UNIVERSITÄT MANNHEIM

Data Mining II
Optimization & Parameter Tuning

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Short Addendum to Neural Networks

- word2vec and its relatives

Why Parameter Tuning?

- What we have seen so far
  - many learning algorithms for classification, regression, ...
- Many of those have parameters
  - k and distance function for k nearest neighbors
  - splitting and pruning options in decision tree learning
  - hidden layers in neural networks
  - C, gamma, and kernel function for SVMs
  - ...
- But what is their effect?
  - hard to tell in general
  - rules of thumb are rare

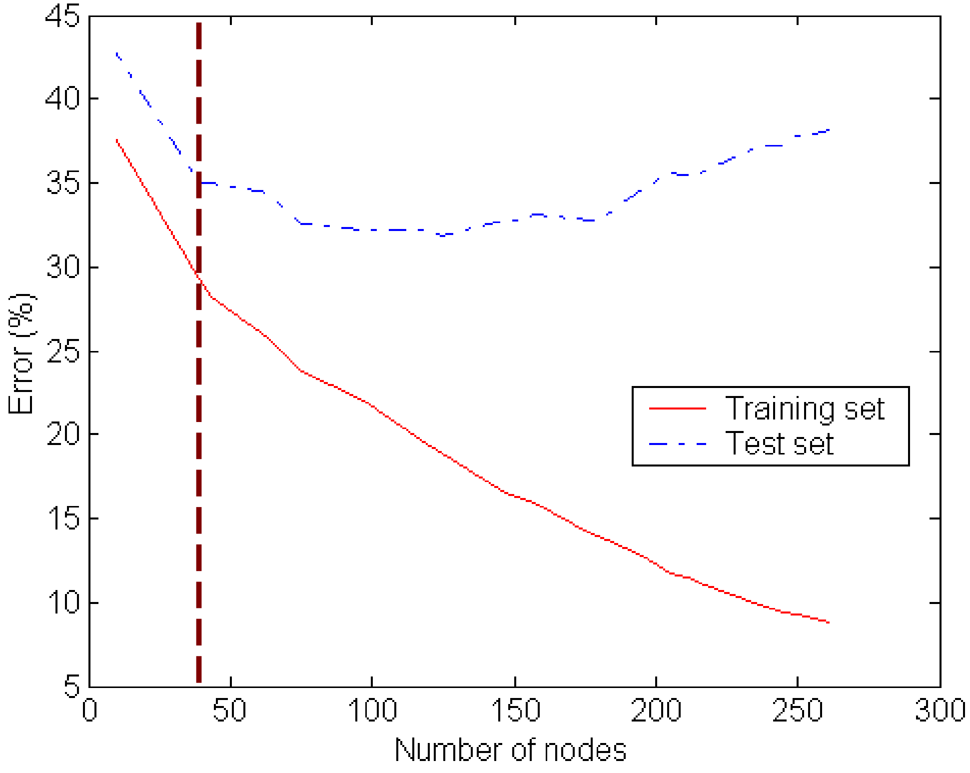
Parameter Tuning – a Naive Approach

- You probably know that approach from the exercises
  1. run classification/regression algorithm
  2. look at the results (e.g., accuracy, RMSE, …)
  3. choose different parameter settings, go to 1

- Questions:
  - when to stop?
  - how to select the next parameter setting to test?

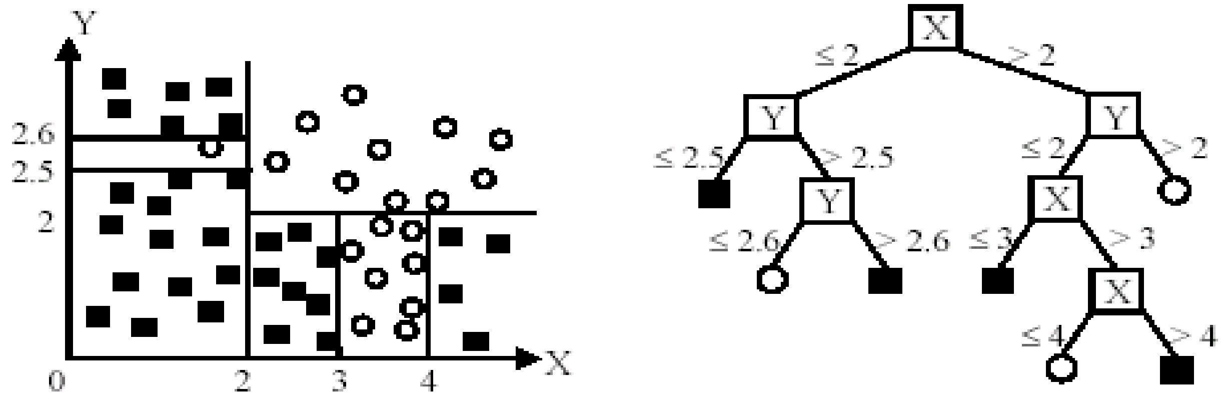
Parameter Tuning – Avoid Overfitting!

- Recap overfitting:
  - classifiers may overadapt to training data
  - the same holds for parameter settings
- Possible danger:
  - finding parameters that work well on the training set
  - but not on the test set
- Remedy:
  - use cross-validation for testing parameter settings



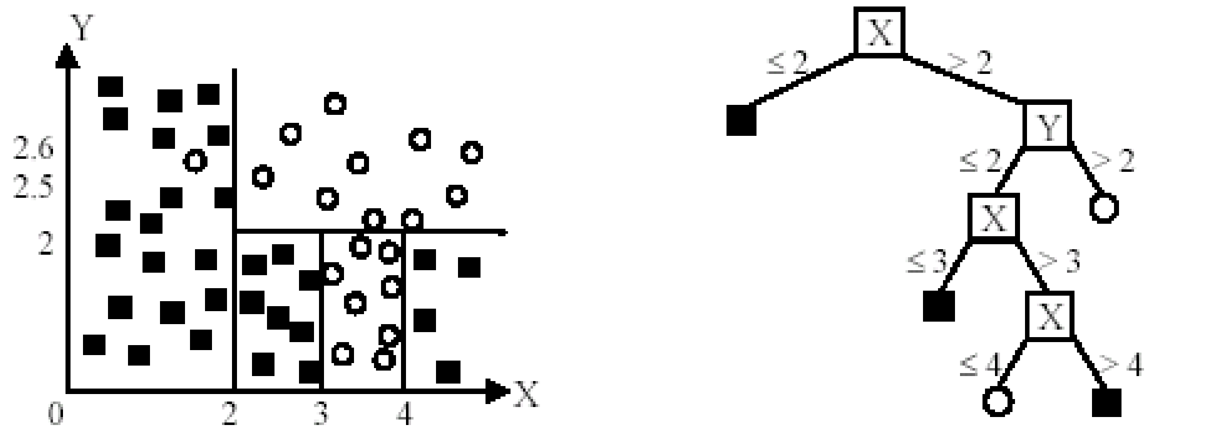
Parameter Tuning – Avoid Overfitting!

