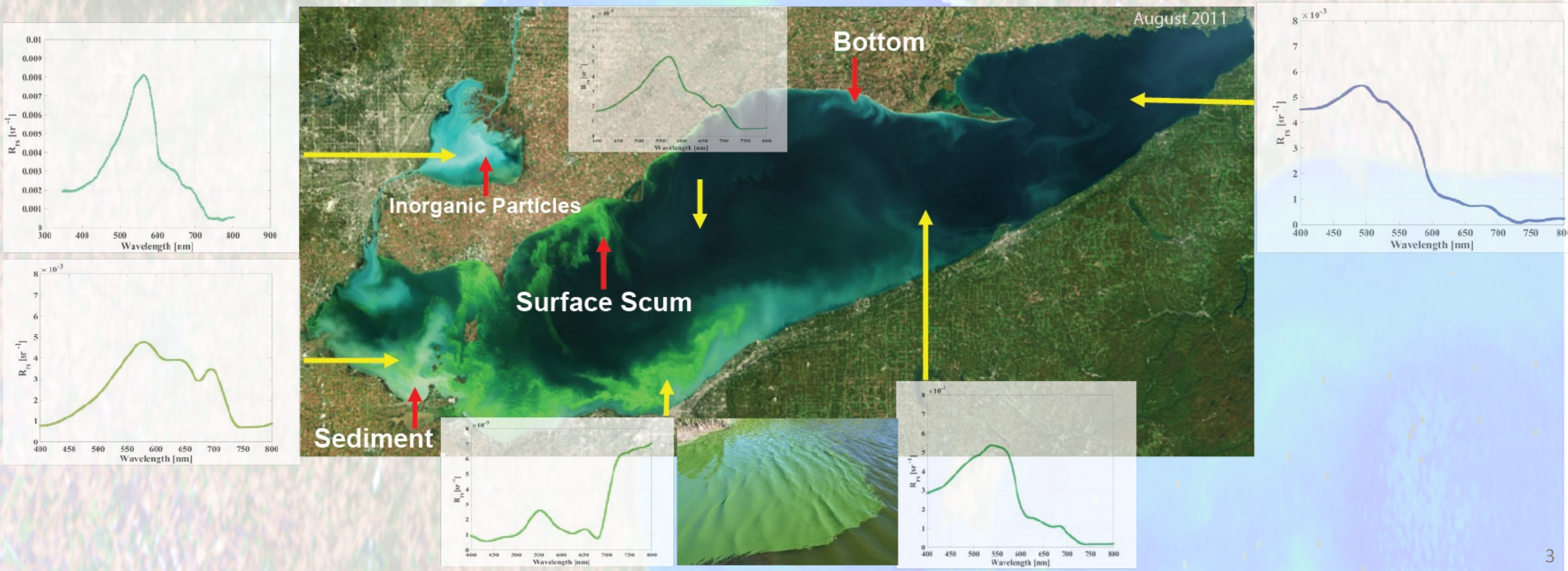
3. What are Mixture Density Networks (MDNs)? How to perform uncertainty estimation for MDNs?

4. Do ML estimated uncertainty metrics need calibration?

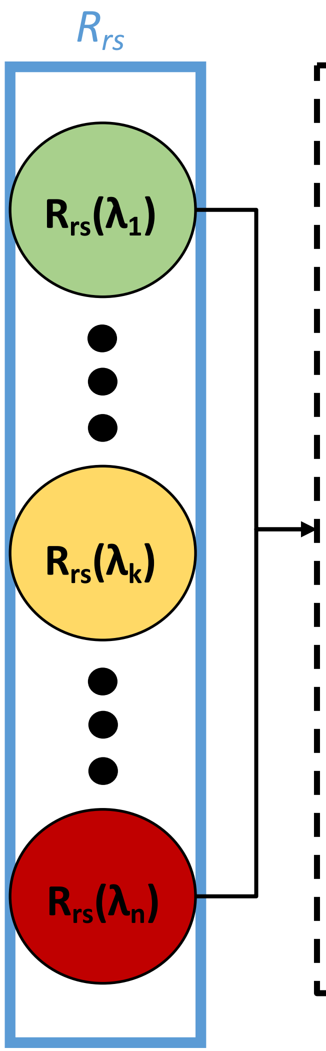
5. How do MDN-derived uncertainties appear in satellite products?

Monitoring water bodies using spectral remote sensing data

- Spectral datasets allow for clear discrimination of water column components.
- Data available from a variety of sensors at different spectral resolutions.



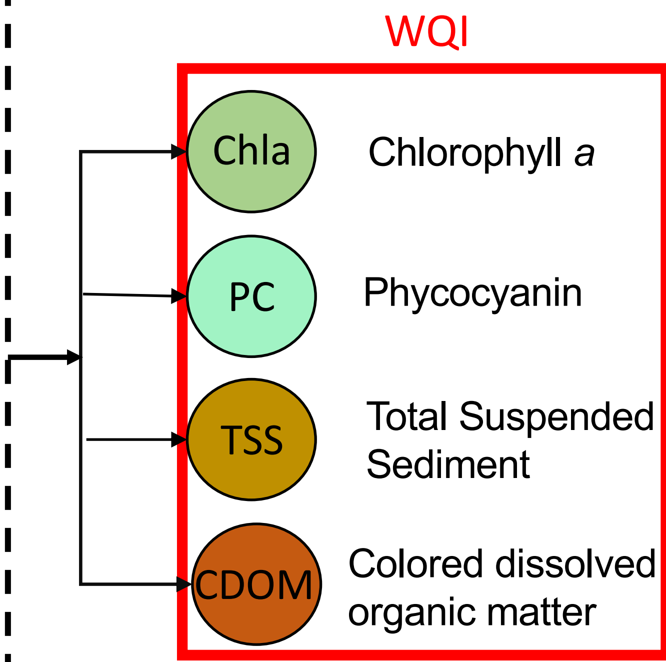
Machine learning based spectral inversion framework



Machine Learning (ML) tools commonly used for the estimation of Water Quality Indicators (WQI) from remote sensing reflectance (R_{rs}).

- **Mixture Density Networks (MDN)[1]**
- Bayesian Neural Networks with MC-dropout (BNN-MC)[2]
- eXtreme Gradient Boosted Trees (XGB)[3]
- Support Vector Machines/Regression (SVM)[4]

ML approaches show excellent WQI estimation on available labeled datasets.



[1] **MDN References**
Pahlevan et al. 2020, Smith et al. 2021, O'Shea et al. 2021, Pahlevan et al. 2022

[2] **BNN-MC References**
Werther et al. 2022

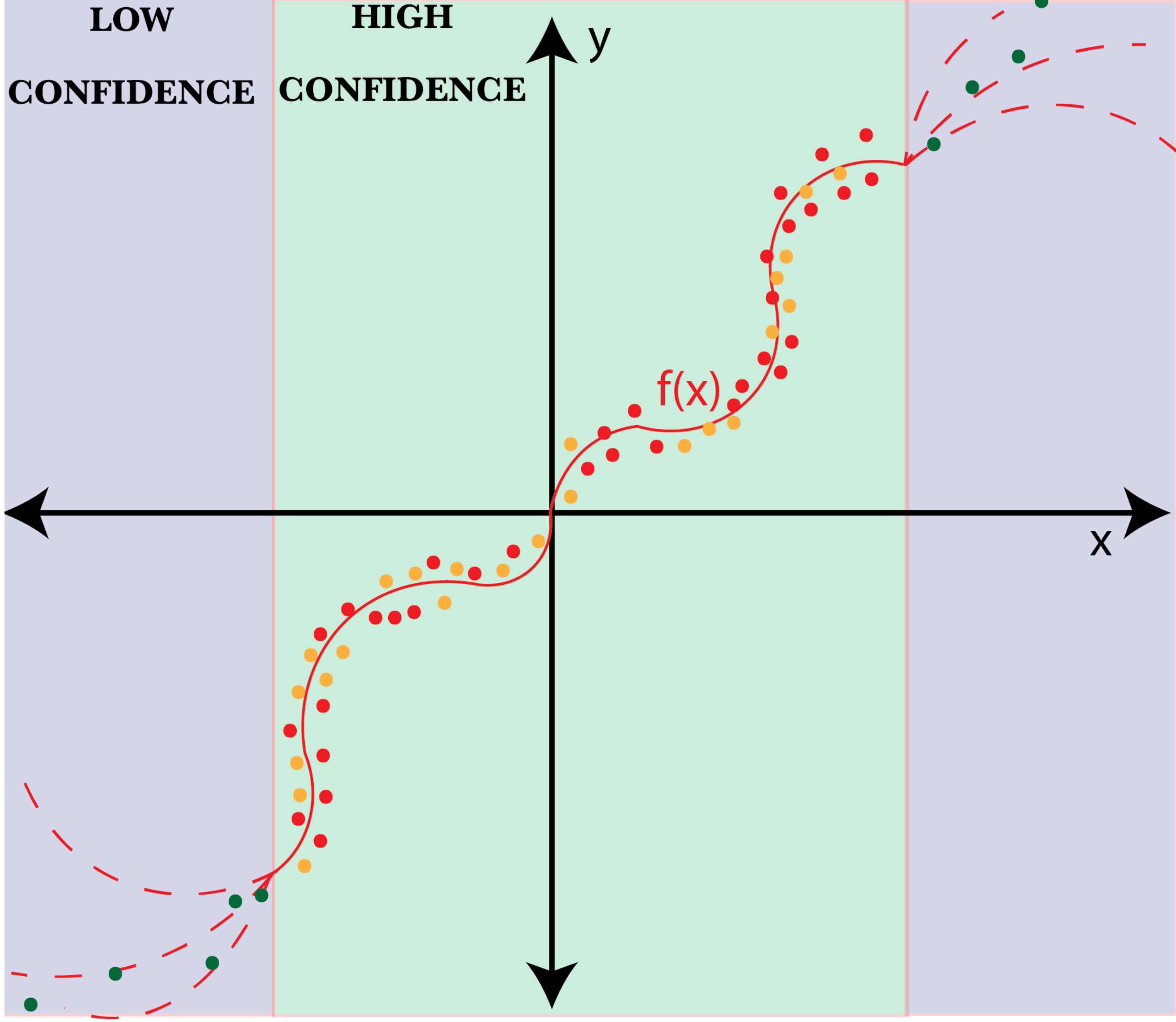
[3] **xGB References**
Cao et al. 2020

[4] **SVM References**
Kwiatkowska et al., 2003, Zhan et al. 2003

The need for uncertainty

- ML models function as black boxes
  - Performance only guaranteed for test samples like the training samples.
  - For practical applications need a way to identify Out-of-distribution (OOD) samples.

