# Neural Network Development for Radiative Transfer Model Simulation

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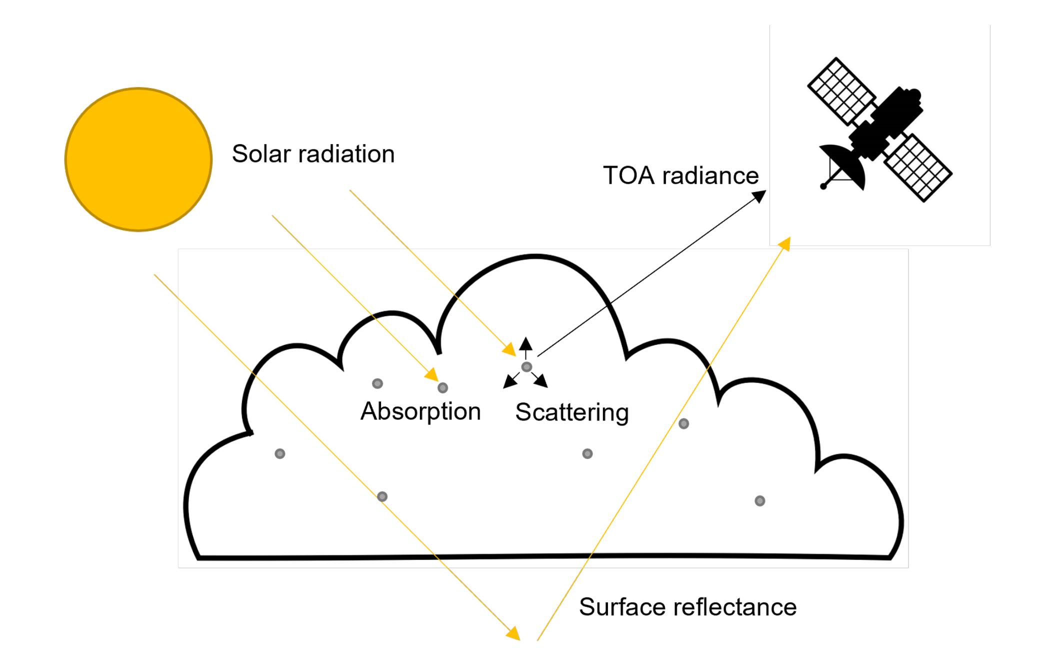
## Introduction

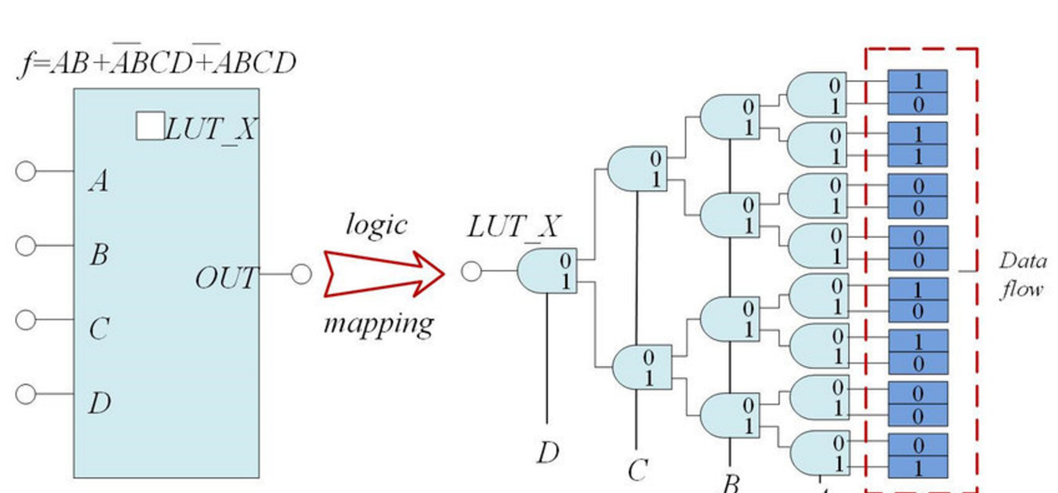
- Satellites observe the top of atmosphere (TOA) solar radiation reflectance to retrieve the characteristics of Earth's atmosphere.
- This retrieval is done using a look-up table (LUT) simulated by a radiative transfer model to show the quantitative dependence of TOA radiation on atmospheric parameters (e.x. aerosol optical depth, $CO_2$ concentration).
- Analyzing massive amounts of satellite data (well above millions of datapoints) requires a fast and efficient retrieval algorithm.
- A LUT strongly prefers linearity when retrieving data since any intermediate datapoint must be interpolated.
- In this work a neural network (NN) was trained on the LUT to be used as its replacement in the retrieval algorithm.
- Neural networks are highly non-linear by nature and do not require interpolation.
- Neural networks also offer improvements in the speed of the retrieval algorithm through a quicker prediction process allowing for near real-time applications and more timely predictions.