- Parameter option: pruning (yes/no)



(A) A partition of the data space

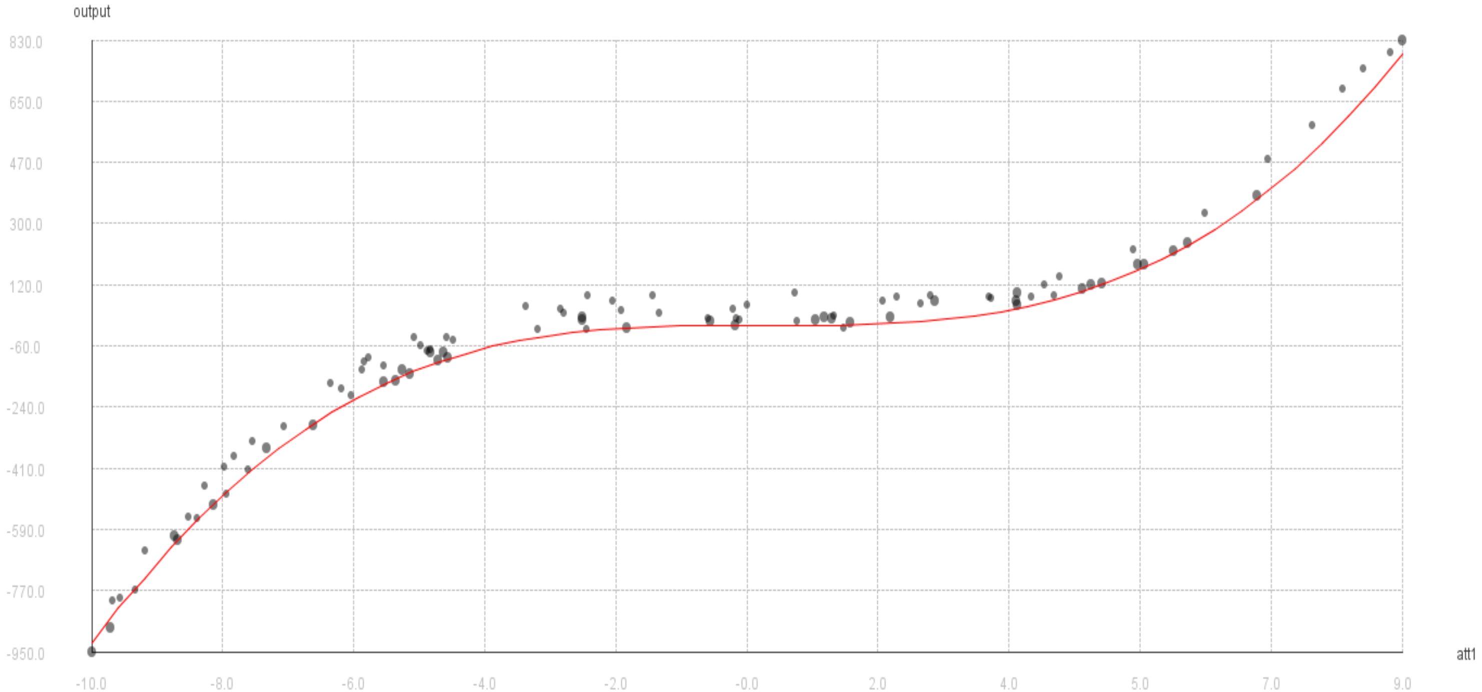
(B). The decision tree



Parameter Tuning – Avoid Overfitting!

- Real example: train a local polynomial regression model
  - Parameter to tune: find the optimal maximum degree of the polynomial

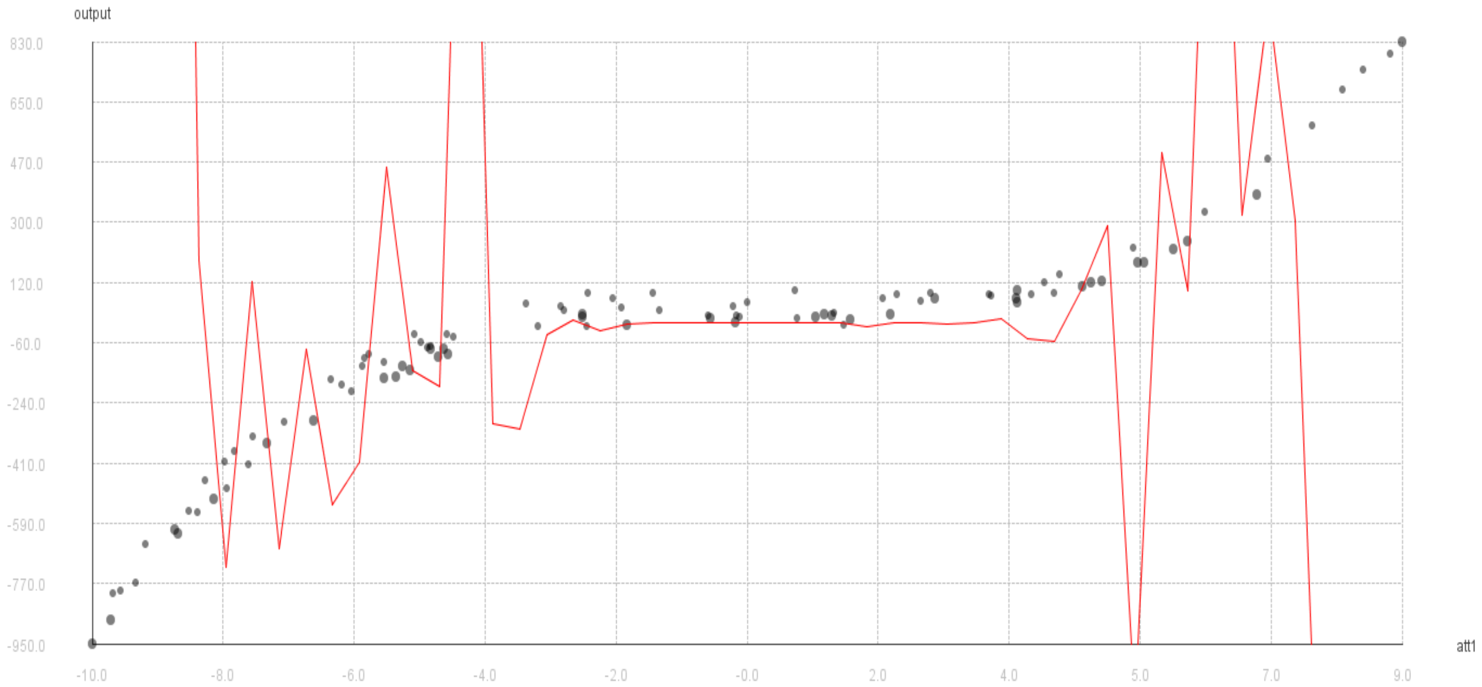
- Tuning with cross validation: degree = 3



Parameter Tuning – Avoid Overfitting!

