Speedup Techniques for Hyperparameter Optimization

Meta-Learning

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Introduction

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  - Many models are periodically re-fit to track changes in the data
  - Many models are re-fit to perform well on new tasks
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For a good introduction to meta-learning in general, see [AutoML Book: Chapter 2]

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Goal of meta-learning:

- use meta-data $\mathcal{D}_{\text{meta}}$ to choose $\theta_i \in \Theta$ for t_{new} better than only based on $\mathcal{D}_{\text{new}}$.

[adapted from AutoML Book: Chapter 2]

The Role of Meta-Features

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- Each task t_j can be described by a vector of K meta-features:

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$$m(t_j) = (m_{j,1}, \ldots, m_{j,K})$$

- This vector can be used to define a similarity measure between two tasks
  - e.g., calculating the Euclidean distance between $m(t_i)$ and $m(t_j)$
  - Based on similarity, we can transfer information from the most similar tasks to new task t_{new}

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- Others - not included in the previous groups
  - e.g., time related measures, clustering and distance-based measures

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- Can we learn from meta-data $\mathcal{D}_{\text{meta}}$ how to initialize HPO?
- Note: just a single default configuration often does not perform great on a new dataset
  - Otherwise there would be no point in HPO

Meta-Learning for HPO Approach 2: Model-Warmstarting

- Many HPO methods use a predictive model (e.g., Bayesian optimization)
- By running HPO on different datasets, we learn something about the search landscape
  - E.g., what are bad regions of the configuration space in general

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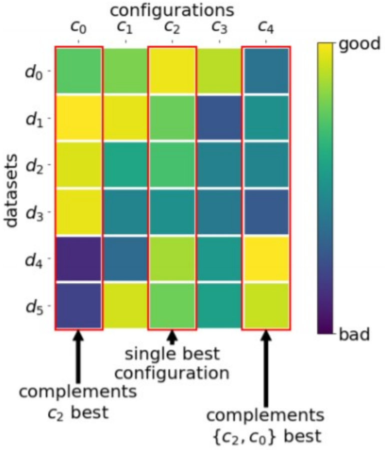
- By running HPO on different datasets, we learn something about the search landscape
  - E.g., what are bad regions of the configuration space in general
- Given: n predictive models $\hat{c}_{\mathcal{D}_i} : \mathbf{\Lambda} \rightarrow \mathbb{R}$ from HPO on $\mathcal{T}_{\text{meta}}$
- How can we use these $\hat{c}_{\mathcal{D}_i}$ to speed up HPO?

Meta-Learning for HPO Approach 3: Task-independent Recommendations

- *Idea:* learn a sorted list of defaults
- *Method:* mostly greedy on $\mathcal{T}_{\text{meta}}$
- *Results:* surprisingly strong, better than Bayesian Optimization



[Wistuba et al. 2017; Feurer et al. 2018; Pfisterer et al. 2018]

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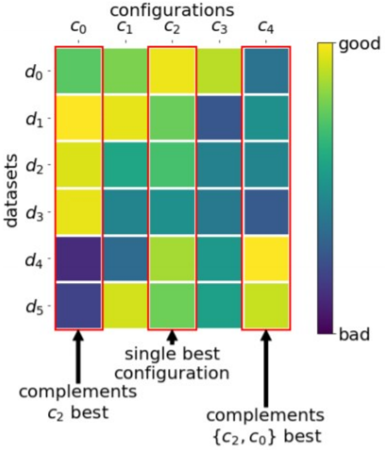
Advantages

- Easy to share and use
- Strong anytime performance
- Embarrassingly parallel

Disadvantages

- Not adaptive



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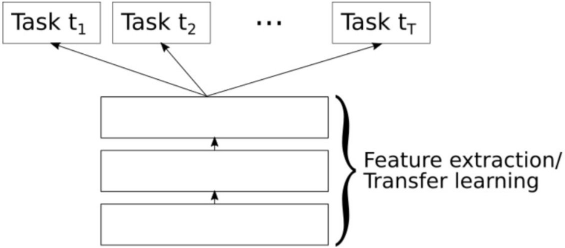

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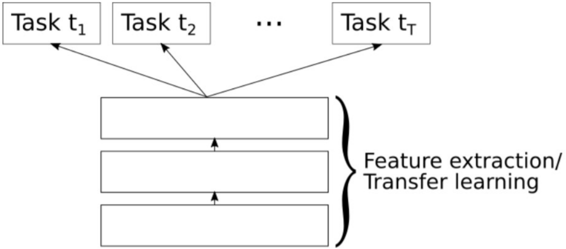

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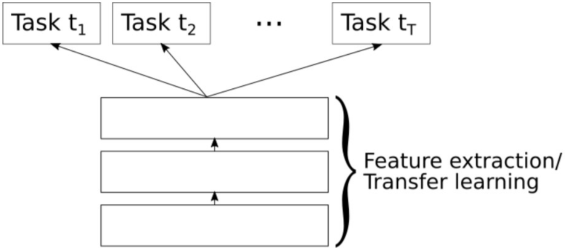
- This uses meta-learning for feature extraction on the hyperparameter configurations



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Meta-Learning for HPO Approach 5: Learning a Black-box Optimization Algorithm from Data

- Learning a blackbox optimization algorithm
  - Use $\mathcal{D}_{\text{meta}}$ to learn a mapping from $\mathcal{D}_{\text{new}}$ to the next configuration $\boldsymbol{\lambda}$ to evaluate
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  - Reinforcement learning [Li and Malik. 2016]
    - ★ Can be harder to get to work, but does not require differentiable f

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  - Also depend on the $\boldsymbol{\lambda}$ value: $u_\phi(\boldsymbol{\lambda}) = u_\phi(\mu_t(\boldsymbol{\lambda}), \sigma_t(\boldsymbol{\lambda}), \boldsymbol{\lambda})$
    - This allows to fine-tune to the characteristics of $\mathcal{D}_{\text{meta}}$ (e.g., avoid poor parts of the space)

Questions to Answer for Yourself / Discuss with Friends

- Repetition. What are the different kinds of meta-features which can be used to describe machine learning datasets?
- Repetition. List all the different ways of using the meta data for HPO you recall
- Discussion. In the various meta-learning approaches, what will happen if all prior tasks are dissimilar to the target task?