Ensembles of Neural Surrogates for Parametric Sensitivity in Ocean Modeling

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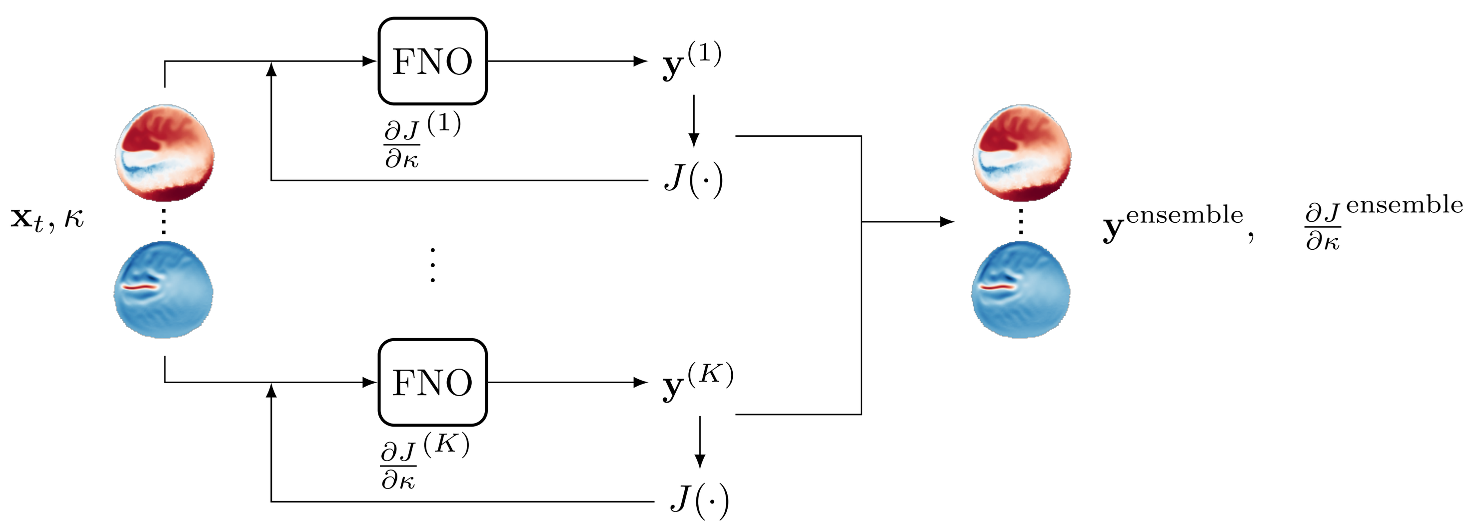
Motivation

