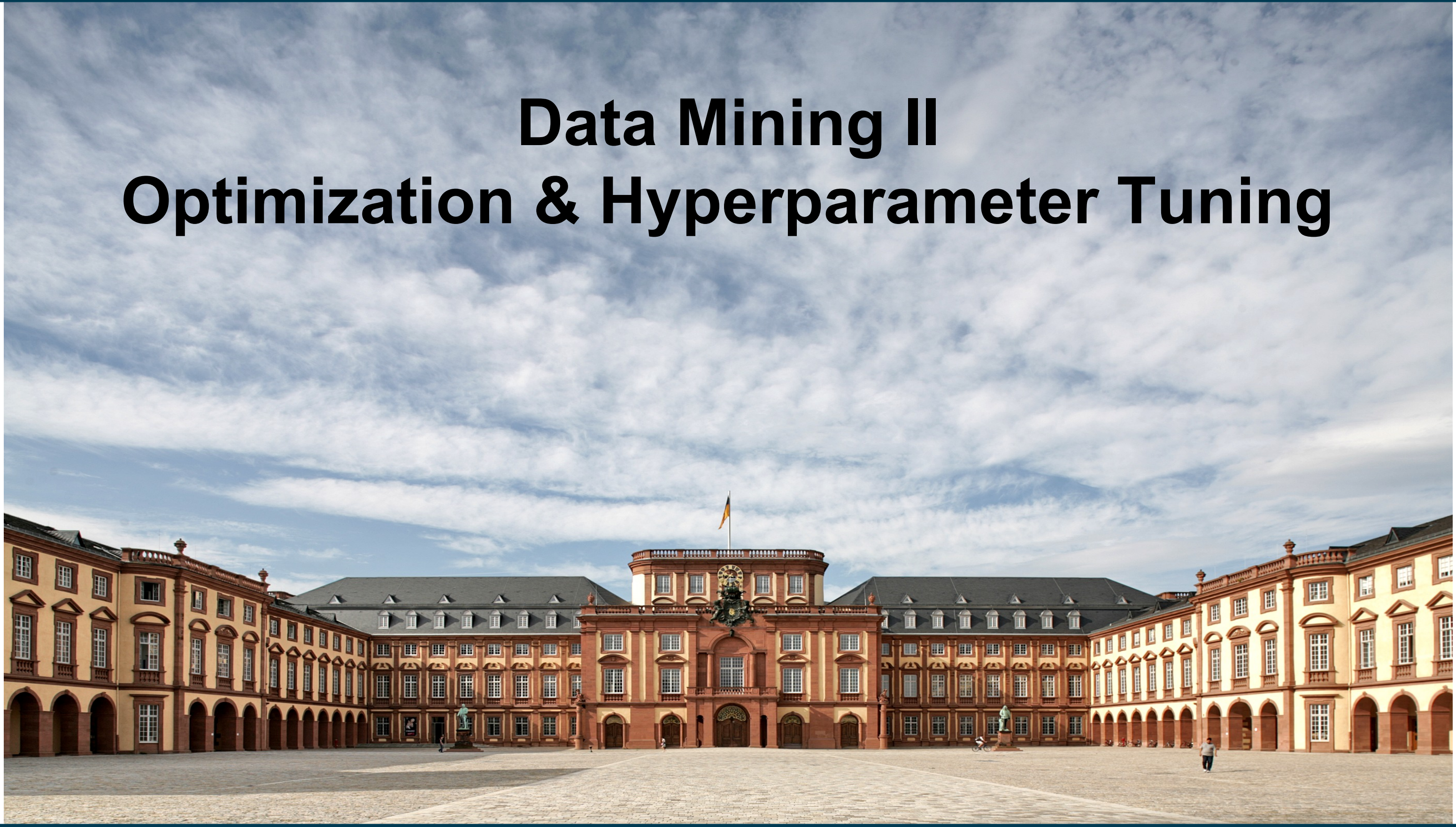


Data Mining II
Optimization & Hyperparameter Tuning

Heiko Paulheim

Why Hyperparameter Tuning?

- What we have seen so far
  - many learning algorithms for classification, regression, ...
- Many of those have hyperparameters
  - 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

Parameters vs. Hyperparameters

- Parameters
  - ...are learned during training
  - Typical examples:
    - Coefficients in (linear) regression
    - Weights in neural networks
    - …
  - Training:
    - Find set of of parameters so that objective function is minimized/maximized
      - (on a holdout set)

Parameters vs. Hyperparameters

- Hyperparameters
  - ...are fixed *before* training
  - Typical examples:
    - Network layout and learning rate in neural netwo
    - k in kNN
    - …
  - Training:
    - Find set of of parameters so that objective function is minimized/maximized
      - (on a holdout set)
      - given a previously fixed set of hyperparameters

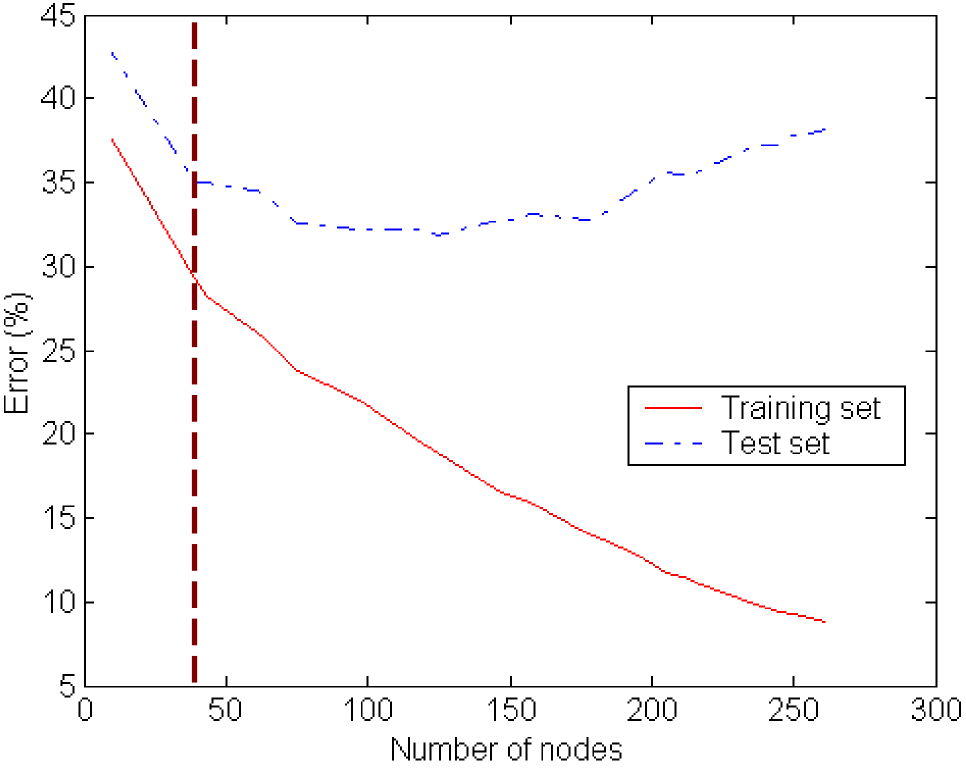
Hyperparameter Tuning – a Naive Approach

- 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?