- Real example: train a local polynomial regression model
  - Parameter to tune: find the optimal maximum degree of the polynomial

- Tuning without cross validation: degree = 9



Parameter Tuning: Brute Force

- Try all parameter combinations that exist

- Consider, e.g., the k-NN classifier in RapidMiner
  - try 30 different distance measures
  - try all k from 1 to 100
  - use weighting or not

    → 6,000 runs of k-NN

- Plus: we use 10-fold CV for evaluating the parameter settings

    → that makes a total of 60,000 runs of k-NN

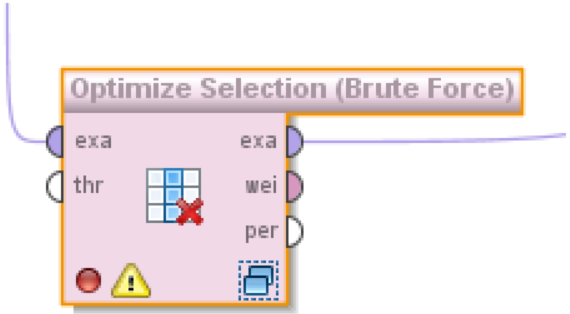
→ we need a better strategy than brute force!

Intermezzo: Beyond Parameter Tuning

- Parameter tuning is an optimization problem
- Finding optimal values for N variables
- Properties of the problem:
  - the underlying model is unknown
    - i.e., we do not know changing a variable will influence the results
  - we can tell how good a solution is when we see it
    - i.e., by running a classifier with the given parameter set
  - but looking at each solution is costly
    - e.g., 60,000 runs of k-NN

- Such problems occur quite frequently

Intermezzo: Beyond Parameter Tuning



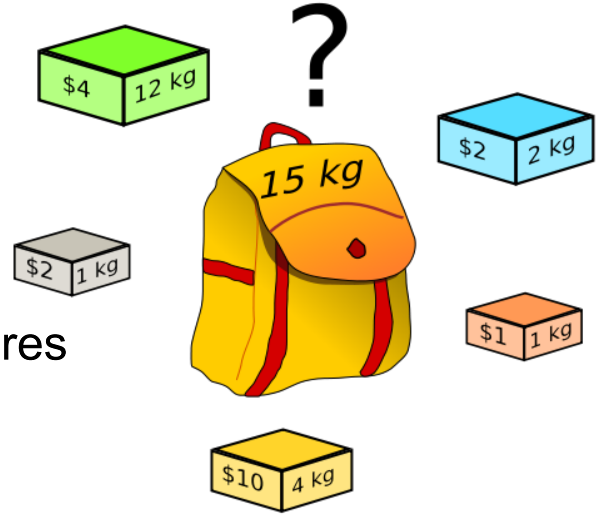
- Related problem:
  - feature subset selection
  - cf. Data Mining 2, first lecture

- Given n features, brute force requires 2^n evaluations
  - for 20 features, that is already one million
    → ten million with cross validation

Intermezzo: Beyond Parameter Tuning

- Knapsack problem
  - given a maximum weight you can carry
  - and a set of items with different weight and monetary value
  - pack those items that maximize the monetary value

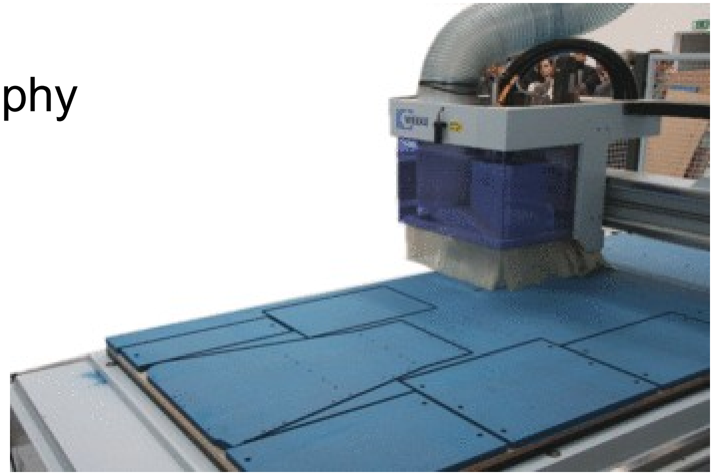
- Problem is NP hard
  - i.e., deterministic algorithms
    require an exponential amount of time
  - Note: feature subset selection for N features
    requires 2^n evaluations