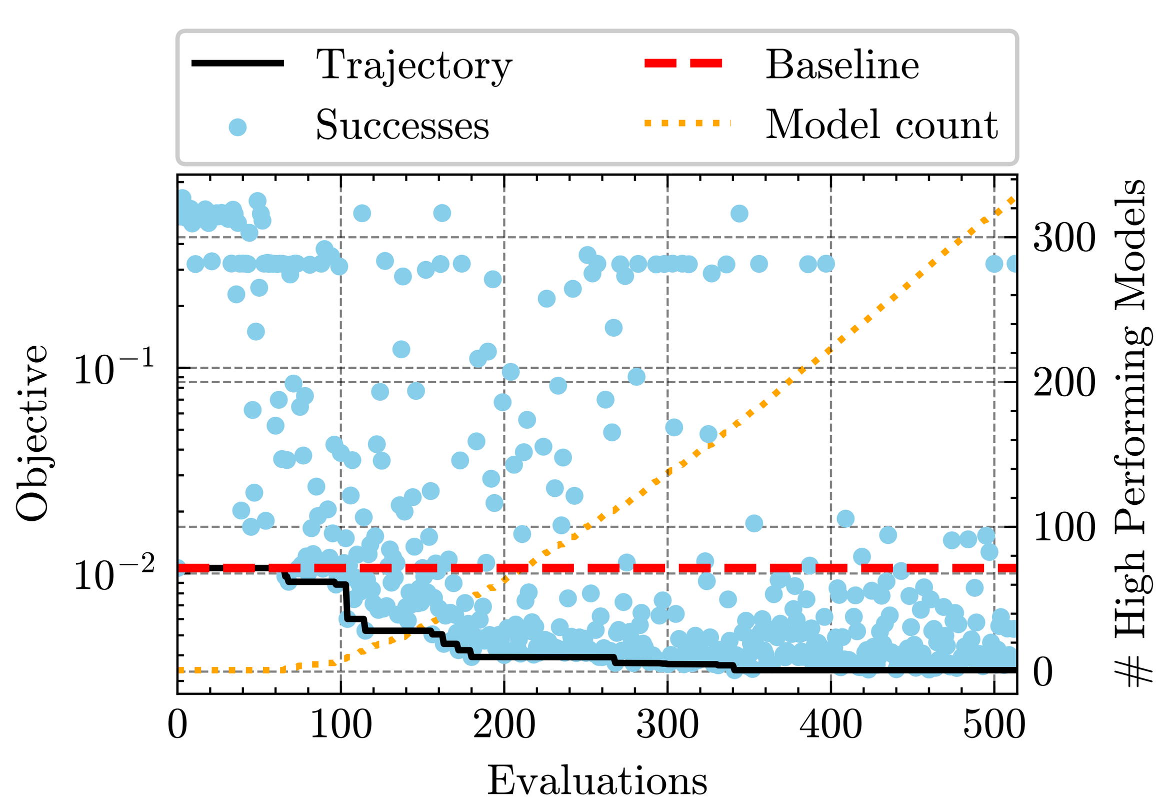
Ocean simulations at lower resolutions must rely on various *uncertain parameterizations* to account for unresolved processes. However, model sensitivity to parameterizations is difficult to quantify, making it challenging to tune these parameterizations *to reproduce observations*. Deep learning surrogates have shown promise for efficient computation of the parametric sensitivities in the form of partial derivatives, but their *reliability is difficult to evaluate* without ground truth derivatives. We propose an ensemble learning framework to improve both the function value predictions and its derivative estimates.



Ocean State Forecasting

We build an ensemble of neural surrogates constructed from a large-scale hyperparameter optimization (HPO) using DeepHyper. The ensemble improves both the forward prediction performance and derivative estimates.

- Form ensembles with two weighting schemes using the top models from the HPO.
- Improve the forward single-stepping predictions compared to the baseline model and best model from the HPO for all five ocean states investigated.