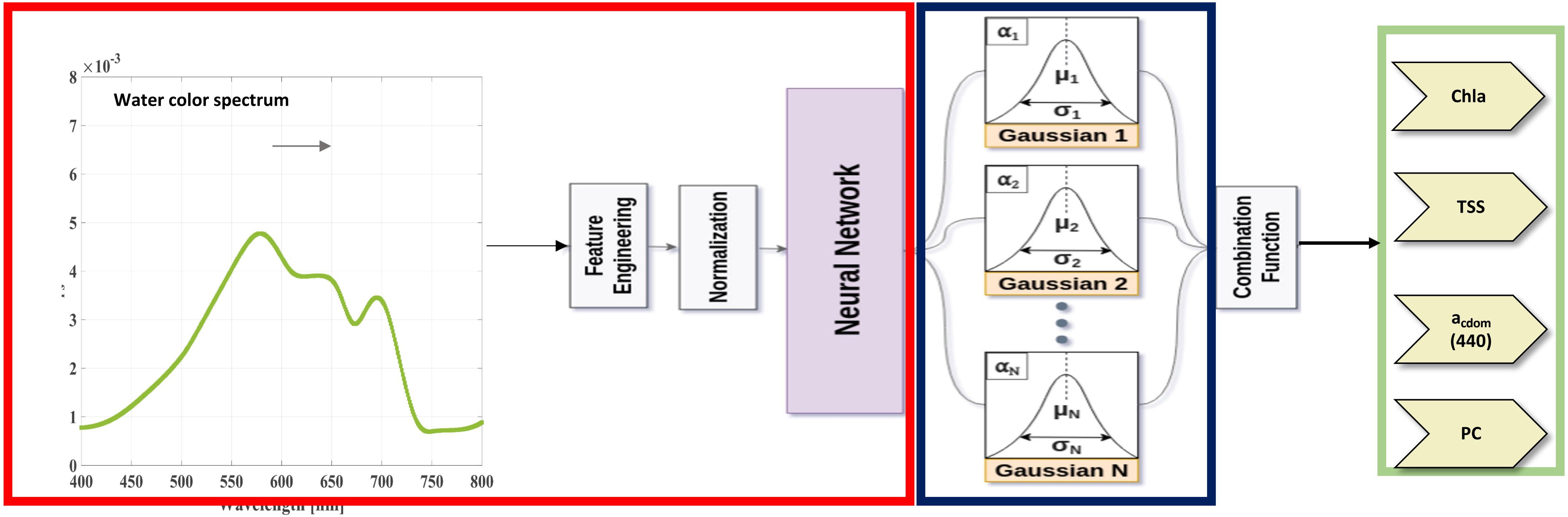
- Sources of uncertainty in ML
  - *Aleatoric* (or random) uncertainty
  - *Epistemic* (or knowledge based) uncertainty



TASK: Estimate f(x) such that it minimizes the mean squared error:

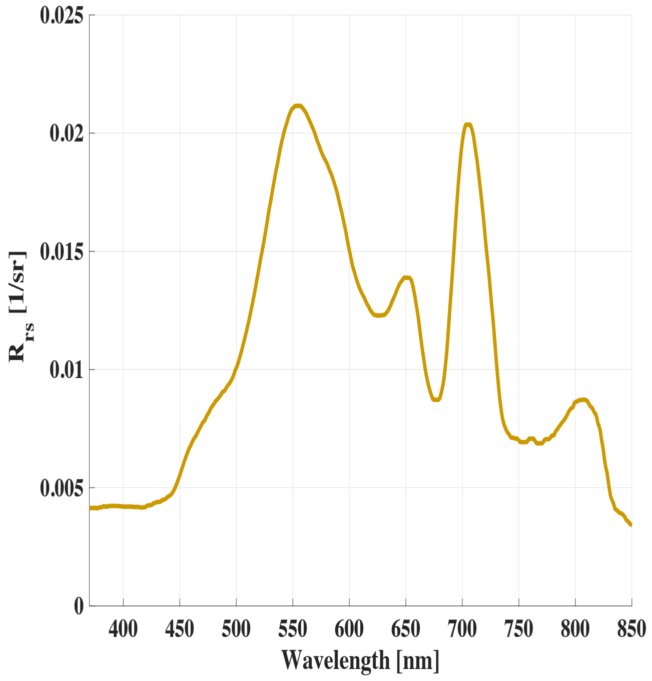
$\boxed{\operatorname{argmin}_f \ (1/N)||y - f(x)||^2}$ SCORE

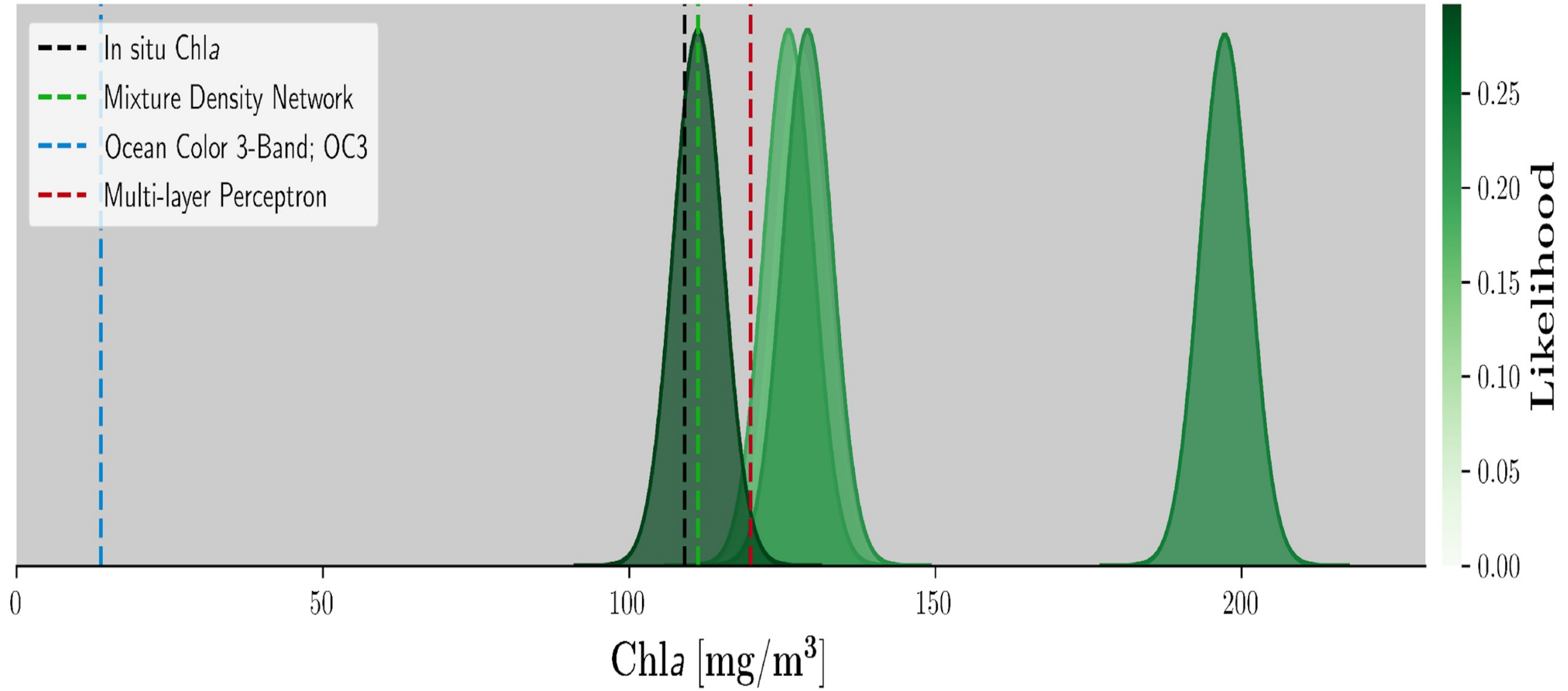
Mixture Density Networks (MDNs)



- Neural network variant that estimates the output as mixture of Gaussians.
  - The Gaussians are chosen to maximize the probability of the expected output for the training samples.
  - Designed for scenarios wherein the output distribution is expected to be multimodal.

Mixture Density Networks (MDNs)





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  - The Gaussians are chosen to maximize the probability of the expected output for the training samples.
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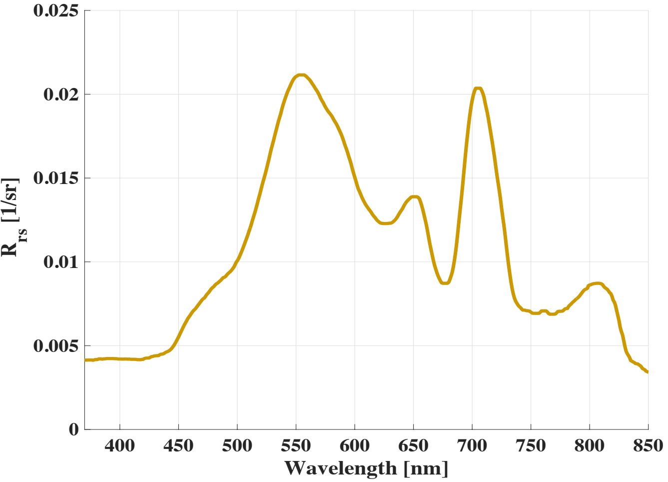
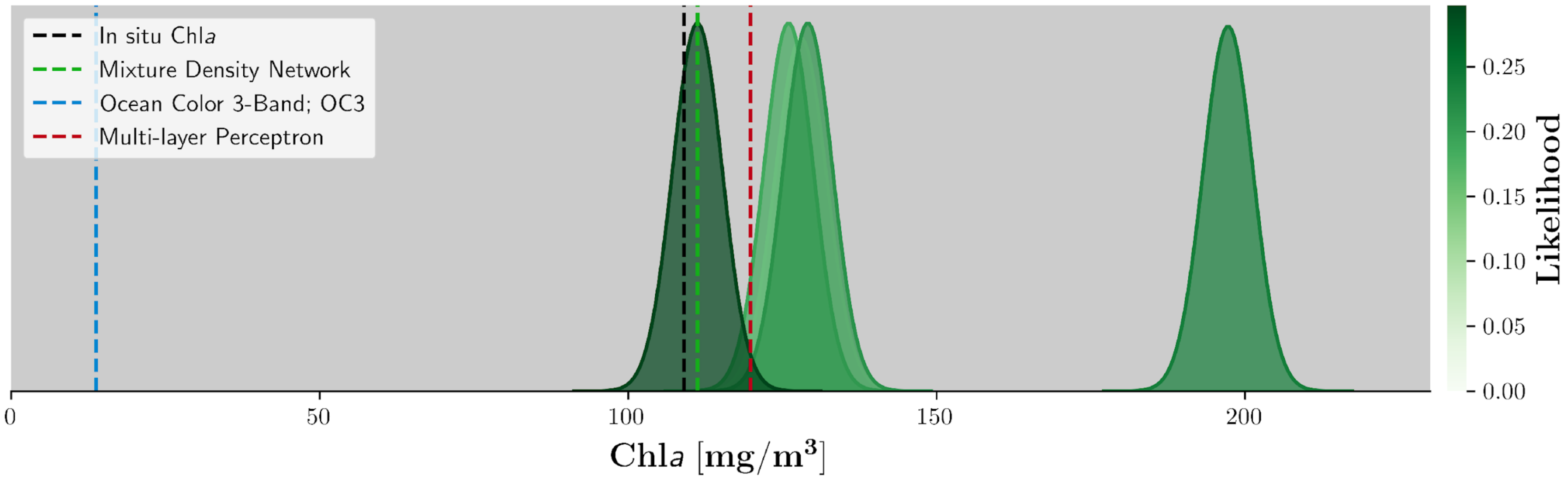
Uncertainty Estimation for MDNs[5]





