OAK RIDGE National Laboratory

Ensembles of Networks Produced from Neural Architecture Search

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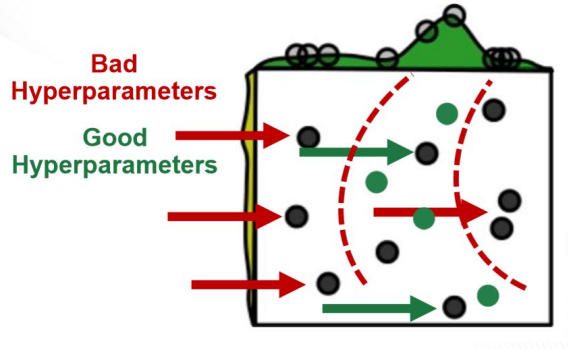
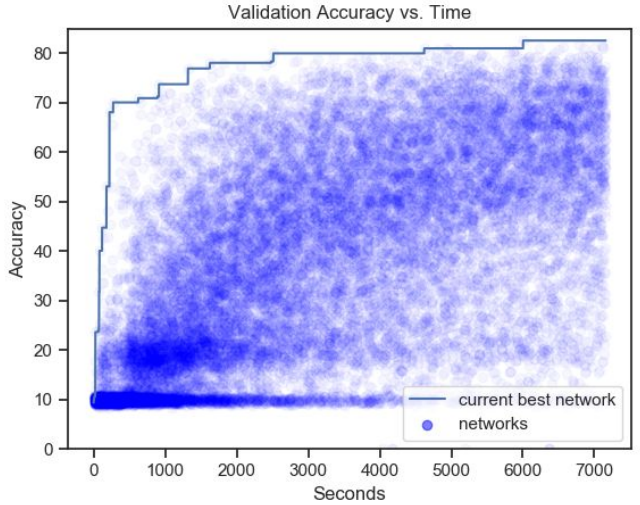
Problem Overview

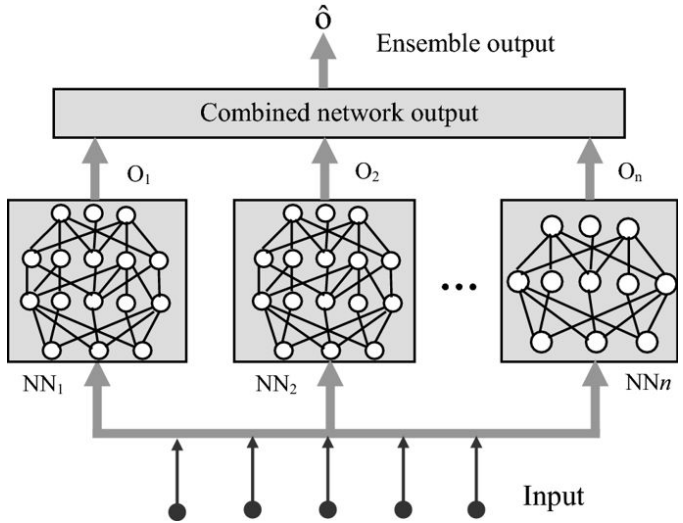
- Neural architecture search automatically designs neural networks for various challenges, focusing on single best network
- Single network with optimal performance may have limited knowledge of data distribution or over/under-fitted to training data.
- Many networks created & evaluated throughout NAS, providing opportunity to assemble network ensembles.
- Neural network ensembles combine outputs from neural networks with different parameters, offering improved prediction accuracies.





Problem Overview

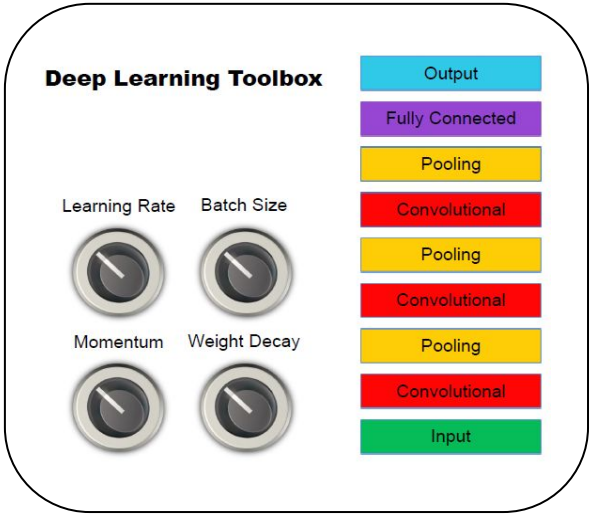
- We produced network ensembles with results from one or more runs of **M**ulti-node **E**volutionary **N**eural **N**etworks for **D**eep **L**earning (MENNDL)
- Two approaches considered and applied to two traditional image dataset benchmarks.
- We detail effects of ensembling networks from NAS method including:
  - Ensembles created from multiple instantiations of method.
  - Size of ensemble on performance.
  - Performance measured with accuracy & ensemble diversity.

