HEURISTIC OPTIMIZATION

Automatic Algorithm Configuration

Thomas Stützle

The algorithmic solution of hard optimization problems is one of the OR/CS success stories!

- Exact (systematic search) algorithms
  - Branch&Bound, Branch&Cut, constraint programming, ...
  - powerful general-purpose software available
  - guarantees on optimality but often time/memory consuming
- Approximate algorithms
  - heuristics, local search, metaheuristics, hyperheuristics ...
  - typically special-purpose software
  - rarely provable guarantees but often fast and accurate

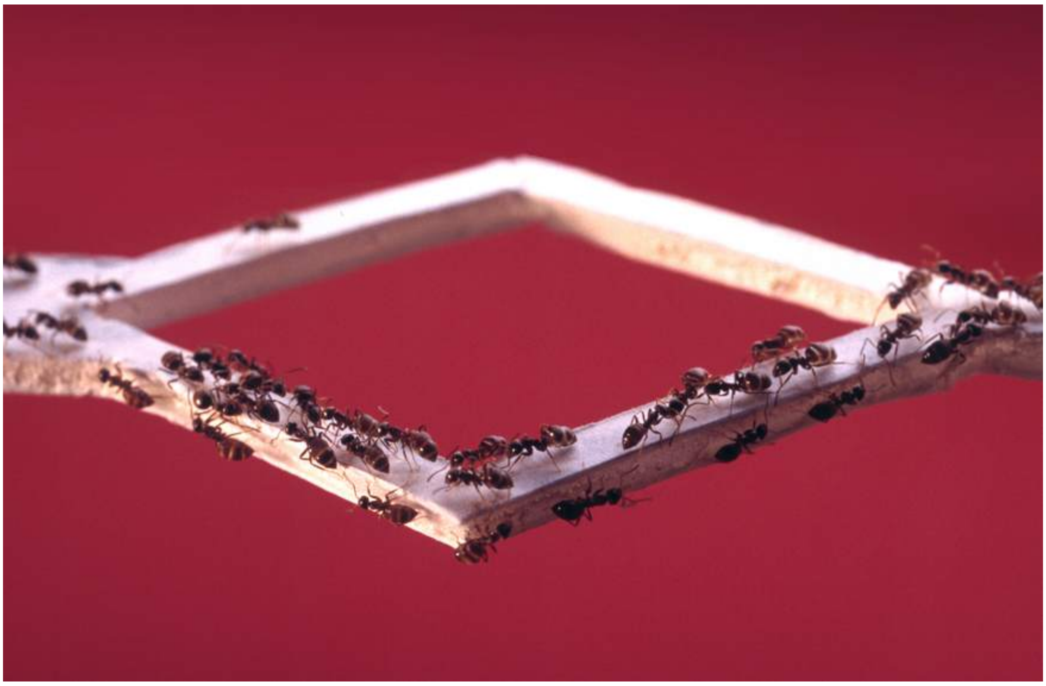
Much active research on hybrids between
exact and approximate algorithms!

Design choices and parameters everywhere

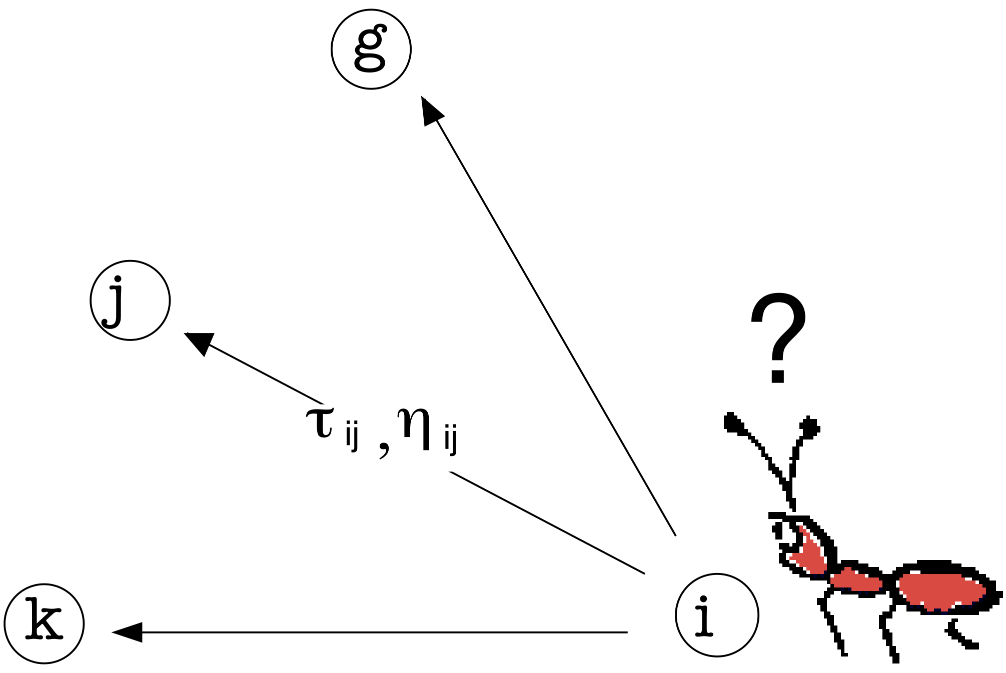
Todays high-performance optimizers involve a large number of design choices and parameter settings