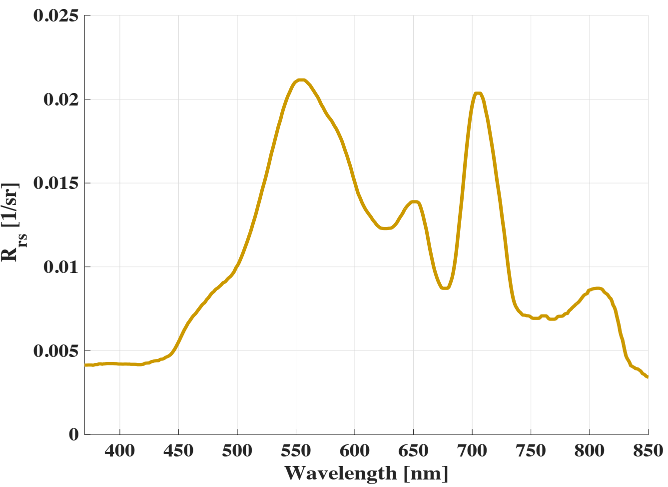
Since the MDN output is probabilistic in nature, the uncertainty can be estimated from the predicted distribution:

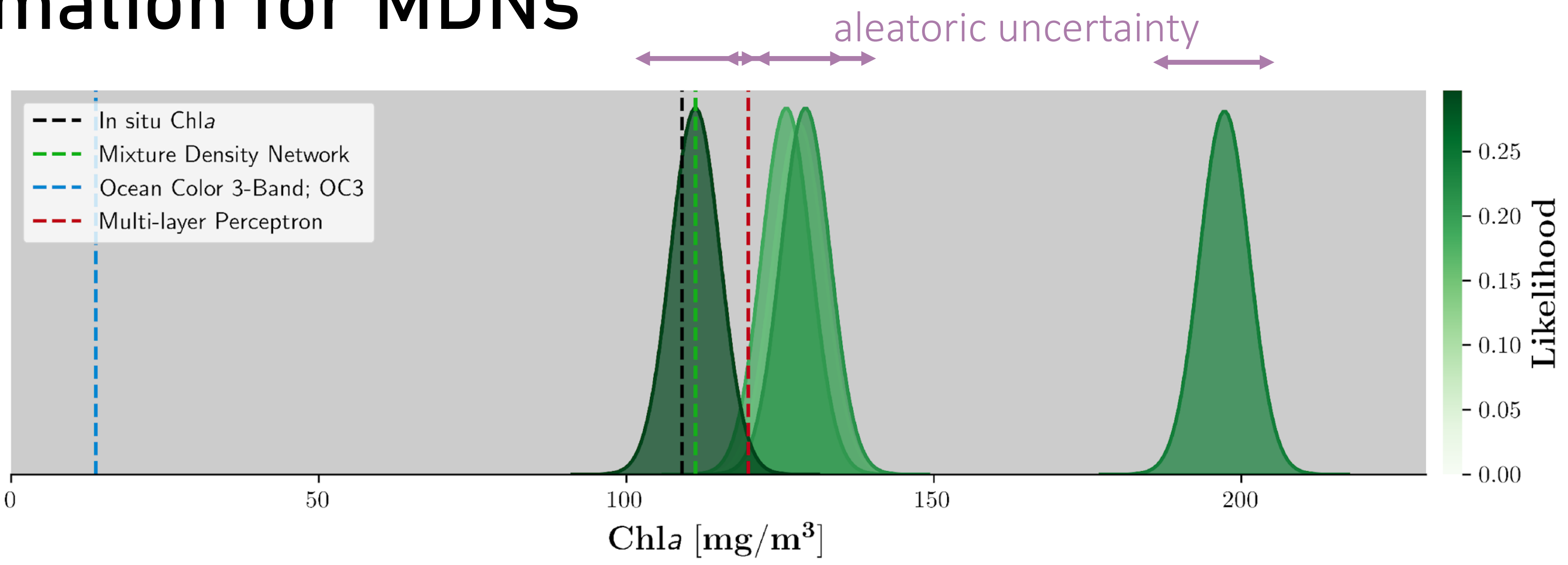
$$\sigma^2_{UNC} = \mathbb{V}(y_i | x_i) = \sigma^2_{alt}(x) + \sigma^2_{eps}(x)$$

- Prediction uncertainties have been shown to be well approximated by the variance of the estimated distribution.
- Further, the variance can be decomposed in aleatoric and epistemic components.

[5] **MDN-uncert References**
Choi et al., 2018
Saranathan et al., 2023

Uncertainty Estimation for MDNs





$$\sigma^2_{UNC} = \mathbb{V}(y_i|x_i) = \sigma^2_{alt}(x) + \sigma^2_{eps}(x)$$

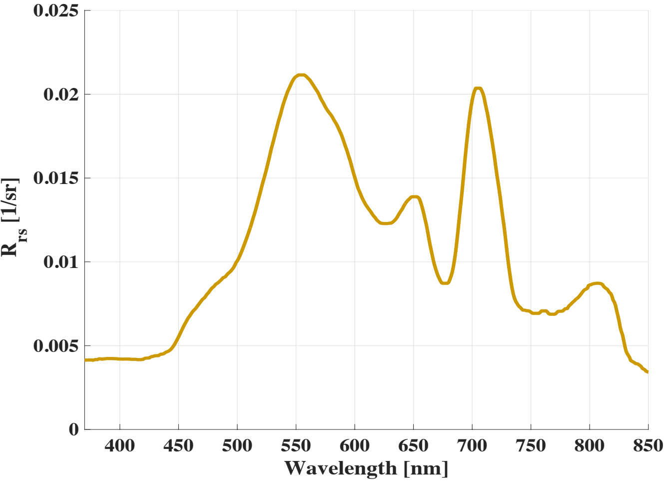
$$\sigma^2_{UNC} = \mathbb{V}(y_i|x_i) = \mathbb{E}_{k\sim\pi}(\mathbb{V}(y|x,k)) + \mathbb{V}_{k\sim\pi}(\mathbb{E}(y|x,k))$$

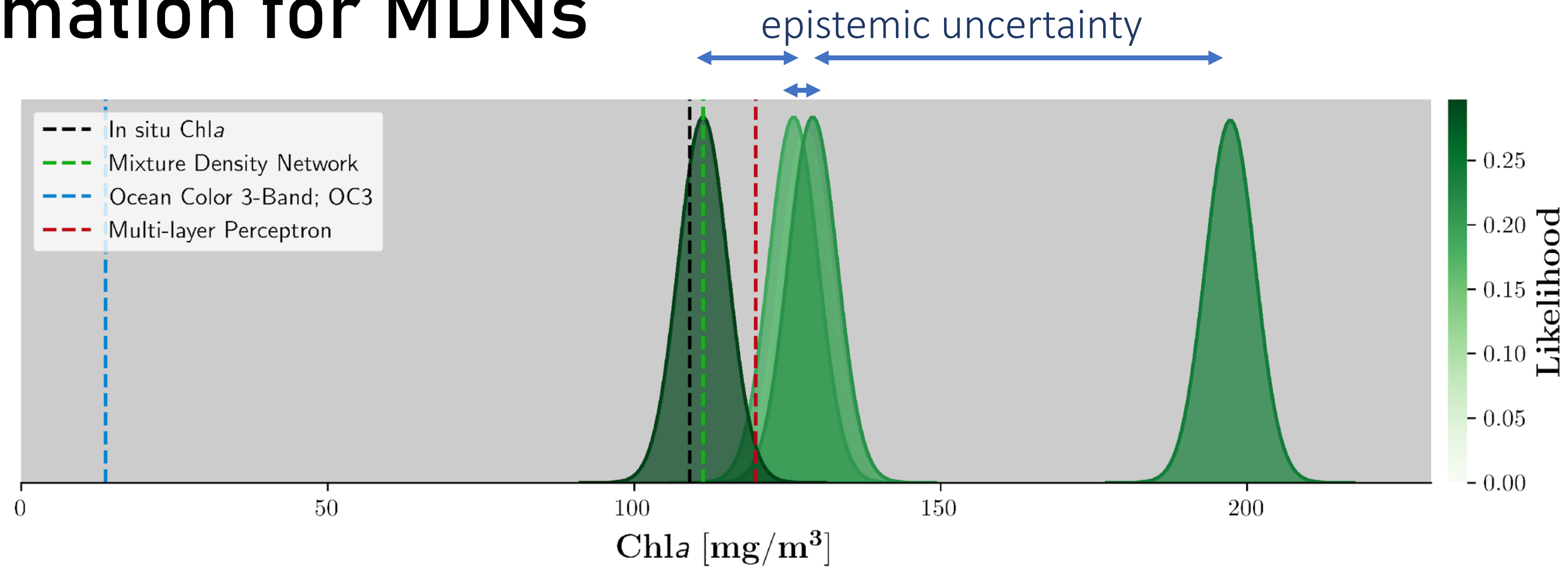
$$= \underbrace{\boxed{\sum_{j=1}^{K} \pi_j(x)\Sigma_j(x)}}_{\text{aleatoric}} + \sum_{j=1}^{K} \pi_j(x) \left\| \mu_j(x) - \sum_{k=1}^{K} \pi_k(x)\mu_k(x) \right\|^2$$