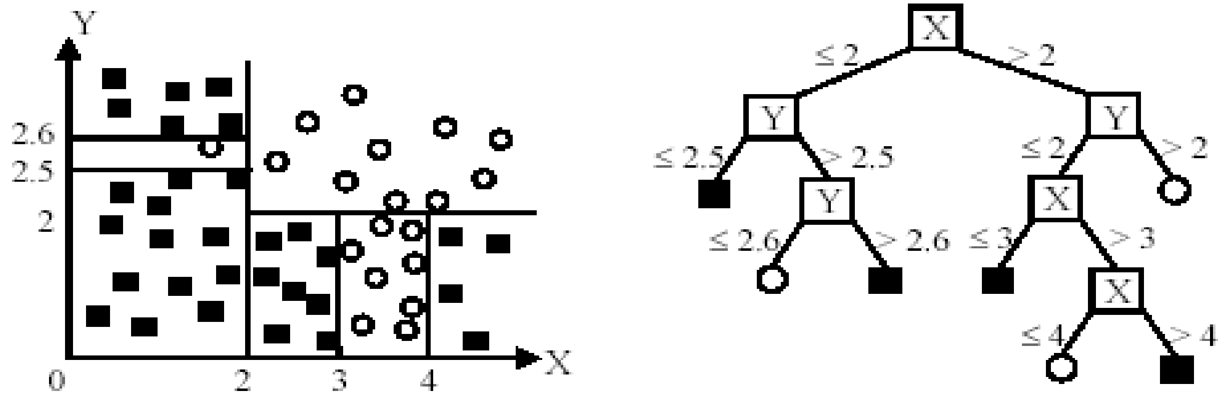
Hyperparameter Tuning – Avoid Overfitting!

- 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



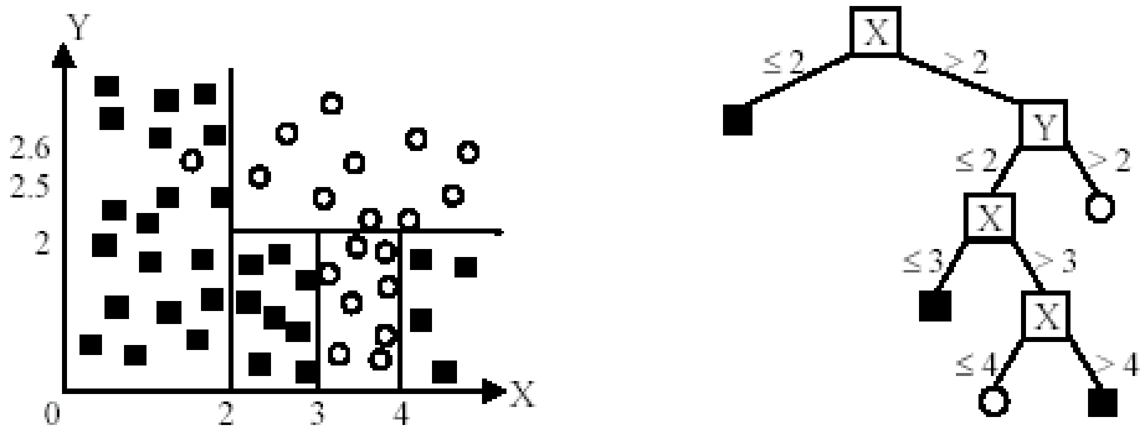
Hyperparameter Tuning – Avoid Overfitting!

- Parameter option: pruning (yes/no)



(A) A partition of the data space

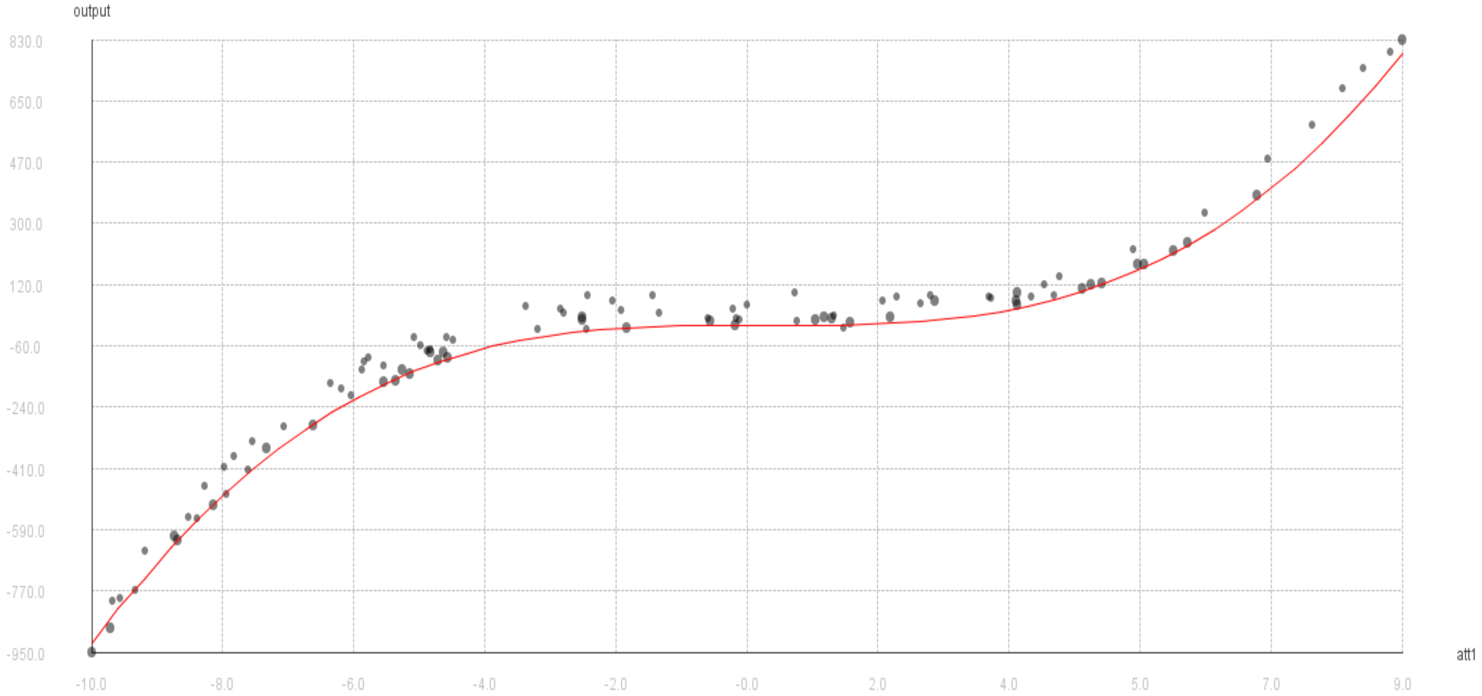
(B). The decision tree



Hyperparameter Tuning – Avoid Overfitting!

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

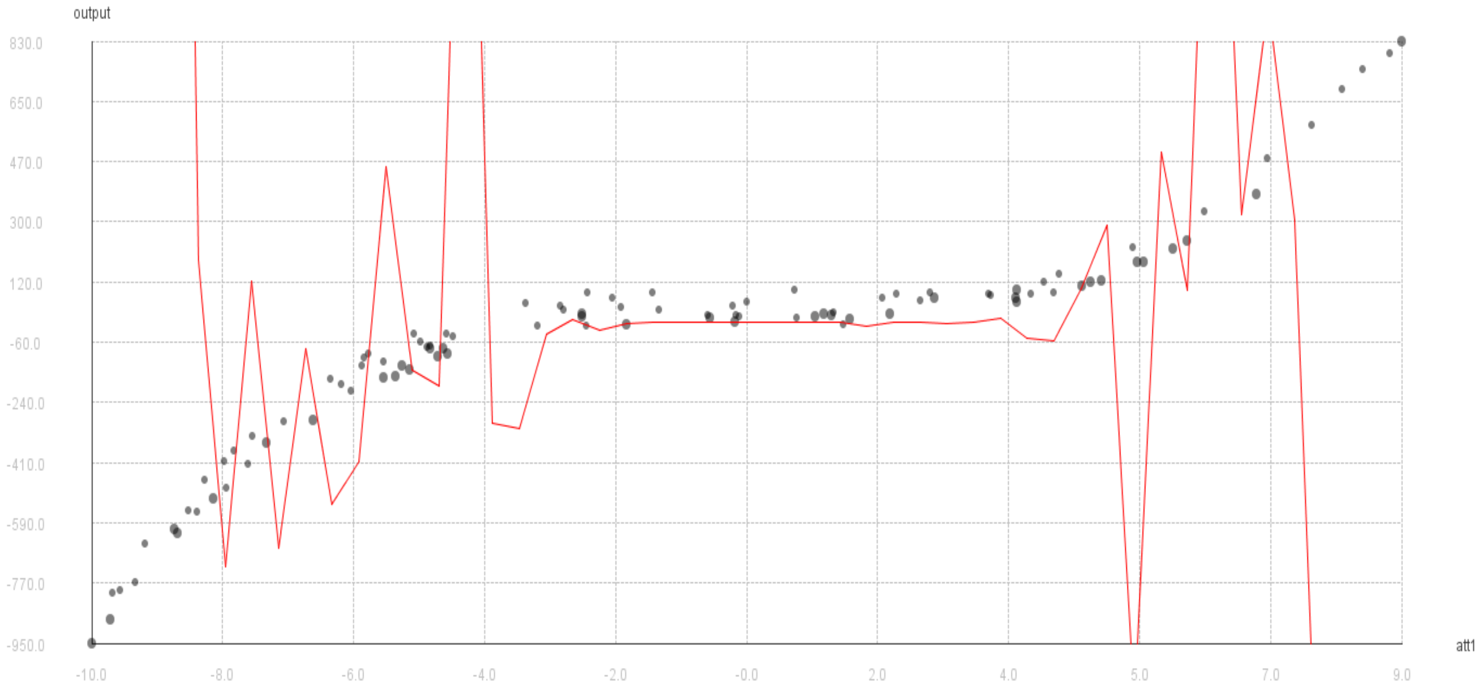
- Tuning with proper validation: degree = 3



