VU Machine Learning

WS 2024/2025

Exercise 3.3

Automated Machine Learning

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This is one of possible topics for exercise 3. See other possible topics from my colleague in tuwel. You have to select only one topic for exercise 3

Exercise 3.3

- Automated Machine Learning
  - Implementation of a simulated annealing algorithm for automated selection/configuration of machine learning algorithms
  - Comparison with other state of the art approaches
  - Group work (like in the first two assignments)
  - Presentations: after the submission

Implementation of algorithm

- Implement a simulated annealing algorithm that searches for the best machine learning technique (and best hyperparameters) for a particular classification/regression data set

Implementation of algorithm

- Search space:
  - At least five available machine learning algorithms
  - Most important hyperparameters that should be tuned for each of these algorithms. You can specify for each hyperparameter a reasonable range of possible values
  - The aim is to find a solution (the best algorithm/hyperparameters) in the search space that optimizes an evaluation score (e.g., classification accuracy or RMSE)
- Please write me an email if you have any questions

Comparison with other approaches

- Compare you approach with two state of the art AutoML systems (e.g. auto-sklearn, TPOT…)
- Use for comparison four classification or regression data sets (you can also use the data sets from the previous assignments)
- Time limit: you should use at least 1h per data set

Submission

- Your implementation
- More than 20 slides with this structure
  - Main information for your implementation: representation of solution, neighborhoods, evaluation function, parameters used for implemented technique…
  - Selected state of the art AutoML systems for comparison
  - Discussion of results/Lessons learned
- No report (only slides) needed for this assignment
- Submission deadline:
  - Submission: 30.01.2025, Presentations: 31.01.2025

  OR
  - Submission: 26.02.2025, Presentations: 27.02.- 03.03.2025

Presentations/Discussion of assignment

- Discussion of code
- Implementation issues
- Discussion of results and your findings

Appendix: Simulated Annealing

Definition of search problem

- Given e search space S together with its feasible part

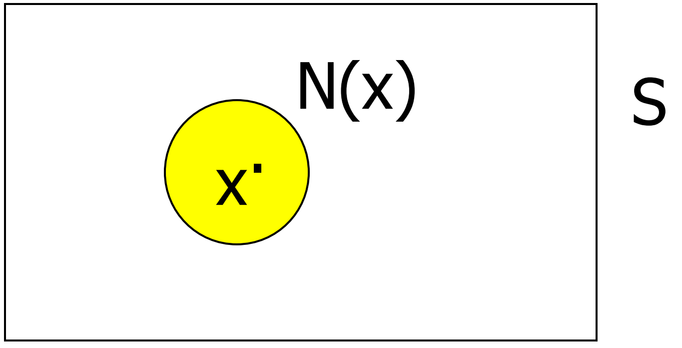
  $F \subseteq S$, find $x \in F$ such that

  $eval(x) \leq eval(y)$ for all $y \in F$

- x that satisfies the above condition is called global optimum (for minimization problem)

Neighbourhood and local optima

- Region of the search space that is near particular point in the space



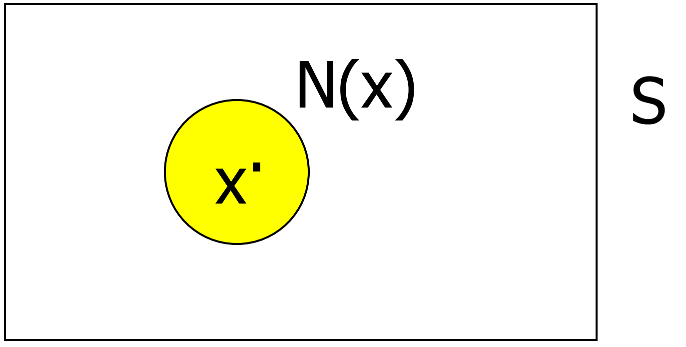
- A potential solution $x \in F$ ia a local optimum with respect to the neighborhood *N*, if and only if

  $eval(x) \leq eval(y),$

  for all $y \in N(x)$

Local Search Techniques

- Are based on the neighbourhood of the current solution



- The solution is changed iteratively with so called neighbourhood relations (moves) until an acceptable or optimal solution is reached

Simulated Annealing

- Is based on the analogy from the thermodynamics
- To grow a crystal, the row material is heated to a molten state
- The temperature of the crystal melt is reduced until the crystal structure is frozen in
- Cooling should not be done two quickly, otherwise some irregularities are locked in the crystal structure

Simulated Annealing

```
Prozedure simulated annealing
 begin
    t=0
    Intialize T
    select a current solution v_c at random
   evaluate v_c
    repeat
     repeat
        select a new solution v_n in the neighborhood of v_c
         if eval(v_c) < eval(v_n) then  v_c =v_n
          else if random[0,1) < e^((eval(v_n)-eval(v_c))/T) then v_c=v_n
     until (termination-condition)
     T=g(T,t)
     t=t+1
    until (halting-criterion)
 end
```

SA – problem specific questions

- What is a solution?
- What are the neighbors of a solution?
- What is a cost of a solution
- How do we determine the initial solution

SA – specific questions

- How do we determine the intial “temperature” T”
- How do we determine the cooling ration g(T,t)?
- How do we determine the termination condition?
- How do we determine the halting criterion?

- STEP 1: $T=T_{max}$

  select v_c at random

- STEP 2: pick a point v_n from the neighborhood of v_c

  if *eval*(v_n) *is better than the val*(v_c)
  then select it $(v_c=v_n)$
  else select it with probability $e^{\frac{-\Delta eval}{T}}$
  repeat this step k_T times

- STEP 3: set $T=rT$

  if $T \geq T_{\min}$
  then goto STEP 2
  else goto STEP 1