## Methodology

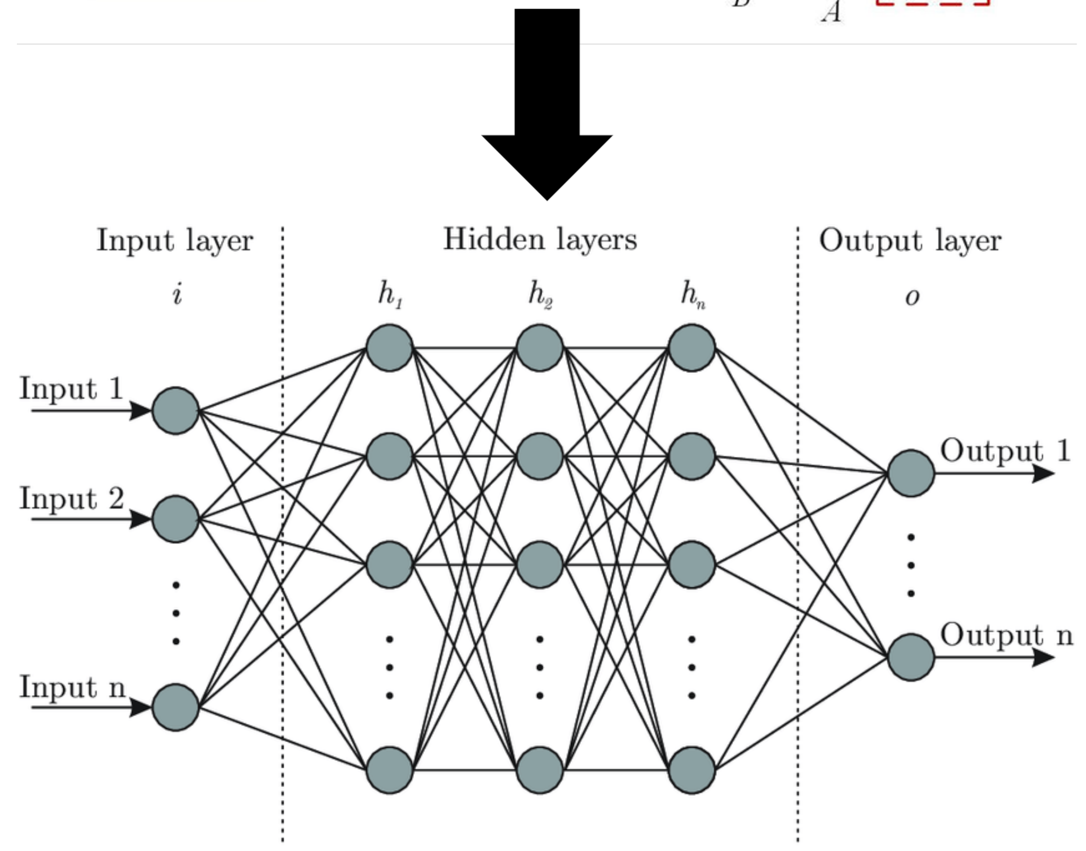
- UNL-VRTM was used to simulate this radiative transfer process and generate a LUT to relate atmospheric parameters to the satellite observed TOA reflectance.
- Atmospheric parameters used in the simulation process were:
  - Surface pressure
  - Surface reflectance
  - Aerosol optical depth
  - Height
  - Viewing zenith angle
  - Solar zenith angle
  - Relative azimuth




- TOA reflectances were considered at the following wavelengths:
  - R443
  - R551
  - R680
  - Ratio of R688/R680
  - Ratio of R764/R780
  - R780
- These values were used as targets, or tasks, for a feedforward neural network, and the atmospheric conditions related to those TOA reflectances were used as the input features.