<u>Key:</u>

x_i: Remote Sensing Reflectance
y_i: Water optical parameters
σ: standard deviation
π_i: likelihood of the ith MDN component
μ_i: mean of the ith MDN component
Σ_i: variance of the ith MDN component

Uncertainty Estimation for MDNs





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x_i: Remote Sensing Reflectance

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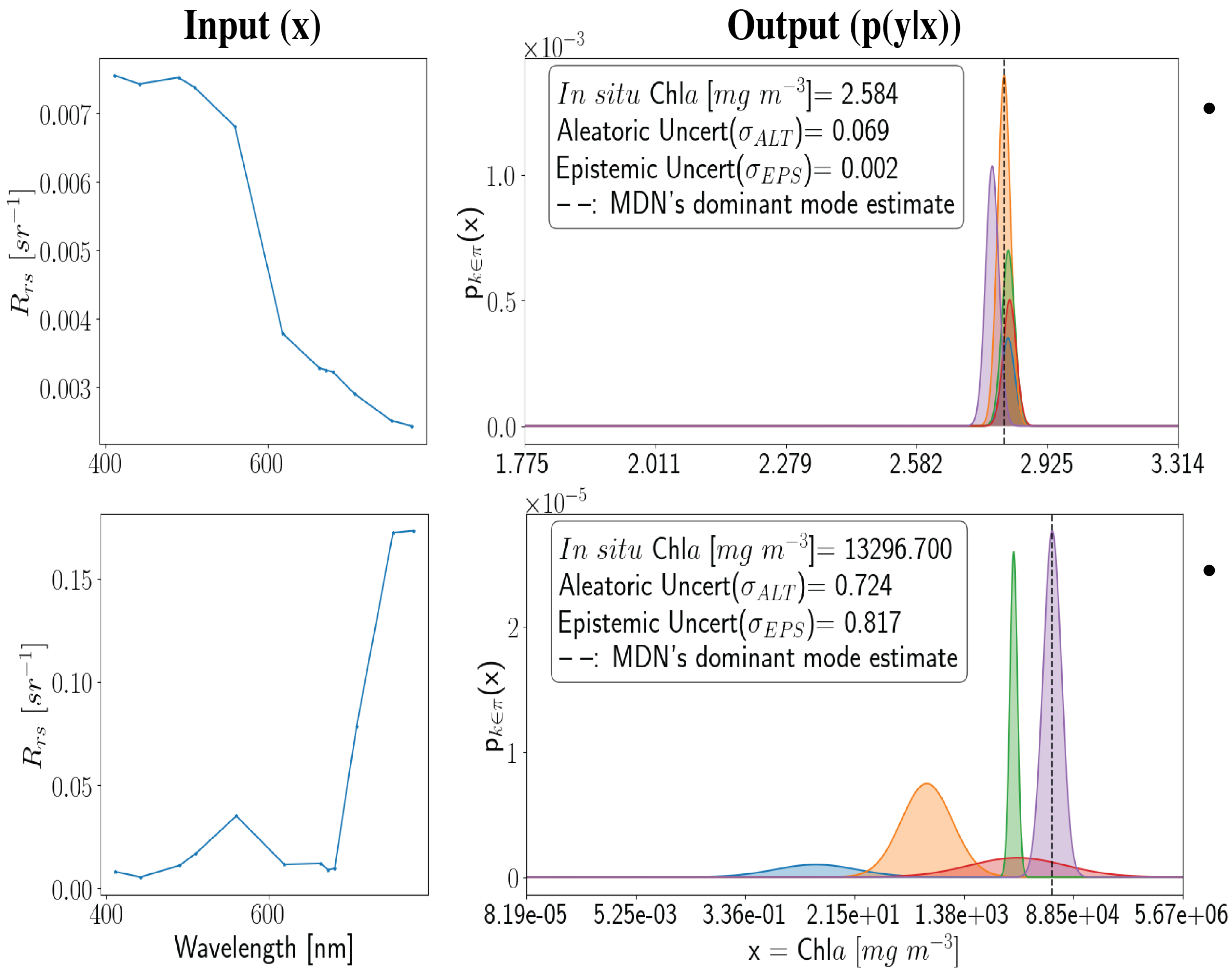
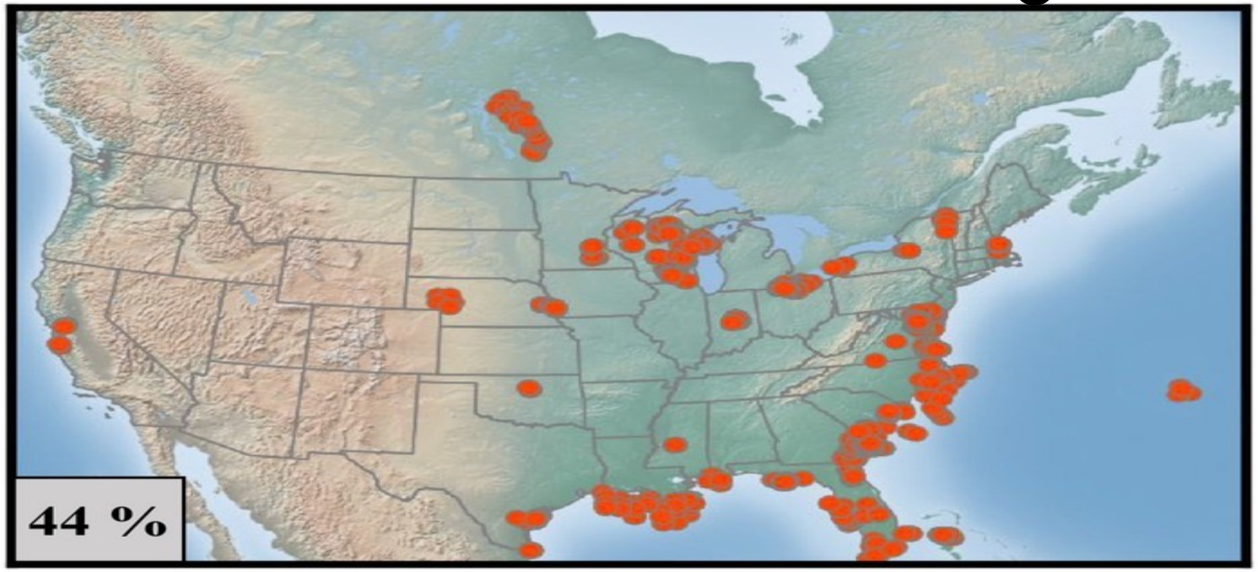
Sample MDN estimated uncertainties



- High confidence samples
  - Distribution appears unimodal.
  - Low variance in individual components.

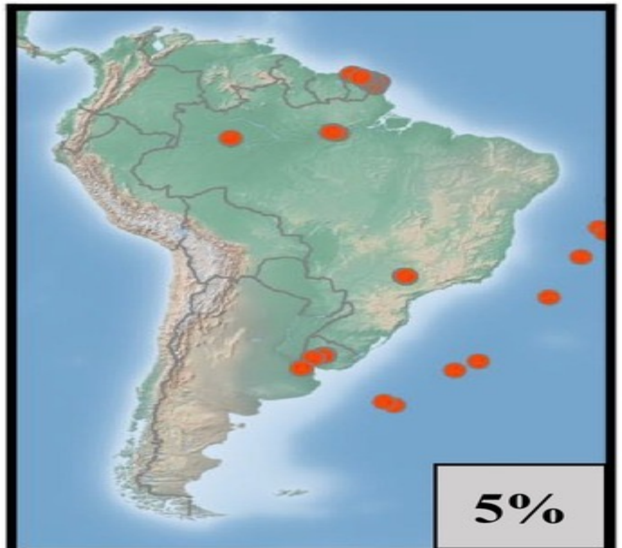
- Low confidence samples
  - Distribution appears to have many well-separated modes (peaks).
  - Components with a very large spread (variance) indicating model uncertainty.

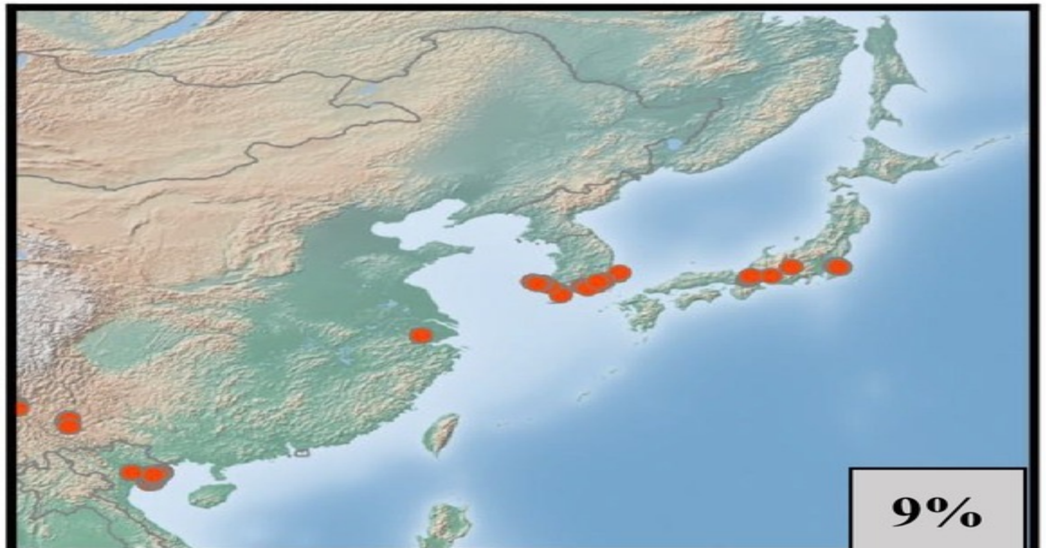
GLORIA[6]: A Large (N=~8,237) Globally Distributed *In situ* Dataset for training and testing the MDNs

