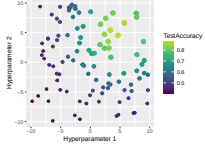
Introduction to Machine Learning

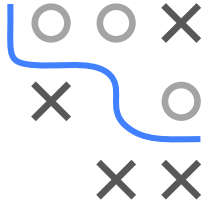
Hyperparameter Tuning - Basic Techniques



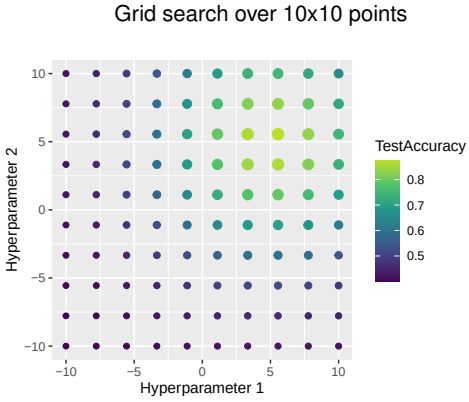
Learning goals

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

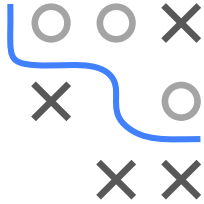
GRID SEARCH



- 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 / 2



Advantages

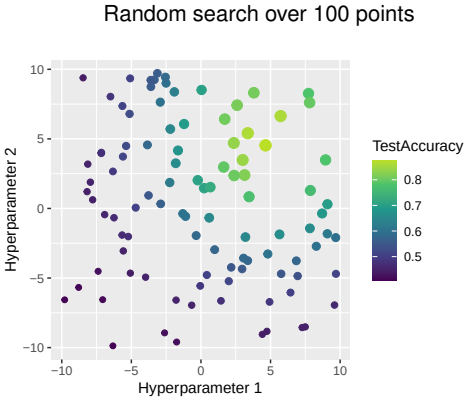
- Very easy to implement
- All parameter types possible
- Parallelizing computation is trivial

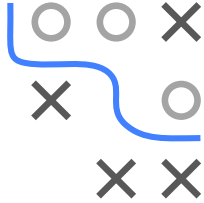
Disadvantages

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

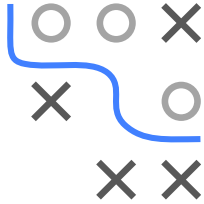
RANDOM SEARCH

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





RANDOM SEARCH / 2



Advantages

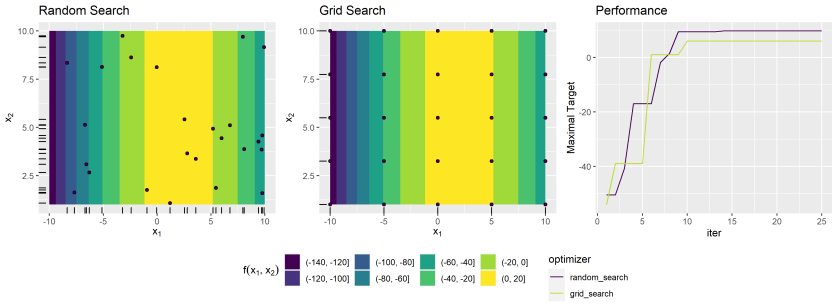
- Like grid search: very easy to implement, all parameter types possible, trivial parallelization
- Anytime algorithm: can stop the search whenever our budget for computation is exhausted, or continue until we reach our performance goal.
- No discretization: each individual parameter is tried with a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

Hyperparameter	Type	Min	Max
`num.trees`	integer	3	500
`mtry`	integer	5	50
`min.node.size`	integer	10	100