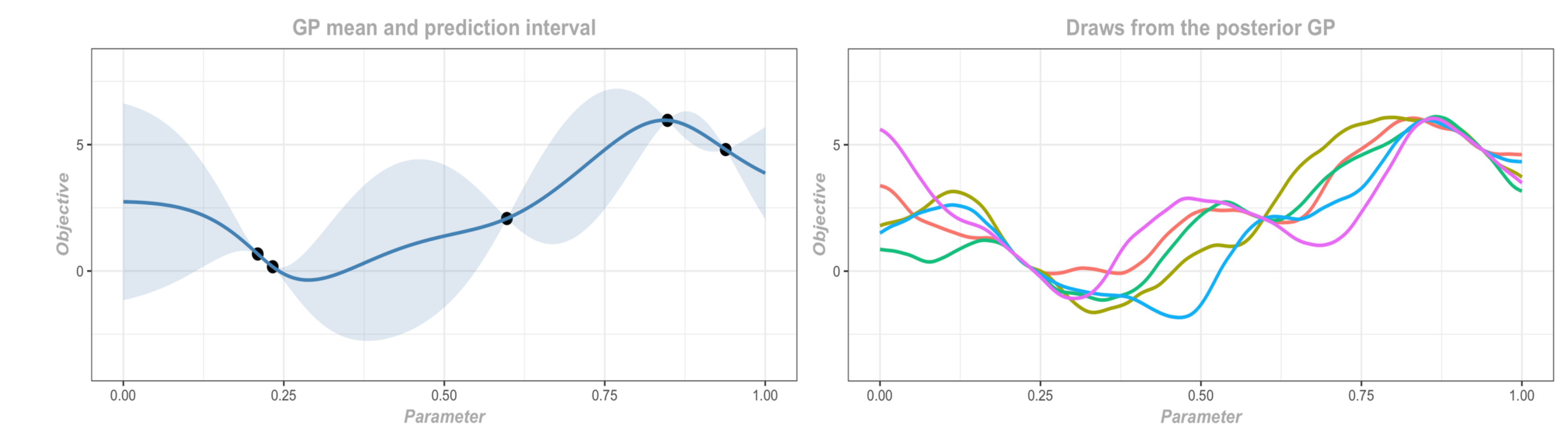



- A multitask neural network was trained to predict TOA reflectance at all wavelengths and ratios considered with the same output. Additionally, single task models were trained to predict each task as a single output.