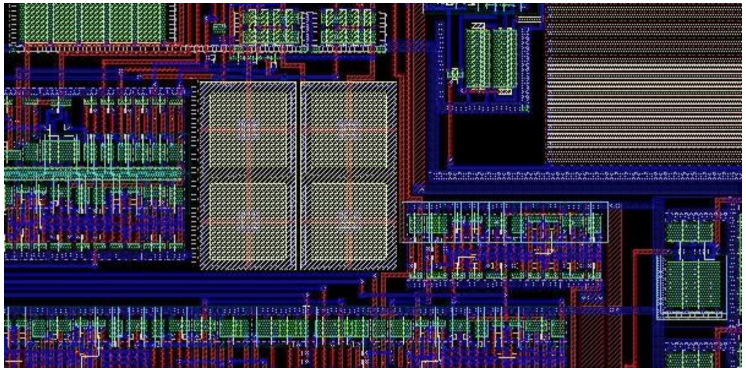


Intermezzo: Beyond Parameter Tuning

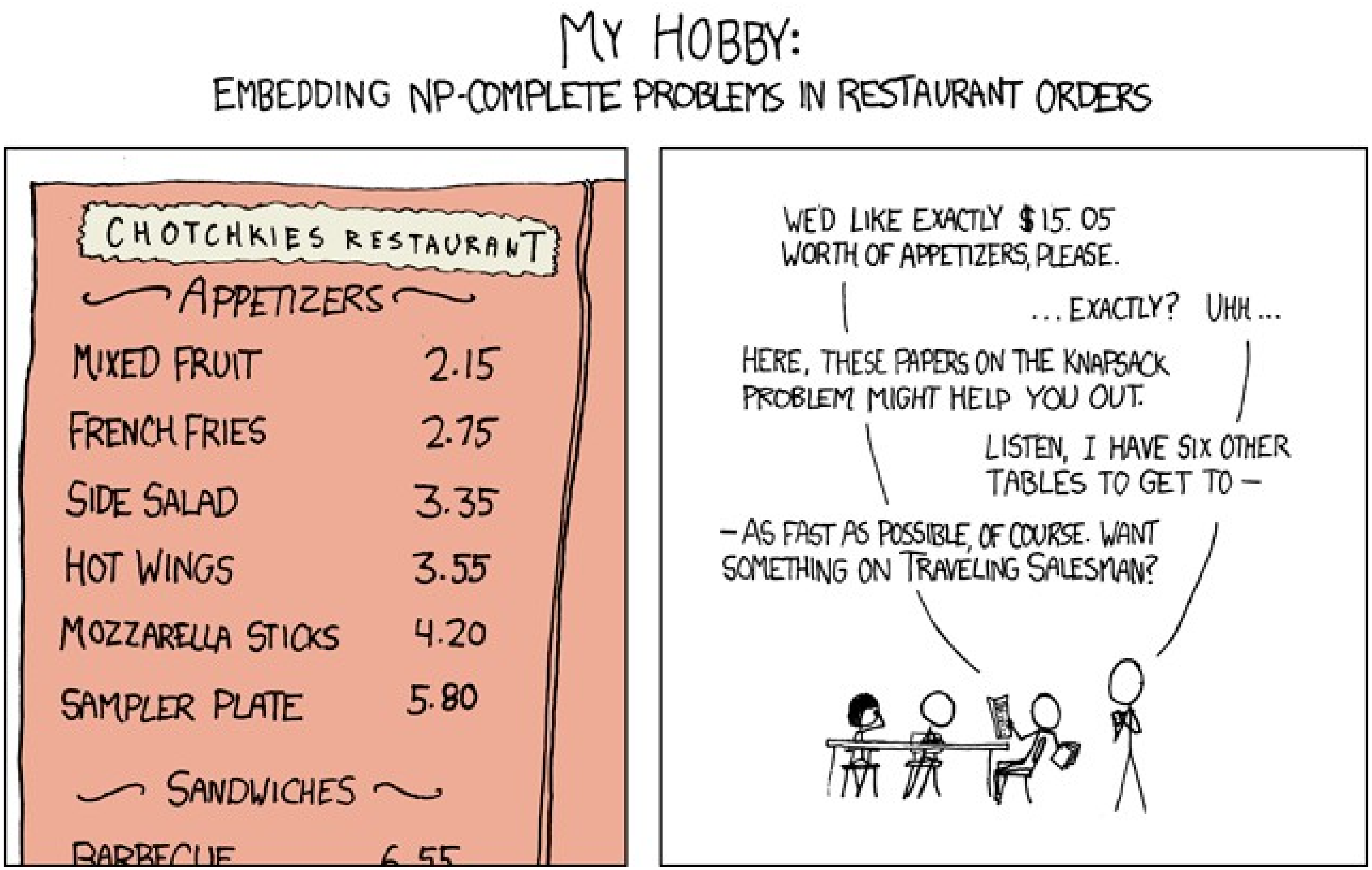
- Many optimization problems are NP hard
  - Routing problems (Traveling Salesman Problem)
  - Integer factorization

    hard enough to be used for cryptography
  - Resource use optimization
    - e.g., minimizing cutoff waste
  - Chip design
    - minimizing chip sizes





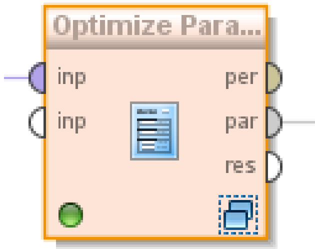
Intermezzo: Beyond Parameter Tuning



http://xkcd.com/287/

Parameter Tuning: Brute Force

- Properties of Brute Force search
  - guaranteed to find the best parameter setting
  - too slow in most practical cases



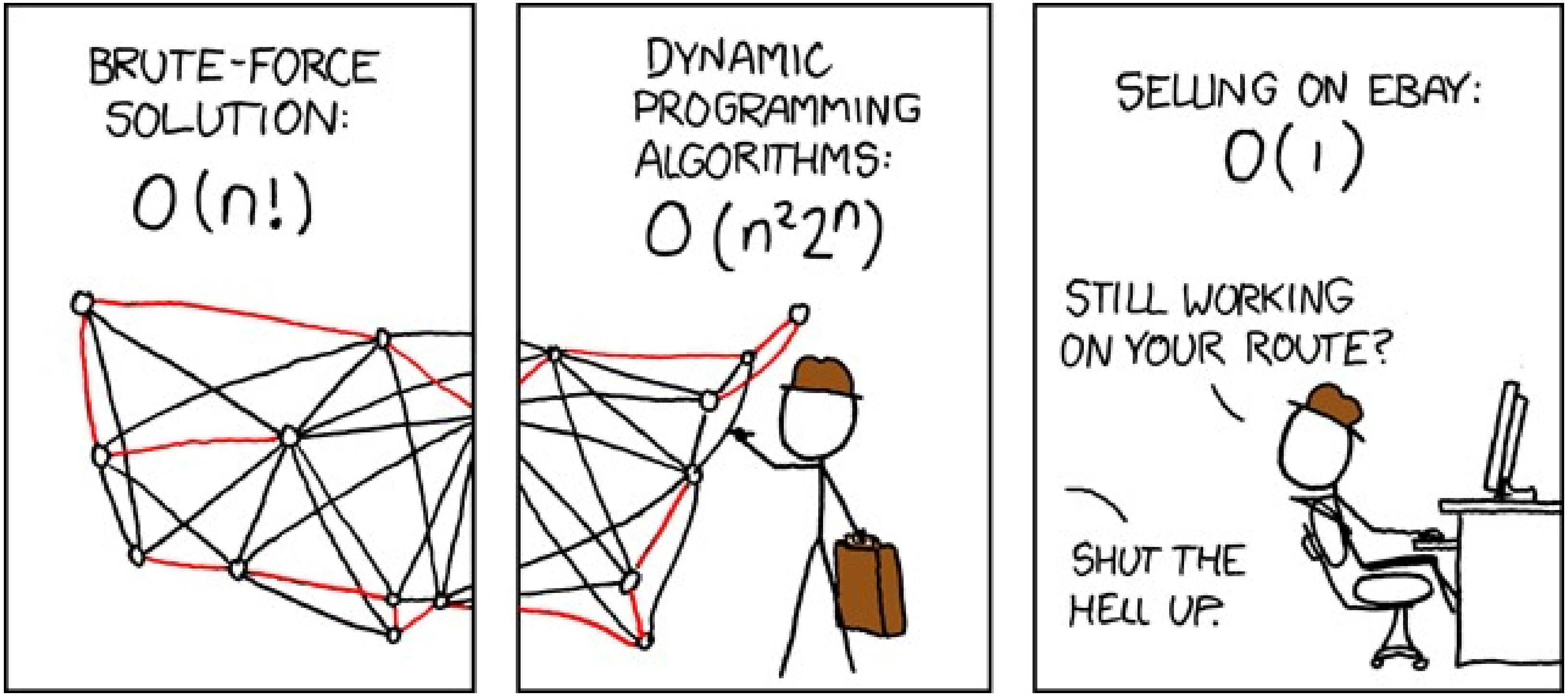
- Grid Search in RapidMiner:
  - performs a brute force search
  - with equal-width steps on non-discrete numerical attributes (e.g., 10,20,30,..,100)
- Parameters with a wide range (e.g., 0.0001 to 1,000,000)
  - with ten equal-width steps, the first step would be 1,000
  - but what if the optimum is around 0.1?
  - logarithmic steps may perform better

