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Data Mining II
Optimization & Parameter Tuning

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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

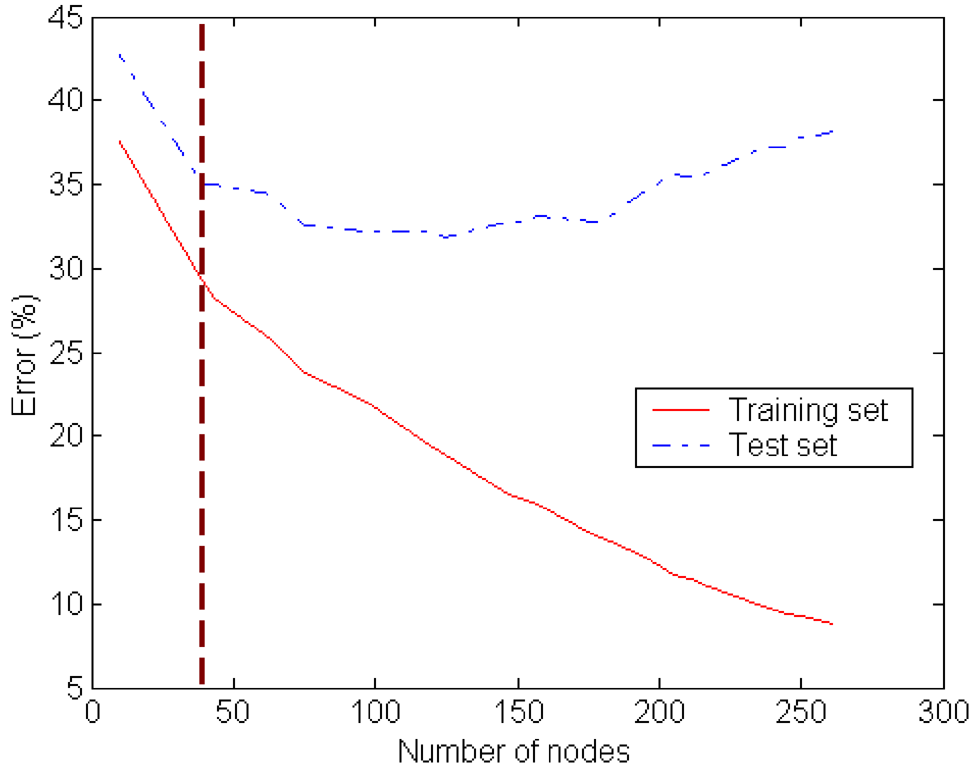
Parameter Tuning – a Naive Approach

- 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?

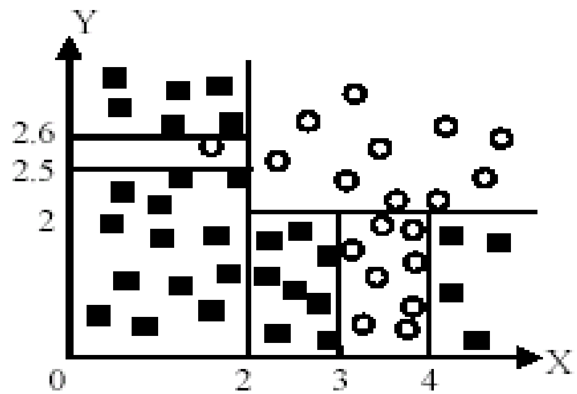
Parameter Tuning – Avoid Overfitting!

- 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:
  - train / test / validation split

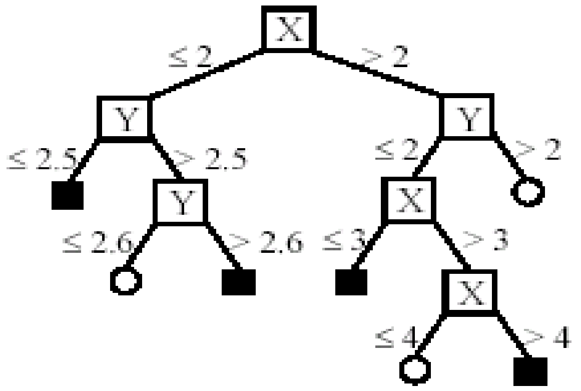


Parameter Tuning – Avoid Overfitting!

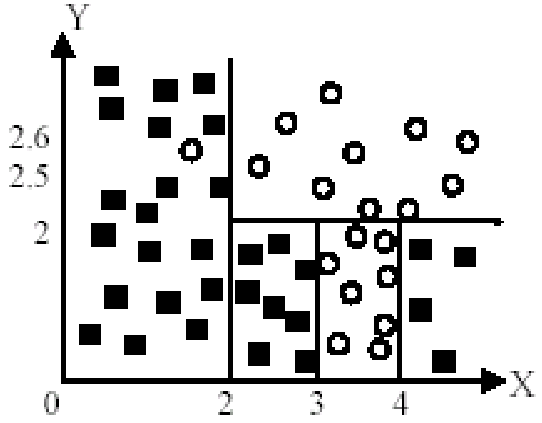
- Parameter option: pruning (yes/no)

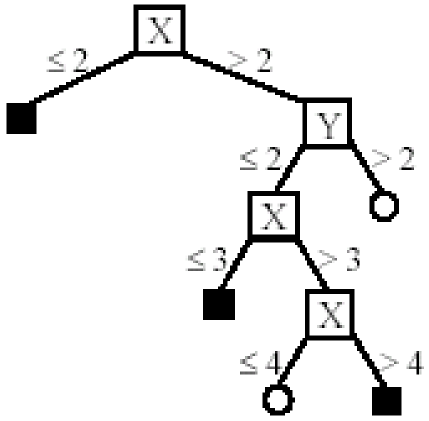


(A) A partition of the data space



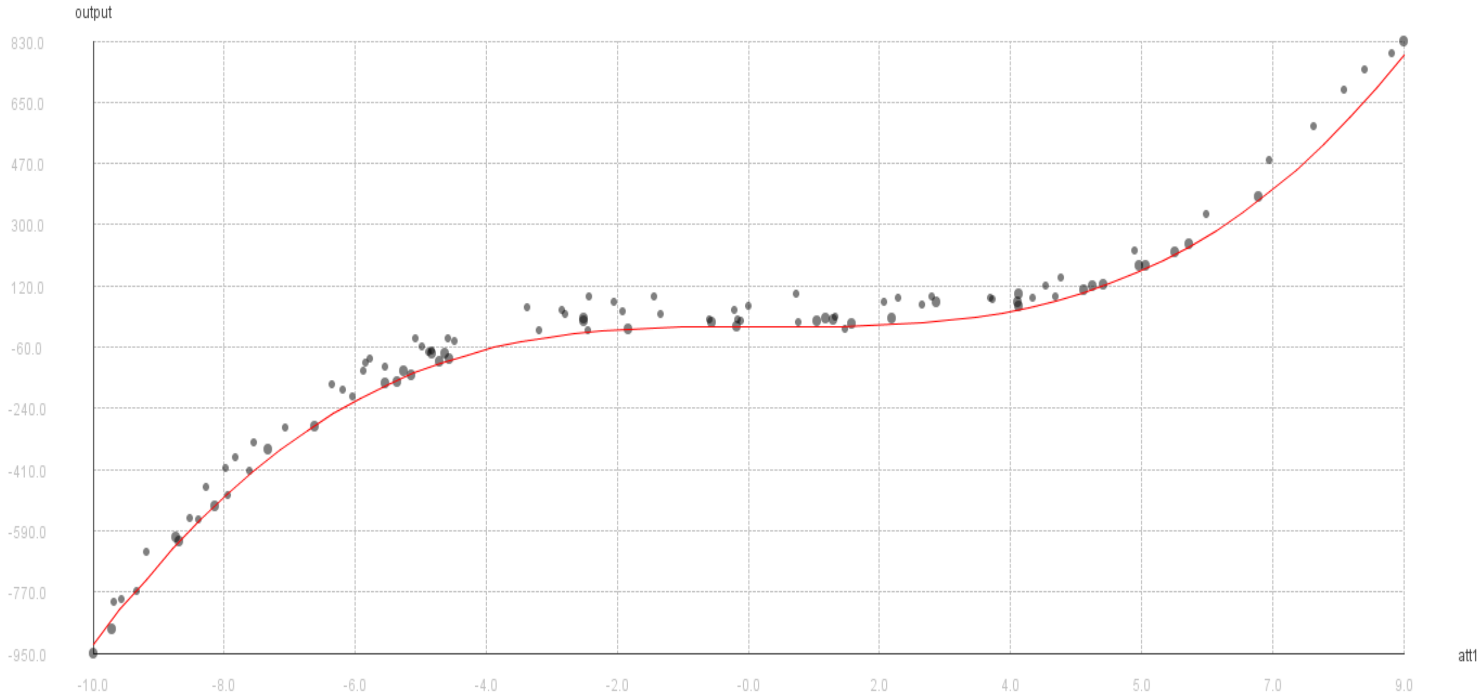
(B). The decision tree





Parameter Tuning – Avoid Overfitting!