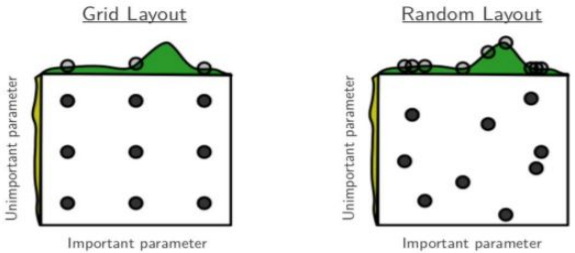


Alam, K, Siddique, N., Adeeli, H. A dynamic ensemble learning algorithm for neural networks, Neural Computing and Applications. Jul. 2019

Neural Architecture Search

- Features & learning capacity of deep convolutional neural networks (CNN) controlled by hyperparameters
- Tailoring architecture to data set is computationally expensive & time-consuming
- Hyperparameters traditionally selected manually or by grid or random search.
- We use MENNDL- evolutionary optimization approach to NAS
  - HPC framework that uses evolutionary algorithm to parallelize large-scale network evaluation.
  - Allows efficient hyperparameter search, by considering previous results, produces networks with increased accuracy & efficiency

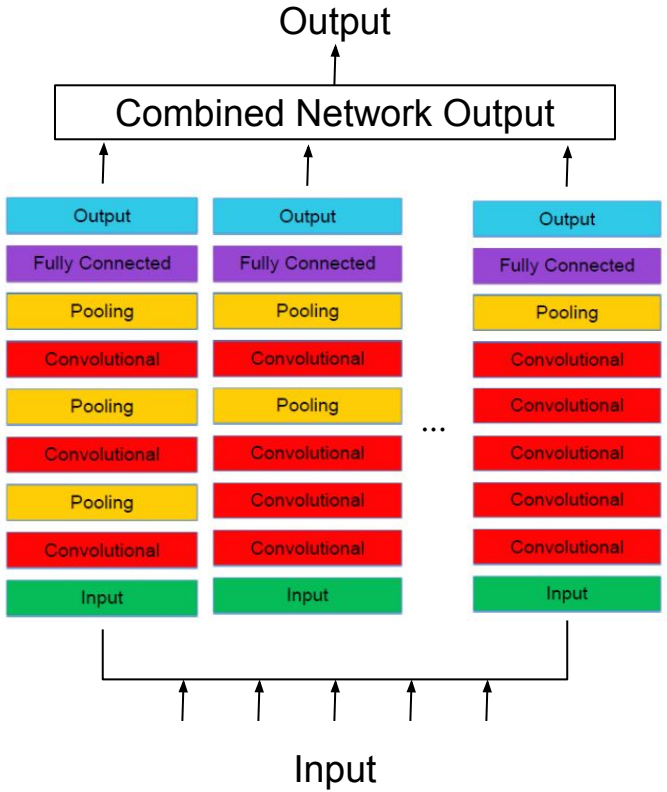




Bergstra, J, and Bengio, Y. Random Search for Hyperparameter Optimization, Journal of Machine Learning Research, Feb. 2012

