On the Effectiveness of Bayesian AutoML methods for Physics Emulators

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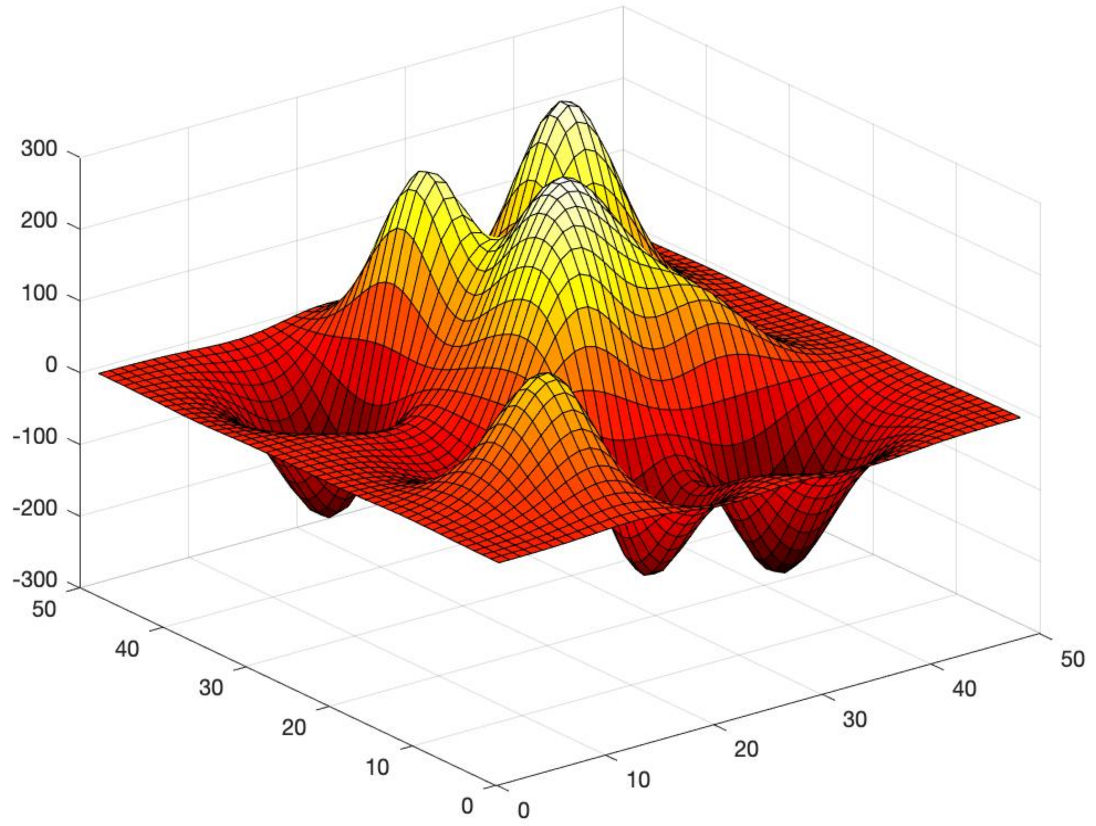
NEURAL INFORMATION PROCESSING SYSTEMS
ML4Eng Paper