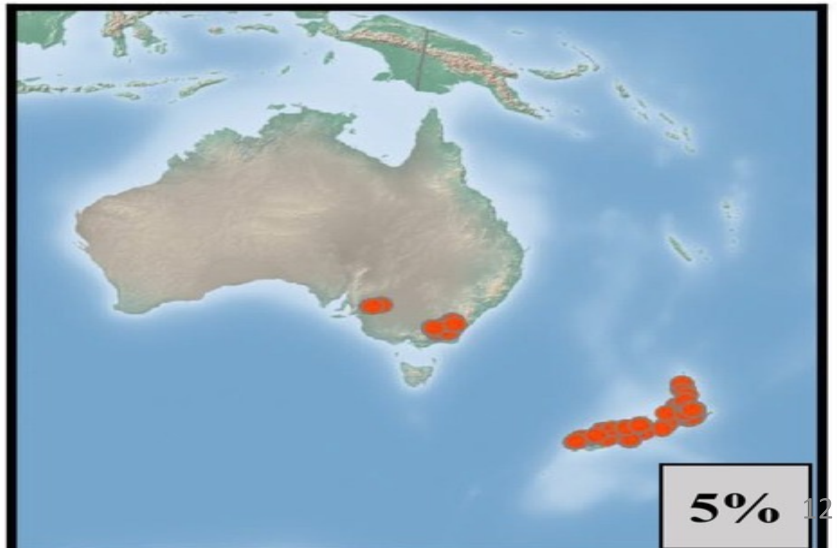


***In situ* measurements**

[6] **GLORIA**
Lehmann et al. (2023)







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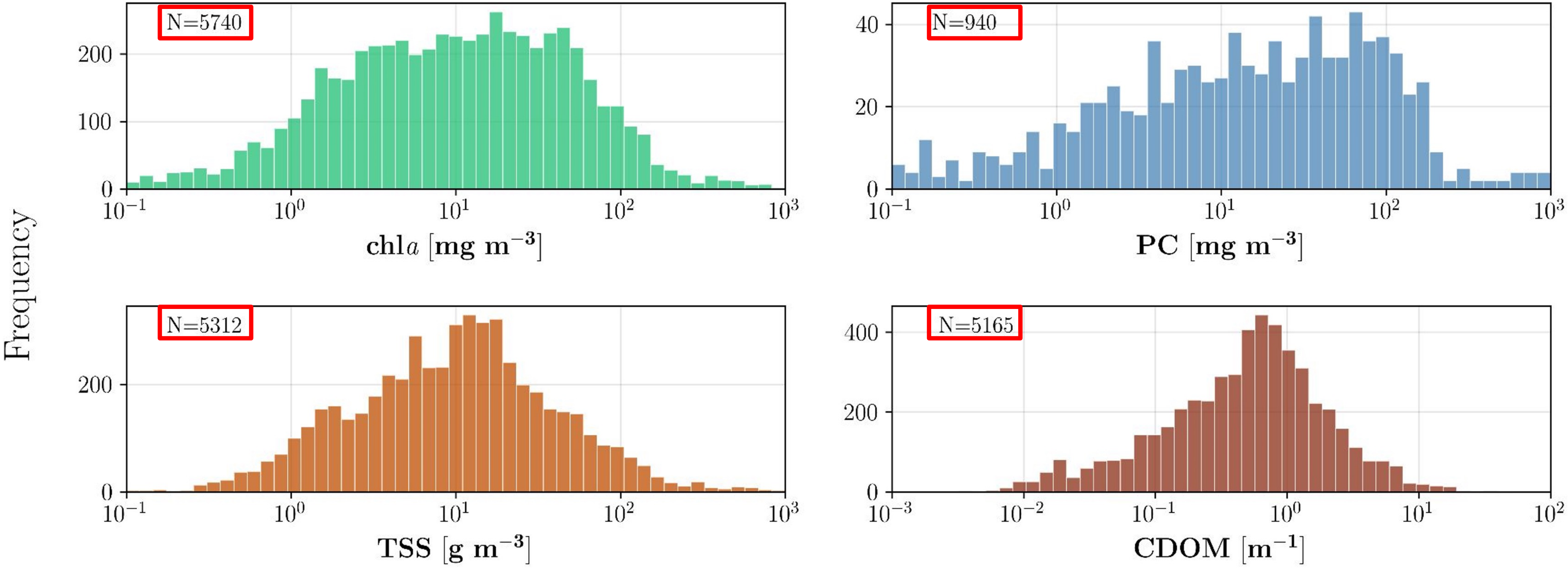


- Contains samples over ~3-4 orders of magnitude concentration range

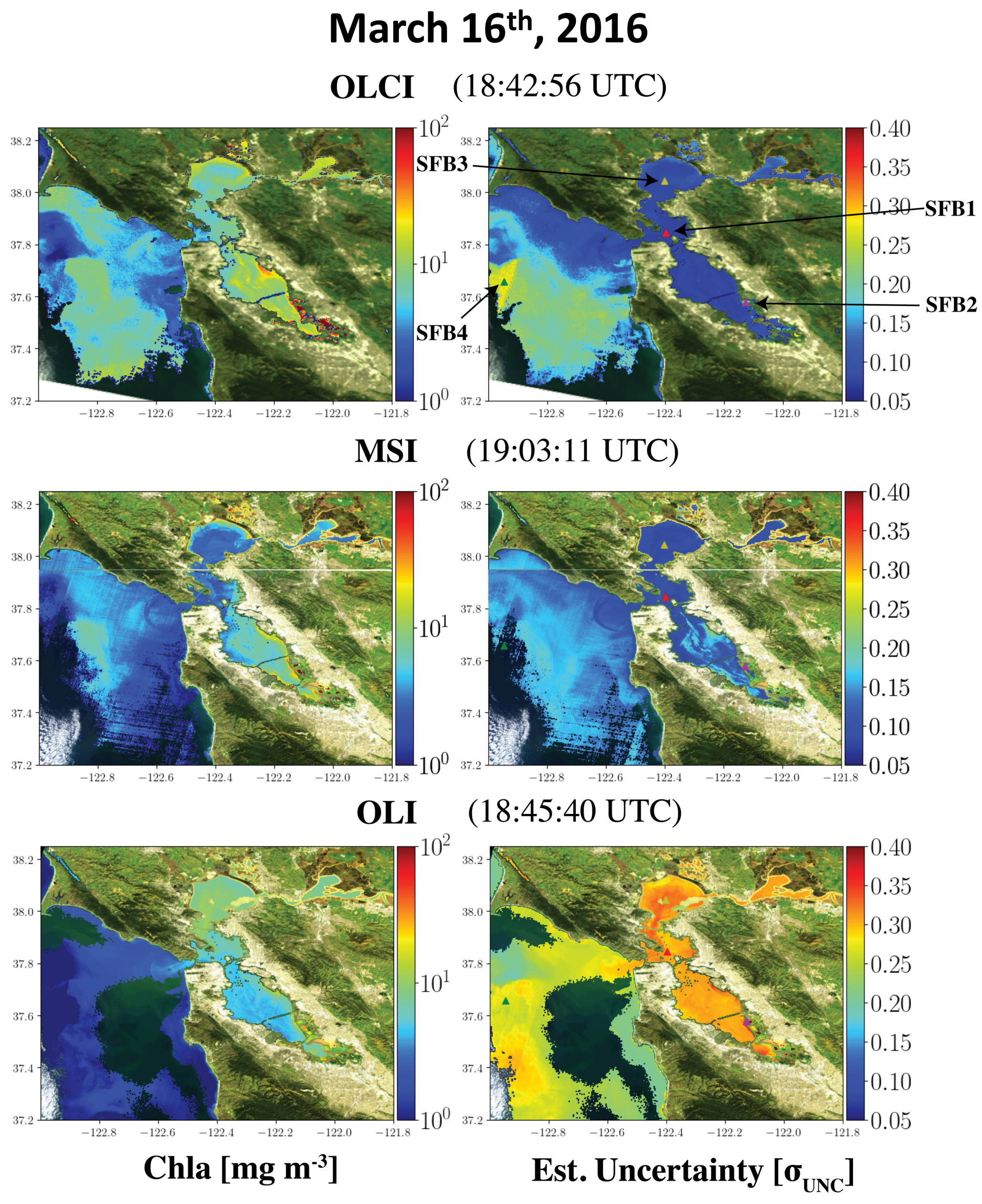
[6] **GLORIA**
Lehmann et al. (2023)

Validate the estimated uncertainty

- The MDN uncertainty metric successfully identifies unexpected data conditions, such as:
  - Noisy Test Data
  - Noisy Training Data
  - Out-of-Distribution samples
  - Atmospheric Distortion

- The uncertainty metrics also show a clear correlation between the error and uncertainty.
  - Allows the use of uncertainty as a proxy for error in some cases.