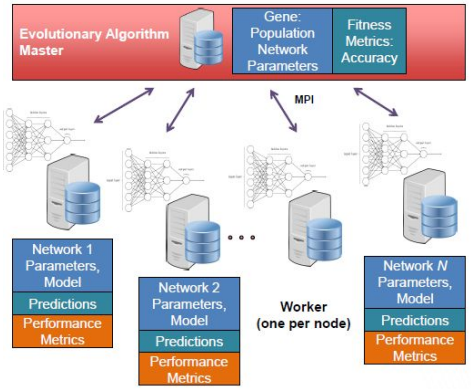
Neural Network Ensembles

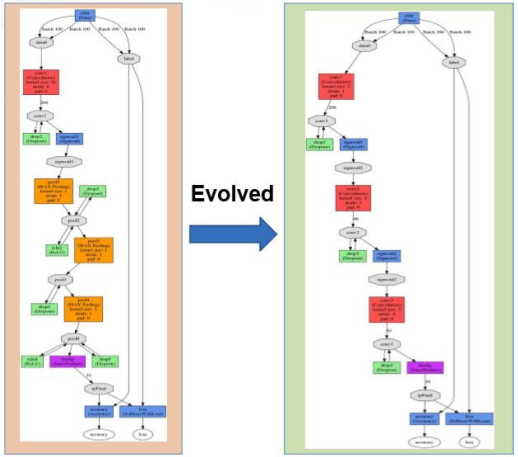
- Collection of neural networks trained on same task; results combined to produce model high generalization ability
- Successful deep learning models learn distribution of dataset; single models often overfit
- Network ensembles with different parameters and architectures learn varying aspects of training set
- Ensemble networks with randomly generated topologies, weights, or that learn random subsets of training data to encourage training error diversity.



MENNDL Overview

- **M**ulti-node **E**volutionary **N**eural **N**etworks for **D**eep **L**earning (MENNDL)- software framework that implements evolutionary algorithm for optimizing neural network topology & hyperparameters.
- Optimizes number of layers, layer type for each layer, and the corresponding layer hyperparameters.
- Utilizes asynchronous approach to evaluate the networks it generates in parallel in order to maximize utilization of leadership scale HPC