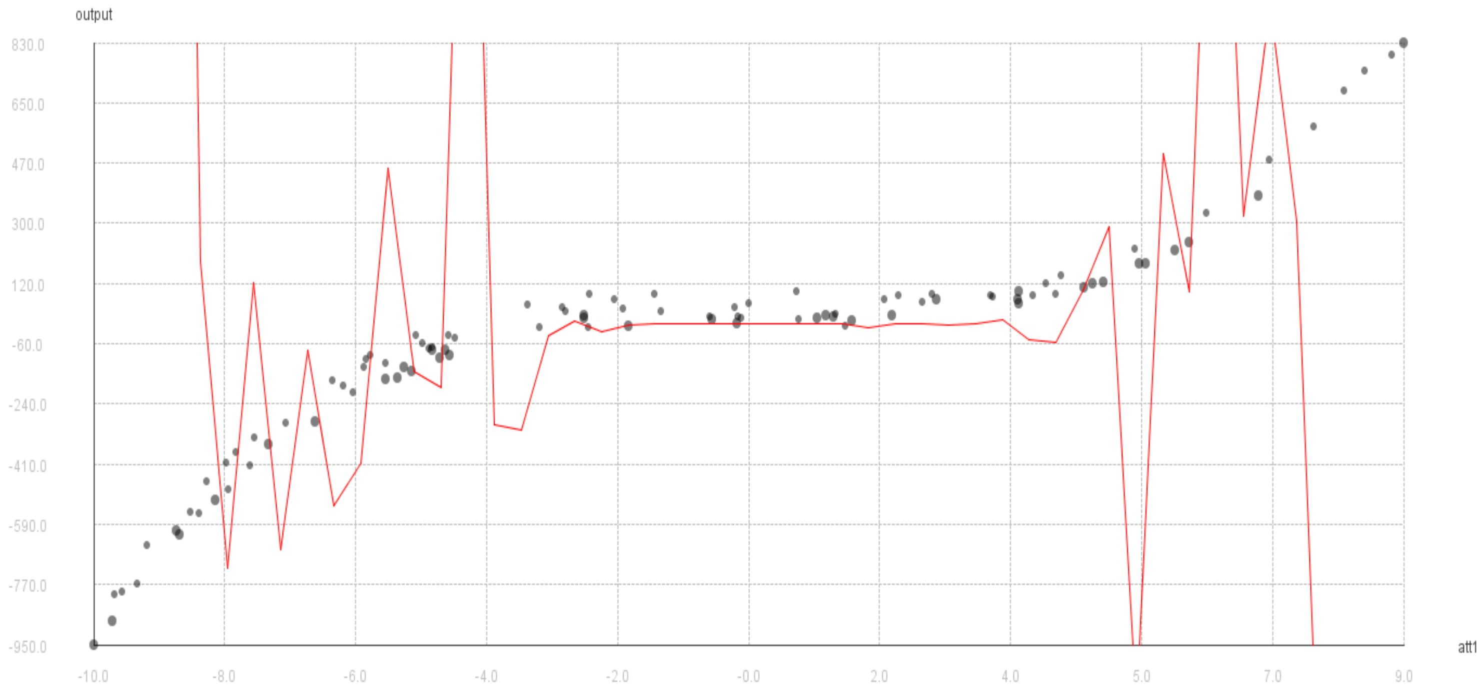
- Real example: train a local polynomial regression model
  - Parameter to tune: find the optimal maximum degree of the polynomial
- Tuning with proper validation: degree = 3



Parameter Tuning – Avoid Overfitting!

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

- Tuning overfitting: degree = 9



Parameter Tuning: Brute Force

- Try all parameter combinations that exist

- Consider, e.g., a k-NN classifier
  - try 30 different distance measures
  - try all k from 1 to 1,000
  - use weighting or not

    → 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

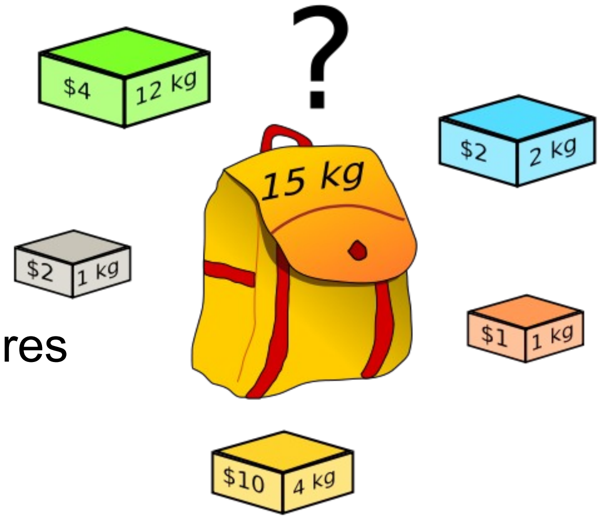
- Related problem:
  - feature subset selection
  - cf. Data Mining 2, first lecture

- 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

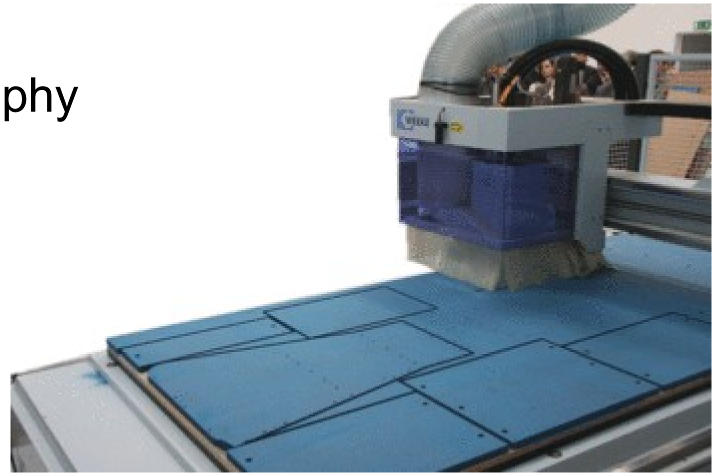
- Problem is NP hard
  - i.e., deterministic algorithms
    require an exponential amount of time
  - Note: feature subset selection for N features
    requires 2^n evaluations