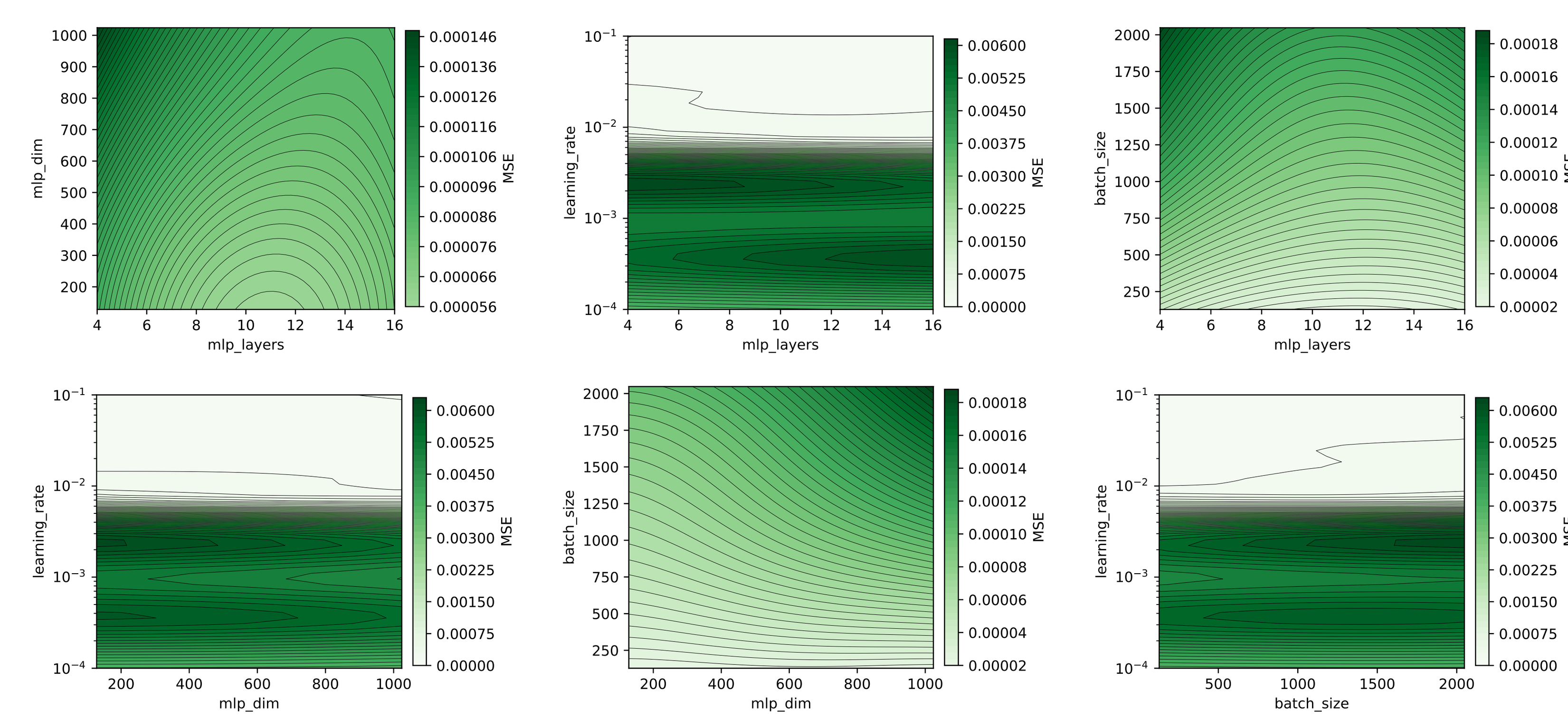



## Hyperparameter Optimization

- Neural network hyperparameters were tuned using Bayeisan optimization for both the single task and multitask models.
- Hyperparameter model evaluation was performed on a validation dataset withheld from model training.
- Bayesian optimization was implemented using the Ax Experimentation Platform.
- A surrogate model of model performance is created from a Gaussian process based on previous observations.
- Parameters are selected from the surrogate model allowing for informed exploration of parameter space and reducing the number of models that must be trained compared to methods like grid searching.




- Results and parameters selected from each trial during optimization can be saved and plotted.
- Models were optimized to improve mean squared error (MSE)
- Optimized model configurations saw massive improvements in performance.
- The average MSE of the top 5 scoring models run was 1.6E-5 compared to an average of the lowest 5 of 5.6E-3
- Contour plots of performance allow insight into parameter spaces and relationships, allowing for informed experiment design.




## Future Work

- Replacement of the LUT currently being used in the retrieval algorithm with the NN model.
- Implementation of an end-to-end GPU-accelerated retrieval using NN model to improve speed.
- Improvement of other components of the overall retrieval algorithm, such as cloud masking, using machine learning methods.