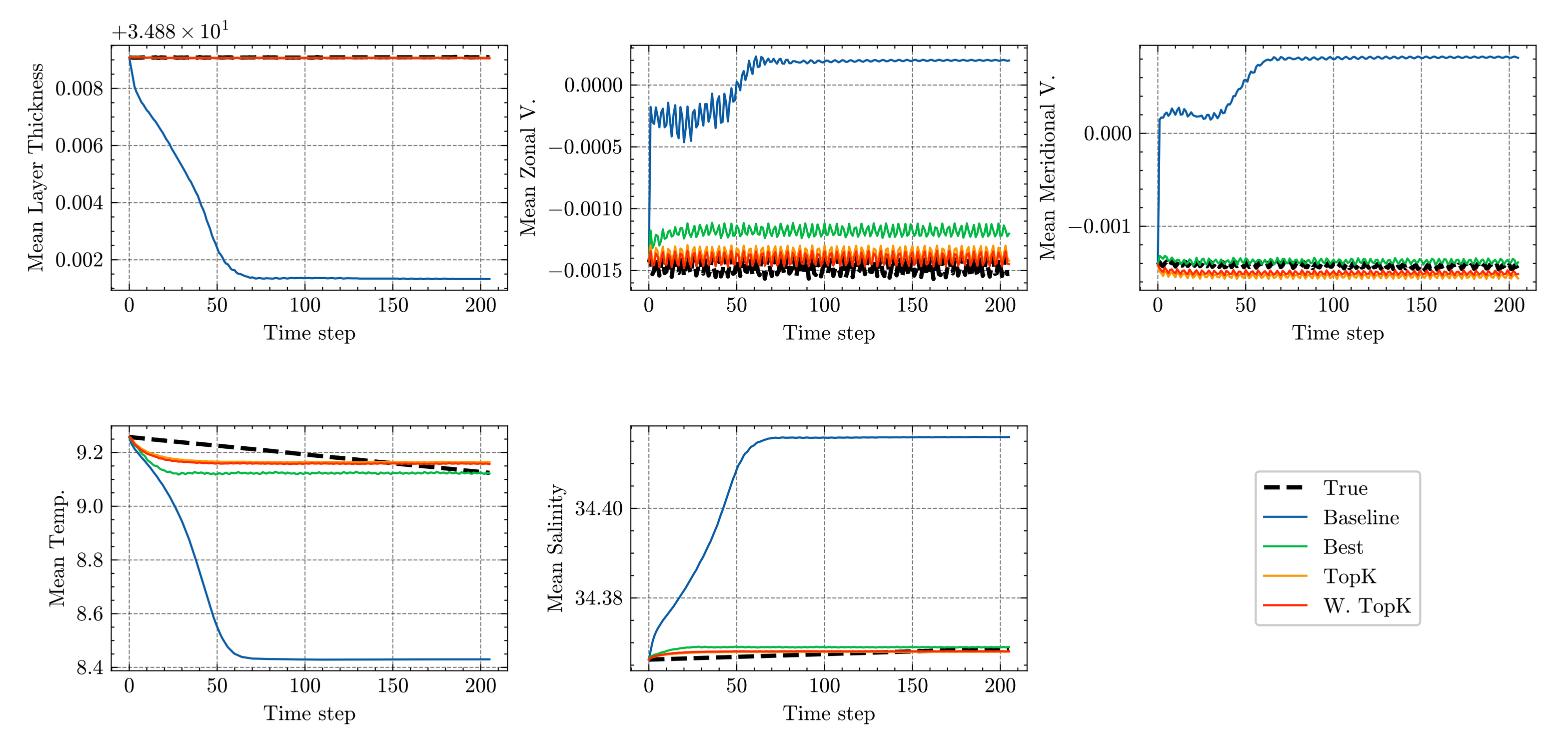


Hyperparameter search trajectory. Starting with the baseline configuration, the search balances the exploration and exploitation which leads to increasingly better models depicted by the solid black line. The number of high performing models increases accordingly.

Table 1: RMSE (↓) of single step forward predictions.