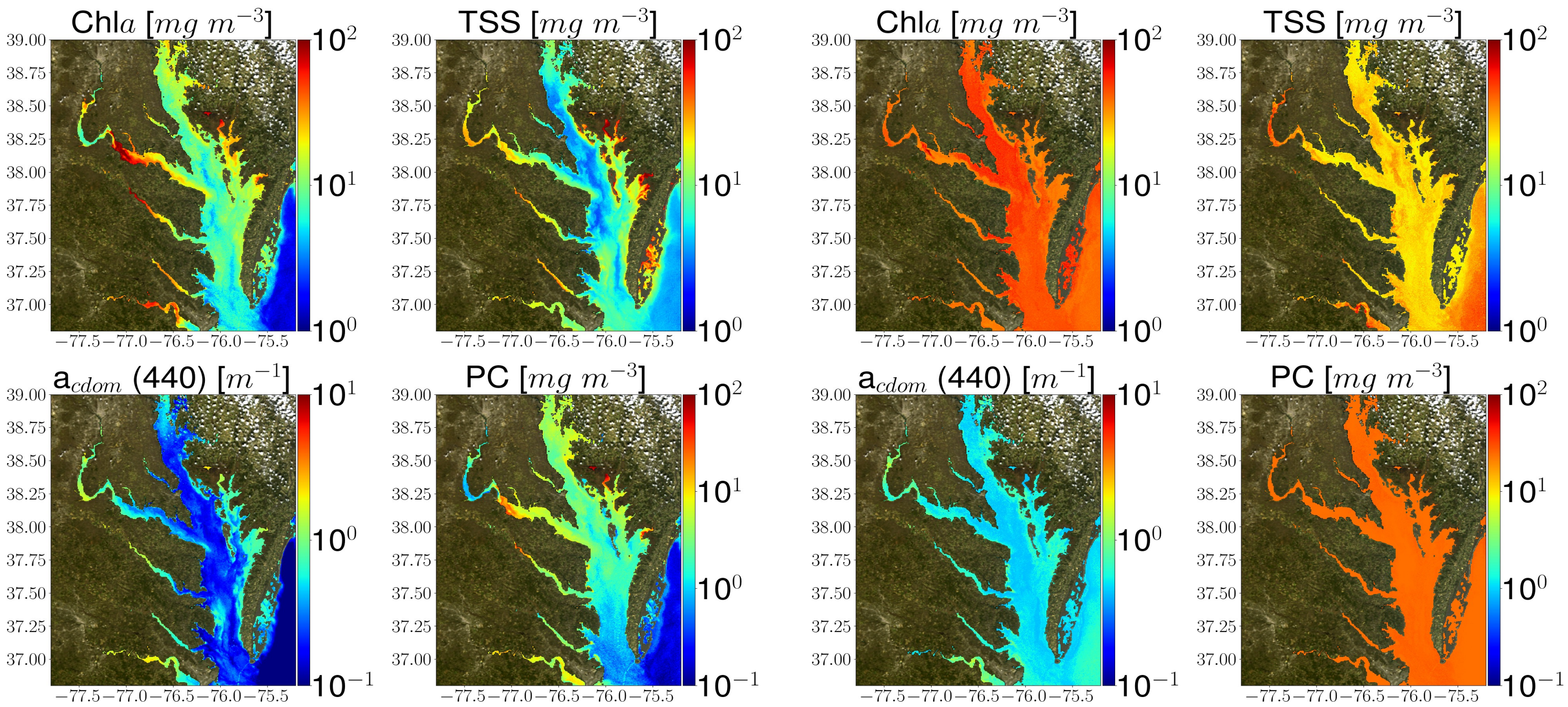
- Even for satellite data can qualitatively verify that prediction uncertainty is related to test-training similarity.



MDN estimated Chl*a* and associated uncertainty maps over near concurrent measurements over San Francisco Bay from Saranathan et al, 2022 (TGRS).

Interpret the MDN estimated uncertainty metric

March 4th, 2017

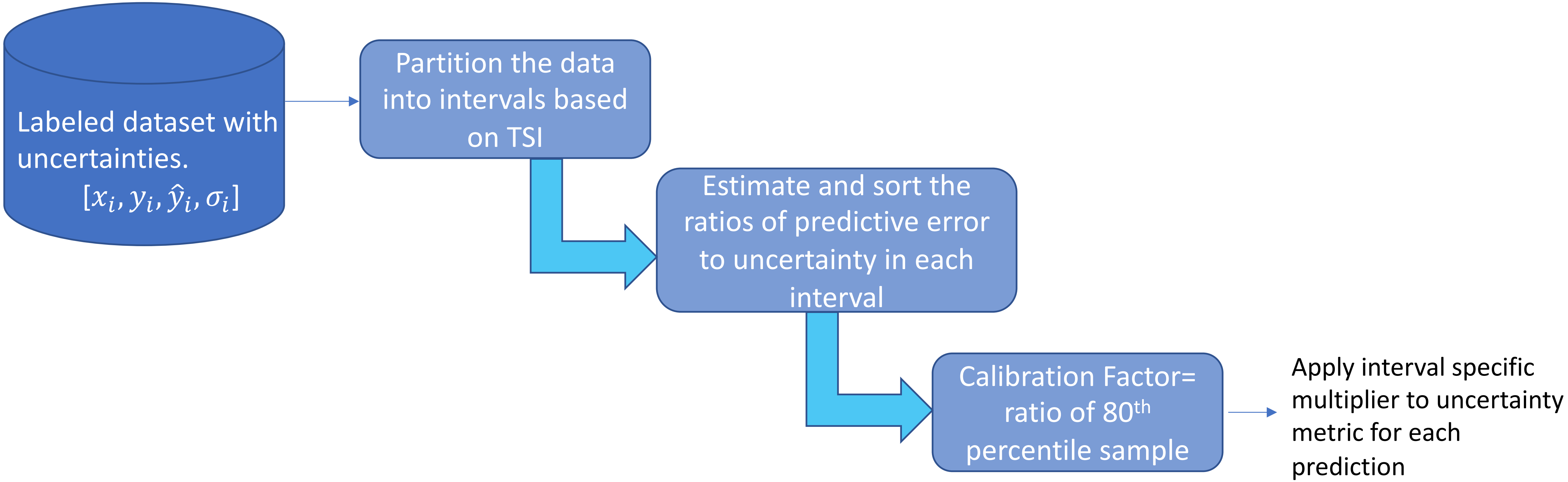


Product Estimates **Unscaled uncertainty**

MDN estimated WQI products and associated (unscaled) uncertainty maps from OLCI data over Chesapeake Bay.

- The MDN uncertainty metric while valuable is **hard to interpret**
  - The scale of the metric is based on properties of the model.
  - Understanding/Interpreting the maps takes identification of a map-specific scaling.
  - The scale of the original metric is not intuitive.
- Need to modify/calibrate the metric to make it "human-friendly".

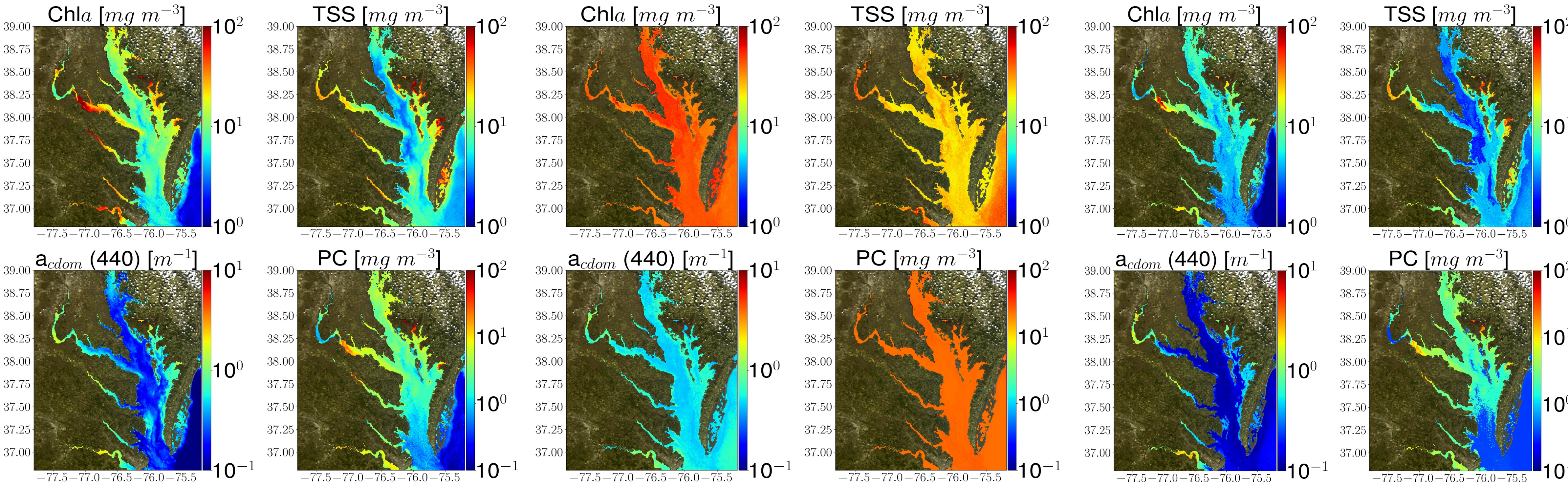
Calibrate the estimated uncertainty for human interpretability



- Identify a simple multiplicative factor based on the predicted value to map the uncertainty into a usable space.
- The calibration translates the uncertainty to the same space as the predicted values making interpretation more intuitive.

Estimate uncertainty for satellite data over Chesapeake Bay: OLCI Data

March 4th, 2017



Product Estimates | **Unscaled uncertainty** | **Calibrated uncertainty**

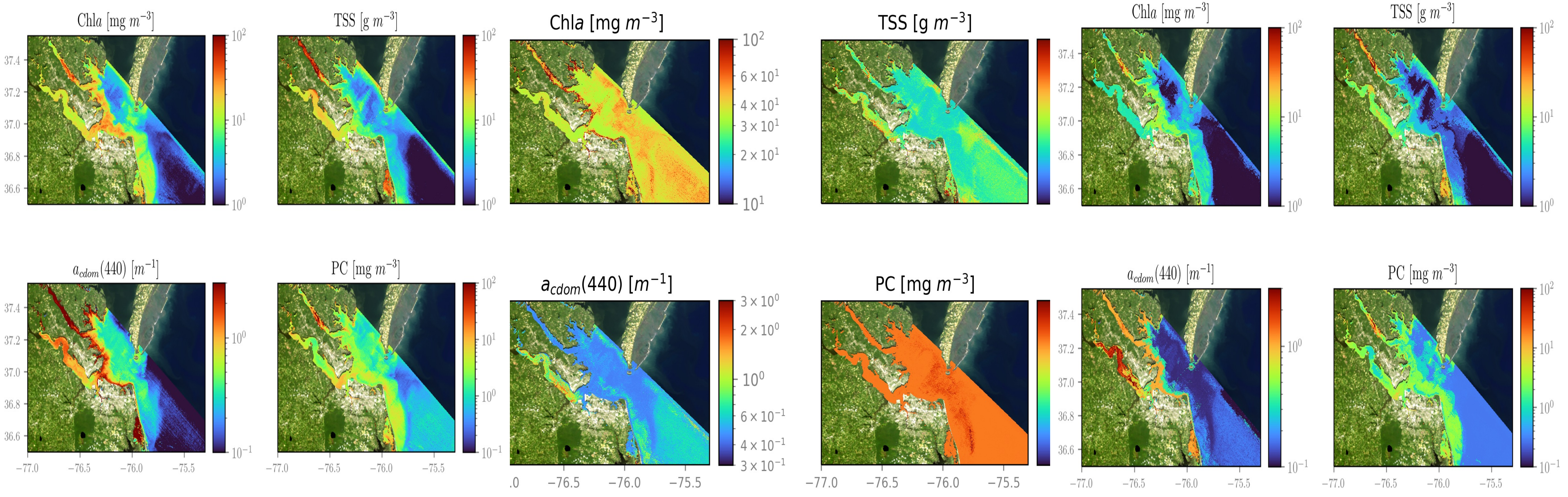
- Currently, generating scaled and unscaled uncertainty products for many different sensor/spectral resolutions
  - Showing the OLCI results as a proxy for the expected results on the PACE mission

Acolite-processed imagery

PACE

Estimate uncertainty for satellite data over Chesapeake Bay: HICO Data

April 1st, 2010



Product Estimates **Unscaled uncertainty** **Calibrated uncertainty**

Similar products can also be extracted for hyperspectral data extracted from the HICO sensor

L2GEN-processed imagery

Conclusions

- The MDN uncertainty metric clearly addresses the missing component of confidence associated with the model's prediction.
  - Very useful for identifying unexpected data conditions (noisy/distorted data or OOD samples).
  - Clear correlation between error and MDN estimated uncertainty.