Parameter Tuning: Heuristics

- Properties of Brute Force search
  - guaranteed to find the best parameter setting
  - too slow in most practical cases

- Needed:
  - solutions that take less time/computation
  - and *often* find the best parameter setting
  - or find a *near-optimal* parameter setting

Beyond Brute Force



https://xkcd.com/399/

Parameter Tuning: One After Another

- Given n parameters with m degrees of freedom
  - brute force takes m^n runs of the base classifier

- Simple tweak:
  1. start with default settings
  2. try all options for the first parameter
     2a. fix best setting for first parameter
  3. try all options for the second parameter
     3a. fix best setting for second parameter
  4. ...

- This reduces the runtime to n*m
  - i.e., no longer exponential!
  - but we may miss the best solution

Parameter Tuning: Interaction Effects

- Interaction effects make parameter tuning hard
  - i.e., changing one parameter may change the optimal settings for another one

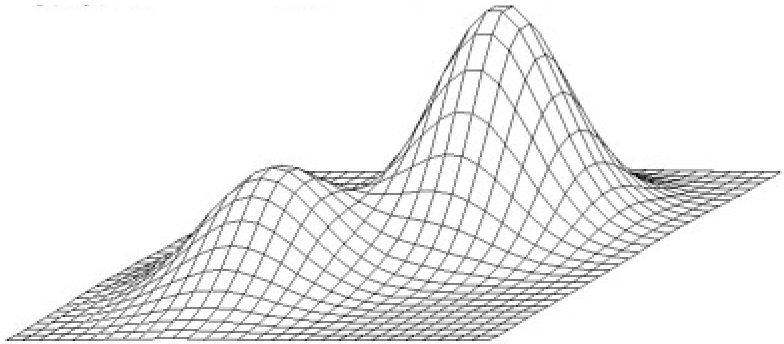
- Example: two parameters p and q, each with values 0,1, and 2
  - the table depicts classification accuracy

	p=0	p=1	p=2
q=0	0.5	0.4	0.1
q=1	0.4	0.3	0.2
q=2	0.1	0.2	0.7

Parameter Tuning: Interaction Effects

- If we try to optimize one parameter by another (first p, then q)
  - we end at p=0,q=0 in six out of nine cases
  - on average, we investigate 2.3 solutions

	p=0	p=1	p=2
q=0	0.5	0.4	0.1
q=1	0.4	0.3	0.2
q=2	0.1	0.2	0.7



Hill-Climbing Search

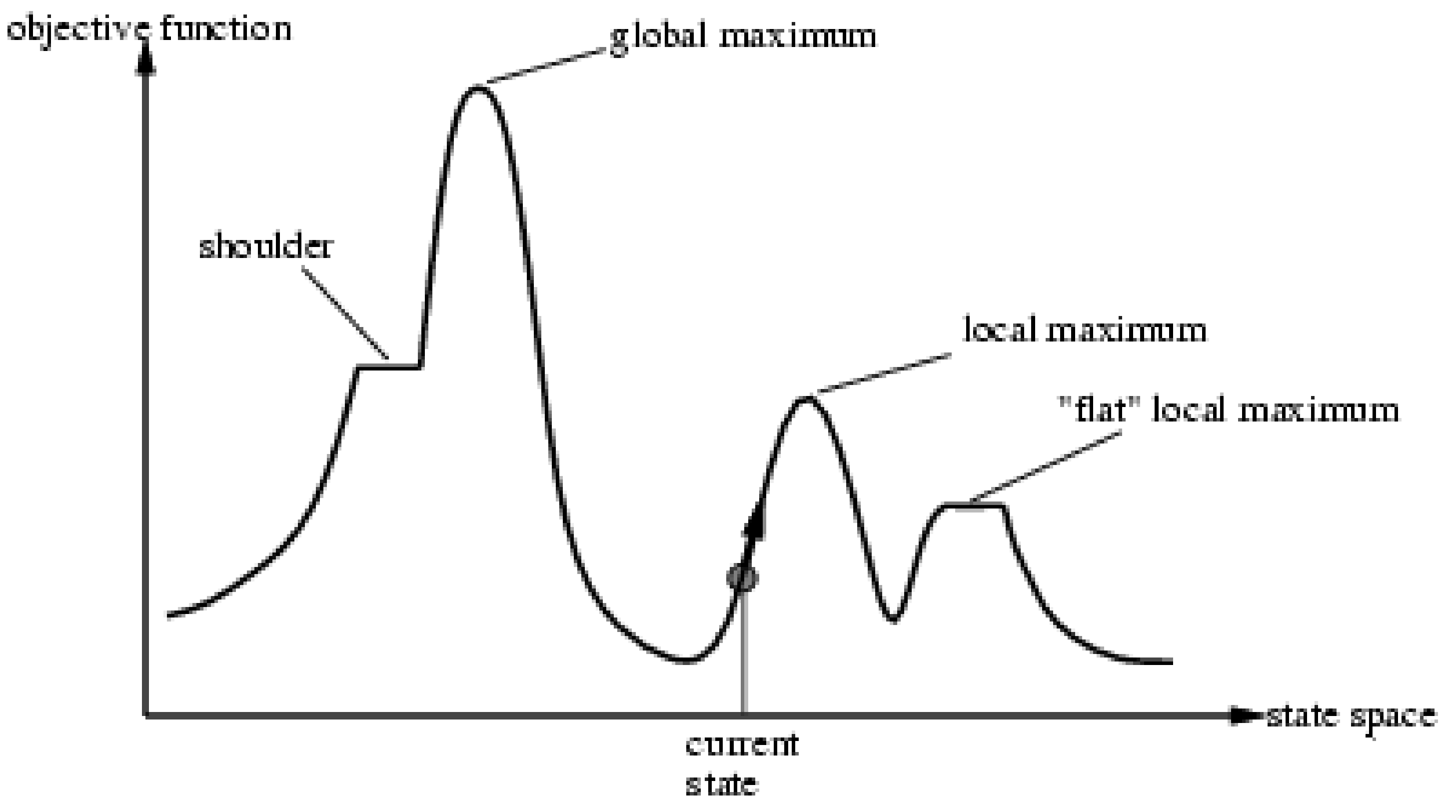
- a.k.a. *greedy local search*
- always search in the direction of the steepest ascend
  - "Like climbing Everest in thick fog with amnesia"

```
function HILL-CLIMBING(problem) returns a state that is a local maximum
   inputs: problem, a problem
   local variables: current, a node
                    neighbor, a node

   current ← MAKE-NODE(INITIAL-STATE[problem])
   loop do
      neighbor ← a highest-valued successor of current
      if VALUE[neighbor] ≤ VALUE[current] then return STATE[current]
      current ← neighbor
```

