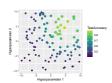
Introduction to Machine Learning

Hyperparameter Tuning - Basic Techniques



Learning goals

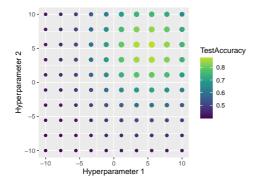
- Understand the idea of grid search
- Understand the idea of random search
- Be able to discuss advantages and disadvantages of the two methods



GRID SEARCH

- Simple technique which is still quite popular, tries all HP combinations on a multi-dimensional discretized grid
- For each hyperparameter a finite set of candidates is predefined
- Then, we simply search all possible combinations in arbitrary order

Grid search over 10x10 points





GRID SEARCH / 2

Advantages

- Very easy to implement
- All parameter types possible
- Parallelizing computation is trivial

Disadvantages

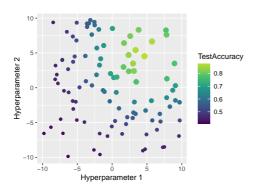
- Scales badly: combinatorial explosion
- Inefficient: searches large irrelevant areas
- Arbitrary: which values / discretization?



RANDOM SEARCH

- Small variation of grid search
- Uniformly sample from the region-of-interest

Random search over 100 points





RANDOM SEARCH / 2

Advantages

- Like grid search: very easy to implement, all parameter types possible, trivial parallelization
- Anytime algorithm: can stop the search whenever our budget for computation is exhausted, or continue until we reach our performance goal.
- No discretization: each individual parameter is tried with a different value every time

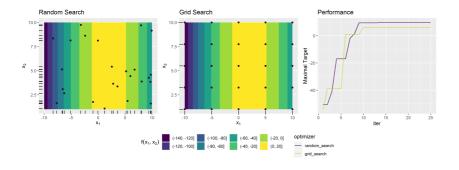
Disadvantages

- Inefficient: many evaluations in areas with low likelihood for improvement
- Scales badly: high-dimensional hyperparameter spaces need lots of samples to cover.



RANDOM SEARCH VS. GRID SEARCH

We consider a maximization problem on the function $f(x_1,x_2)=g(x_1)+h(x_2)\approx g(x_1)$, i.e. in order to maximize the target, x_1 should be the parameter to focus on.



 \Rightarrow In this setting, random search is more superior as we get a better coverage for the parameter x_1 in comparison with grid search, where we only discover 5 distinct values for x_1 .



TUNING EXAMPLE

Tuning random forest with grid search/random search and 5CV on the ${
m sonar}$ data set for AUC:

Hyperparameter	Туре	Min	Max
$_{ m num.trees}$	integer	3	500
mtry	integer	5	50
$\min.node.size$	integer	10	100