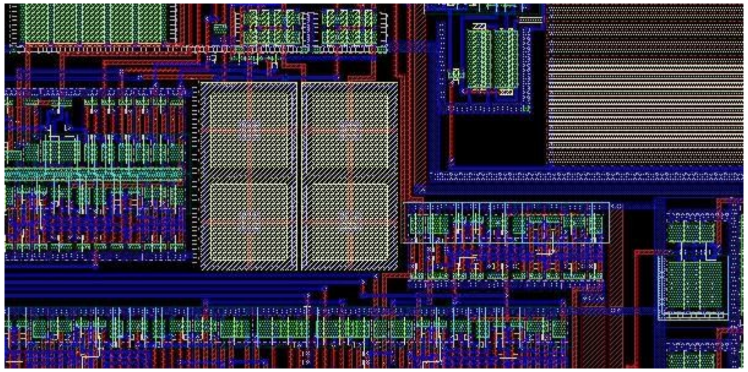


Intermezzo: Beyond Parameter Tuning

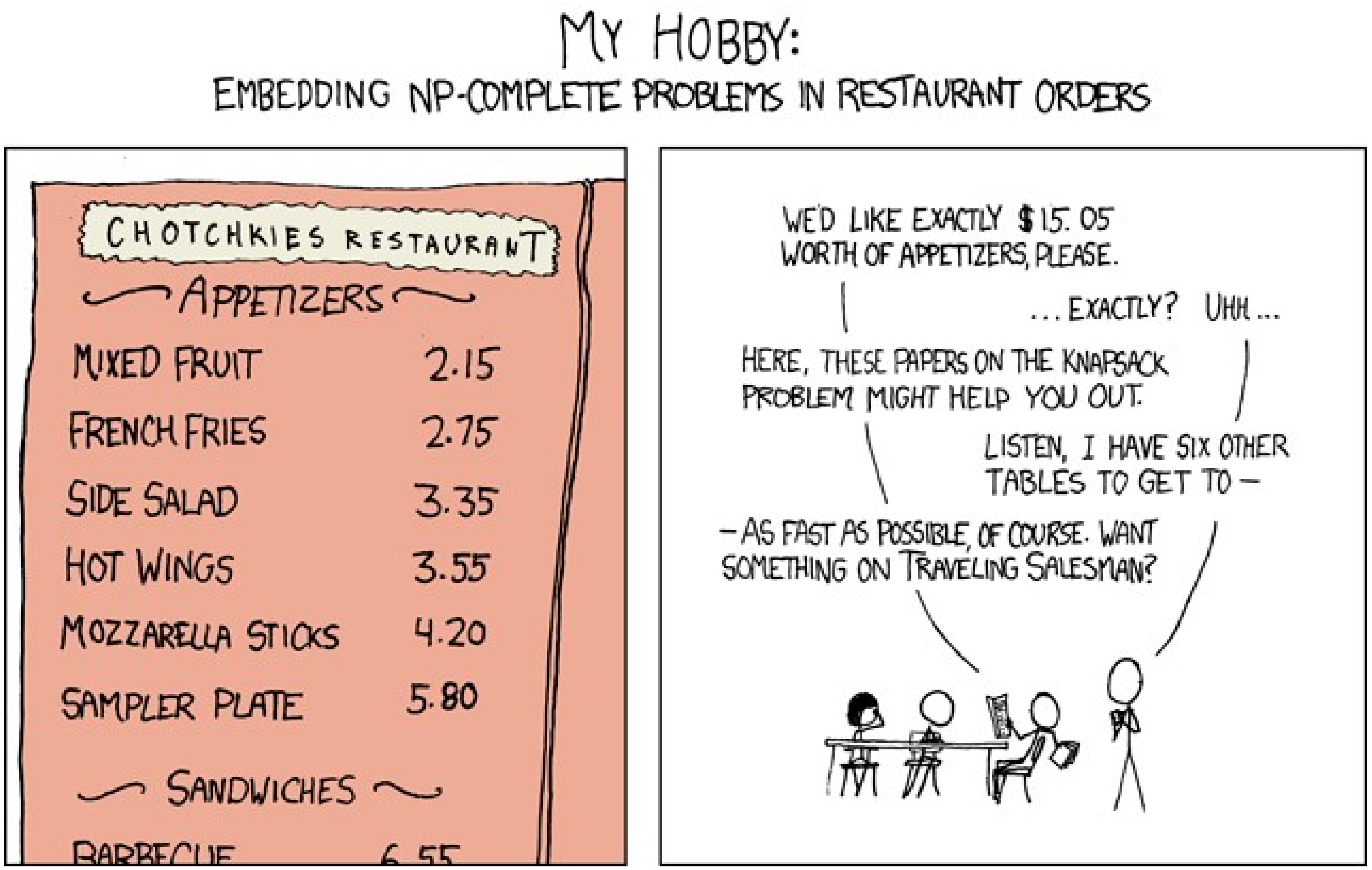
- Many optimization problems are NP hard
  - Routing problems (Traveling Salesman Problem)
  - Integer factorization

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





Intermezzo: Beyond Parameter Tuning


MY HOBBY:
EMBEDDING NP-COMPLETE PROBLEMS IN RESTAURANT ORDERS
CHOTCHKIES RESTAURANT
APPETIZERS
MIXED FRUIT 2.15
FRENCH FRIES 2.75
SIDE SALAD 3.35
HOT WINGS 3.55
MOZZARELLA STICKS 4.20
SAMPLER PLATE 5.80
SANDWICHES
BARBECUE 6.55
WE'D LIKE EXACTLY $15.05 WORTH OF APPETIZERS, PLEASE.
...EXACTLY? UHH...
HERE, THESE PAPERS ON THE KNAPSACK PROBLEM MIGHT HELP YOU OUT.
LISTEN, I HAVE SIX OTHER TABLES TO GET TO –
– AS FAST AS POSSIBLE, OF COURSE. WANT SOMETHING ON TRAVELING SALESMAN?

http://xkcd.com/287/

Parameter Tuning: Brute Force

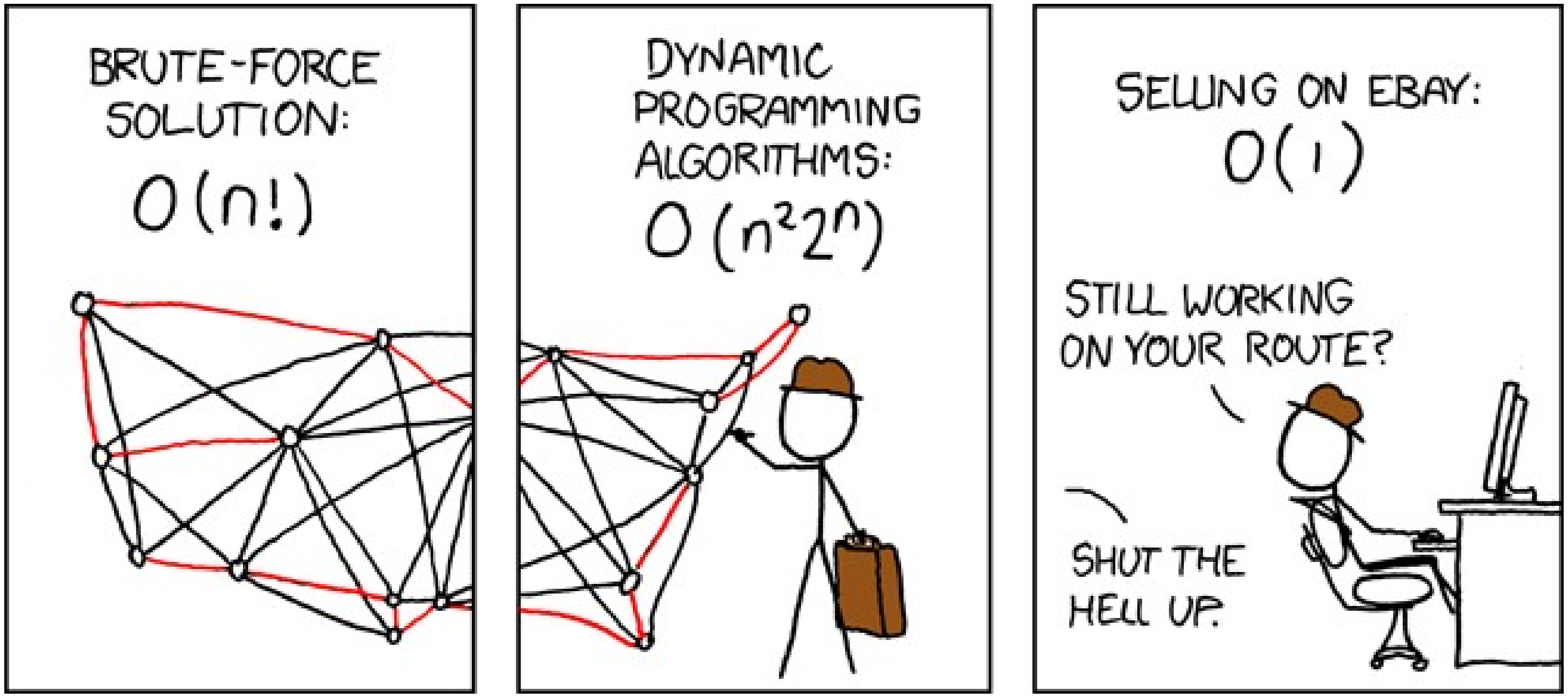
- Properties of Brute Force search
  - guaranteed to find the best parameter setting
  - too slow in most practical cases
- Grid Search
  - performs a brute force search
  - with equal-width steps on non-discrete numerical attributes (e.g., 10,20,30,..,100)
- Parameters with a wide range (e.g., 0.0001 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

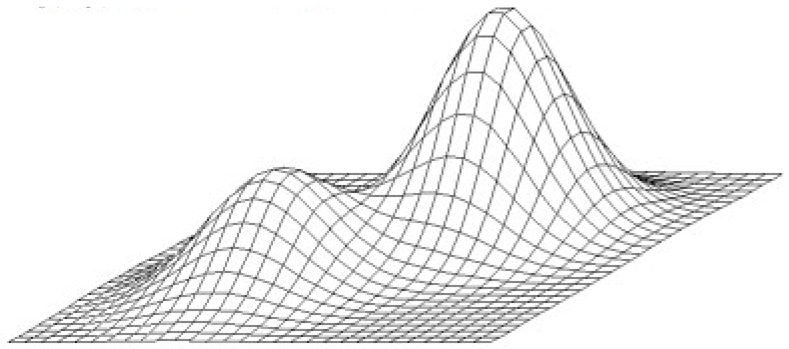
- Example: two parameters p and q, each with values 0,1, and 2
  - the table depicts classification accuracy

