ORIE 4741: Introduction to AutoML

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October 28, 2019

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?

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 $\{y_j\}$?

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

Model selection is important

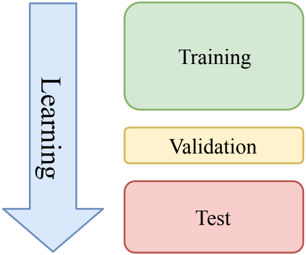
A naive exhaustive search that runs all models wastes

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

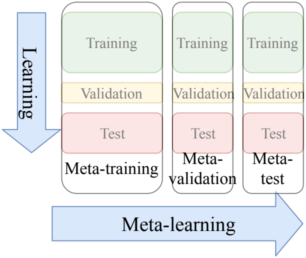
Approaches to avoid exhaustive search:

- 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$^+$17, ZBSS16, THHLB13] ...
- auto-sklearn [FKE$^+$15]: meta-learning + Bayesian optimization
- TPOT [OUA$^+$16]: genetic programming
- H2O AutoML
- Hyperband [LJD$^+$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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