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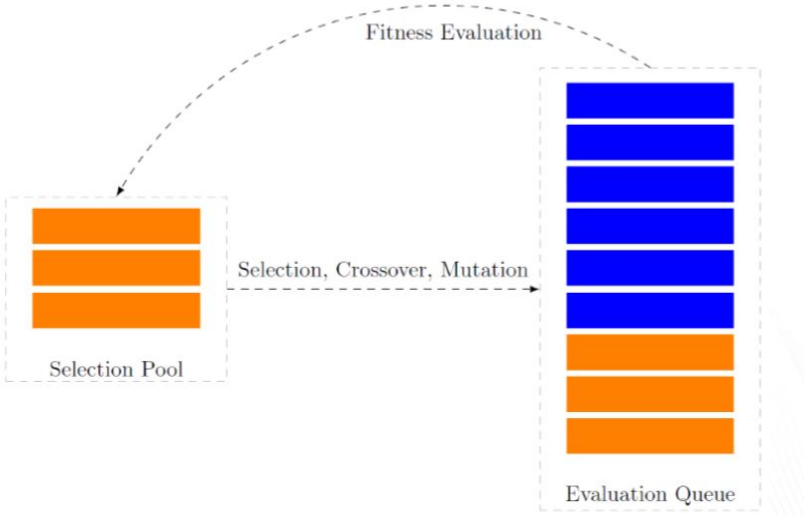
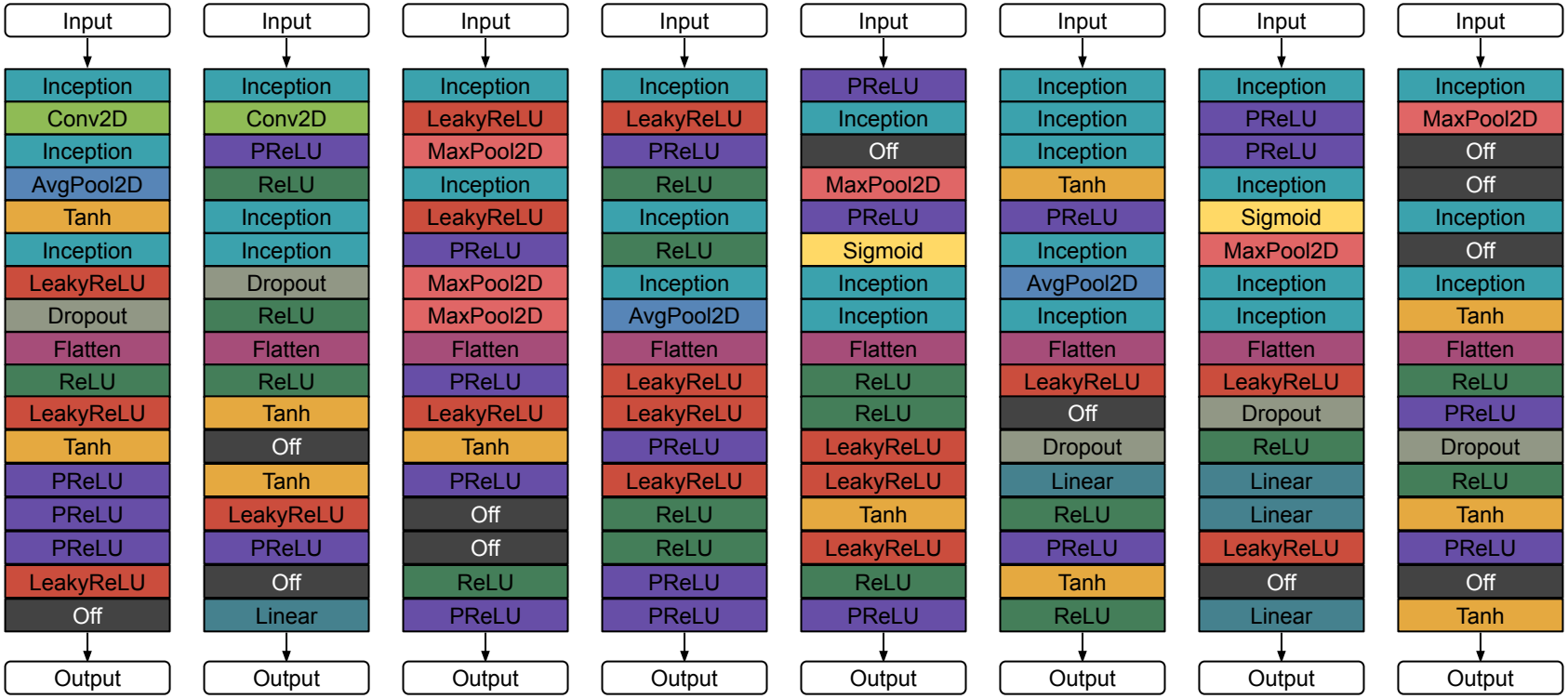
MENNDL

- Evolutionary algorithms mimic natural selection
  - Neural network population as individuals each with set of architectural hyperparameters or genes.
- Evolutionary algorithms are good for global search of spaces with many local minima.
- Basic evolutionary process:
  - Fitnesses of individuals in each generation evaluated (e.g. validation accuracy)
  - selection → mutation → crossover