- exact solvers
  - design choices include alternative models, pre-processing, variable selection, value selection, branching rules ...
  - many design choices have associated numerical parameters
  - example: SCIP 3.0.1 solver (fastest non-commercial MIP solver) has more than 200 relevant parameters that influence the solver's search mechanism
- approximate algorithms
  - design choices include solution representation, operators, neighborhoods, pre-processing, strategies, ...
  - many design choices have associated numerical parameters
  - example: multi-objective ACO algorithms with 22 parameters (plus several still hidden ones)

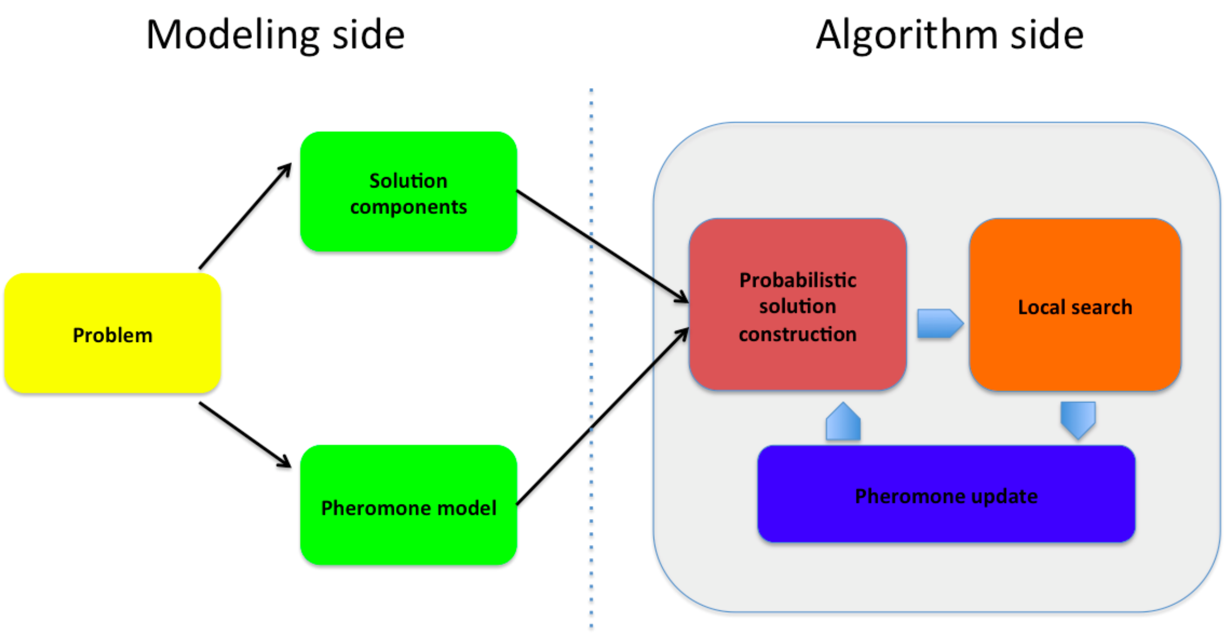
Example: Ant Colony Optimization



ACO, Probabilistic solution construction



Applying Ant Colony Optimization



ACO design choices and numerical parameters

- solution construction
  - choice of constructive procedure
  - choice of pheromone model
  - choice of heuristic information
  - numerical parameters
    - α, β influence the weight of pheromone and heuristic information, respectively
    - q_0 determines greediness of construction procedure
    - m, the number of ants
- pheromone update
  - which ants deposit pheromone and how much?
  - numerical parameters
    - ρ: evaporation rate
    - τ_0: initial pheromone level
- local search
  - ... many more ...