	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

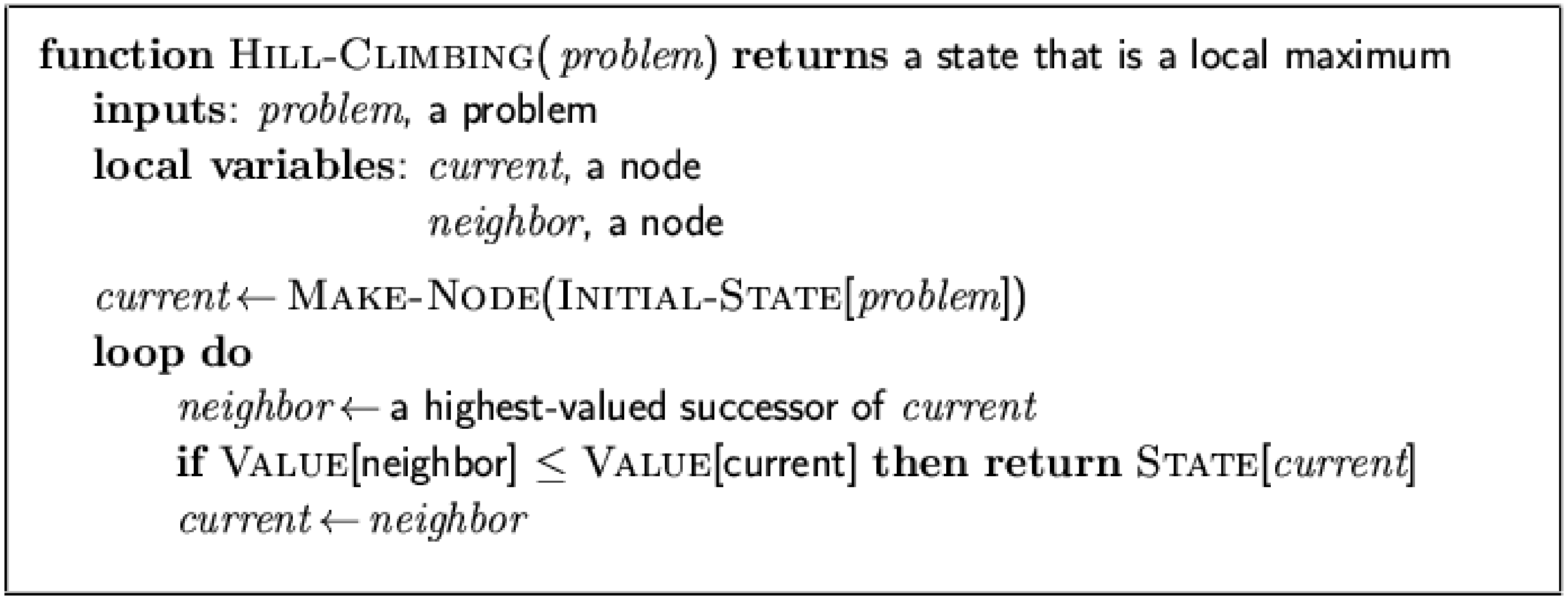
- If we try to optimize one parameter by another (first p, then q)
  - we end at p=0,q=0 in six out of nine cases
  - on average, we investigate 2.3 solutions

	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"

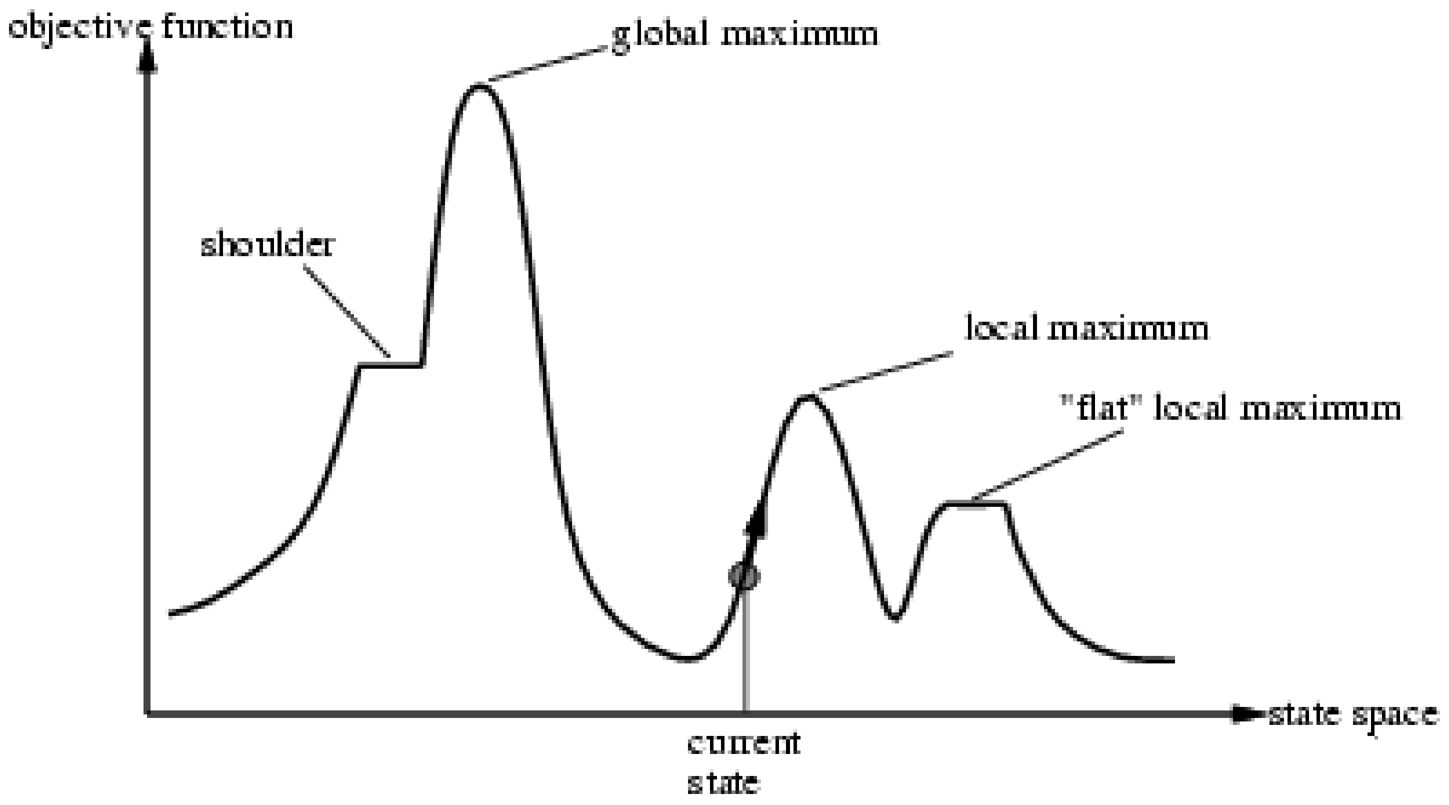


```
function HILL-CLIMBING(problem) returns a state that is a local maximum
    inputs: problem, a problem
    local variables: current, a node
                     neighbor, a node

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

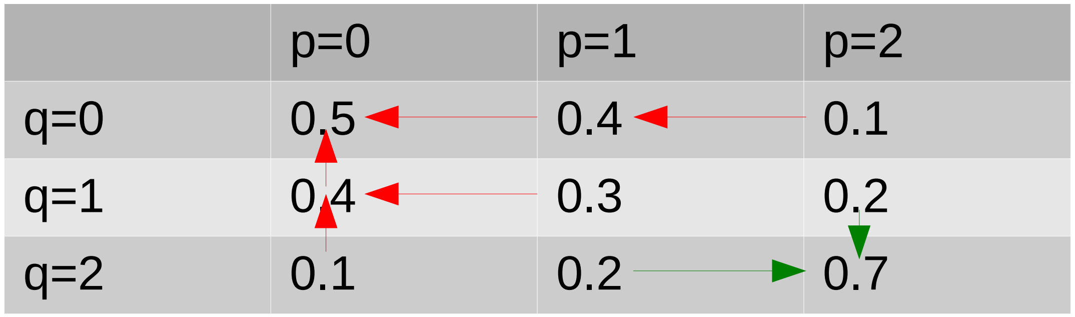
Hill-Climbing Search

- 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

Local Beam Search

- Keep track of k states rather than just one
- Start with k randomly generated states
- At each iteration, all the successors of all k states are generated
- Select the k best successors from the complete list and repeat

Simulated Annealing

- Escape local maxima by allowing “bad” moves
  - Idea: but gradually decrease their size and frequency
- Origin: metallurgical annealing

- Bouncing ball analogy:
  - Shaking hard (= high temperature)
  - Shaking less (= lower the temperature)
- If T decreases slowly enough, best state is reached

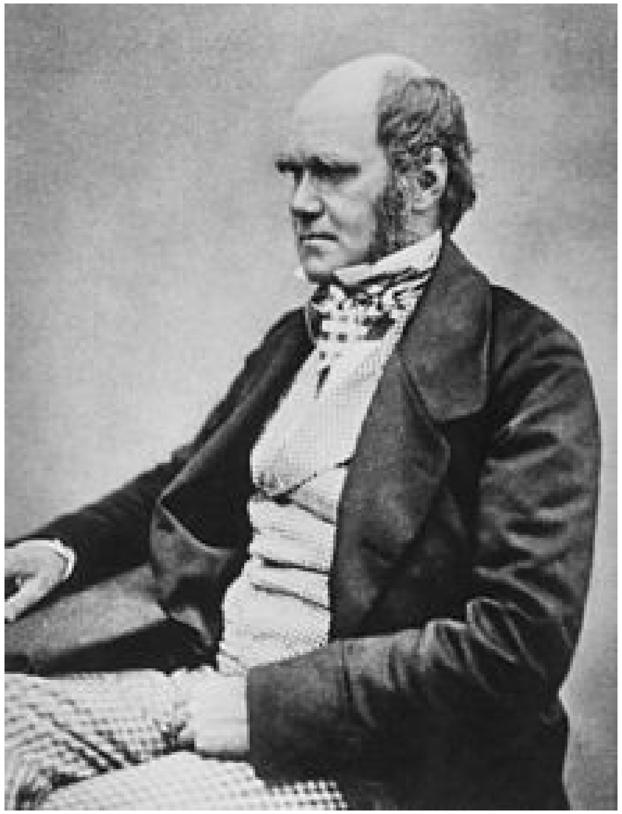
Simulated Annealing