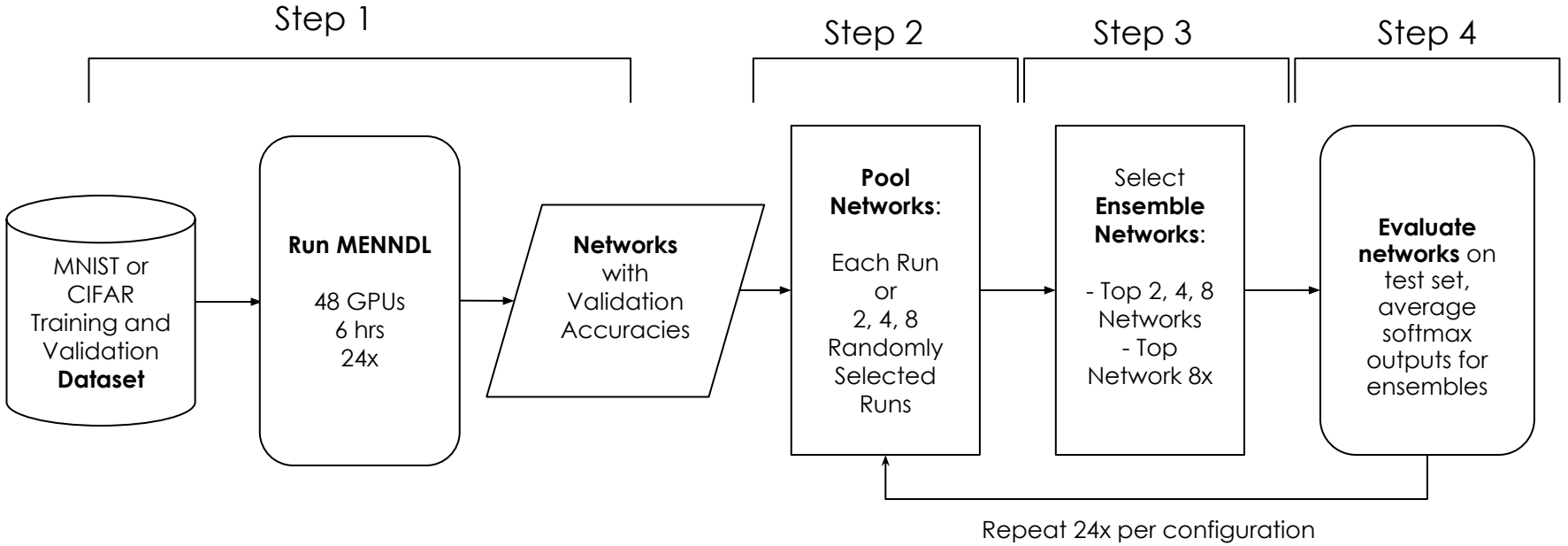
MENNDL Algorithm



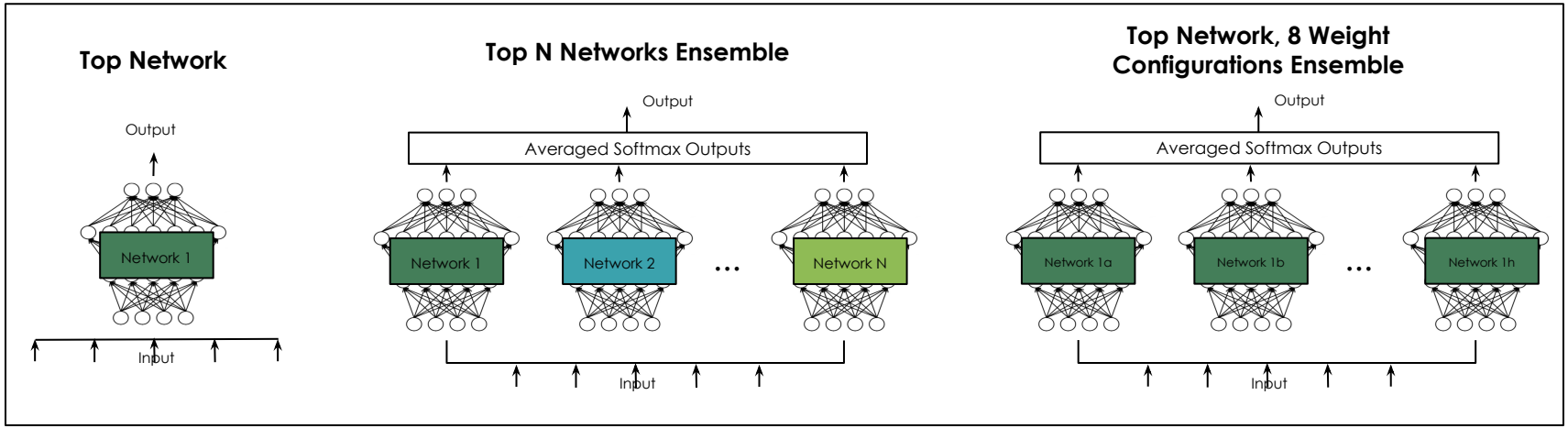
CIFAR-10 MENNDL Top Networks Runs 1-8

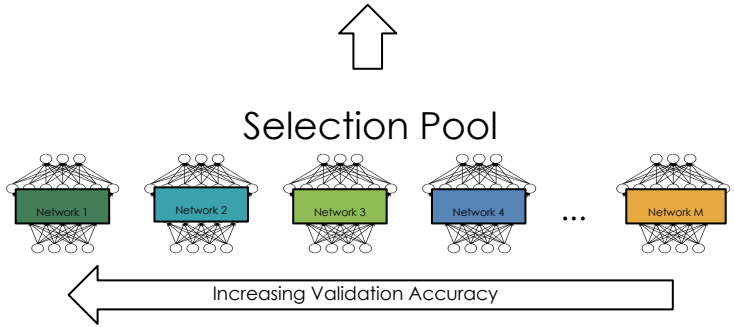


MENNDL Network Ensembles



Ensemble Configurations





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Measuring Ensemble Diversity

- Ensemble diversity measured by averaging total disagreement between predicted outputs for each sample
- Result is value that measures probability two networks in ensemble disagree with one another on given test sample.

