NEURAL INFORMATION PROCESSING SYSTEMS

AutoML for Climate Change

A Call to Action

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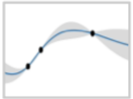
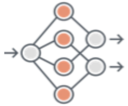
A Call to Action

- ❖ Climate Change AI initiative presents diverse challenges

- ❖ Opportunity to use **AutoML techniques**
  - ➢ Hyperparameter optimization - HPO (*model training*)
  - ➢ Neural architecture search - NAS (*model selection*)

- ❖ Future challenge: **Spatiotemporal data / Physics-constrained settings**

Evaluating AutoML Out-of-the-box

AutoML Methods
 Hyperparameter Optimization **(Optuna)**
 Neural Architecture Search **(SMAC3)**

CCAI Benchmarks	Metrics of Interest
 ClimART (**CA**)	Accuracy, Inference Latency
 Open Catalyst Project (**OC20**)	Mean Absolute Error Between Energies
 Wind Power Forecasting (**SDWPF**)	Average Accuracy Across Turbines

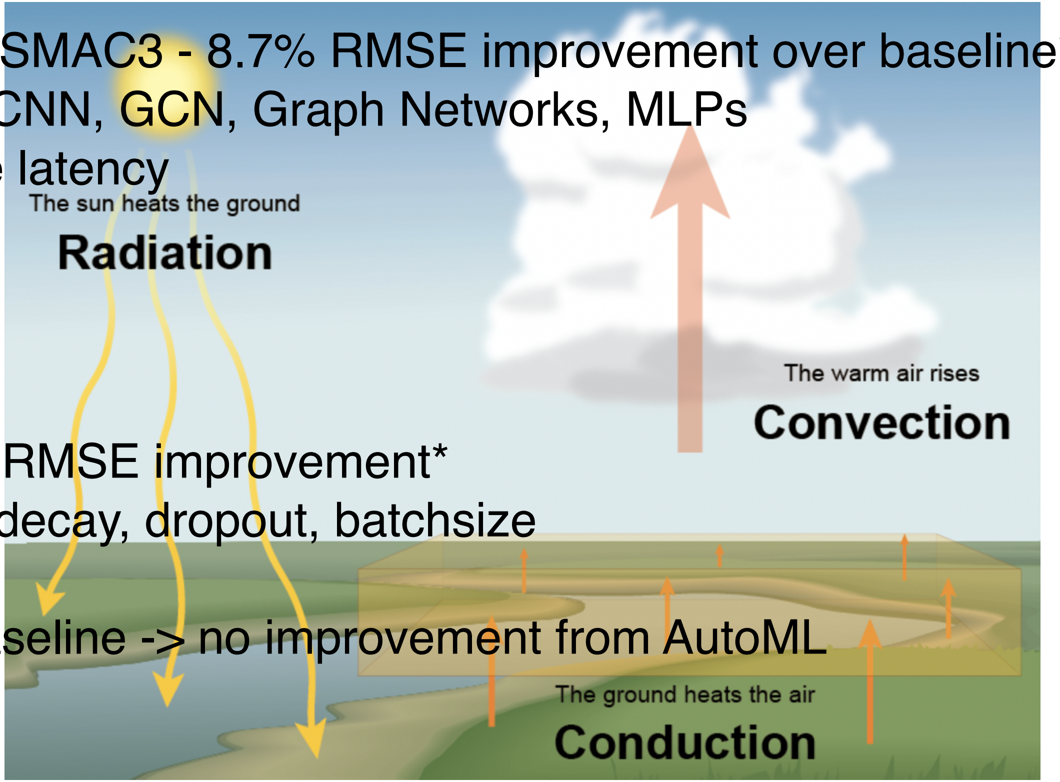
Benchmark #1: ClimART (NeurIPS DBT 2021)

Multi-objective NAS with SMAC3 - 8.7% RMSE improvement over baseline*
- ❖ Model selection from CNN, GCN, Graph Networks, MLPs
- ❖ Comparable inference latency