```
function SIMULATED-ANNEALING( problem, schedule) return a solution state
    input: problem, a problem
           schedule, a mapping from time to temperature
    local variables: current, a node.
                     next, a node.
                     T, a “temperature” controlling the probability of downward steps

    current $\leftarrow$ MAKE-NODE(INITIAL-STATE[problem])
    for t $\leftarrow$ 1 to $\infty$ do
           T $\leftarrow$ schedule[t]
           if T = 0 then return current
           next $\leftarrow$ a randomly selected successor of current
           $\Delta$E $\leftarrow$  VALUE[next] - VALUE[current]
           if $\Delta$E > 0 then current $\leftarrow$ next
           else current $\leftarrow$ next only with probability $e^{\Delta E / T}$
```

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

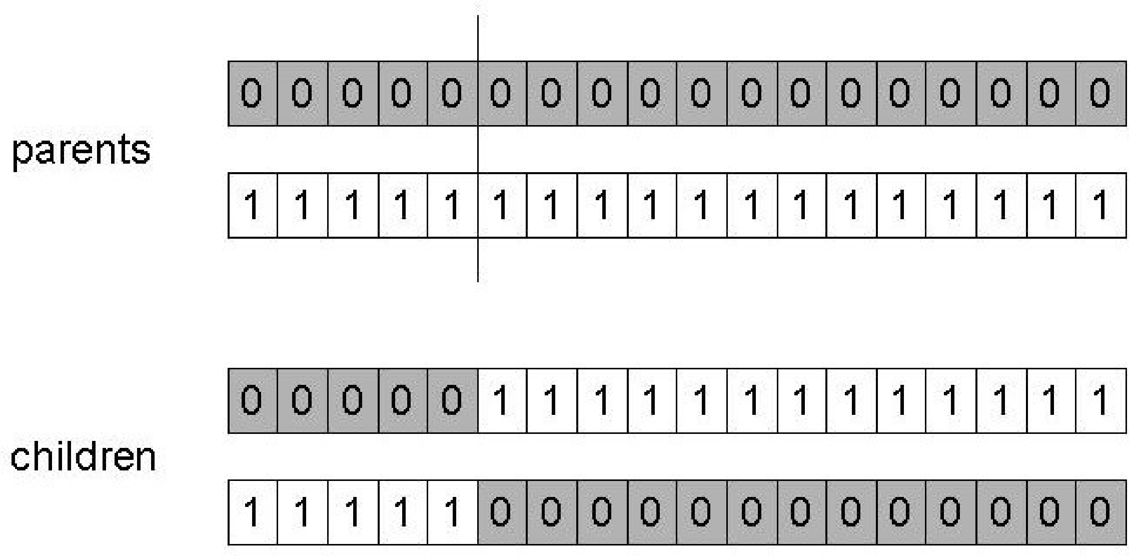
SGA Reproduction Cycle

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

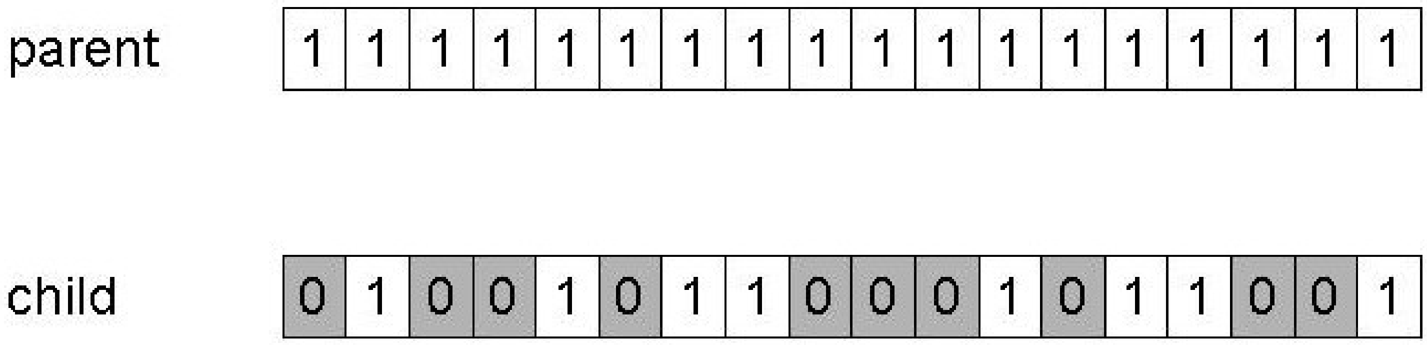
SGA Operators: 1-point crossover

- 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)



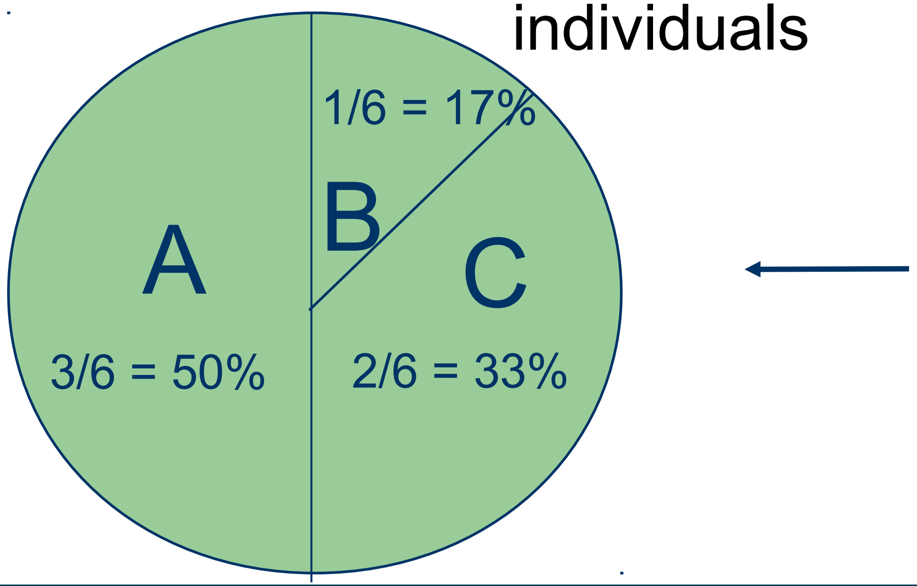
SGA Operators: Mutation

- 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



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 ...

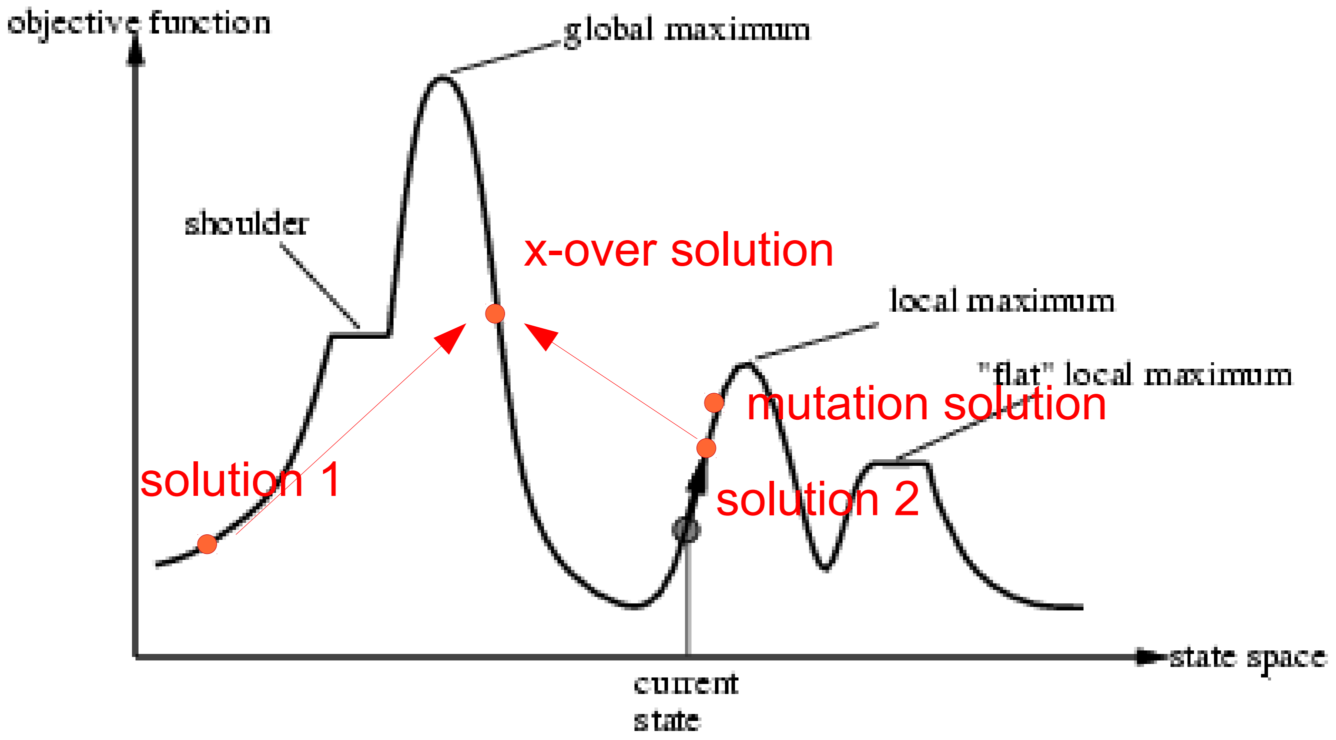
- Answer (at least, rather wide agreement):
  - it depends on the problem, but
  - in general, it is good to have both
  - both have another role
