

Wifi ensembles for nsbi4hep

Nathan Kang

ANL

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Introduction

- ▶ Opened PR for the refactoring and HPO enhancements I worked on at

<https://github.com/hep-cce/nsbi4hep/pull/2>

- ▶ Working on implementing wifi ensembling (<https://arxiv.org/abs/2506.00113>) based on the example from ML4FP ensembling tutorial <https://github.com/ml4fp/2025-lbnl/blob/main/sessions/day2/ensembling-tutorial/ensembling.ipynb>

Ensemble training

- ▶ Train N models (f_i) with identical hyperparameters but bootstrap resample the training dataset based on different random seeds
- ▶ Implemented within the framework by re-using part of the Ray Tune machinery for the HPO, but instead we scan over different seeds while keeping model parameters the same between trials; makes it straightforward to do the scaling to multiple GPUs/nodes for running the training for ensemble members in parallel

Example for job with 8 models running in parallel on 2 nodes x 4 GPUs

Trial status: 8 RUNNING

Current time: 2026-07-14 19:33:08. Total running time: 1min 30s

Logical resource usage: 16.0/128 CPUs, 8.0/8 GPUs (0.0/2.0 accelerator_type:A100)

Current best trial: a2127_00001 with val_loss=0.6926648020744324 and params={'member_seed': 43}

Trial name	status	member_seed	iter	total time (s)	val_loss
member_0	RUNNING	42	3	63.3497	0.692797
member_1	RUNNING	43	3	63.0916	0.692665
member_2	RUNNING	44	3	62.921	0.692797
member_3	RUNNING	45	3	63.0848	0.69278
member_4	RUNNING	46	3	61.4479	0.69303
member_5	RUNNING	47	3	61.0118	0.692761
member_6	RUNNING	48	3	60.5434	0.692712
member_7	RUNNING	49	3	61.739	0.692836

Weight fitting

- ▶ Now move to fit weights (w_i) for each of the models in the ensemble
- ▶ Added additional split for data in datamodule `wi_fit_size` besides train/val/test for doing the fit
- ▶ Minimize against symmetrized MLC loss (currently working on validating this part works properly)
- ▶ Still need to include the following steps for evaluating uncertainty
- ▶ Hopefully will be ready by the time I present on the framework at DPF next week