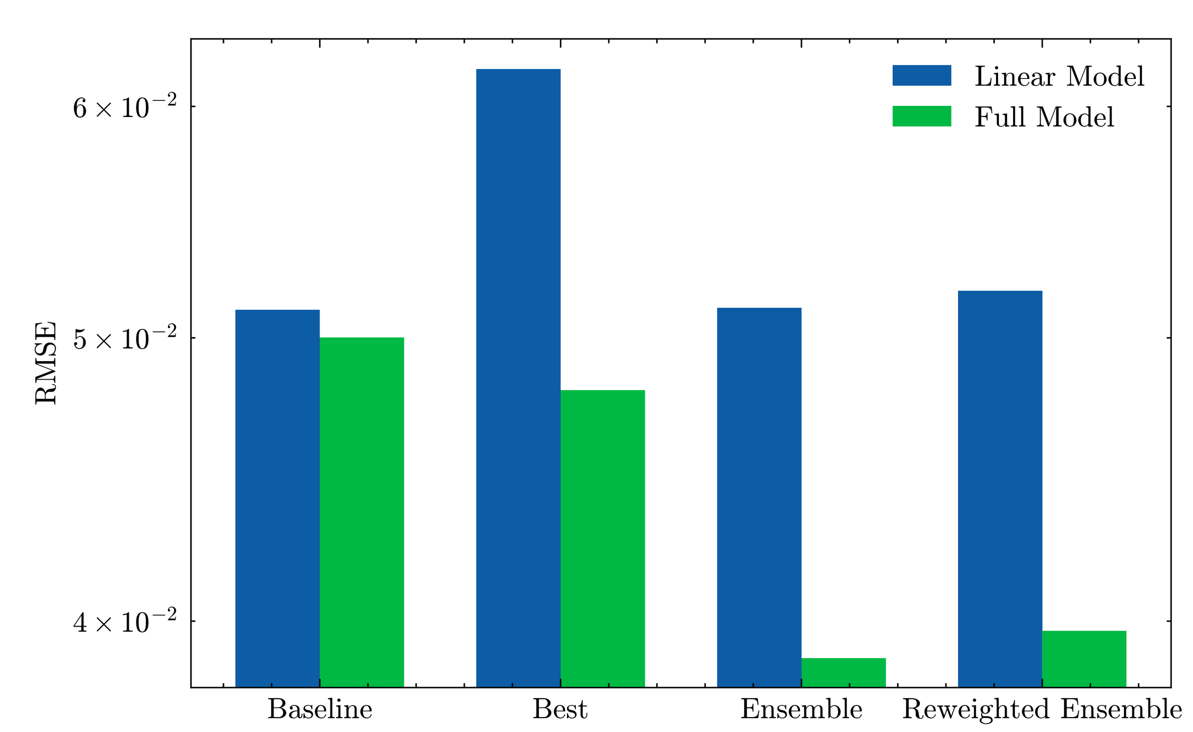
	Constant Pred.	Baseline	Top-1	Top10 Ensemble
Layer Thickness	**0.0004**	0.0011	0.0008	**0.0004**
Zonal V.	0.0122	0.0022	0.0024	**0.0016**
Meridional V.	0.0075	0.0024	0.0019	**0.0013**
Temp.	0.3876	0.0494	0.0484	**0.0385**
Salinity	0.0072	0.0026	0.0024	0.0018

- Such superior accuracy in the single-stepping predictions results in more stable autoregressive rollouts for all five ocean states.
- Provides epistemic uncertainty of function value predictions and their derivatives, improving reliability of the neural surrogates in decision making.