Diversity Metric

$$d(p_i, p_j) = \frac{1}{m} \sum_{k=1}^{m} \psi(p_{ik}, p_{jk})$$

$$\psi(p_{ik}, p_{jk}) = \begin{cases} 0, & p_{ik} = p_{jk} \\ 1, & \text{otherwise} \end{cases}$$

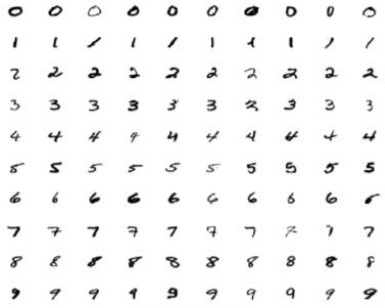
$$\frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} d(p_i, p_j)$$

Experiment Details

- Each MENNDL run and ensemble experiment carried out on Summit supercomputer at Oak Ridge National Laboratory
- System has 4608 nodes, each with 2 IBM POWER9 CPUs and 6 NVIDIA Volta GPUs

Datasets

- CIFAR-10 dataset consists of 10 classes of 60,000 32 by 32 multicolor images
- MNIST consists of 70,000 28 by 28 grayscale images of handwritten digits ranging 0 to 9
- Dataset samples normalized; no data augmentation
- 10% random training samples as validation set per network.
- Individual networks trained with batch size of 64 on remaining training samples.
- Networks evaluated on validation set to obtain fitnesses for selection
- Ensemble accuracies based on test sets



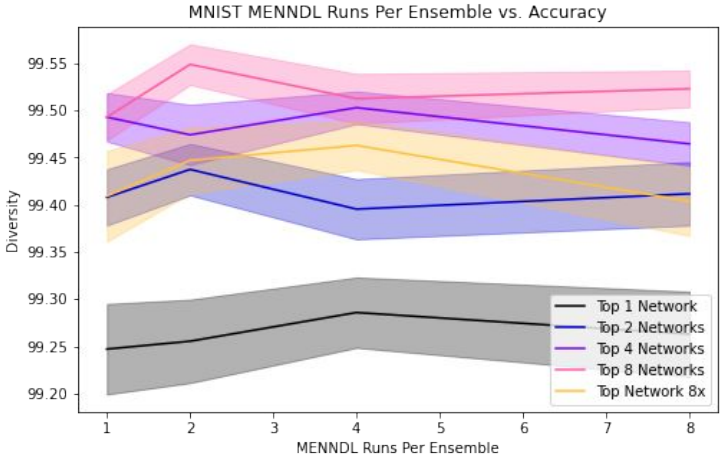
MNIST

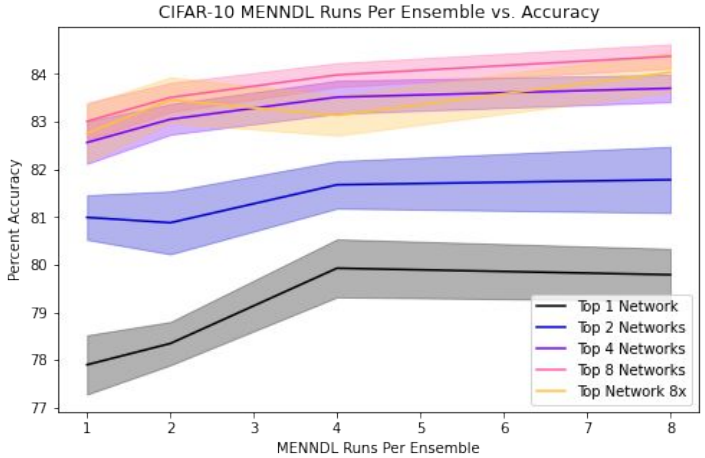
CIFAR

Results

MENNDL Run Statistics

Statistic	Dataset	
	MNIST	CIFAR-10
Total Networks	589.63±73.71	607.63±86.35
Generations	13.08±1.61	13.54±1.76
Best Network Fitness	99.33±0.10	78.47±1.26