  - mutation-only-EA is possible, crossover-only-EA would not work

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

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

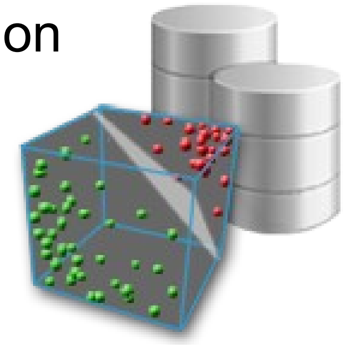
- A similar problem is *selecting* a learner for the task at hand
- Again, we could go with *search*
- Another approach is *meta learning*

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

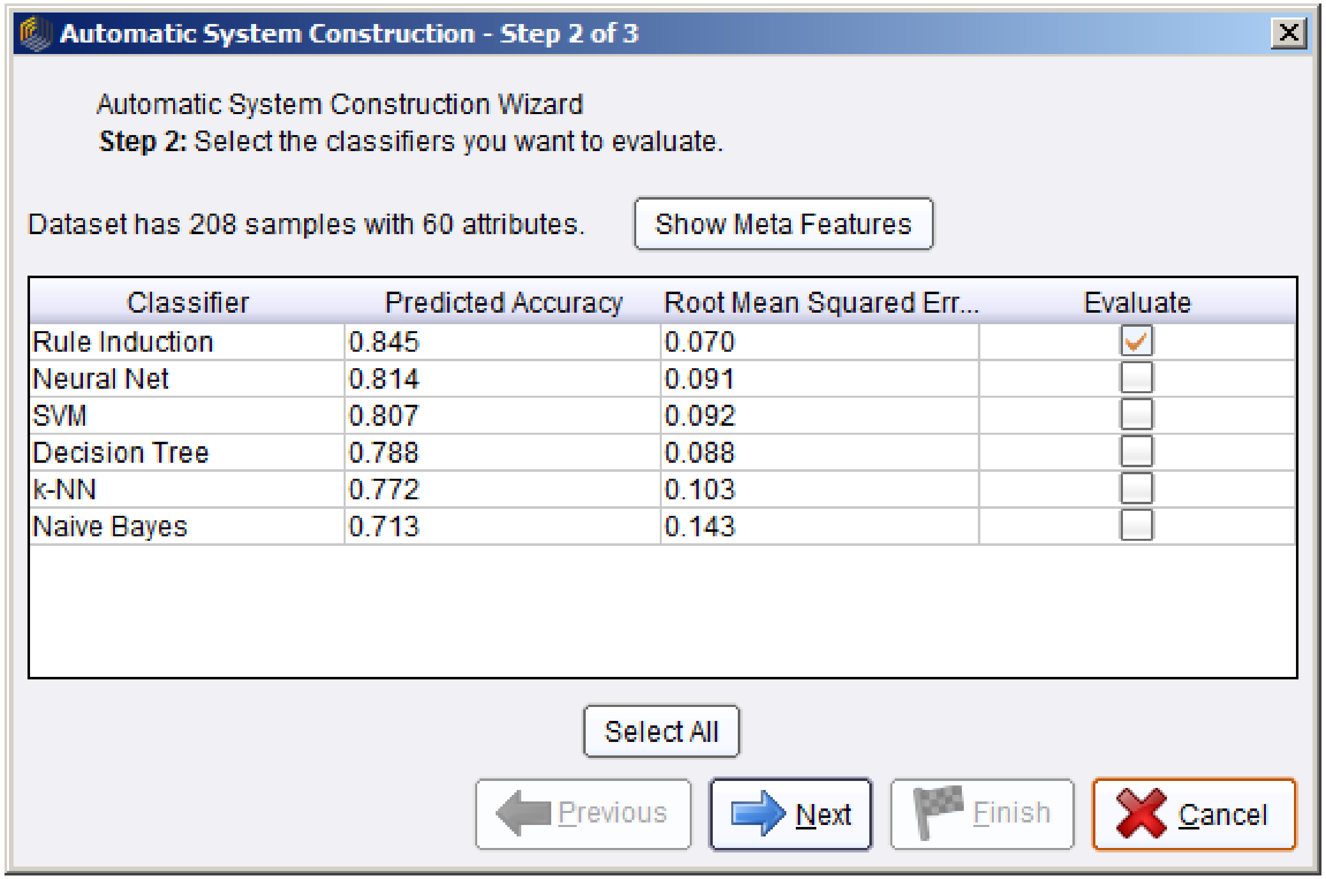
- Used in the *Automatic System Construction* extension
- regression trained on
  - 90 datasets
  - 54 features



- 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



Automatic System Construction Wizard
Step 2: Select the classifiers you want to evaluate.

Dataset has 208 samples with 60 attributes.

Classifier	Predicted Accuracy	Root Mean Squared Err...	Evaluate
Rule Induction	0.845	0.070	✓
Neural Net	0.814	0.091	☐
SVM	0.807	0.092	☐
Decision Tree	0.788	0.088	☐
k-NN	0.772	0.103	☐
Naive Bayes	0.713	0.143	☐

...and now for something completely different.

- Recap: search heuristics are good for problems where...
  - finding an optimal solution is difficult
  - evaluating a solution candidate is easy
  - the search space of possible solutions is large
- Possible solution: genetic programming

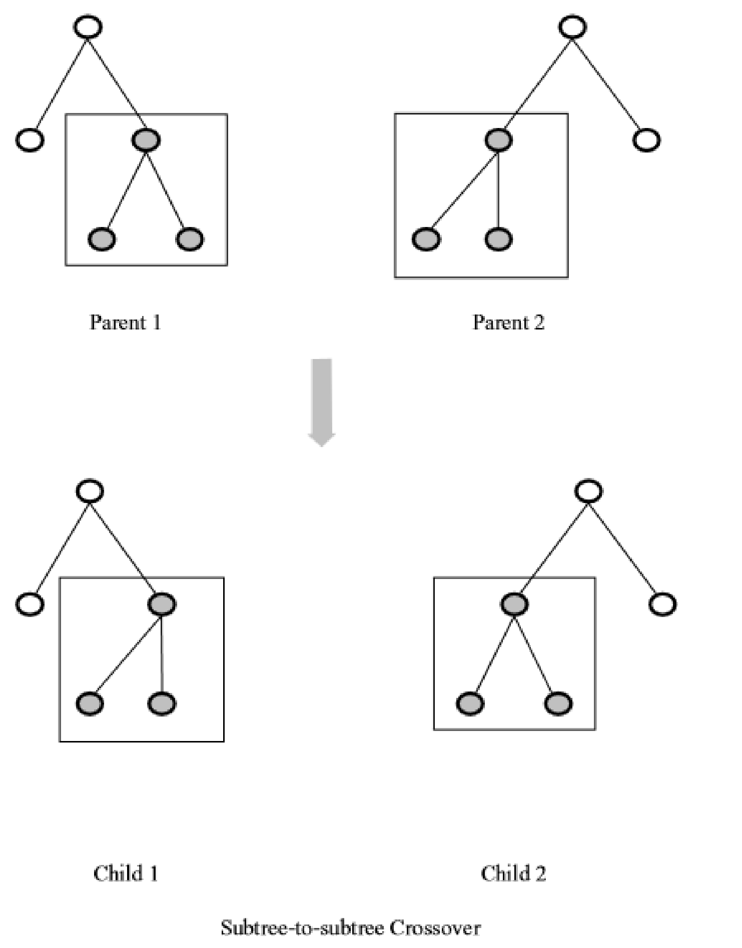
- We have encountered such problems quite frequently
- Example: learning an optimal decision tree from data

Genetic Decision Tree Learning