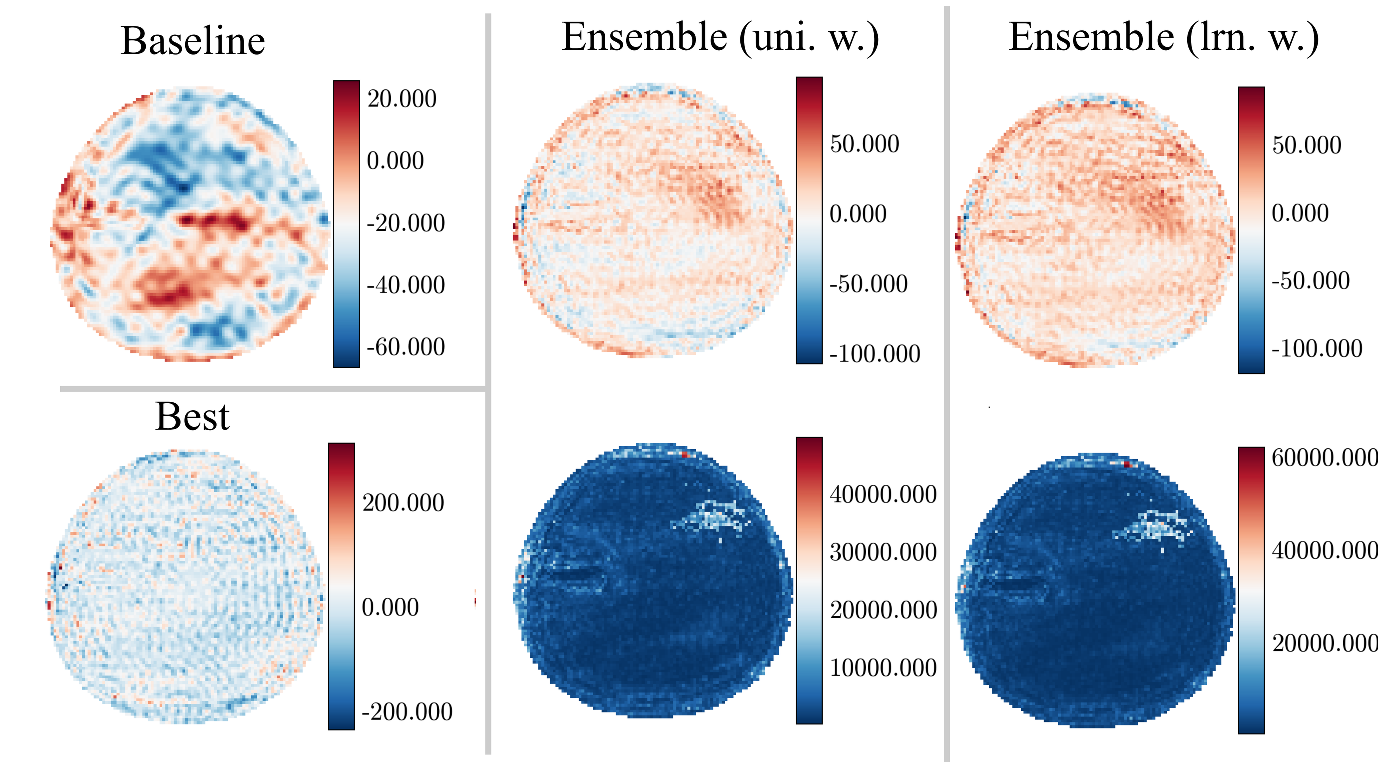


Autoregressive rollout performance comparisons among the three models. The curves are the spatially averaged ocean states for 8 years. For the baseline model, the forecasts quickly diverge from the true state due to error accumulation, whereas the ensembles generate stable prediction for all ocean states.

Parametric Sensitivity



RMSE of the temperature predictions from linearized models. We indirectly validate the estimated sensitivity using the linearized models to make predictions for nearby points. We expect the model having a better sensitivity estimation to produce a more accurate linear model.



Time averaged model estimated sensitivity of J calculated using the temperature fields to κ.

- Demonstrate that a model accurate for forward function values may still be inaccurate in its derivative estimates.
- Through linearization, the ensemble framework shows a better estimated first order derivatives compared to the best single model from the HPO, while maintaining the lowest errors in forward predictions.

Conclusion

- Improves both forward predictions and derivative estimates without requiring ground truth sensitivities.
- Potentially enables systematic exploration and calibration of parameterizations in low-resolution ocean simulations.
- Promise to helps reduce biases in parameterized eddy effects, improving the fidelity of large-scale ocean and climate models.
- Accelerates the optimization and calibration workflow, making it easier to align simulations with observations.
- Provides a generalizable framework for constructing neural surrogates that are consistent in both function and derivative estimation.
- Enhances the trustworthiness of machine learning–based emulators for scientific discovery and policy-relevant climate projections.

Future Directions

- Extend the framework to multiple parameterizations, allowing simultaneous treatment of several parameterizations determining the ocean dynamics at mesoscales.
- Evaluate sensitivities via numerical differentiation of the physical model, providing a reference to validate neural surrogate–based derivatives in the absence of analytic ground truth.
- Incorporate data assimilation approaches to integrate observational constraints, further refining both forward predictions and sensitivity estimates.
- Broaden applicability beyond ocean modeling, exploring the use of this framework in other climate and Earth system components where parameterization uncertainties are significant.