Hill-Climbing Search

- Problem: depending on initial state, one can get stuck in local maxima



Hill Climbing Search

- Given our previous problem
  - we end up at the optimum in three out of nine cases
  - but the local optimum (p=0,q=0) is reached in six out of nine cases!
  - on average, we investigate 2.1 solutions

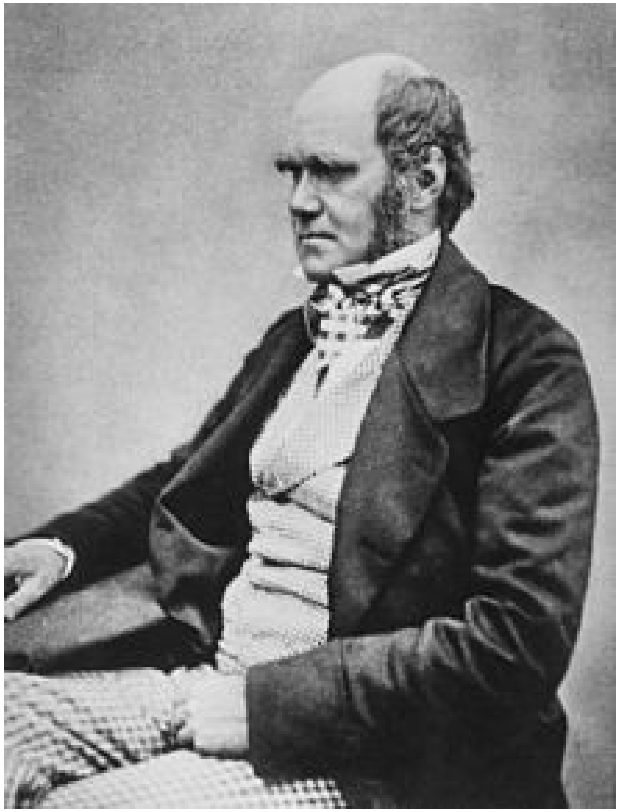
	p=0	p=1	p=2
q=0	0.5	0.4	0.1
q=1	0.4	0.3	0.2
q=2	0.1	0.2	0.7

Variations of Hill Climbing Search

- Stochastic hill climbing
  - random selection among the uphill moves
  - the selection probability can vary with the steepness of the uphill move
- First-choice hill climbing
  - generating successors randomly until a better one is found, then pick that one
- Random-restart hill climbing
  - run hill climbing with different seeds
  - tries to avoid getting stuck in local maxima

Genetic Algorithms

- Inspired by *evolution*
- Overall idea:
  - use a population of individuals (solutions)
  - create new individuals by crossover
  - introduce random mutations
  - from each generation, keep only the best solutions ("survival of the fittest")
- Developed in the 1970s
- John H. Holland:
  - Standard Genetic Algorithm (SGA)



Charles Darwin (1809-1882)

Genetic Algorithms

- Basic ingredients:
  - individuals: the solutions
    - parameter tuning: a parameter setting
  - a fitness function
    - parameter tuning: performance of a parameter setting (i.e., run learner with those parameters)
  - a crossover method
    - parameter tuning: create a new setting from two others
  - a mutation method
    - parameter tuning: change one parameter
  - survivor selection

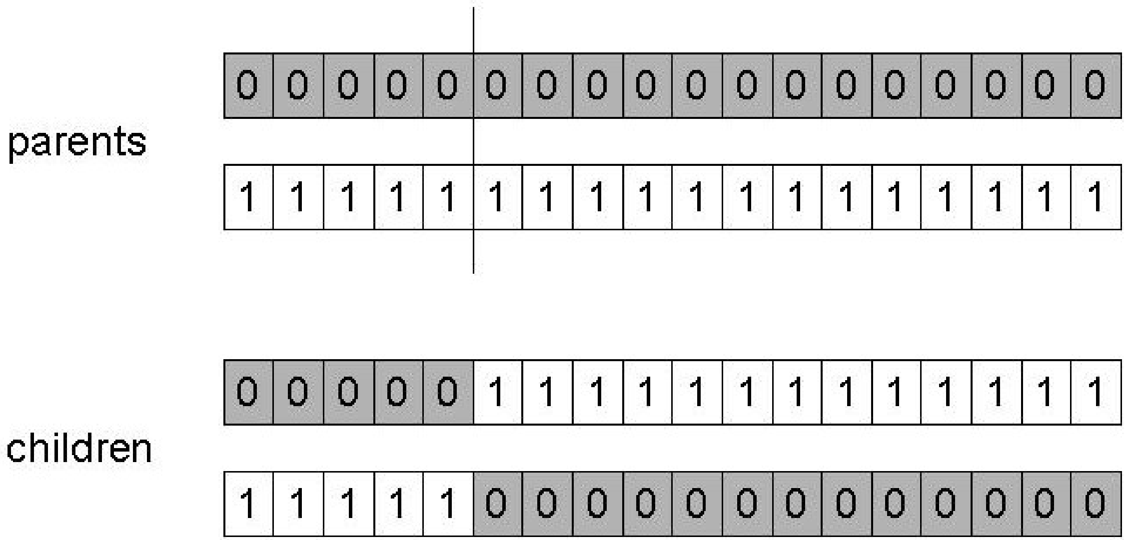
SGA Reproduction Cycle

1. Select parents for the mating pool

   (size of mating pool = population size)
2. Shuffle the mating pool
3. For each consecutive pair apply crossover with probability p_c, otherwise copy parents
4. For each offspring apply mutation
   (bit-flip with probability p_m independently for each bit)
5. Replace the whole population with the resulting offspring

SGA Operators: 1-point crossover

- Choose a random point on the two parents
- Split parents at this crossover point
- Create children by exchanging tails
- P_c typically in range (0.6, 0.9)



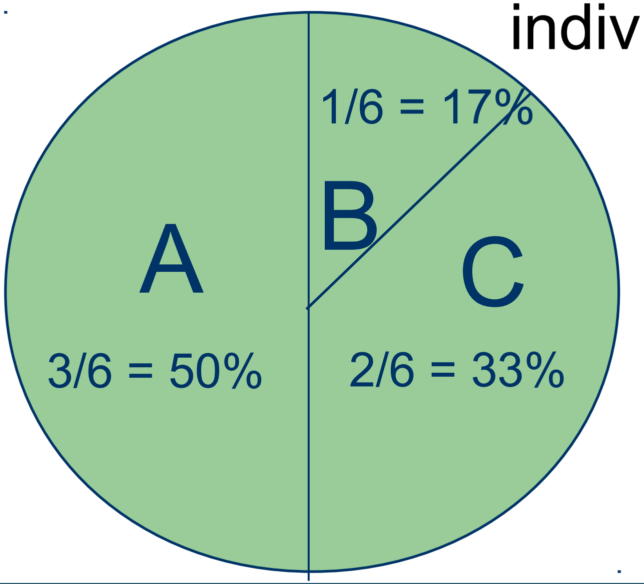
SGA Operators: Mutation

- Alter each gene independently with a probability p_m
- p_m is called the mutation rate
  - Typically between 1/pop_size and 1/ chromosome_length

parent	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
child	0	1	0	0	1	0	1	1	0	0	0	1	0	1	1	0	0	1

SGA Operators: Selection

- Main idea: better individuals get higher chance
  - Chances proportional to fitness
  - Implementation: roulette wheel technique
    - » Assign to each individual a part of the roulette wheel
    - » Spin the wheel n times to select n individuals



fitness(A) = 3

fitness(B) = 1

fitness(C) = 2

Crossover OR Mutation?