Hyperparameter 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



Hyperparameter 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 Hyperparameter Tuning

- Hyperparameter 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 Hyperparameter Tuning

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

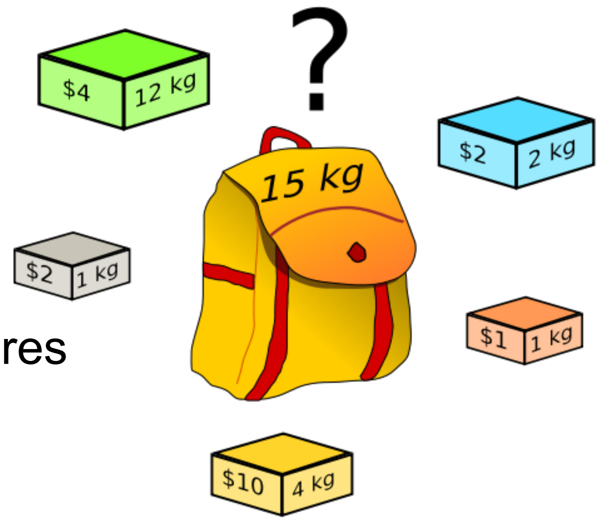
- Given n features, brute force requires 2^n evaluations
  - for 20 features, that is already one million
    → ten million with cross validation

Intermezzo: Beyond Hyperparameter 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

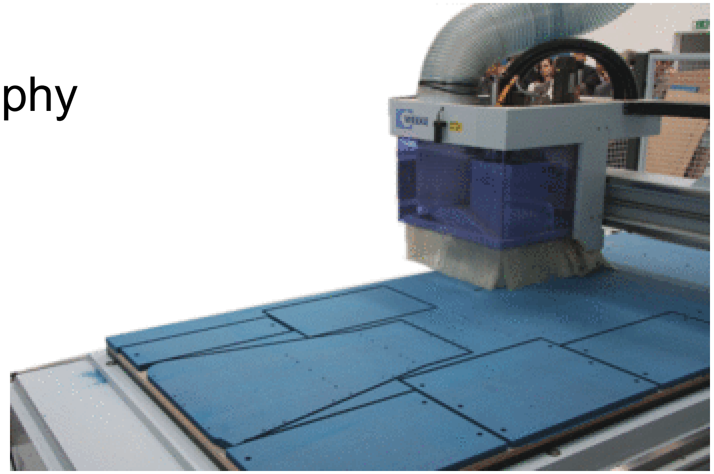
- Problem is NP hard
  - i.e., deterministic algorithms
    require an exponential amount of time

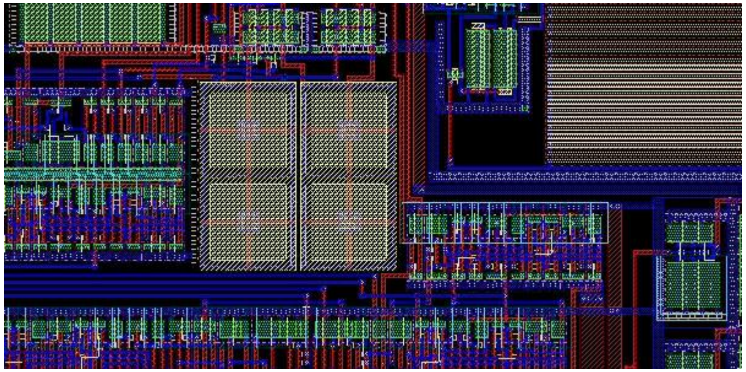
  - Note: feature subset selection for N features
    requires 2^n evaluations



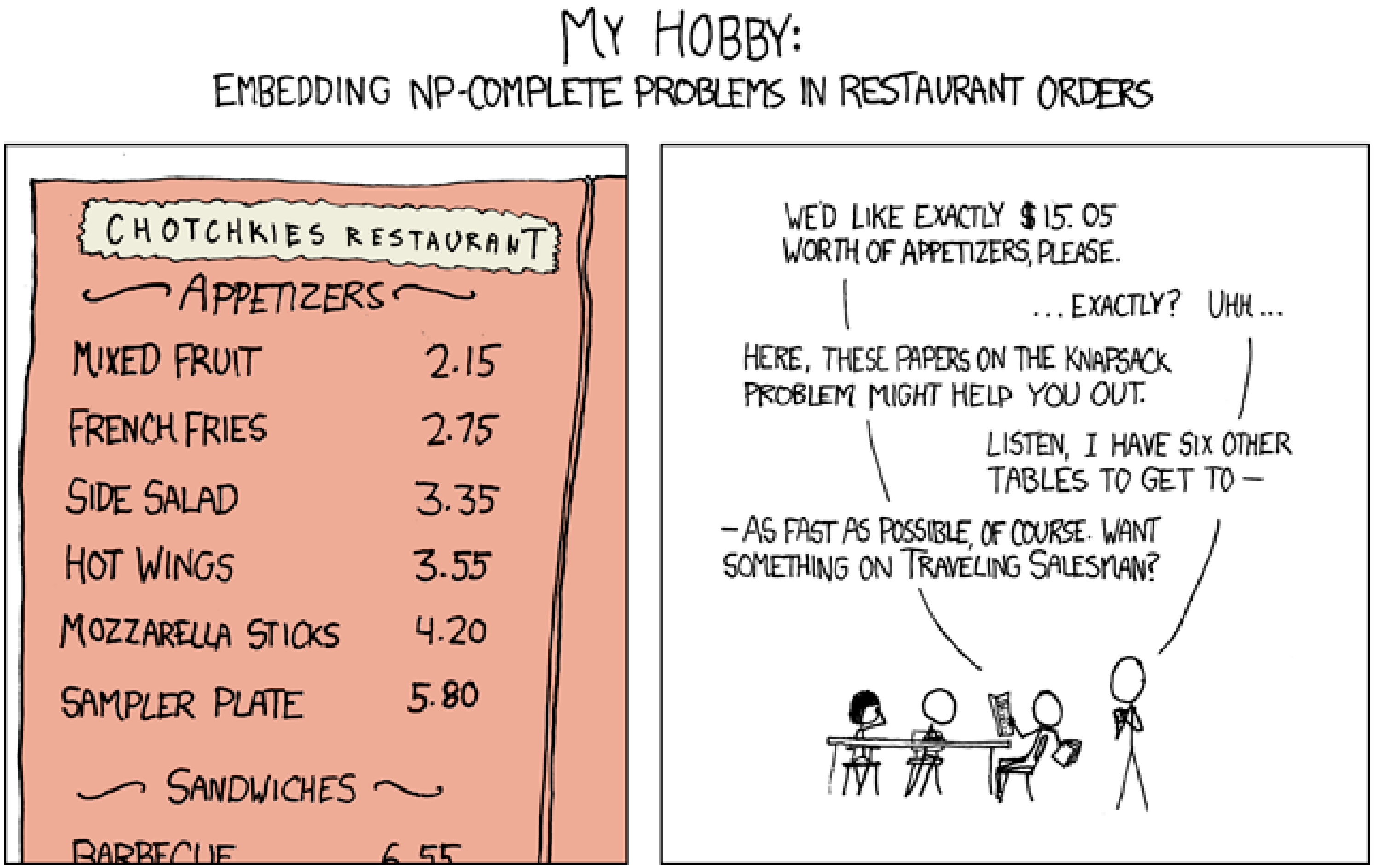
Intermezzo: Beyond Hyperparameter Tuning