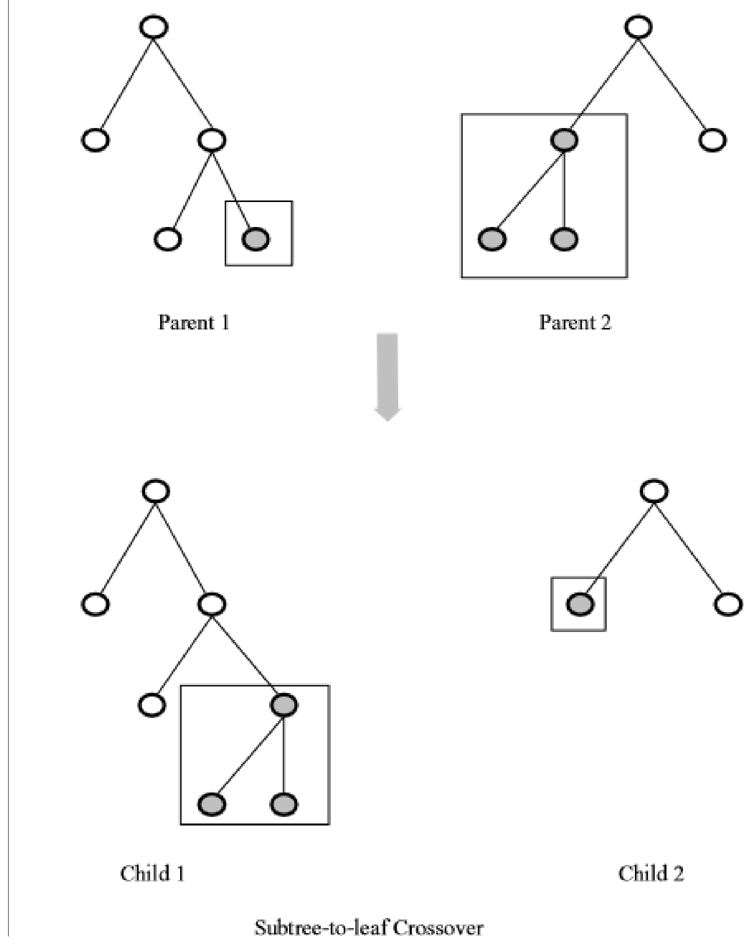
- e.g., GAIT (Fu et al., 2003)
  - also the source of the pictures on the following slides
- Population: candidate decision trees
  - initialization: e.g., trained on small subsets of data
- Create new decision trees by means of
  - crossover
  - mutation
- Fitness function: e.g., accuracy

Genetic Decision Tree Learning

- Crossover:



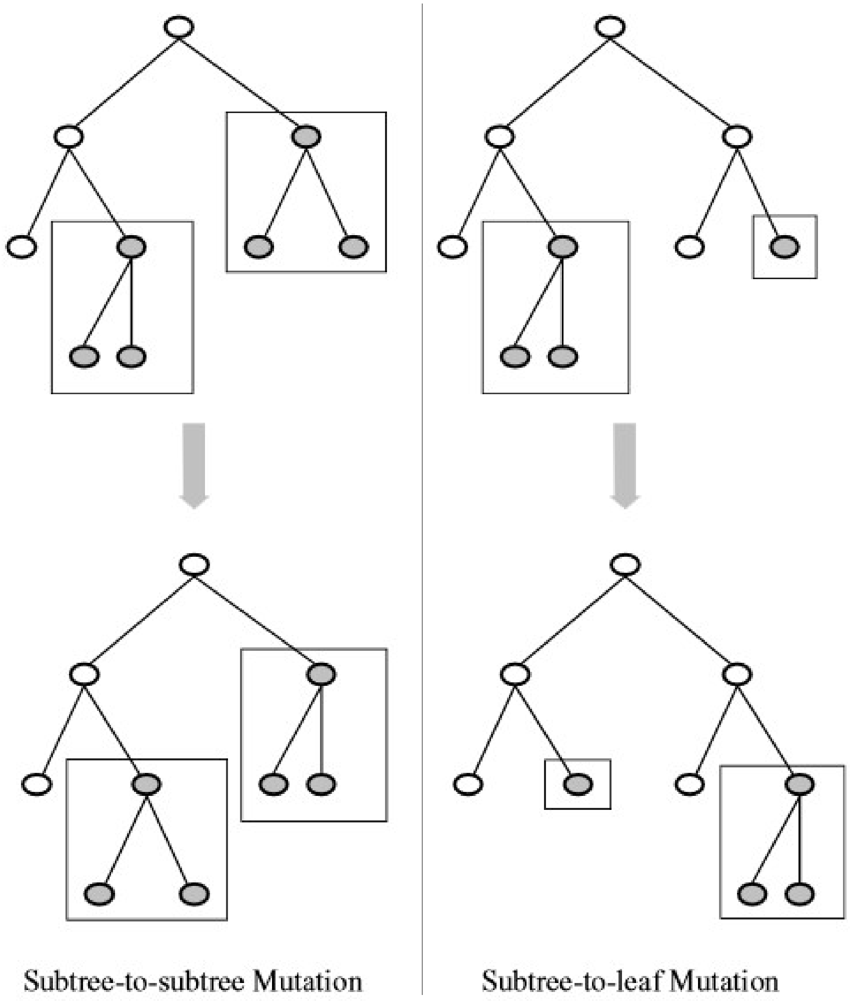
Subtree-to-subtree Crossover



Subtree-to-leaf Crossover

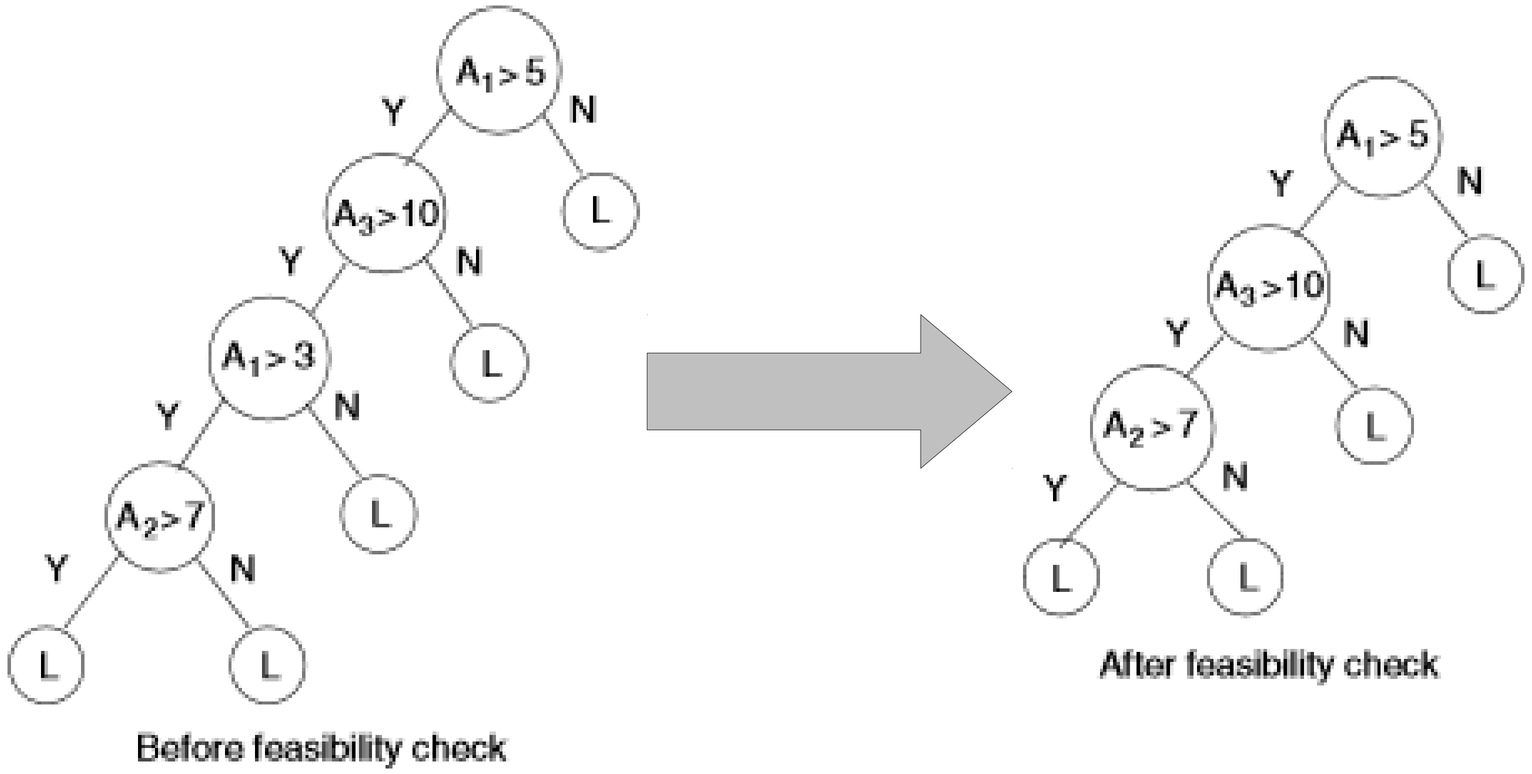
Genetic Decision Tree Learning

- Mutation:



Genetic Decision Tree Learning

- Feasibility Check:



Combination of GP with other Learning Methods

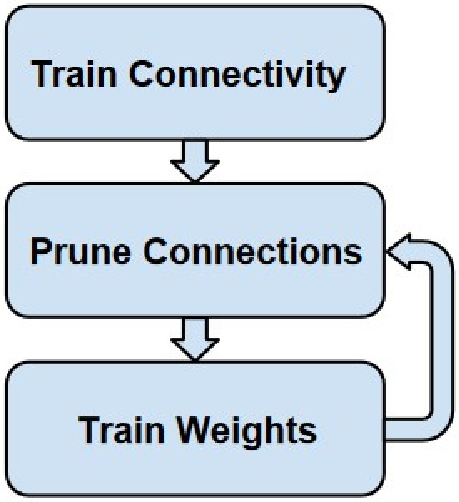
- Rule Learning (“Learning Classifier Systems”), since late 70s
  - Population: set of rule sets (!)
  - Crossover: combining rules from two sets
  - Mutation: changing a rule

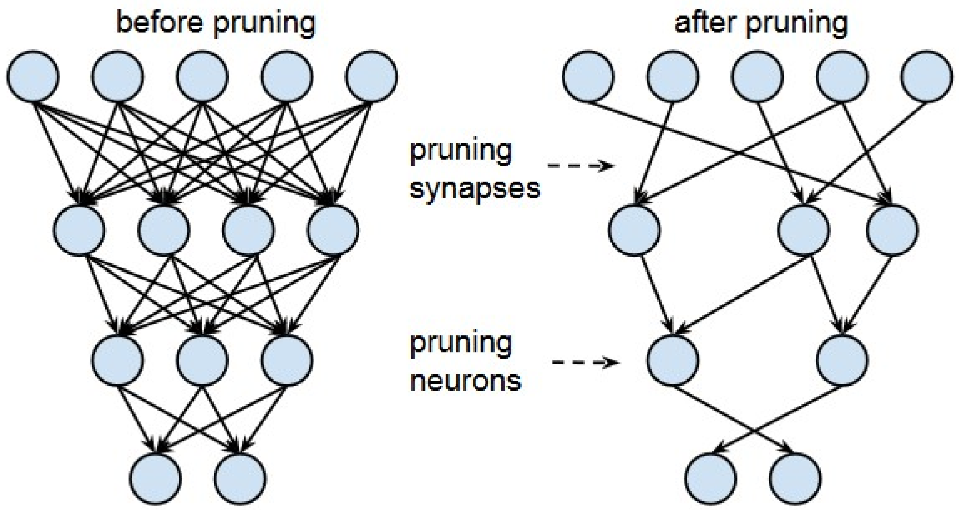
- Artificial Neural Networks
  - Easiest solution: fixed network layout
  - The network is then represented as an ordered set (vector) of weights e.g., [0.8, 0.2, 0.5, 0.1, 0.1, 0.2]
  - Crossover and mutation are straight forward
  - Variant: AutoMLP
    - Searches for best combination of hidden layers and learning rate

Parameter Optimization vs. Pruning

- Architecture of a neural network can be seen as parameters
  - How many hidden layers? Which size?

- Pruning approaches: train large network, then start eliminating connections