- The calibration technique appears to make the estimated uncertainty metric more intuitive for the end-users.
  - ***Operational Caveat***: Most of the model creation and validation is performed using low noise *in situ* data and statistical guarantees may not extend to satellite data products.

Future Work

- Uncertainty Estimation
    - Compare the MDN-specific uncertainty estimates to estimates from other machine learning methods such as BNN-MC, ensemble of MLP’s, etc..
    - Identify/isolate the main factors affecting the amount of uncertainty seen in these models.

- Uncertainty Metric Calibration
    - Experiment with other non-interval based methods for uncertainty calibration.
    - Include end-user suggestion into the calibration process to generate the most useful/informative products

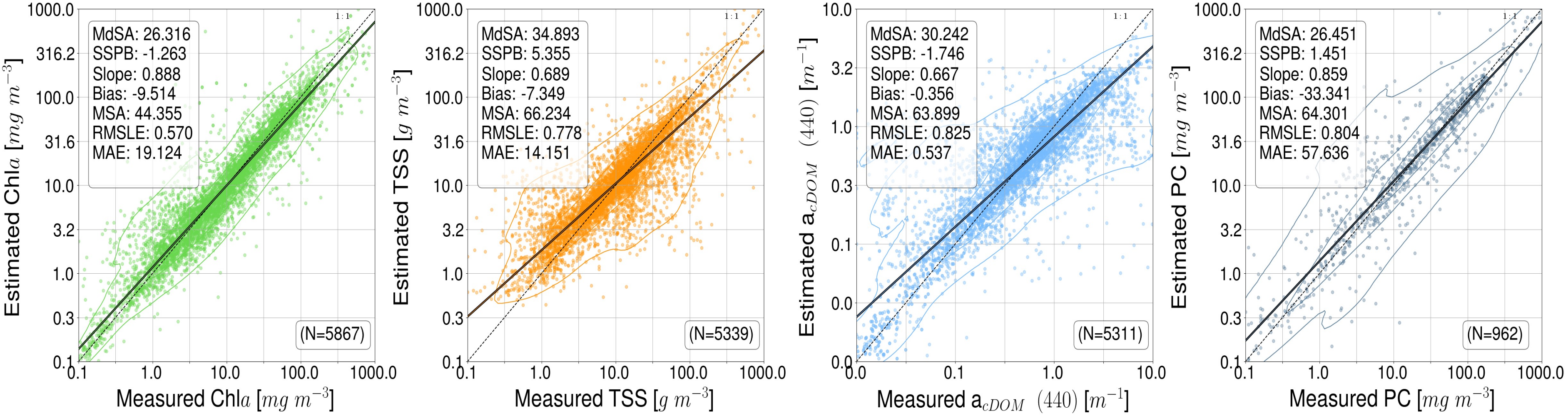
- For any questions/comments or general interest, please contact me at arun.saranathan@ssaihq.com

Acknowledgement: This work was funded by the NASA PACE Science and Applications Team.

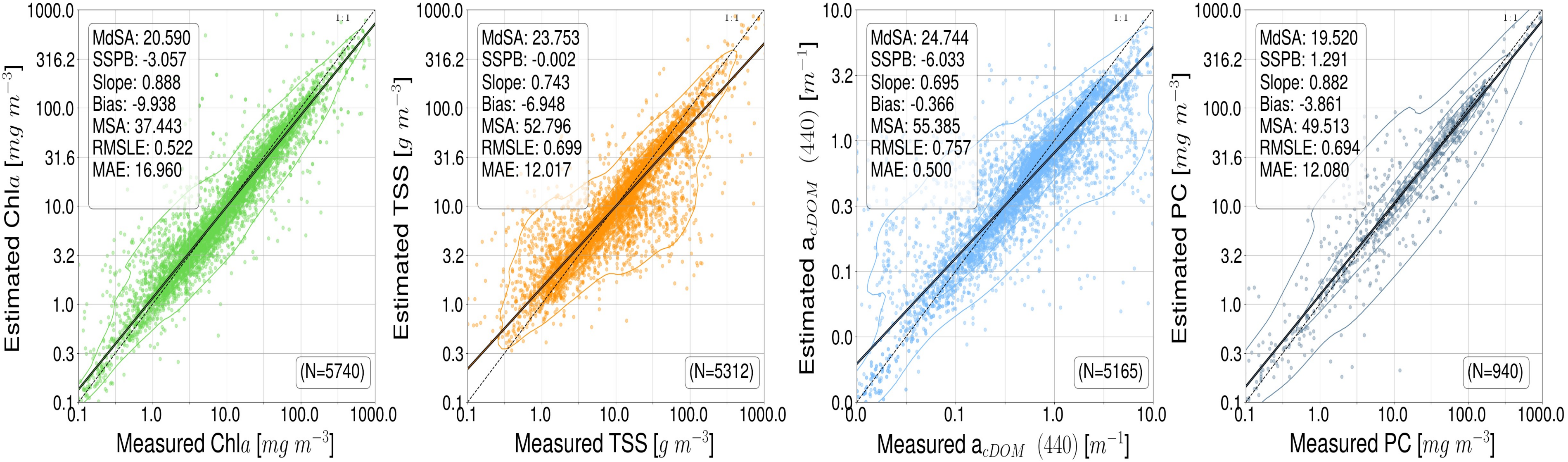
Additional Slides

MDN model prediction performance for WQI

MDN Test Perfromance-S3A



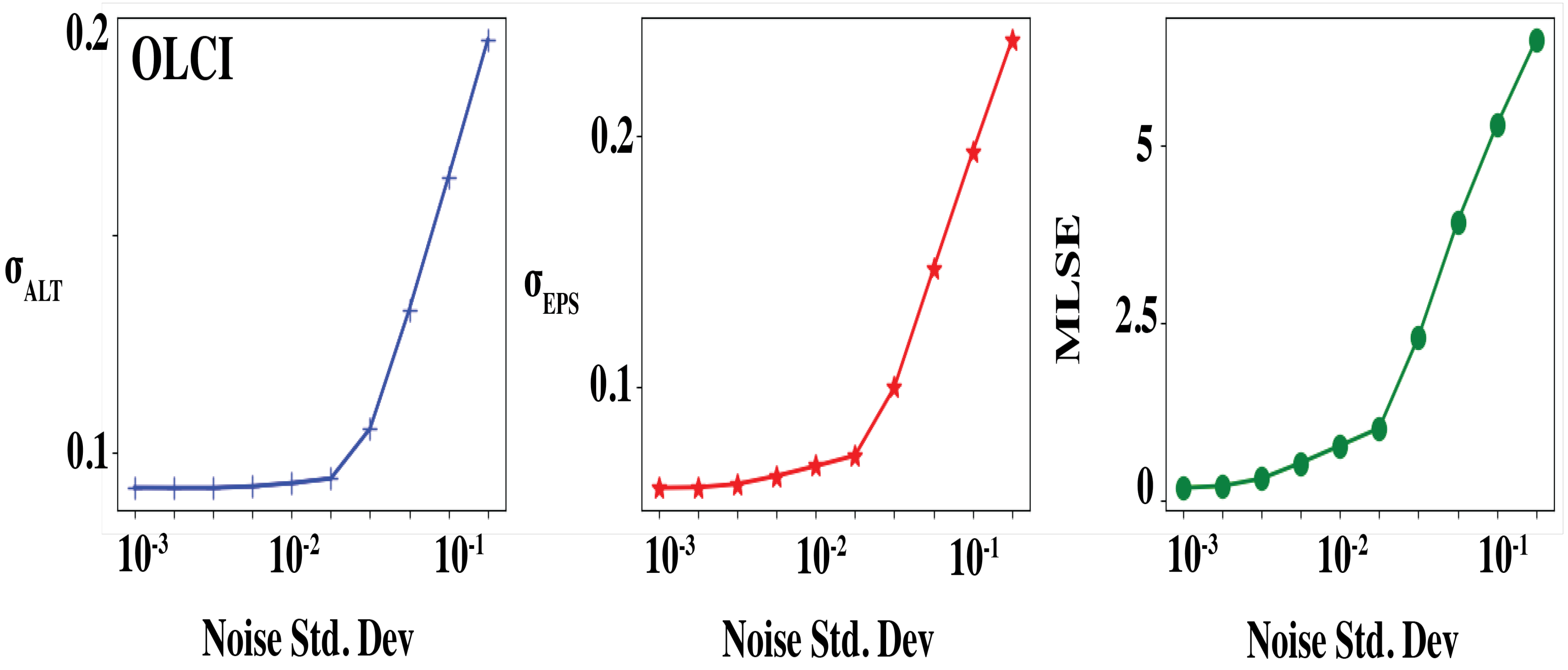
MDN Test Perfromance-HICO



MDNs perform admirably on in-distribution test samples for many different sensors.

