AutoML: Hyperparameter Optimization

Example and Practical Hints

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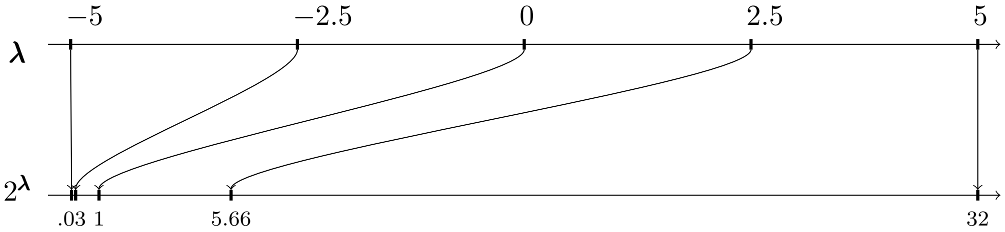
Scaling and Ranges I

- Knowledge about hyperparameters can help to guide the optimization
- E.g., it can be beneficial to optimize hyperparameters on a non-uniform scale.

Example: regularization hyperparameter on log-scale

- Many ML algorithms have non-neg. hyperparameters (e.g. regularization constant), for which it can make sense to try out very small and very large values during tuning
- Usual trick: put on log-scale: C of SVM: $[2^{-15}, 2^{15}] = [0.00003, 32768]$



Scaling and Ranges II

- Similar to the scale, e.g., linear or logarithmic, upper and lower bounds for hyperparameters have to be specified as many optimizers require them
- Setting these correctly usually requires deeper knowledge about the inner workings of the ML method and a lot of practical experience
- Furthermore, if $\hat{\boldsymbol{\lambda}}$ is close to the border of $\boldsymbol{\Lambda}$ the ranges should be increased (or a different scale should be selected), but many algorithms do not do this automatically
- Meta-Learning can help to decide which hyperparameters should be tuned in which ranges

Default Heuristics

- Instead of using static defaults, we sometimes can compute hyperparamter defaults heuristically, based on simple data characteristics.
- A lot faster than tuning and sometimes can work well, although not many guarantees exists and it is often unclear how well this works across many different data scenarios
- Well-known example: Number of random features to consider for splitting in random forest: mtry $= \sqrt{p}$, where p is total number of features.
- For the RBF-SVM a data dependent default for the γ parameter (inverse kernel width) can be computed by using the (inverse of the) median of the pairwise distances $\|\mathbf{x} - \tilde{\mathbf{x}}\|$ between data points (or a smaller random subset for efficiency)

Tuning Example - Setup

We want to train a *spam detector* on the popular Spam dataset[1].

- The learning algorithm is a support vector machine (SVM) with RBF kernel.
- The hyperparameters we optimize are
  - Cost parameter cost $\in [2^{-15}, 2^{15}]$.
  - Kernel parameter $\gamma \in [2^{-15}, 2^{15}]$.
- We compare four different optimizers
  - Random search
  - Grid search
  - A $(1+1)$-selection EA and Gauss mutation with $\sigma = 1$.
  - *CMAES* - efficient EA that generates offspring from a multivariate Gaussian
- We use a 5-fold CV for tuning on the inside, to optimize accuracy (ACC) and 10-fold on the outside for nested CV
- All methods are allowed a budget of 100 evaluations

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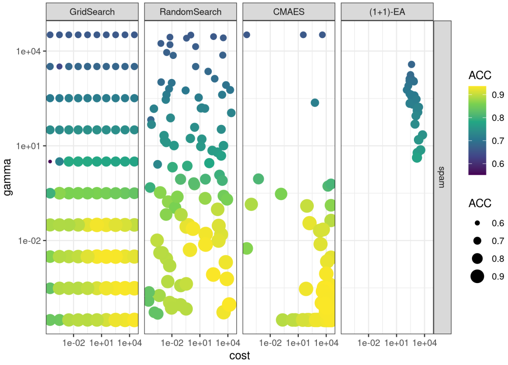
[1] `https://archive.ics.uci.edu/ml/datasets/spambase`

Tuning Example

We notice here:

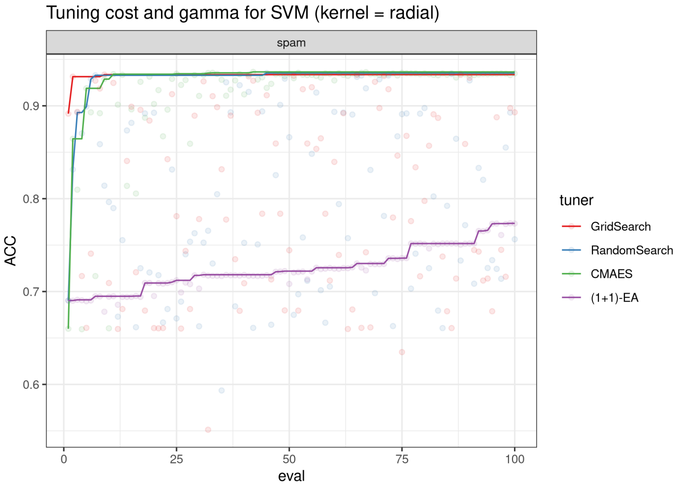
- Both *Grid search* and *random search* have many evaluations in regions with bad performance ($\gamma > 1$)
- *CMAES* only explores a small region
- *(1+1)-EA* does not converge, we probably set its control parameters in a suboptimal manner
- May we should increase ranges?
- Such a visual analysis is a lot harder for more than 2 hyperparameters



Tuning Example cont.

The *optimization trace* shows the best obtained performance until a given time point.

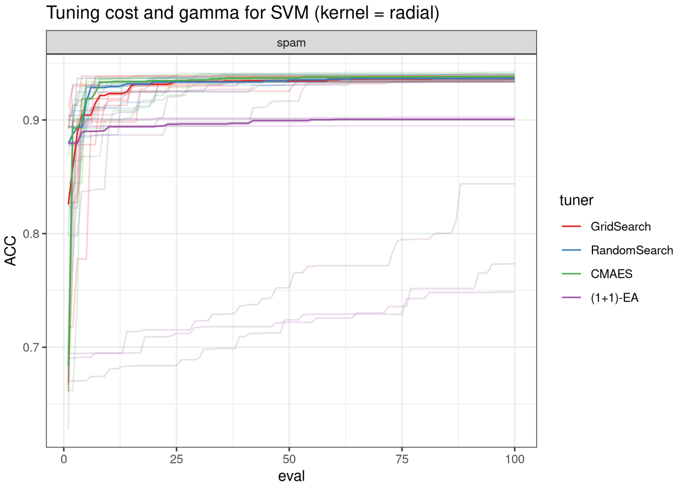
- For *random search* and *grid search* the chronological order of point evaluation is somewhat arbitrary
- The curve shows the performance on the tuning validation (*inner resampling*) on a single fold



Tuning Example cont.

The *optimization trace* shows the best obtained performance until a given time point.

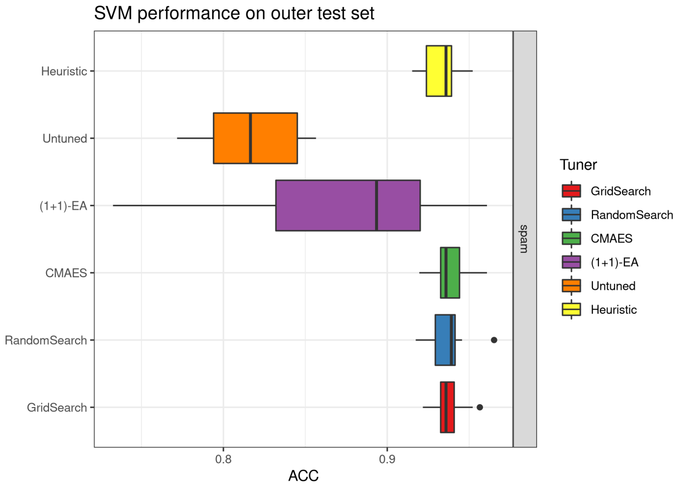
- The outer 10-fold CV gives us 10 optimization curves.
- The median at each time point gives us an estimate of the average optimization progress.



Tuning Example: Validation

Distribution of the ACC-values on *outer test sets* with a 10-fold CV.

- We compare with SVM in (unreasonable) defaults ($\text{cost} = 1, \gamma = 1$) and the previously discussed heuristic with $\text{cost} = 1$
- We abstained from proper statistical testing here
- The performance is somewhat lower than indicated by the results on the inner resampling



Challenges and Final Comments I

1. Getting it right which hyperparameters to tune, in what ranges, and where defaults and where heuristics might be ok.
2. Choosing and balancing out budget for tuning and inner and outer resampling.
3. Dealing with multi criteria-situations, where multiple performance metrics are of interest
4. Dealing with parallelization and time-heterogeneity
5. Ensuring the computational stability of the tuning process and dealing with crashes

Challenges and Final Comments II

6. Post-Hoc analysis of all obtained tuning results
7. Exploiting the multi-fidelity property of ML training (suppress bad configurations early without investing too much time)
8. Including preprocessing and full pipelining into the tuning process, and dealing with complex hierarchical spaces