- 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 Hyperparameter Tuning



http://xkcd.com/287/

Hyperparameter Tuning: Brute Force

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

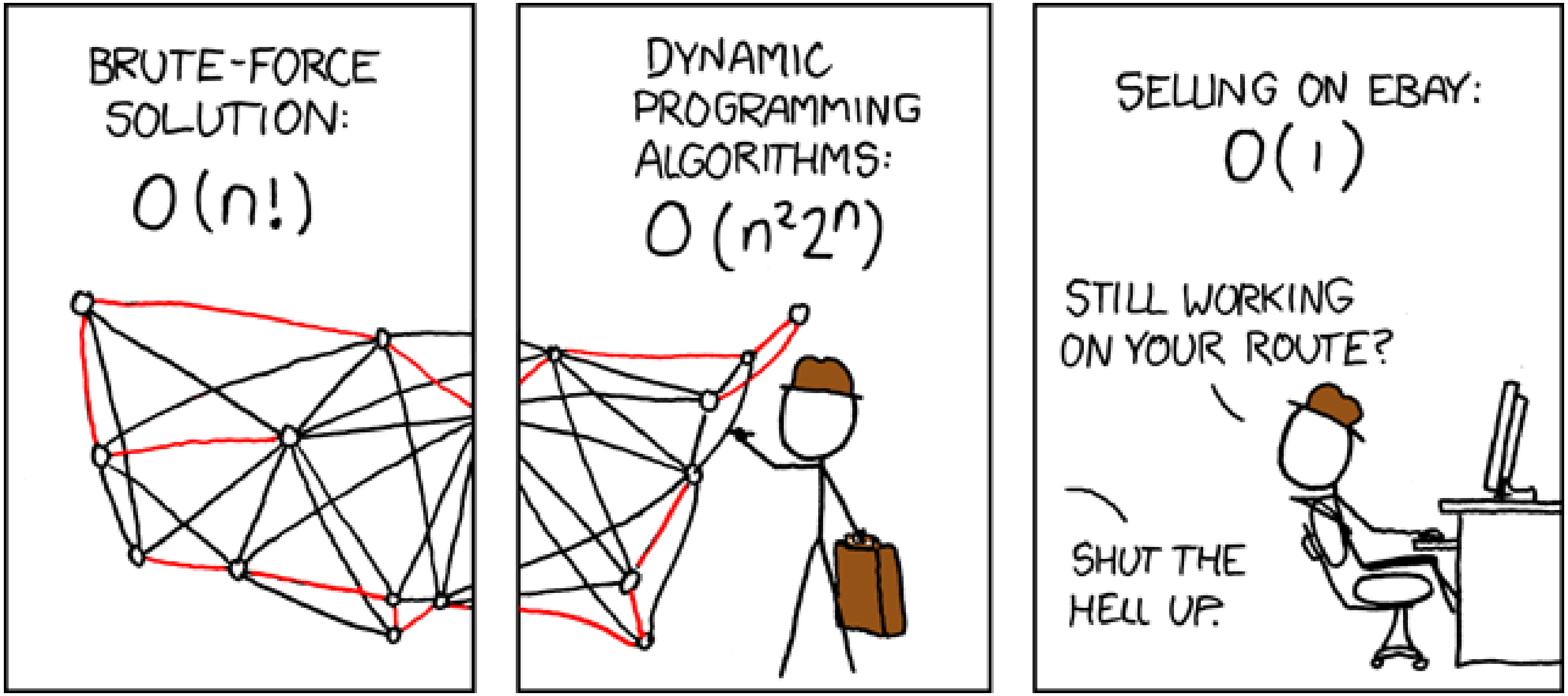
- Grid Search
  - performs a brute force search
  - with equal-width steps on non-discrete numerical attributes (e.g., 10,20,30,..,100)
- Hyperparameter with a wide range (e.g., 0.0001 to 1,000,000)
  - with ten equal-width steps, the first step would be 1,000
  - but what if the optimum is around 0.1?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

Hyperparameter 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/

Hyperparameter 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

Hyperparameter Tuning: Interaction Effects

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

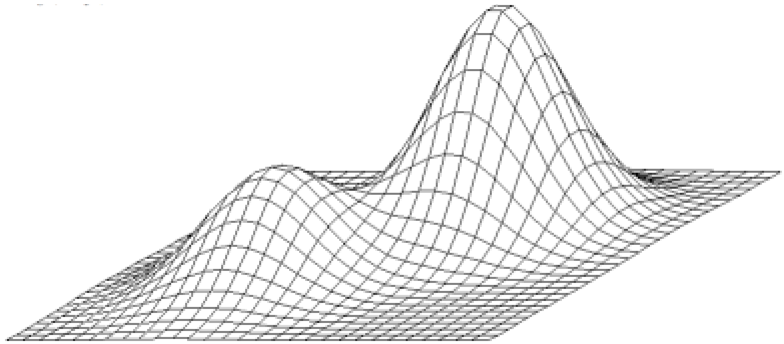
- Example: two parameters p and q, each with values 0,1, and 2
  - the table depicts classification accuracy