Han et al. (2015): Learning both Weights and Connections for Efficient Neural Network

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

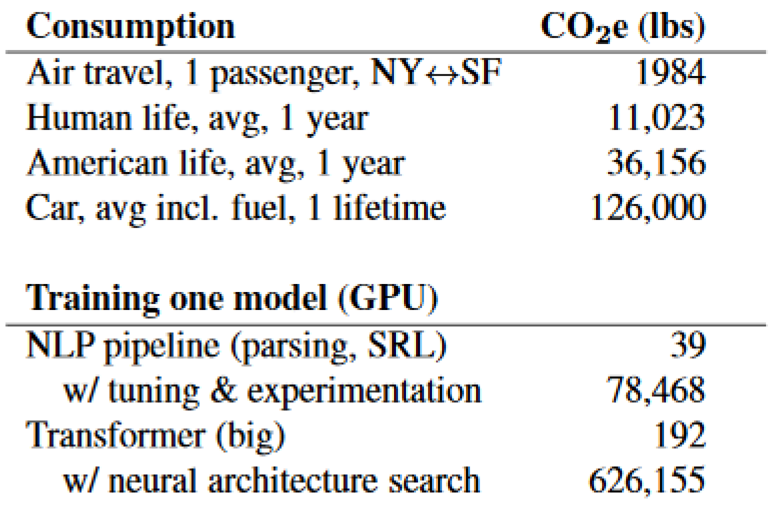
Wrap-Up

- Heuristic Methods
  - Hill climbing with variations
  - Beam search
  - Simulated Annealing
  - Genetic Programming

- Other uses of genetic programming
  - Feature subset selection
  - Model fitting

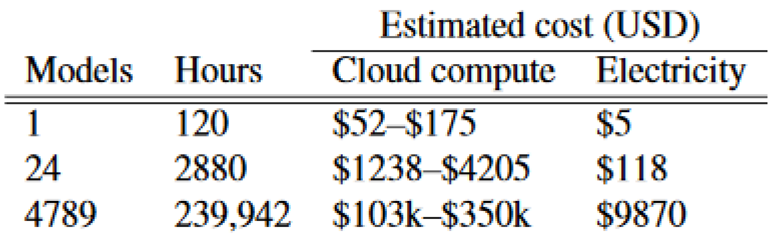
Parameter Tuning: Criticism

- Just let those numbers sink…
  - ...think: carbon footprint
  - ...think: fair chances?



Consumption	CO_2e (lbs)
Air travel, 1 passenger, NY↔SF	1984
Human life, avg, 1 year	11,023
American life, avg, 1 year	36,156
Car, avg incl. fuel, 1 lifetime	126,000
Training one model (GPU)	
NLP pipeline (parsing, SRL)	39
w/ tuning & experimentation	78,468
Transformer (big)	192
w/ neural architecture search	626,155

Table 1: Estimated CO_2 emissions from training common NLP models, compared to familiar consumption.[1]



Models	Hours	Estimated cost (USD)	
		Cloud compute	Electricity
1	120	\$52–\$175	\$5
24	2880	\$1238–\$4205	\$118
4789	239,942	\$103k–\$350k	\$9870

Table 4: Estimated cost in terms of cloud compute and electricity for training: (1) a single model (2) a single tune and (3) all models trained during R&D.

Strubell et al. (2019): Energy and Policy Considerations for Deep Learning in NLP

Questions?

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