- Decade long debate: which one is better / necessary ...

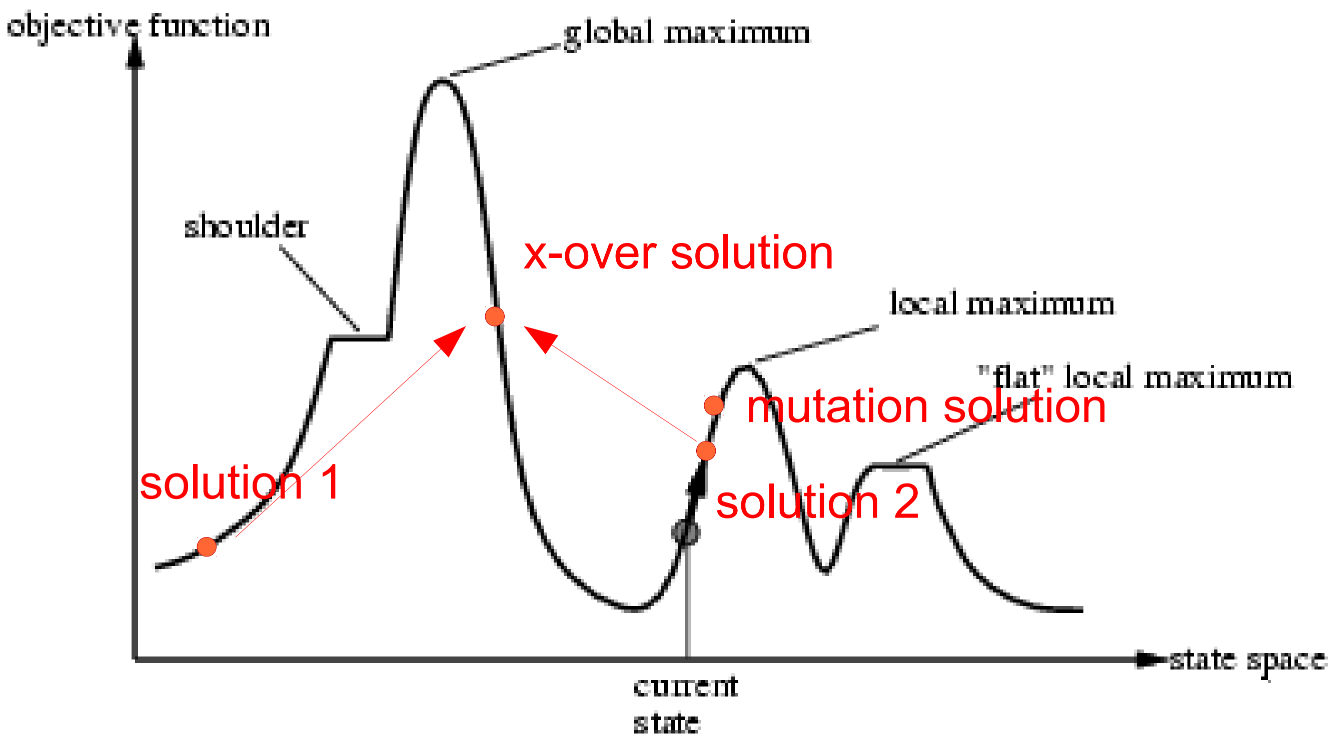
- Answer (at least, rather wide agreement):
  - it depends on the problem, but
  - in general, it is good to have both
  - both have another role
  - mutation-only-EA is possible, crossover-only-EA would not work

Crossover OR Mutation? (cont'd)

- Exploration: Discovering promising areas in the search space, i.e. gaining information on the problem
- Exploitation: Optimising within a promising area, i.e. using information
- There is co-operation AND competition between them
  - Crossover is explorative, it makes a *big* jump to an area somewhere "in between" two (parent) areas
  - Mutation is exploitative, it creates random *small* diversions, thereby staying near (in the area of) the parent

Crossover OR Mutation? (cont'd)

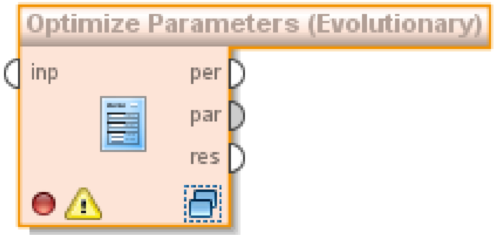
- Recall the solution space example from Hill Climbing
  - crossover makes big jumps
  - mutation makes small steps

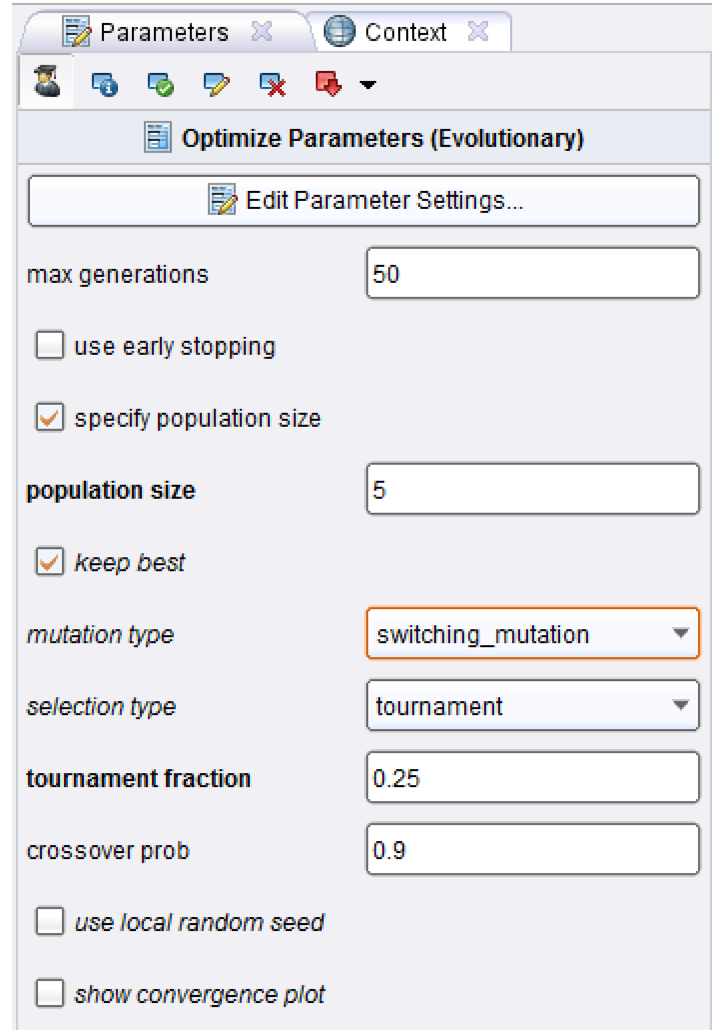


Crossover OR Mutation? (cont'd)