	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

Hyperparameter 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

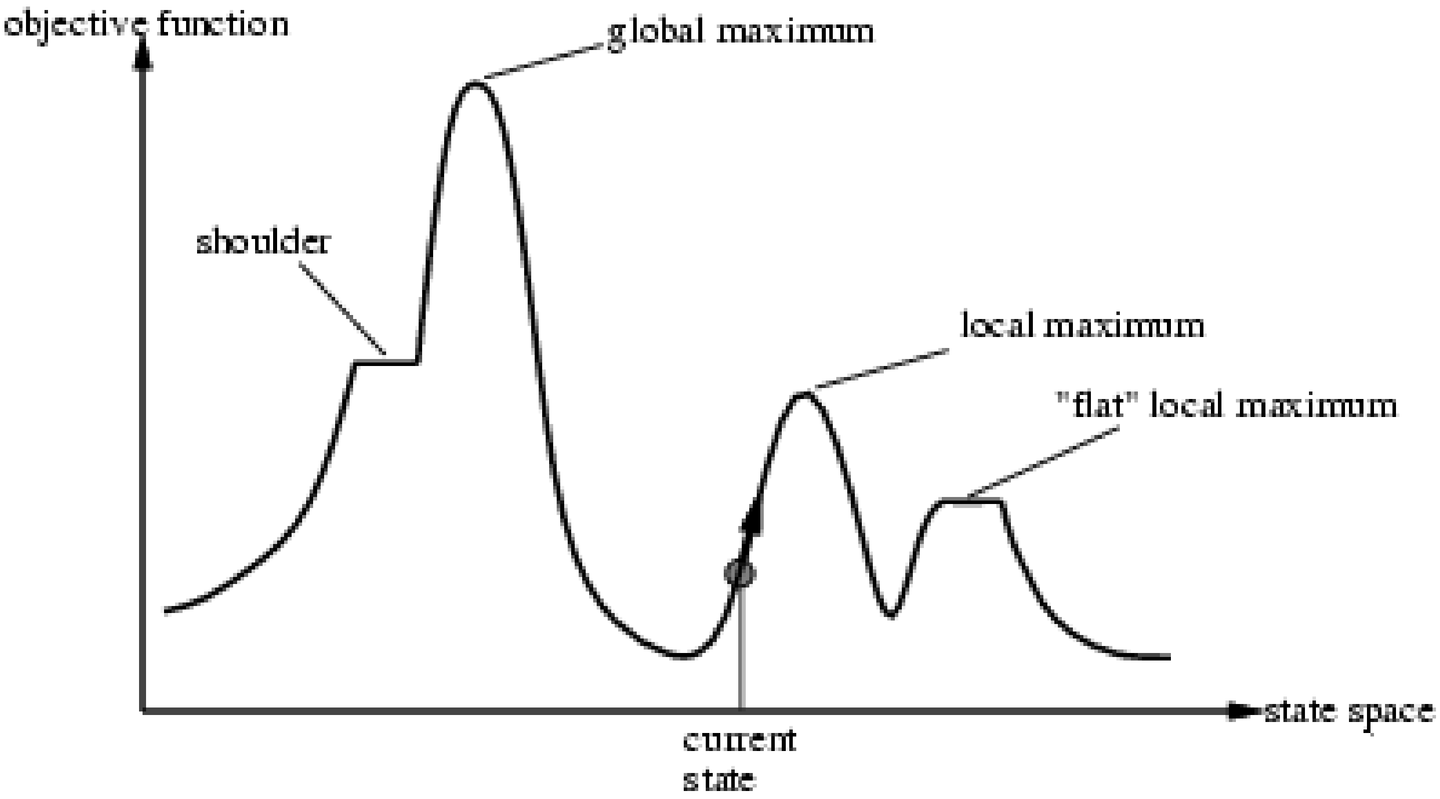
- a.k.a. *greedy local search*
- always search in the direction of the steepest ascend
  - "Like climbing Everest in thick fog with amnesia"

```
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

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

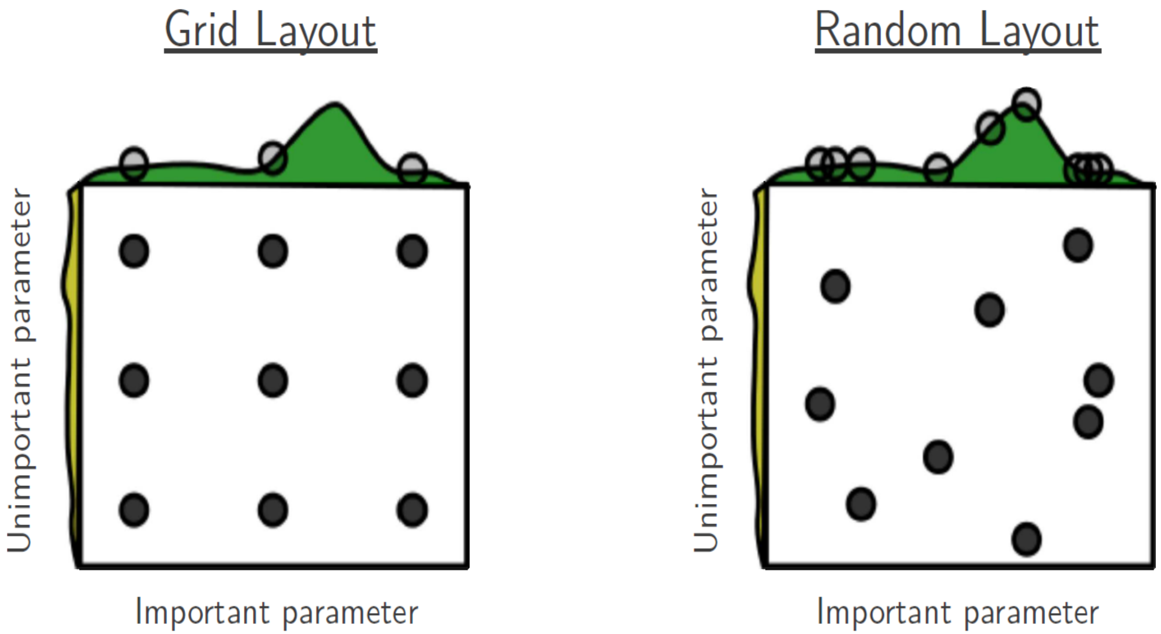
Grid Search vs. Random Search

- All the examples discussed so far use *fixed* grids
  - e.g., an interval from 0 to 1 with a step size of 0.05

- Challenges:
  - some hyperparameters are pretty sensitive
    - e.g., 0.02 is a good value, but 0 and 0.05 are not
  - others have little influence
    - but it is hard to know upfront which

Grid Search vs. Random Search

- Paper from 2012 (Bergstra and Bengio):
  - grid search may easily miss best parameters
  - *random search* often yields better results

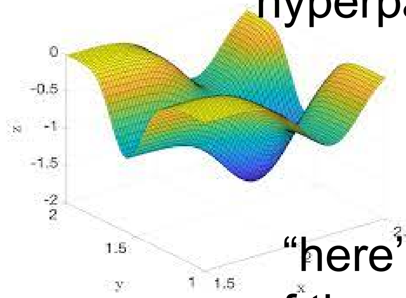


Bergstra & Bengio: Random Search for Hyper-Parameter Optimization, JMLR, 2012

Learning Hyperparameters

- Hyperparameter tuning as a learning problem:
  - Given a set of hyperparameters H, *predict* performance p of model
  - The prediction model is referred to as a *surrogate model* or *oracle*
  - Rationale:
    - Training and evaluating an actual model is costly
    - Learning and predicting with the surrogate model is fast

“test these hyperparameters, please”



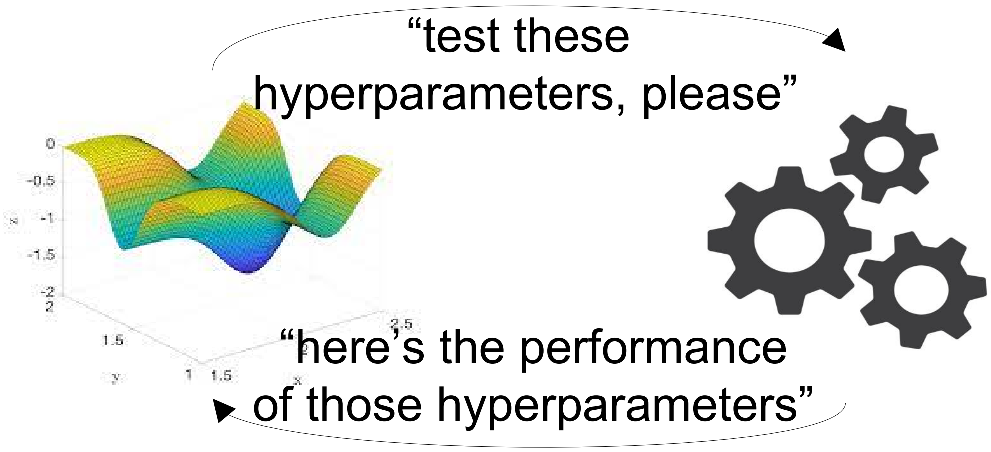
“here’s the performance of those hyperparameters”

Surrogate Model

Actual Model

Learning Hyperparameters

- Note:
  – we want to use not too many runs of the actual model
  – i.e., the surrogate model will have few training points
    - use a simple model
  – Most well-known: *bayesian optimization*



Surrogate Model

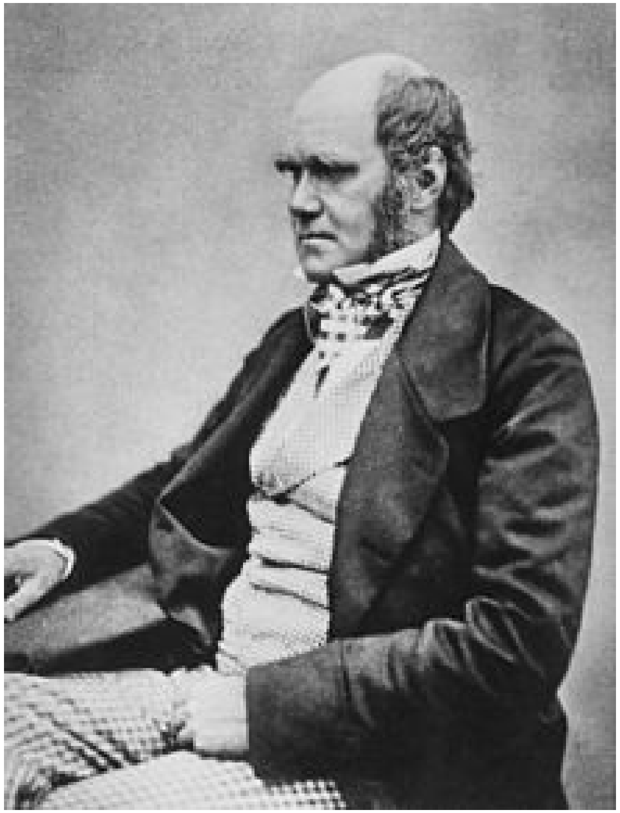
Actual Model

Summary: Grid Search, Random Search, etc.

- Problems of grid search
  - Inefficient
  - Fixed grid sizes may miss good parameters
    - Smaller grid sizes would be even less efficient!
- Random search
  - Often finds good solutions in less time
- Learning hyperparameters / bayesian optimization
  - Sucessively tests hyperparameters close to local optima
  - Similar to hill climbing