Atmospheric
Radiative
Transfer

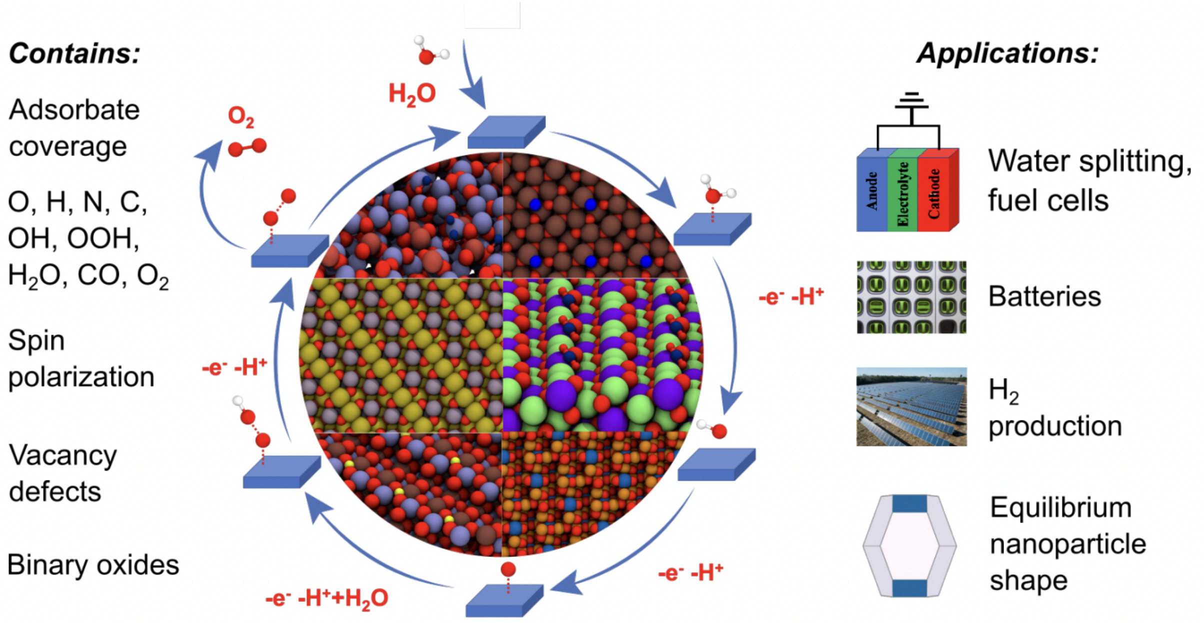
HPO with Optuna - 15.9% RMSE improvement*
- ❖ Learning rate, weight decay, dropout, batchsize

*Authors report a better baseline -> no improvement from AutoML



Benchmark #2: Open Catalyst Project (NeurIPS competition 2021)

New Catalysts for Renewable Energy Storage



Benchmark #2: Open Catalyst Project

GraphNormer (SoTA approach)

+

HPO

{learning rate, warm-up steps, # layers, # attention heads, #blocks}

Only yields **0.65%** improvement in MAE

Benchmark #3: SDWPF - Wind Power Forecasting (KDD Cup 2022)

- **AutoML showed almost no improvement**

- HPO / NAS applied to two winning competition submission
  - Significant cost (up to 50 GPU hours) running AutoML

Promising Future Avenues

- ❖ NAS search spaces for **spatiotemporal data forecasting**
  - ➢ Interpolation between model families: CNN, MLP, GCN, Graph Networks
  - ➢ State-space models for longer sequences

- ❖ Architectures that incorporate **physical constraints**
  - ➢ Drgoňa, Ján, et al. "*Physics-constrained deep learning of multi-zone building thermal dynamics.*"

Checkout our GitHub repo

https://github.com/climate-change-automl/climate-change-automl