- Only crossover can combine information from two parents
- Only mutation can introduce new information (alleles)
- To hit the optimum you often need a 'lucky' mutation

Parameter Tuning Operators in RapidMiner





Genetic Feature Subset Selection

- Feature Subset Selection
  - can also be solved by Genetic Programming
- Individuals: feature subsets
- Representation: binary
  - 1 = feature is included
  - 0 = feature is not included
- Fitness: classification performance
- Crossover: combine selections of two subsets
- Mutation: flip bits

Selecting a Learner

- So far, we have looked at finding good parameters for a learner
  – the learner was always fixed

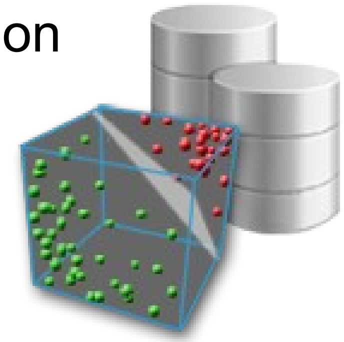
- A similar problem is *selecting* a learner for the task at hand
- Again, we could go with *search*
- Another approach is *meta learning*

Selecting a Learner by Meta Learning

- Meta Learning
  - i.e., *learning about learning*

- Goal: learn how well a learner will perform on a given dataset
  - features: dataset characteristics, learning algorithm
  - prediction target: accuracy, RMSE, ...

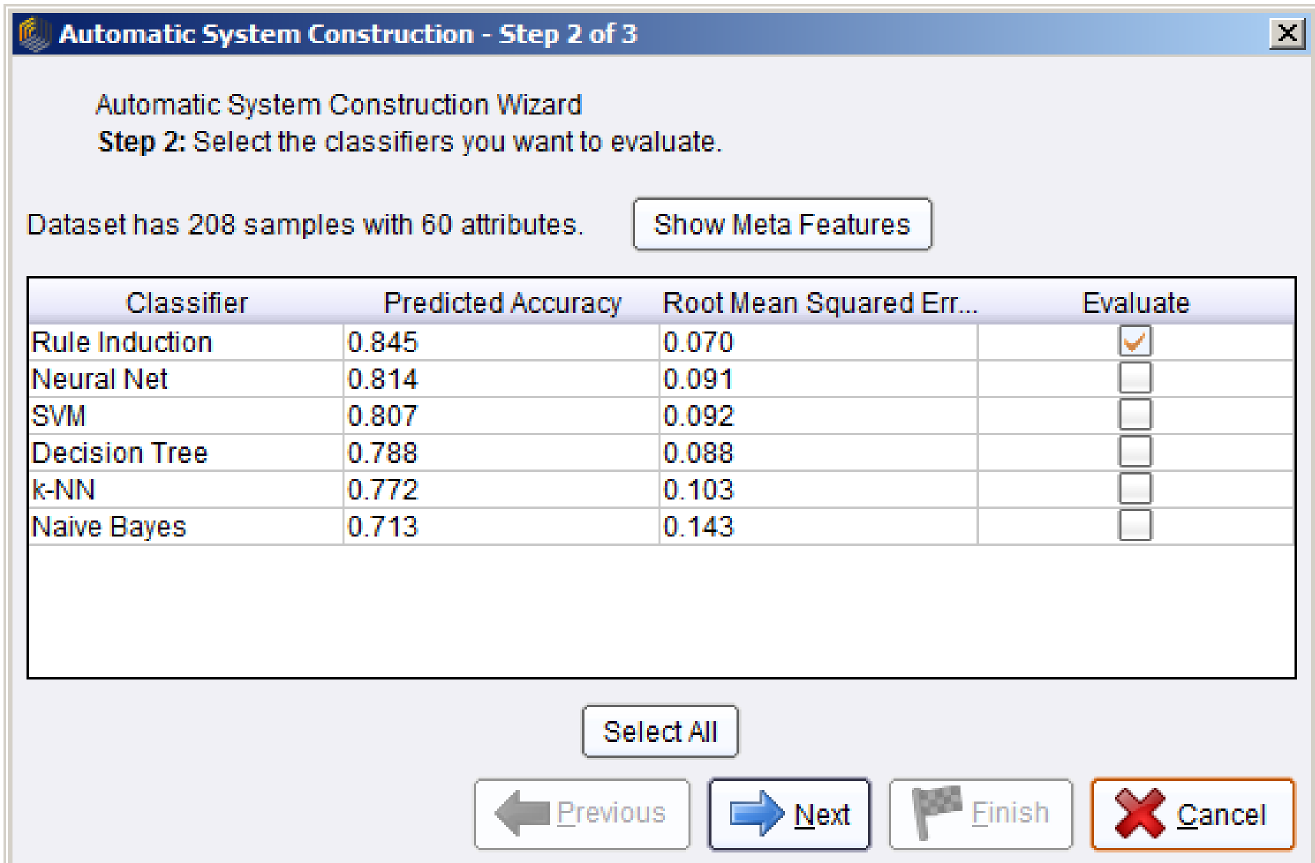
Selecting a Learner by Meta Learning



- Used in the *Automatic System Construction* extension
- regression trained on
  - 90 datasets
  - 54 features
- Examples for features
  - number of instances/attributes
  - fraction of nominal/numerical attributes
  - min/max/average entropy of attributes
  - skewness of classes
  - ...

Selecting a Learner by Meta Learning

- Used in the *Automatic System Construction* extension



Wrap-Up

- Parameter tuning is important
  - many learning methods work poorly with standard parameters
  - often no global optimum, dataset dependent

- Parameter tuning has a large search space
  - trying all combinations is infeasible
  - interaction effects do not allow for one-by-one tuning

Wrap-Up

- Heuristic Methods
  - Hill climbing with variations
  - Beam search
  - Simulated Annealing
  - Genetic Programming
- Other uses of genetic programming
  - Feature subset selection
  - Model fitting

Questions?