Motivation

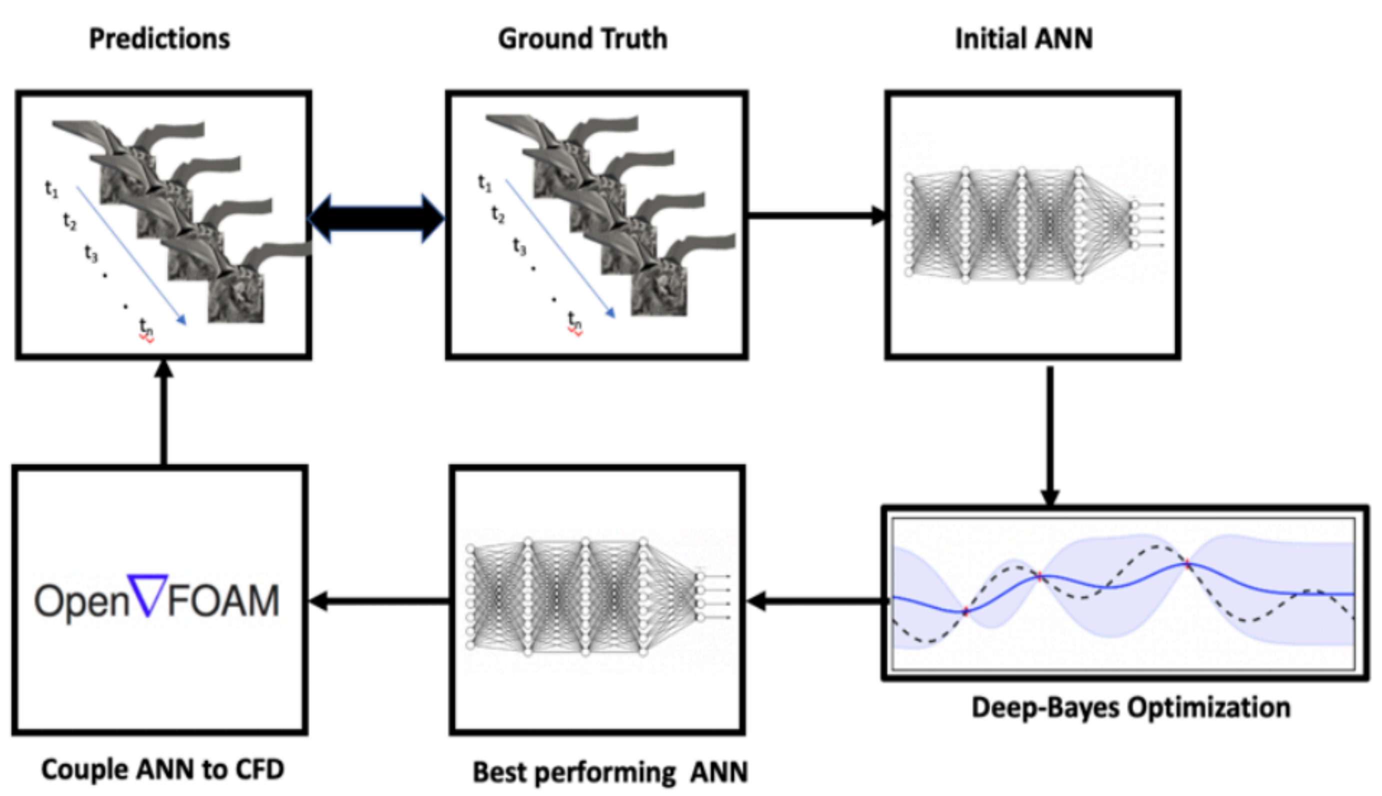
- Scientific data is often high-dimensional, complex, structured, sparse → Complicated loss manifold!
- Best practices in setting up network/hyperparameters translate poorly to scientific data
- Automatic ML methods are promising alternative to robustly train DNNs!



A translating, scaling Gaussian distribution-based loss manifold shows many peaks/troughs

Workflow

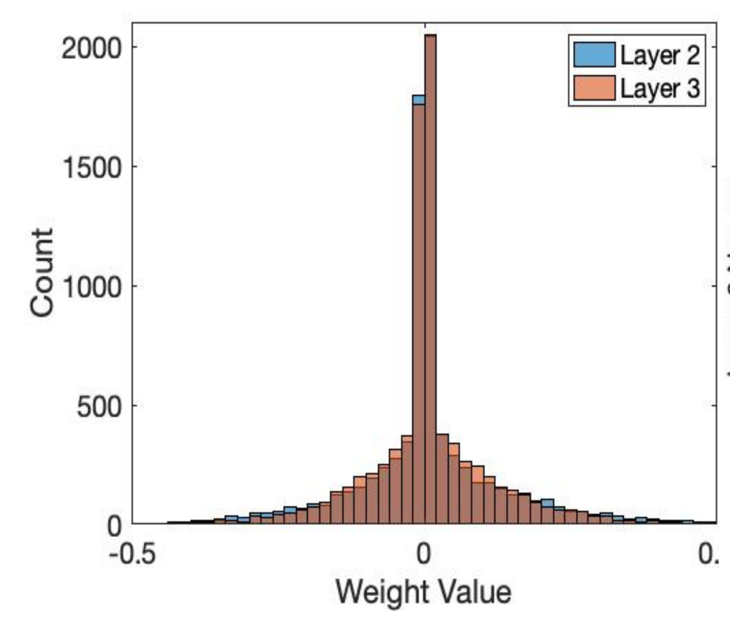
- Bayesian Optimization based AutoML explores parameter space to identify best performing settings, starting with an initial guess
- BayesOpt modeled as Gaussian Process (GP) with Expected Improvement (EI) acquisition function

