

Ensembles of Neural Surrogates for Parametric Sensitivity in Ocean Modeling

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Background

Parametric sensitivity in ocean modeling

- Lower-resolution ocean models depend on uncertain parameterizations.
- Model sensitivity to these parameters is difficult to quantify.
- Manual tuning to match observations is computationally prohibitive.

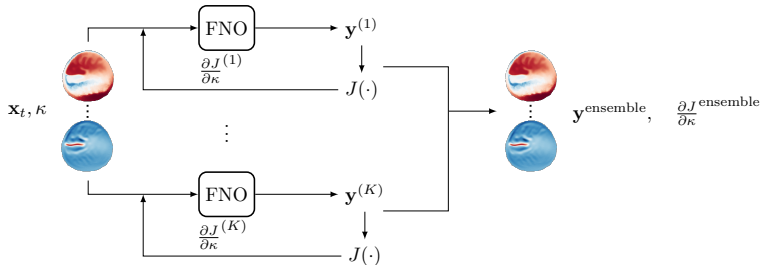
Neural network surrogates offer a promising alternative.

- Deep learning surrogates can efficiently approximate model responses and parametric sensitivities via automatic differentiation.
- However, their reliability is unclear due to the lack of ground truth derivatives to regulate training.

Proposed Method

Deep ensemble framework

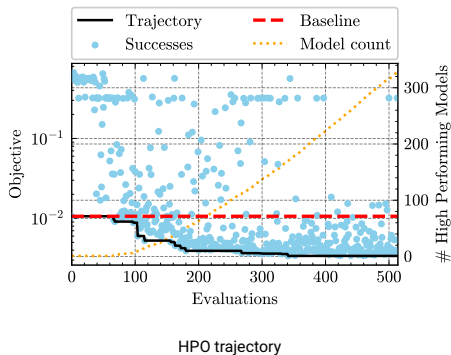
- Large-scale hyperparameter search for ensemble construction
- Ensemble aggregation for improved forward prediction and sensitivity estimation



Overview of deep ensemble of Fourier Neural Operators (FNOs) for ocean parametric sensitivity. We train individual models with diverse hyperparameters to produce time-stepping predictions and parametric sensitivities. We aggregate these outputs to produce ensemble predictions of future ocean states and estimates of the partial derivative of objective J w.r.t. the parameterization κ .

Improved Forward Prediction Performance

- We build an ensemble of neural surrogates from large-scale hyperparameter optimization (HPO) using DeepHyper.
- Ensembles are formed with two weighting schemes: uniform and learned weights.
- Both ensemble types outperform the baseline and best single model across all five ocean states.

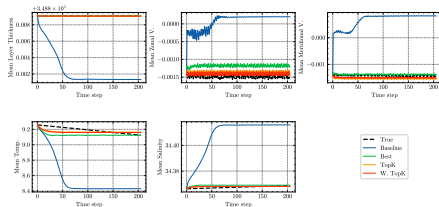


RMSE ($\downarrow$) of single step forward predictions.

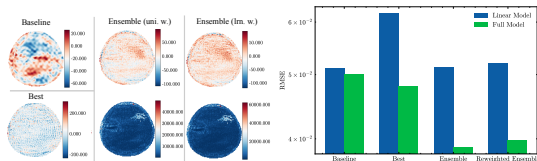
	Constant Pred.	Baseline	Top-1	Top10 Ensemble	Top10 Ensemble (weighted)
Layer Thickness	0.0004	0.0011	0.0008	0.0004	0.0004
Zonal V.	0.0122	0.0022	0.0024	0.0016	0.0016
Meridional V.	0.0075	0.0024	0.0019	0.0013	0.0013
Temp.	0.3876	0.0494	0.0484	0.0385	0.0392
Salinity	0.0072	0.0026	0.0024	0.0018	0.0017

Improved Derivative Estimates and Stability

- Ensembles yield more stable autoregressive rollouts across all ocean states.
- Provide *epistemic uncertainty* in both function and derivative predictions.
- Show that accuracy in forward prediction does not guarantee accuracy in derivatives.
- Linearizing validates the ensembles yield better derivative estimates while maintaining lowest forward errors.



Rollout performance comparison



Sensitivity estimates & linearized models

Key Takeaways

- Proposed a deep ensemble framework for improved parametric sensitivity estimation in ocean models.
- Built ensembles from top-performing HPO models using two weighting strategies.
- Evaluated on single-step prediction, long-range rollout, and sensitivity estimation tasks.
- Outperformed both baseline and best single models across all evaluations.
- Provided uncertainty quantification alongside accurate predictions and sensitivities.

Future work: extend to multiple parameterizations and validate sensitivities via numerical differentiation or data assimilation.