Parameter types

- *categorical* parameters **design**
  - choice of constructive procedure, choice of recombination operator, choice of branching strategy,...
- *ordinal* parameters **design**
  - neighborhoods, lower bounds, ...
- *numerical* parameters **tuning, calibration**
  - integer or real-valued parameters
  - weighting factors, population sizes, temperature, hidden constants, ...
  - numerical parameters may be *conditional* to specific values of categorical or ordinal parameters

Design and configuration of algorithms involves setting categorical, ordinal, **and** *numerical parameters*

Designing optimization algorithms

Challenges

- many alternative design choices
- nonlinear interactions among algorithm components and/or parameters
- performance assessment is difficult

Traditional design approach

- trial–and–error design guided by expertise/intuition $\leadsto$ prone to over-generalizations, implicit independence assumptions, limited exploration of design alternatives

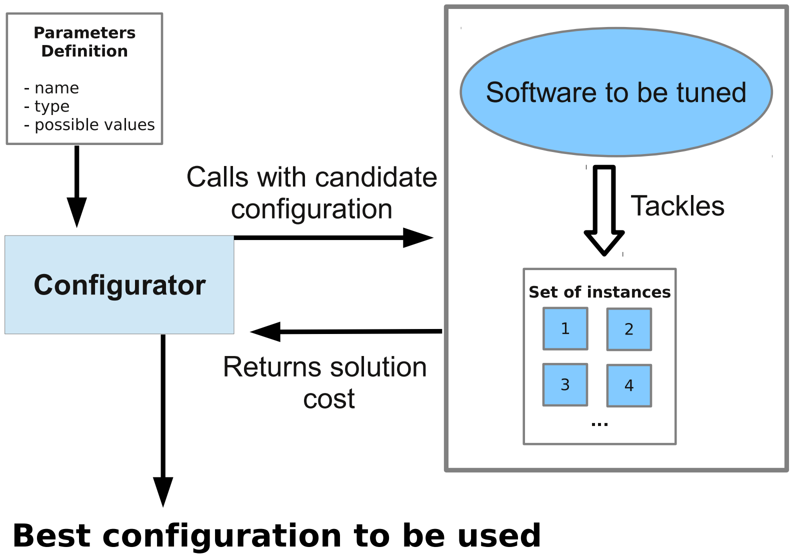
Can we make this approach more principled and automatic?

Towards automatic algorithm configuration

Automated algorithm configuration

- apply powerful search techniques to design algorithms
- use computation power to explore design spaces
- assist algorithm designer in the design process
- free human creativity for higher level tasks

Automatic offline configuration



Typical performance measures

- maximize solution quality (within given computation time)
- minimize computation time (to reach optimal solution)

Offline configuration and online parameter control

Offline configuration

- configure algorithm before deploying it
- configuration on training instances
- related to algorithm design

Online parameter control

- adapt parameter setting while solving an instance
- typically limited to a set of known crucial algorithm parameters
- related to parameter calibration

Offline configuration techniques can be helpful to configure (online) parameter control strategies

Approaches to configuration

- experimental design techniques
  - e.g. CALIBRA [Adenso–Díaz, Laguna, 2006], [Ridge&Kudenko, 2007], [Coy et al., 2001], [Ruiz, Stützle, 2005]
- numerical optimization techniques
  - e.g. MADS [Audet&Orban, 2006], various [Yuan et al., 2012]
- heuristic search methods
  - e.g. meta-GA [Grefenstette, 1985], ParamILS [Hutter et al., 2007, 2009], gender-based GA [Ansótegui at al., 2009], linear GP [Oltean, 2005], REVAC(++) [Eiben & students, 2007, 2009, 2010] . . .
- model-based optimization approaches
  - e.g. SPO [Bartz-Beielstein et al., 2005, 2006, ..], SMAC [Hutter et al., 2011, ..]
- sequential statistical testing
  - e.g. F-race, iterated F-race [Birattari et al, 2002, 2007, . . .]

General, domain-independent methods required: (i) applicable to all variable types, (ii) multiple training instances, (iii) high performance, (iv) scalable

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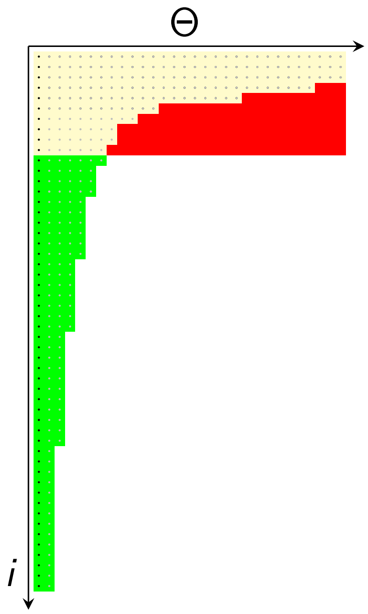
The racing approach



- start with a set of initial candidates
- consider a *stream* of instances
- sequentially evaluate candidates
- discard inferior candidates
  as sufficient evidence is gathered against them
- . . . repeat until a winner is selected
  or until computation time expires

The F-Race algorithm

Statistical testing

1. family-wise tests for differences among configurations
   - Friedman two-way analysis of variance by ranks
2. if Friedman rejects H_0, perform pairwise comparisons to best configuration
   - apply Friedman post-test