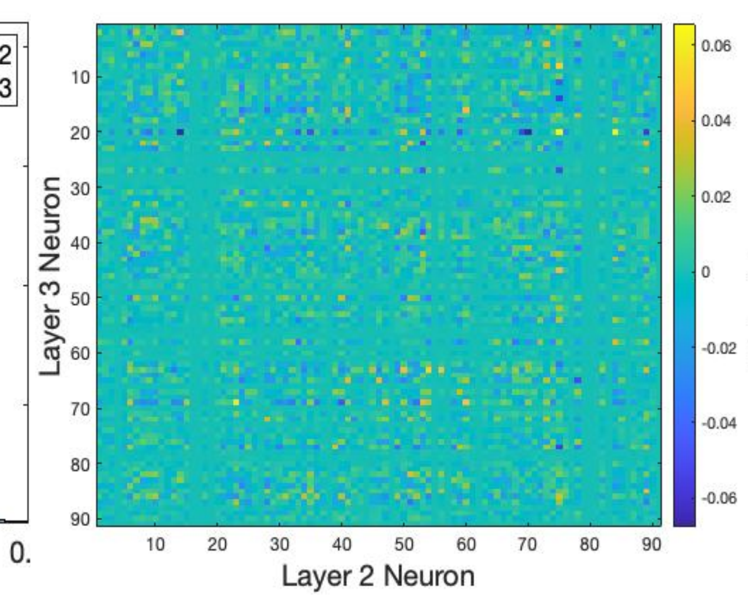


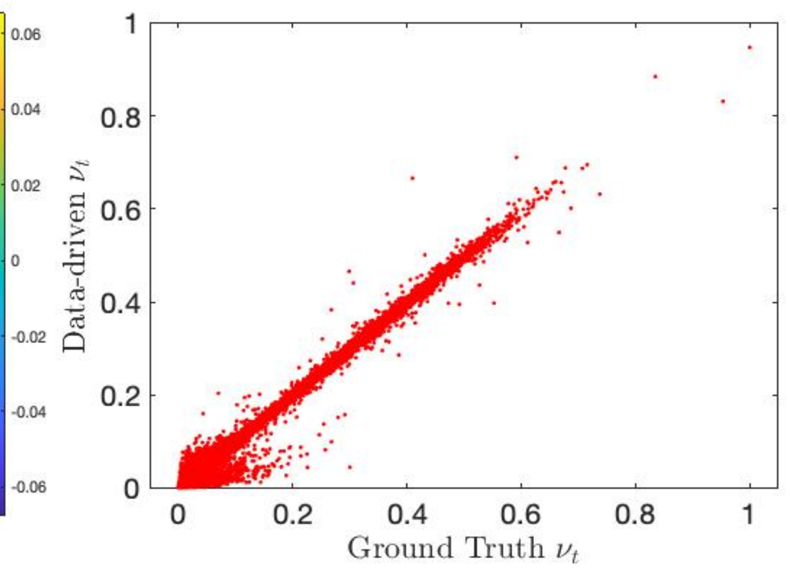
Workflow for AutoML for a physics emulation task. While the final goal of this work is to incorporate machine-learnt model to non-linear PDE solver OpenFOAM, this study will limit to understanding the learning process