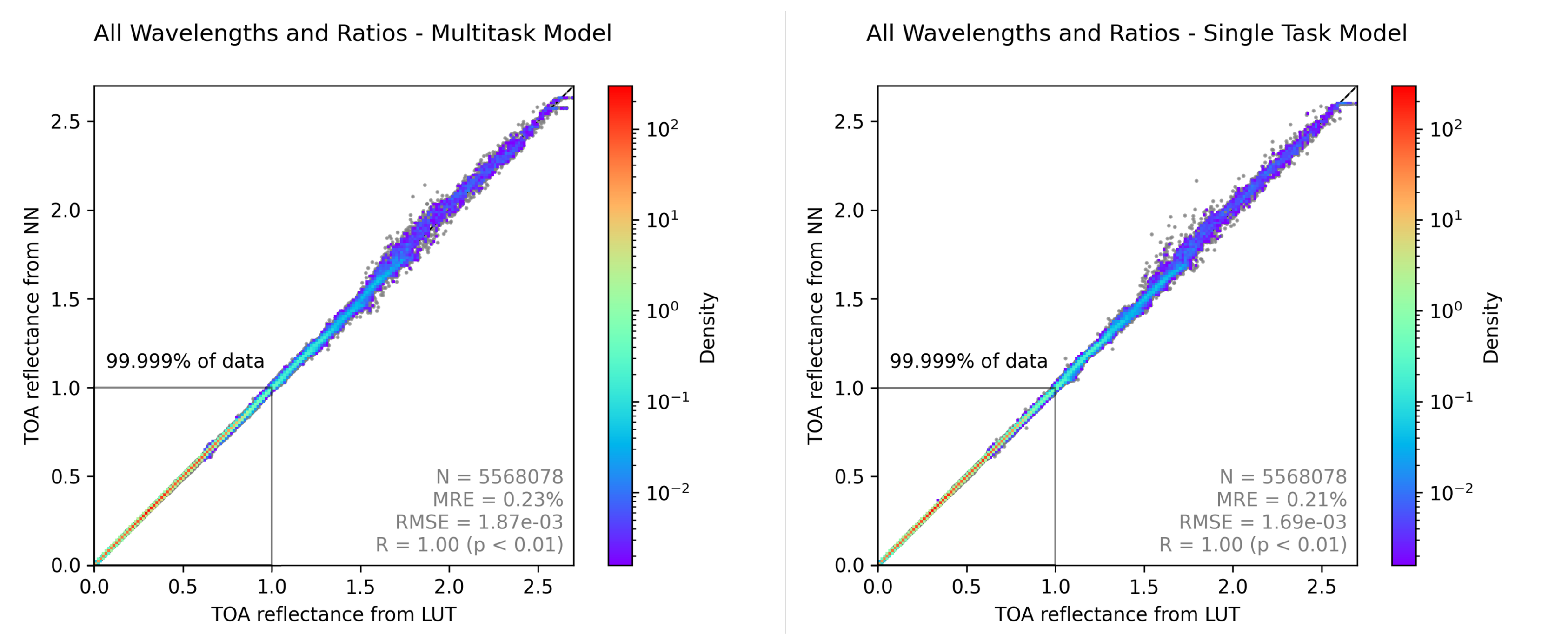
## Acknowledgements

- I would like to thank Xi Chen, Joseph Gomes, and Jun Wang for their invaluable guidance and support in this project, offering advice and assistance when needed and facilitating my development.
- This work was supported by Infrastructure for Data-Advanced Research and Education (I-DARE) and the Iowa Space Grant Consortium. Thank you for allowing me to pursue my academic interests beyond the classroom.