    - Difference: explicit surrogate model

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
    - hyperparameter tuning: a hyperparameter setting
  - a fitness function
    - hyperparameter tuning: performance of a hyperparameter setting (i.e., run learner with those parameters)
  - a crossover method
    - hyperparameter tuning: create a new setting from two others
  - a mutation method
    - hyperparameter 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)

Hyperparameter/ Solution	hp1	hp2	hp3	hp4	hp5	hp6	hp7
s1	true	0.87	0.75	0.01	sgd	0.05	0.72
s2	false	0.75	0.83	0.04	adam	0.04	0.53

Hyperparameter/ Solution	hp1	hp2	hp3	hp4	hp5	hp6	hp7
s1'	true	0.87	0.75	0.01	adam	0.04	0.53
s2'	false	0.75	0.83	0.04	sgd	0.05	0.72

SGA Operators: Mutation

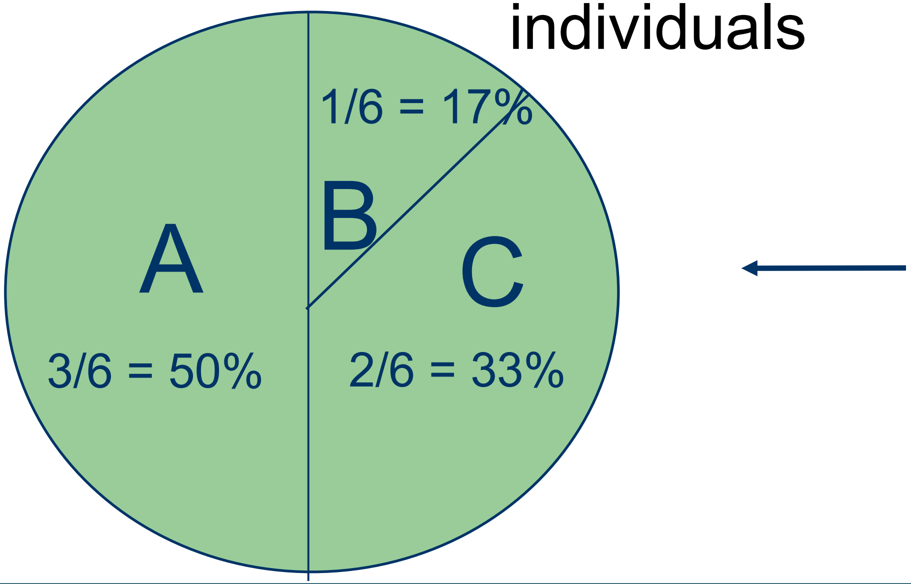
- Alter each gene independently with a probability p_m
- p_m is called the mutation rate
  - Typically between 1/pop_size and 1/ chromosome_length

Hyperparameter/ Solution	hp1	hp2	hp3	hp4	hp5	hp6	hp7
s1	true	0.87	0.75	0.01	sgd	0.05	0.72
s2	false	0.75	0.83	0.04	adam	0.04	0.53

Hyperparameter/ Solution	hp1	hp2	hp3	hp4	hp5	hp6	hp7
s1	true	0.87	0.75	0.01	sgd	0.05	0.72
s2	false	0.75	0.86	0.04	adam	0.04	0.53

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 ...

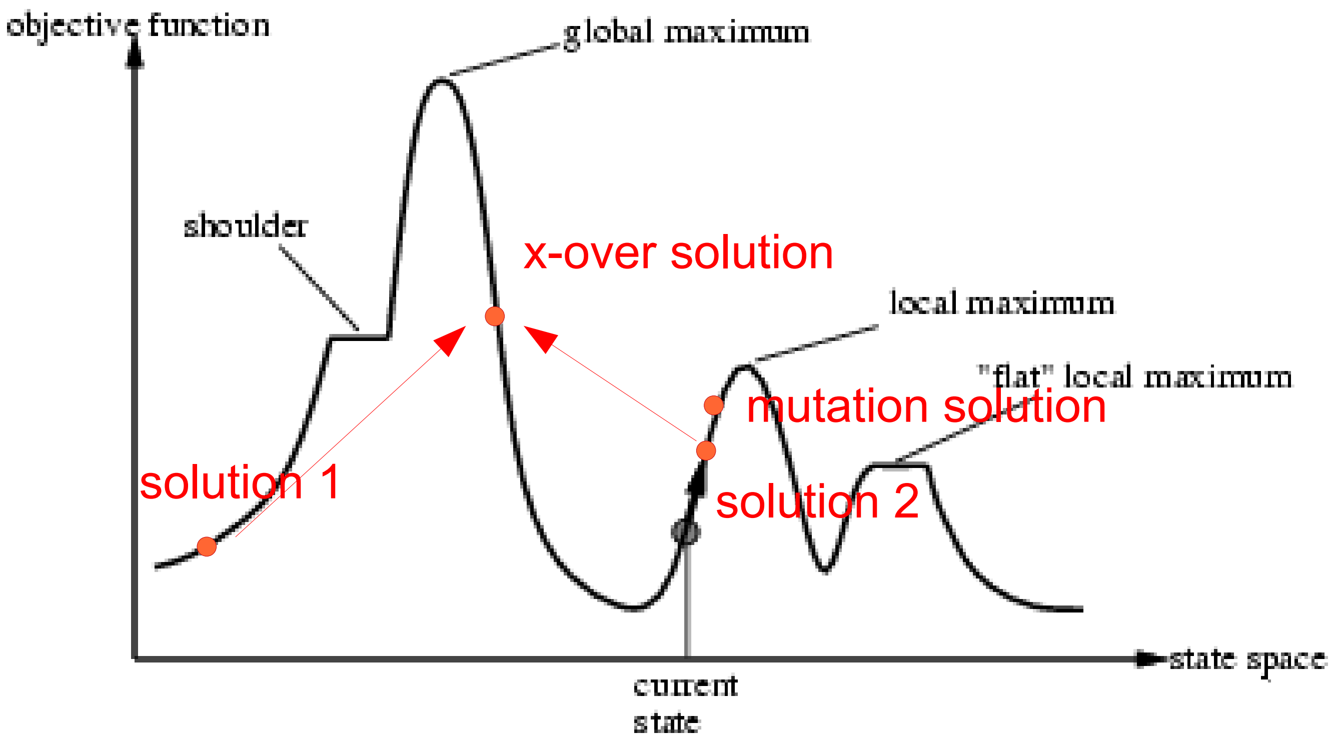
- Answer (at least, rather wide agreement):
  - it depends on the problem, but
  - in general, it is good to have both
  - both have another role
  - mutation-only-EA is possible, crossover-only-EA would not work

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

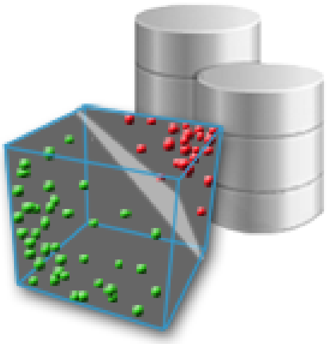
- So far, we have looked at finding good parameters for a learner
  - the learner was always fixed

- 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



- Also known as *AutoML*
- Basic idea: train a regression model
  - data points: individual datasets
    plus ML approach
  - target: expected accuracy/RMSE etc.

- 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

auto-sklearn **0.12.6** Start Releases Installation Manual Examples API Extending Search

auto-sklearn
- Example
- Manual
- License
- Citing auto-sklearn
- Contributing

auto-sklearn

auto-sklearn is an automated machine learning toolkit and a drop-in replacement for a scikit-learn estimator:

```
>>> import autosklearn.classification
>>> cls = autosklearn.classification.AutoSklearnClassifier()
>>> cls.fit(X_train, y_train)
>>> predictions = cls.predict(X_test)
```

auto-sklearn frees a machine learning user from algorithm selection and hyperparameter tuning. It leverages recent advantages in *Bayesian optimization*, *meta-learning* and *ensemble construction*. Learn more about the technology behind *auto-sklearn* by reading our paper published at NIPS 2015 .

NEW: Auto-sklearn 2.0

Auto-sklearn 2.0 includes latest research on automatically configuring the AutoML system itself and contains a multitude of improvements which speed up the fitting the AutoML system.

auto-sklearn 2.0 works the same way as regular *auto-sklearn* and you can use it via

```
>>> from autosklearn.experimental.askl2 import AutoSklearn2Classifier
```

A paper describing our advances is available on arXiv.

...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

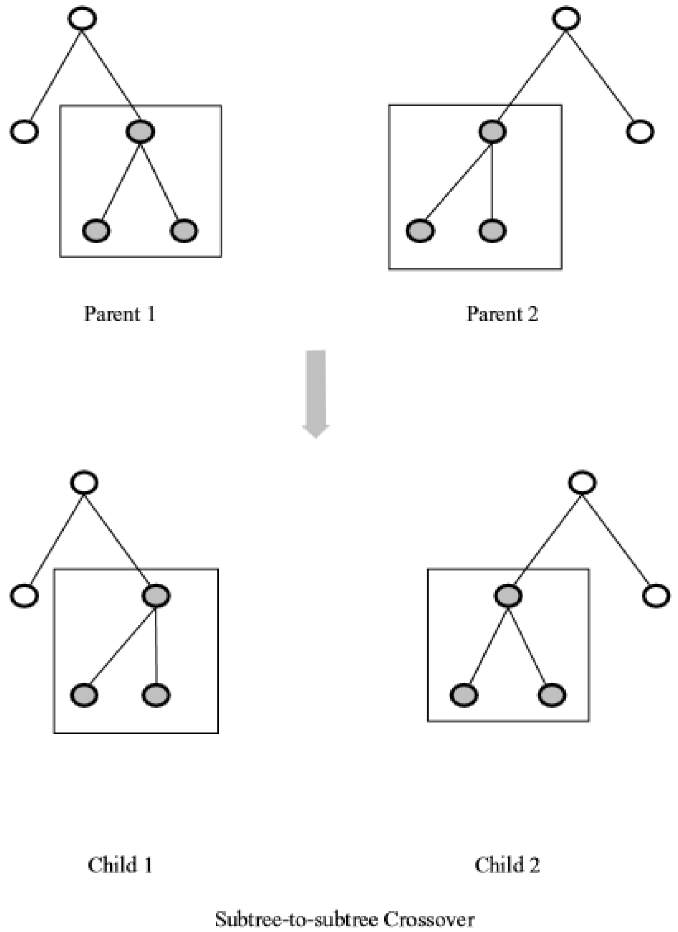
- We have encountered such problems quite frequently
- Example: learning an optimal decision tree from data

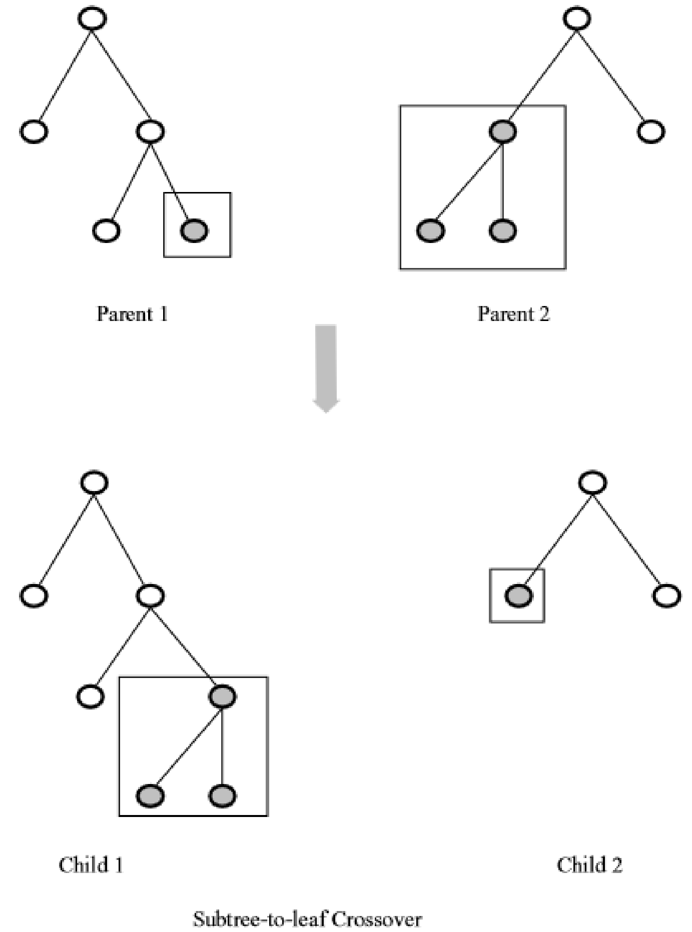
Genetic Decision Tree Learning

- 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

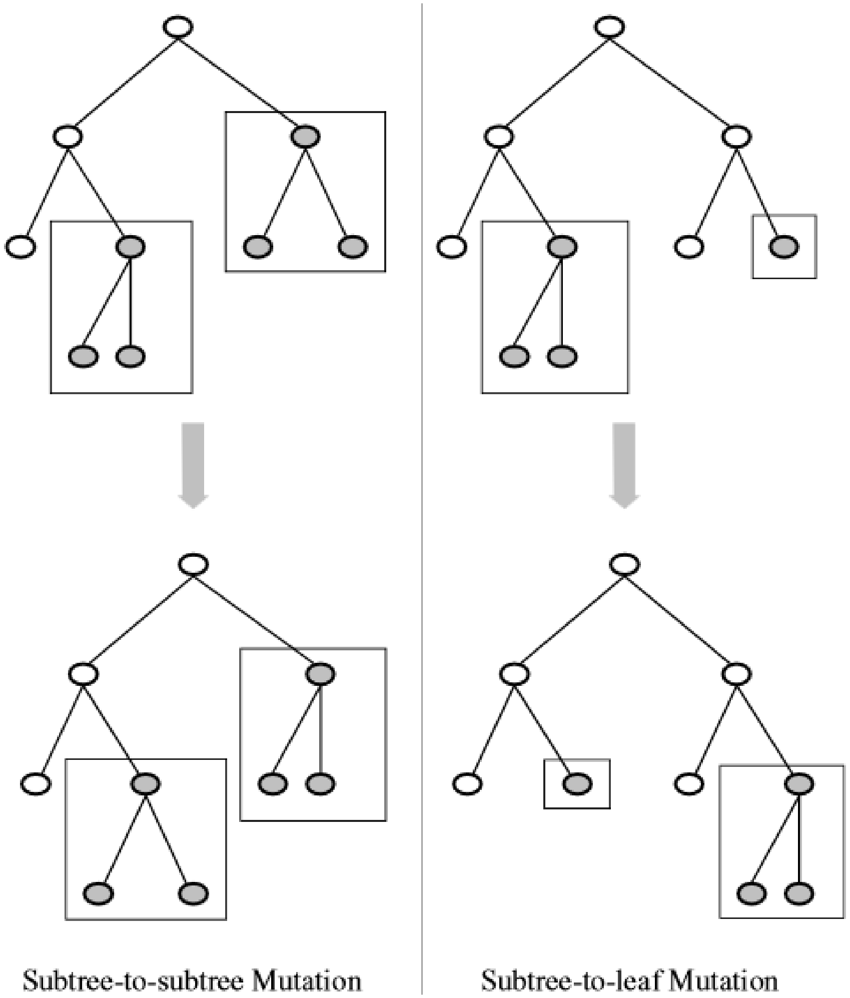
- Crossover:





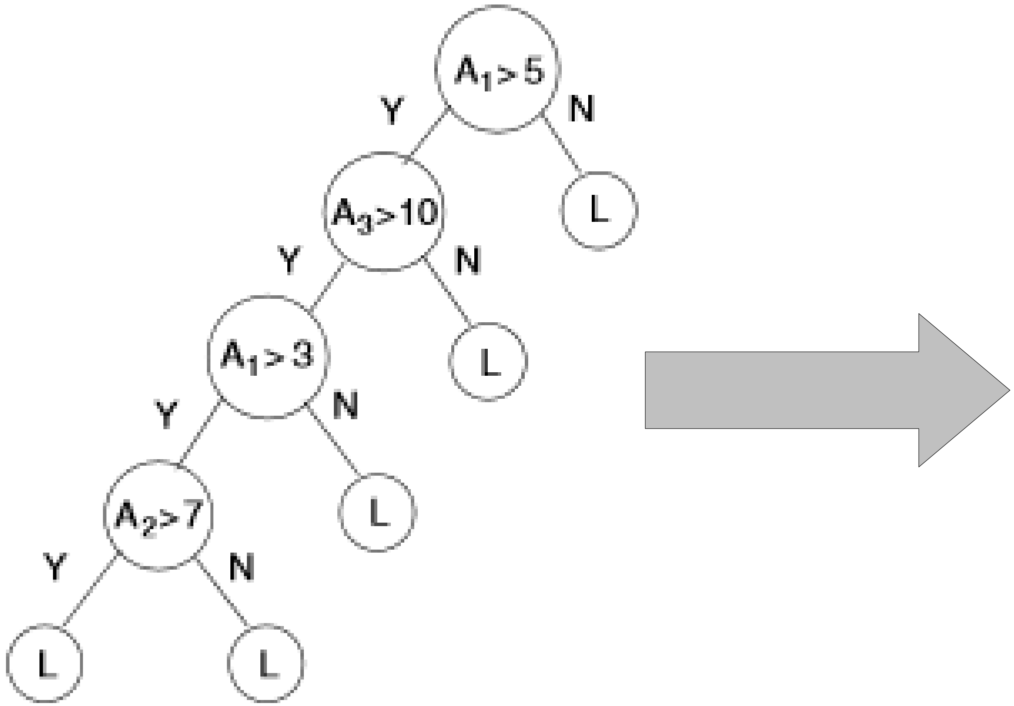
Genetic Decision Tree Learning

- Mutation:

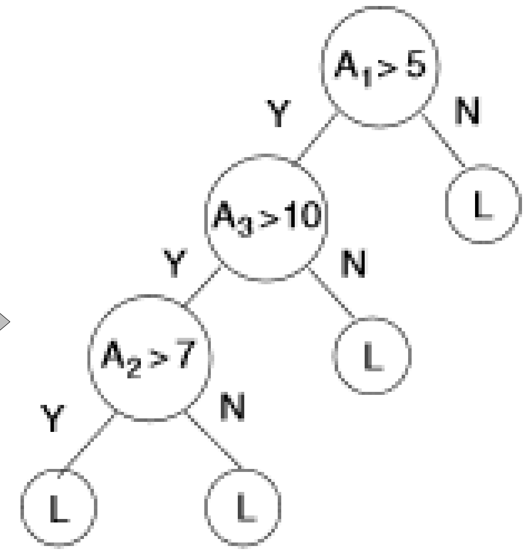


Genetic Decision Tree Learning

- Feasibility Check:



Before feasibility check