Results

Optimizer	Initialization	Batch Size	LR	W	D	$\bar{\varepsilon}$	N
ADAM	Glorot	1426	9.56e-04	91	10	1e-05	84904
ADAM	He	12719	3.77e-04	50	7	2e-04	18207
SGDM	Glorot	6814	0.0098	91	9	2e-03	75812
SGDM	He	1161	0.0098	89	6	1e-03	48778
RMSProp	Glorot	291	1e-04	78	4	8e-04	25432
RMSProp	He	11630	1.86e-05	55	9	1e-03	28004





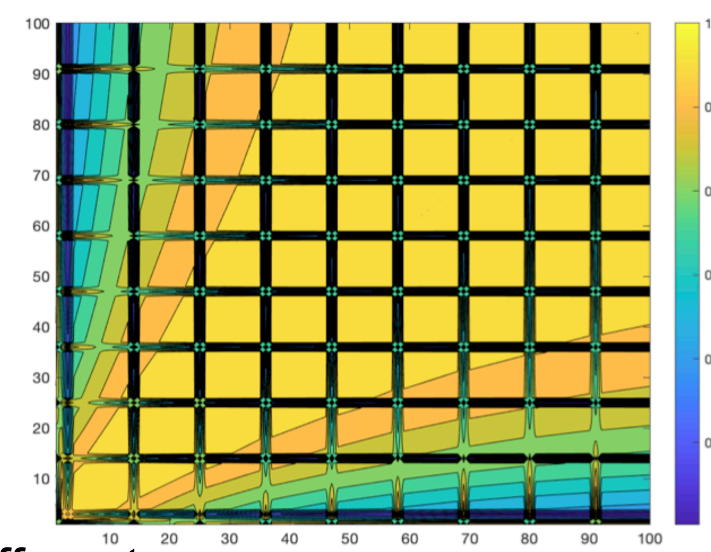


Weight Space Similarity

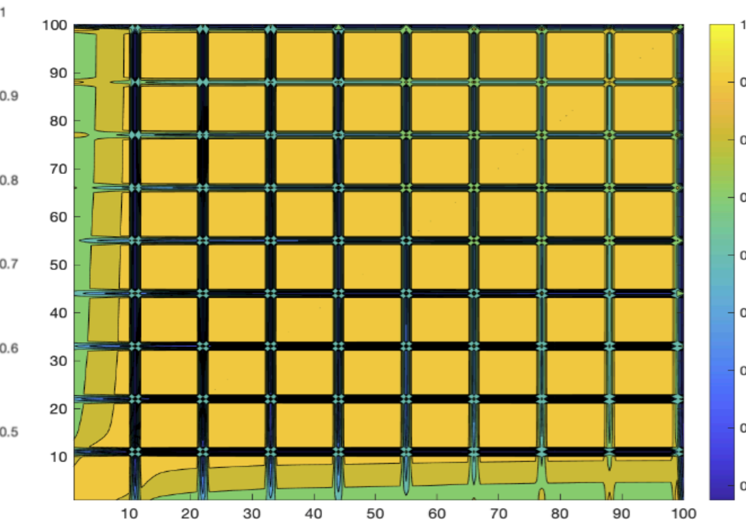
Network checkpointed after every epoch

$$\cos(\theta_1, \theta_2) = \frac{\theta_2 \theta_1^T}{\|\theta_2\| \|\theta_1\|}$$

Self-similar training evolution
Different optimizers have vastly different trajectories