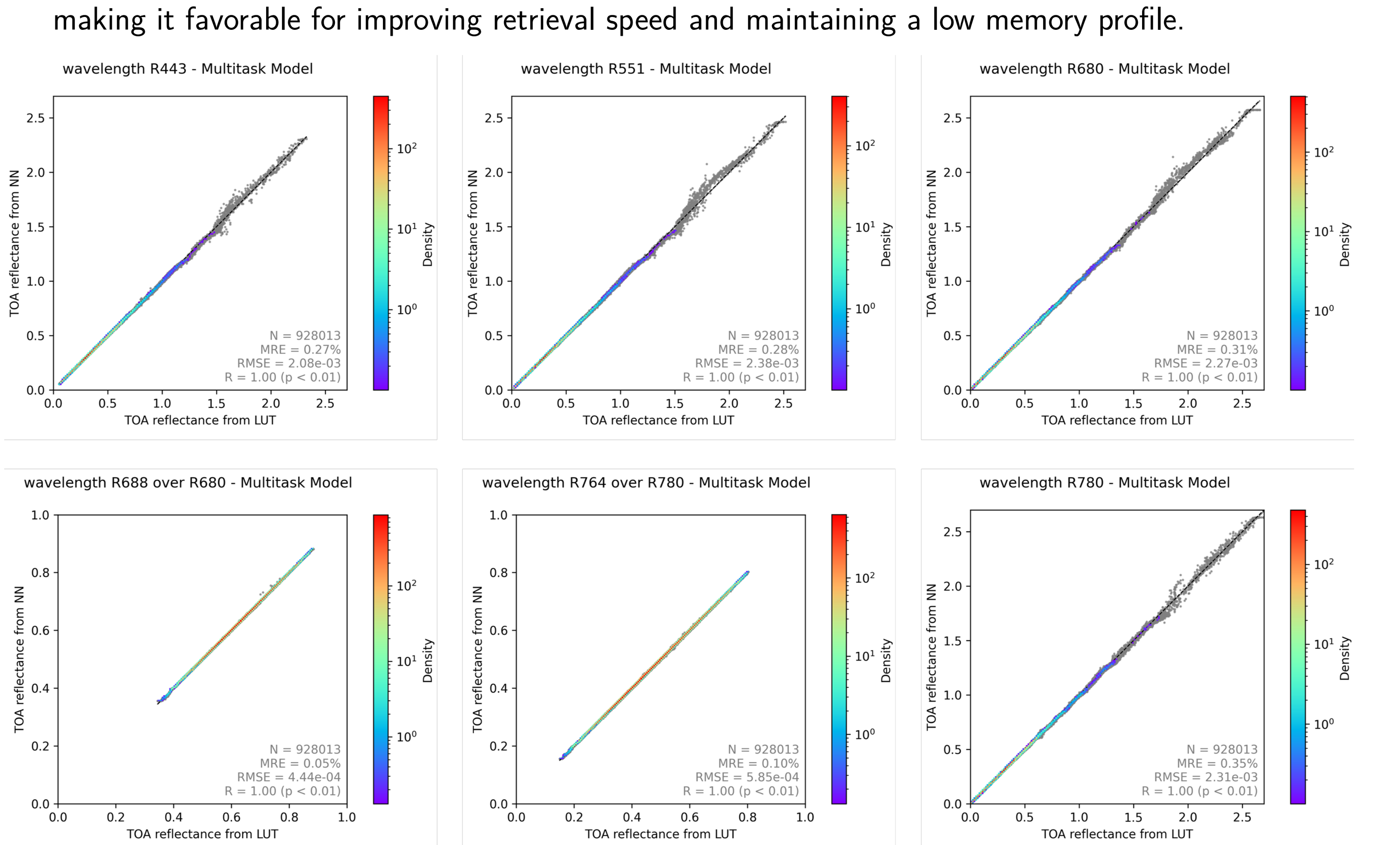
## Model Performance

- Models were evaluated on a testing set withheld from both training and hyperparameter optimization.
- Single task and multitask model performance broken down by individual task and combined performance.

| Prediction task | Multitask model MSE | Single task model MSE |
|---|---|---|
| R443 | 4.33E-6 | 4.49E-6 |
| R551 | 5.66E-6 | 3.72E-6 |
| R680 | 5.15E-6 | 3.50E-6 |
| R688/R680 | 1.97E-7 | 1.83E-7 |
| R764/R780 | 3.42E-7 | 4.40E-7 |
| R780 | 5.34E-6 | 4.84E-6 |
| All tasks | 3.50E-6 | 2.86E-6 |




- All tasks had very similar performance across both models, and there was a difference of only 6.4E-7 between their combined MSE score across all tasks.
- Use of a multitask model only requires loading one NN, and evaluating once to predict all tasks, making it favorable for improving retrieval speed and maintaining a low memory profile.




- It can be observed that above TOA reflectances of 1, the model produces less accurate results. This is due to the scarcity of datapoints at those high TOA values.
- The same scarcity causing the predictions to scatter causes them to have a fairly negligible impact on the overall model performance.
- Each task in the multitask model had a good individual performance, the combined score was not smoothing out any poor performers.
- The results are accurate enough to indicate the model is fit to serve as a functional replacement in the overall retrieval algorithm.