After feasibility check

Combination of GP with other Learning Methods

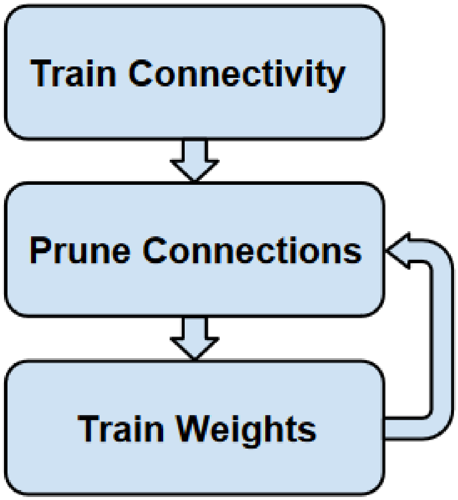
- Rule Learning (“Learning Classifier Systems”), since late 70s
  - Population: set of rule sets (!)
  - Crossover: combining rules from two sets
  - Mutation: changing a rule

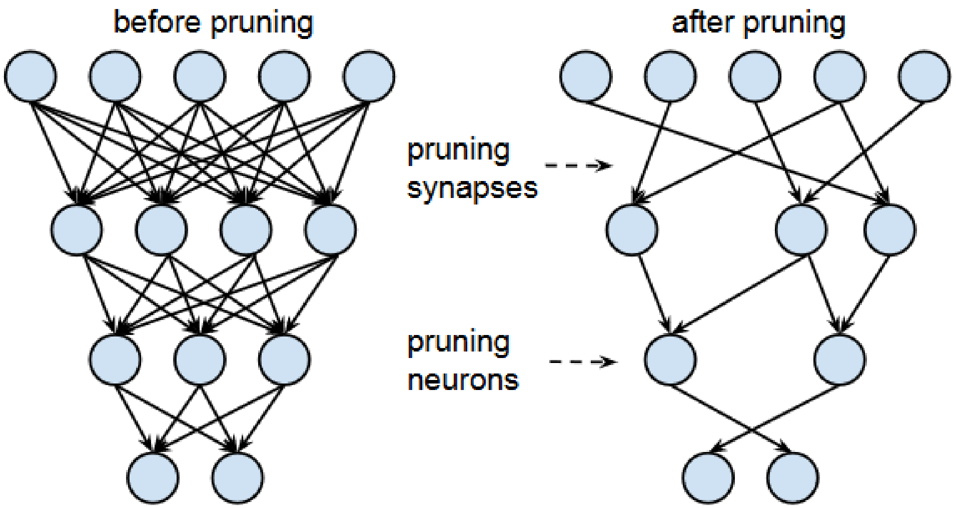
- Artificial Neural Networks
  - Easiest solution: fixed network layout
  - The network is then represented as an ordered set (vector) of weights e.g., [0.8, 0.2, 0.5, 0.1, 0.1, 0.2]
  - Crossover and mutation are straight forward
  - Variant: AutoMLP
    - Searches for best combination of hidden layers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

Hyperparameter 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

- Hyperparameter tuning is important
  - many learning methods work poorly with standard hyperparameters
  - often no global optimum, dataset dependent
- Hyperparameter tuning has a large search space
  - trying all combinations is infeasible
  - interaction effects do not allow for one-by-one tuning
- State of the art
  - Grid search, random search, bayesian optimization

Wrap-Up

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

Hyperparameter 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]

		Estimated cost (USD)	
Models	Hours	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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Data Mining II
Optimization & Parameter Tuning

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