

# ORIE 4741: Introduction to AutoML

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# Outline

Motivation

Some AutoML systems

Demo!

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## What would we do to select models?

Model: algorithm + hyperparameter settings

e.g. ridge regression with  $\lambda = 1$

In supervised learning, given a training set  $\{(x_i, y_i)\}$  and test points  $\{x_j\}$ , how would we get  $\{y_j\}$ ?

## What would we do to select models?

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In supervised learning, given a training set  $\{(x_i, y_i)\}$  and test points  $\{x_j\}$ , how would we get  $\{y_j\}$ ?

- ▶ linear regression?
- ▶ random forest?
- ▶ gradient boosting?
- ▶ ...
- ▶ try all the models in scikit-learn [PVG<sup>+</sup>11], or all the available neural network architectures?

## Model selection is important

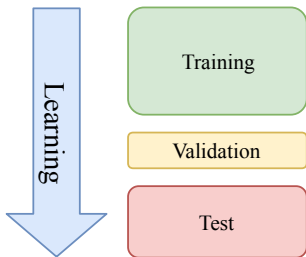
A naive exhaustive search that runs all models wastes

- ▶ programmer time
- ▶ computational time
  - takes long on small datasets
  - is impossible on large datasets

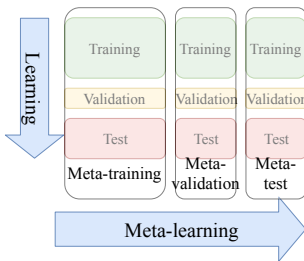
Approaches to avoid exhaustive search:

- ▶ single dataset: surrogate models to predict performance
  - ▶ Gaussian processes
  - ▶ genetic programming
- ▶ learn across datasets: meta-learning

# Learning vs meta-learning



(a) Learning



(b) Meta-learning

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## AutoML frameworks for general models

- ▶ Bayesian optimization frameworks [SLA12, KFB<sup>+</sup>17, ZBSS16, THHLB13] ...
- ▶ auto-sklearn [FKE<sup>+</sup>15]: meta-learning + Bayesian optimization
- ▶ TPOT [OUA<sup>+</sup>16]: genetic programming
- ▶ H2O AutoML
- ▶ Hyperband [LJD<sup>+</sup>18]
- ▶ Probabilistic matrix factorization (PMF) [FSE18]
- ▶ OBOE: matrix factorization + experiment design [YAKU19]
- ▶ ...

# AutoML for neural architecture search

Techniques in use:

- ▶ reinforcement learning [ZL17] ...
- ▶ genetic programming [SSN17] ...
- ▶ Bayesian optimization [JSH19] ...
- ▶ ...

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## Question: When does AutoML overfit?

Recall overfitting: low training error and high test error

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