- **Ensemble accuracies consistently higher when composed of more top networks**.
- Ensemble of top 2 networks offered significant accuracy improvements over individual networks.
- **Ensembles of top 2+ MENNDL runs improve upon generalizability of single best-performing network**.

Results

MNIST Mean Accuracy

MENNDL Runs	Ensemble Method				
	Top Network	Top 2 Networks	Top 4 Networks	Top 8 Networks	Top Network 8x
1	99.2471±0.1225	99.4079±0.0761	99.4929±0.0658	99.4929±0.0624	99.4092±0.1226
2	99.2554±0.1129	99.4375±0.0697	99.4742±0.0815	**99.5487±0.0550**	99.4471±0.0897
4	99.2858±0.0953	99.3954±0.0816	99.5029±0.0443	99.5125±0.0673	99.4629±0.0666
8	99.2629±0.1154	99.4117±0.0860	99.4646±0.0587	99.5229±0.0500	99.4038±0.0933

CIFAR-10 Mean Accuracy

MENNDL Runs	Ensemble Method				
	Top Network	Top 2 Networks	Top 4 Networks	Top 8 Networks	Top Network 8x
1	77.9025±1.5848	80.9925±1.2150	82.5629±1.1345	83.0067±0.9954	82.7583±1.5473
2	78.3483±1.1599	80.8808±1.6867	83.0500±0.8213	83.5075±0.7859	83.4538±1.2226
4	79.9271±1.5532	81.6767±1.2697	83.5146±0.8869	83.9796±0.6361	83.1325±1.0810
8	79.7904±1.3920	81.7825±1.7717	83.6996±0.7334	**84.3708±0.6521**	84.0350±1.0589

- CIFAR-10 ensembles tended to achieve **higher accuracies with larger pools of runs**
- **MNIST ensembles did not**, likely result of low error rates
- Misclassification rate lower with MNIST, little room to add functionally diverse networks to ensemble while maintaining high classification rates

Results

- **Ensembles of top 8 networks** yielded **diversities consistently higher** than 8 retrained copies of top network
- **Decreasing diversity with increasing pool size is an artifact of the diversity metric penalizing agreement even when all networks get the correct answer**

MNIST

MENNDL Runs	Ensemble Runs			
	Top 8 Networks		Top Network 8x	
	Diversity	Accuracy	Diversity	Accuracy
1	0.0610±0.0059	99.4954±0.0536	0.0060±0.0012	99.4083±0.1242
2	**0.0073±0.0007**	**99.5262±0.0569**	0.0055±0.0014	99.4429±0.1129
4	0.0069±0.0006	99.5262±0.0585	0.0058±0.0013	99.4154±0.1126
8	0.0066±0.0006	99.5212±0.0348	0.0060±0.0013	99.4421±0.0826

CIFAR-10

MENNDL Runs	Ensemble Runs			
	Top 8 Networks		Top Network 8x	
	Diversity	Accuracy	Diversity	Accuracy
1	**0.2118±0.0199**	83.0267±1.0399	0.1804±0.0197	82.6771±1.5128
2	0.2008±0.0117	83.7908±0.5655	0.1736±0.0161	82.9808±1.3632
4	0.1885±0.0138	83.8854±0.9317	0.1656±0.0152	83.5458±1.2053
8	0.1777±0.0158	**84.2163±0.6691**	0.1647±0.0158	83.9296±1.1975

Summary & Future Work

- Ensembles of multiple different networks produce better results than best network produced by search method, even when multiple copies of best network retrained several times
- Increased diversity of ensemble network structure produces increased diversity in network predictions, leading to improved ensemble performance.
- As we have demonstrated the diversity of network structures improves performance, we will look to explicitly leverage this by evolving ensembles of networks in NAS approach instead of creating ensemble in post-process, allowing NAS to explicitly identify networks that complement each other

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Questions?