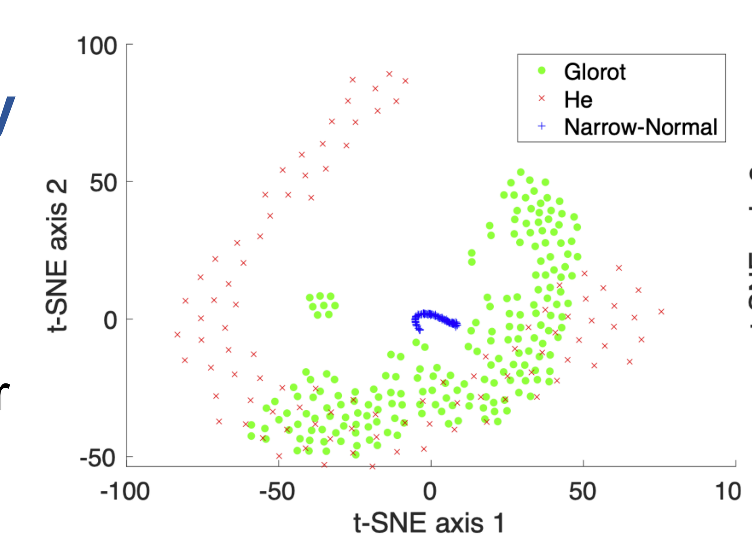
ADAM-Glorot

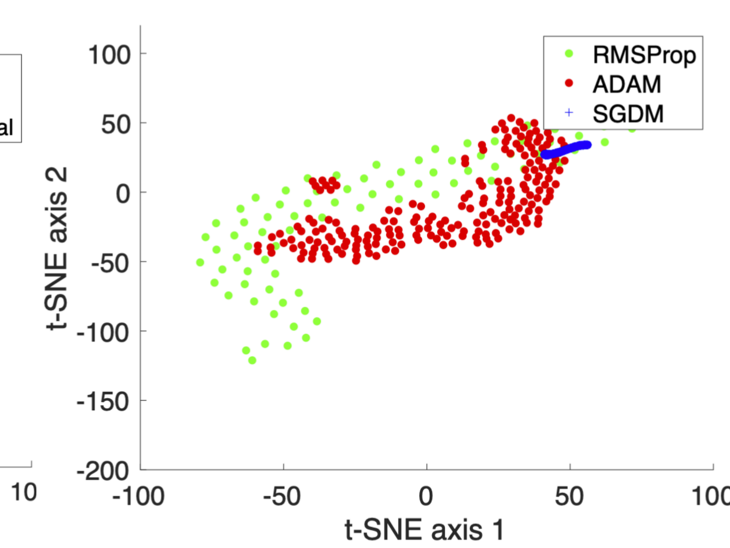


SGDM-Glorot

Function Space Similarity

- t-SNE based dimensionality reduction
- SGDM is stuck in local optima
- ADAM/RMSProp explore larger swaths
- Glorot/He have overlapping exploration