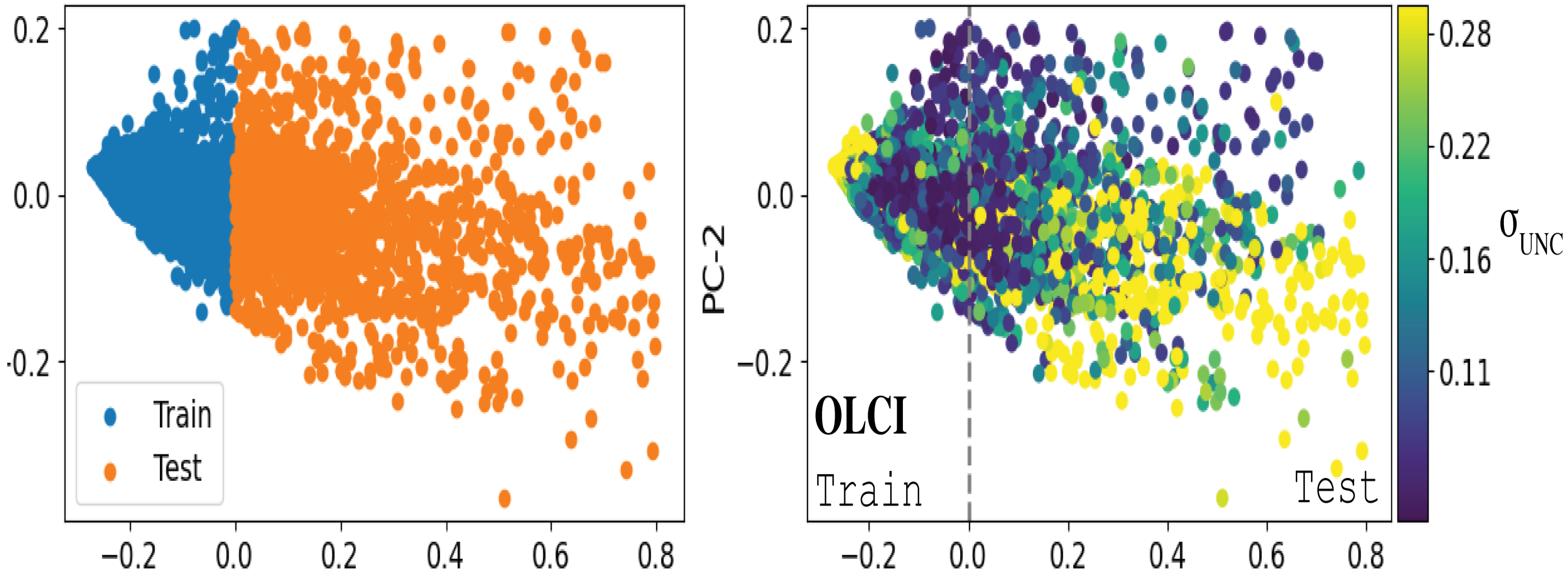
- Showing results @ PACE proxy OLCI (S3A) and HICO resolutions.

Effect of noise on MDN performance and uncertainty



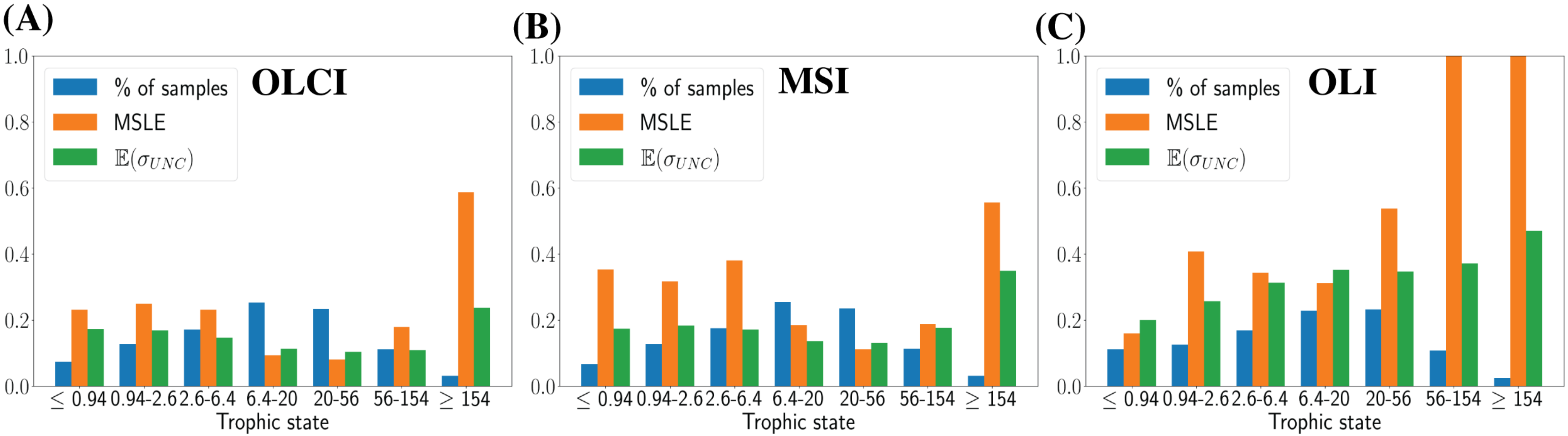
The uncertainty metric is clearly able to track the presence of increased noise in the test samples. Further the increase in uncertainty also corresponds to a decrease in the MDNs prediction performance.

Effect of OOD samples on MDN performance and uncertainty



The uncertainty metric is clearly able to track the presence of OOD samples. Clearly, the uncertainty increases when the distance of the test samples from the training samples increases.

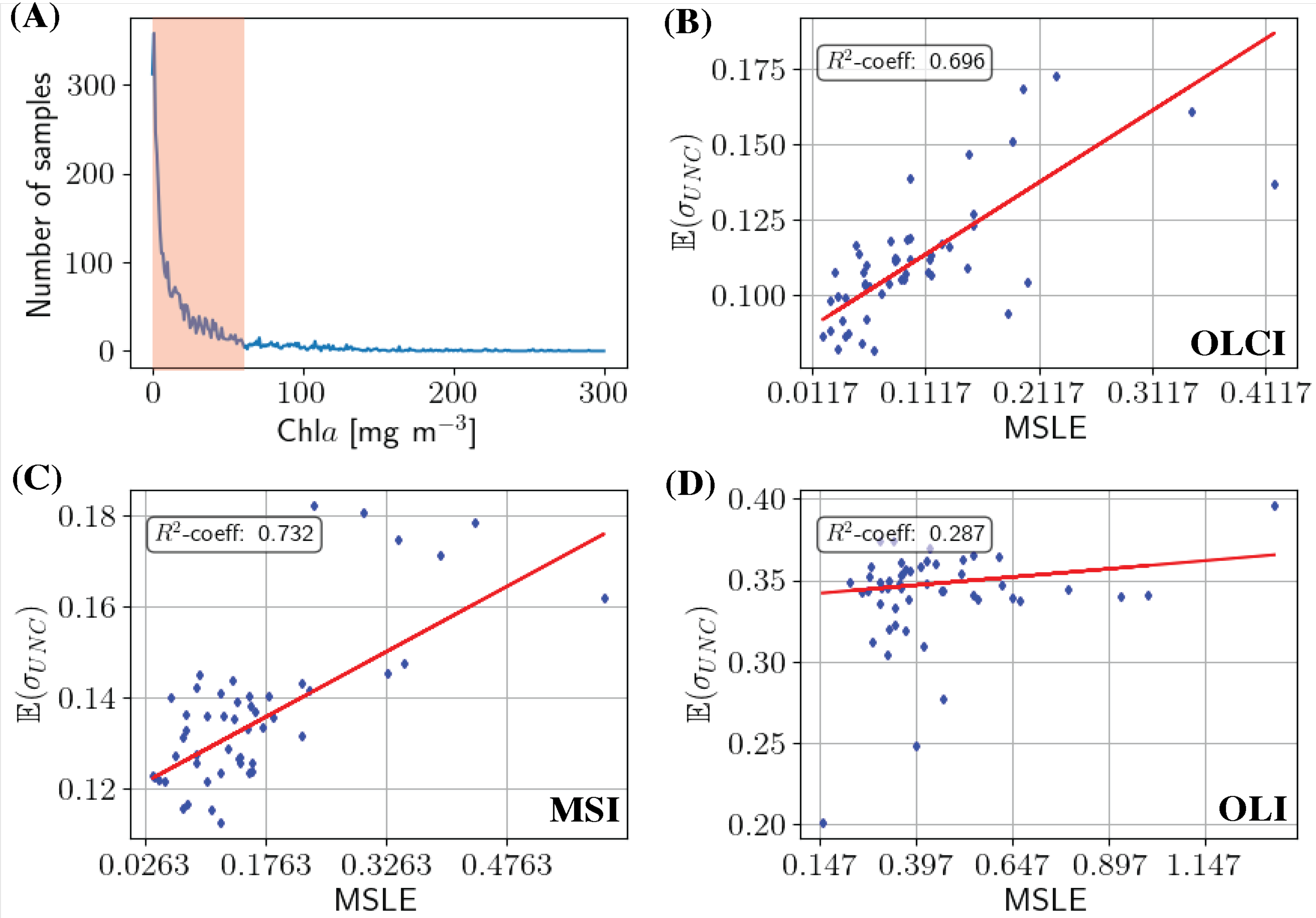
Uncertainty Metric dependance on Data



- The estimated uncertainty metric for samples in specific Chl*a* ranges clearly seems to depend on the number of training samples present in that range.

- The uncertainty metric scale seems very different from the predicted values.

Uncertainty correlation with predicted error



- Even for medium-resolution multispectral sensors there is clear correlation between error and uncertainty

MDN Model properties and Hyperparameters

<u>Data Preprocessing:</u>
Rrs: intra-quartile scaling
WQI: Log-Scaling + MinMax scaling [-1, 1]

Hyperparameter	Chosen Value	Comments
Layers	8	
Nodes/Layer	225	
# of Gaussian Components	5	
Activation	ReLU	
Layer L2-normalization	0.01	
Dropout	N/A	Experiments with this hyperparameter are ongoing
Epochs	250 epochs	
Batch Size	128	
Imputation	Dynamic	Fills in best value based on current model state.

Missing value have no effect of the estimated gradient.

References

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7. E. J. Kwiatkowska and G. S. Fargion , 2003, "***Application of machine-learning techniques toward the creation of a consistent and calibrated global chlorophyll concentration baseline dataset using remotely sensed ocean color data***," IEEE Transactions on Geoscience and Remote Sensing, vol. 41, no. 12, pp. 2844–2860.

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10. Saranathan, A.M., Smith, B. and Pahlevan, N., 2023. "***Per-pixel uncertainty quantification and reporting for satellite-derived chlorophyll-a estimates via mixture density networks***". *IEEE Transactions on Geoscience and Remote Sensing*.