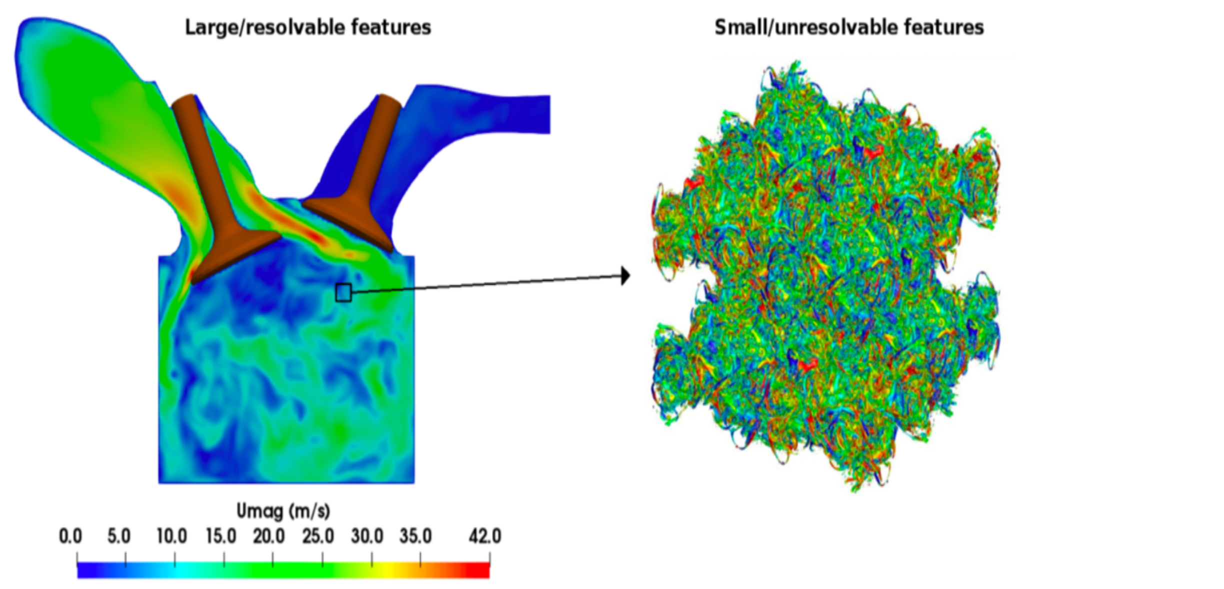


TL;DR

- AutoML methods are successfully in robustly identifying best performing settings for a complicated physics problem
- Network training evolution is heavily dependent on choice of optimizers, adaptive LR optimizers outperform
- Layer-by-Layer learnt weight comparisons reveals complicated nature of network learning

Physics

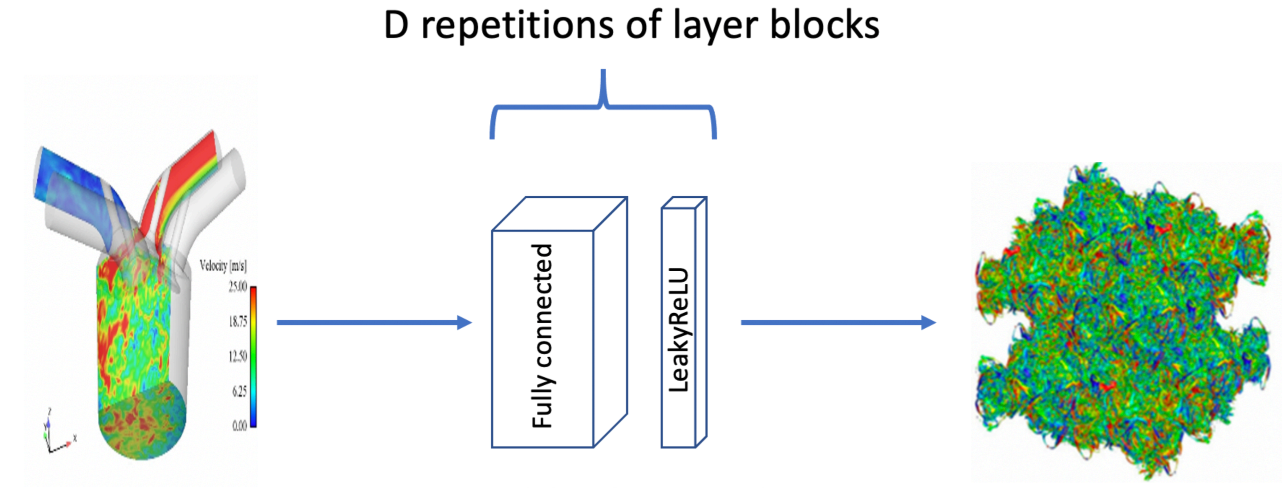
- Accurate turbulence closure is critically important for LES models
- Most methods involve some form of data-fitting, so why not a purely data-driven method!
- Eddy viscosity modeled as a function of large scale filtered variables $\nu_t = f(Re_c, S, \Omega, \nabla K, Y)$



Multiscale nature of a typical Internal Combustion Engine (ICE) simulation. Adopted from Dias Riberio et al.

Network Architecture Search

- NAS, Including optimize for weight initialization and solver



Hyper-parameter	Min. Range	Max. Range	Interpolation
Initial LR	1e-6	1e-2	Logarithmic
LR Drop Factor	10	1000	Integer
Batch Size	100	16000	Logarithmic
Network Depth	2	10	Integer
Network Width	10	100	Integer

References

Dias Ribeiro, Mateus, Alex Mendonça Bimbato, Maurício Araújo Zanardi, José Antônio Perrella Balestieri, and David P. Schmidt. "Large-eddy simulation of the flow in a direct injection spark ignition engine using an open-source framework." *International Journal of Engine Research* (2020): 1468087420903622.Marge Simpson (2010).

Acknowledgements