Iterated race

Racing is a method for the *selection of the best* configuration and independent of the way the set of configurations is sampled

Iterated racing

sample configurations from initial distribution

While not terminate()

apply race

modify sampling distribution

sample configurations

The irace Package

Manuel López-Ibáñez, Jérémie Dubois-Lacoste, Thomas Stützle, and Mauro Birattari. **The irace package, Iterated Race for Automatic Algorithm Configuration.** *Technical Report TR/IRIDIA/2011-004*, IRIDIA, Université Libre de Bruxelles, Belgium, 2011.

http://iridia.ulb.ac.be/irace

- implementation of Iterated Racing in R
  - Goal 1: flexible
  - Goal 2: easy to use
- but no knowledge of R necessary
- parallel evaluation (MPI, multi-cores, grid engine ..)
- initial candidates

irace has shown to be effective for configuration tasks with several hundred of variables

Other tools: ParamILS, SMAC

ParamILS

- iterated local search in configuration space
- requires discretization of numerical parameters
- `http://www.cs.ubc.ca/labs/beta/Projects/ParamILS/`

SMAC

- surrogate model assisted search process
- encouraging results for large configuration spaces
- `http://www.cs.ubc.ca/labs/beta/Projects/SMAC/`

capping: effective speed-up technique for configuration target run-time

Mixed integer programming (MIP) solvers

- powerful commercial (e.g. CPLEX) and non-commercial (e.g. SCIP) solvers available
- large number of parameters (tens to hundreds)

- default configurations not necessarily best for specific problems

Benchmark set	Default	Configured	Speedup
`Regions200`	72	10.5 (11.4 ± 0.9)	*6.8*
`Conic.SCH`	5.37	2.14 (2.4 ± 0.29)	*2.51*
`CLS`	712	23.4 (327 ± 860)	*30.43*
`MIK`	64.8	1.19 (301 ± 948)	*54.54*
`QP`	969	525 (827 ± 306)	*1.85*

FocusedILS tuning CPLEX, 10 runs, 2 CPU days, 63 parameters

Automatic design of hybrid SLS algorithms

Approach

- decompose single-point SLS methods into components
- derive generalized metaheuristic structure
- component-wise implementation of metaheuristic part

Implementation

- present possible algorithm compositions by a grammar
- instantiate grammer using a parametric representation
  - allows use of standard automatic configuration tools
  - shows good performance when compared to, e.g., grammatical evolution [Mascia, Lópes-Ibáñez, Dubois-Lacoste, Stützle, 2014]

General Local Search Structure: ILS

s_0 :=initSolution
s^* := ls(s_0)
repeat
  s' :=perturb(s^*,*history*)
  $s^{*\prime}$:=ls(s')
  s^* :=accept(s^*,$s^{*\prime}$,*history*)
until termination criterion met

- many SLS methods instantiable from this structure
- abilities
  - hybridization
  - recursion
  - problem specific implementation at low-level

Grammar

```
     <algorithm> ::= <initialization> <ils>
<initialization> ::= random | <pbs_initialization>
           <ils> ::= ILS(<perturb>, <ls>, <accept>, <stop>)

<perturb> ::= none | <initialization> | <pbs_perturb>
     <ls> ::= <ils> | <descent> | <sa> | <rii> | <pii> | <vns> | <ig> | <pbs_ls>
 <accept> ::= alwaysAccept | improvingAccept  <comparator>
            | prob(<value_prob_accept>) | probRandom | <metropolis>
            | threshold(<value_threshold_accept>) | <pbs_accept>

<descent> ::= bestDescent(<comparator>, <stop>)
            | firstImprDescent(<comparator>, <stop>)
    <sa>  ::= ILS(<pbs_move>, no_ls,  <metropolis>, <stop>)
    <rii> ::= ILS(<pbs_move>, no_ls, probRandom, <stop>)
    <pii> ::= ILS(<pbs_move>, no_ls, prob(<value_prob_accept>), <stop>)
    <vns> ::= ILS(<pbs_variable_move>, firstImprDescent(improvingStrictly),
                  improvingAccept(improvingStrictly), <stop>)
     <ig> ::= ILS(<deconst-construct_perturb>, <ls>, <accept>, <stop>)

<comparator> ::= improvingStrictly | improving
<value_prob_accept> ::= [0, 1]
<value_threshold_accept> ::= [0, 1]
<metropolis> ::= metropolisAccept(<init_temperature>, <final_temperature>,
                                  <decreasing_temperature_ratio>, <span>)
 <init_temperature> ::= {1, 2,..., 10000}
<final_temperature> ::= {1, 2,..., 100}
<decreasing_temperature_ratio> ::= [0, 1]
<span> ::= {1, 2,..., 10000}
```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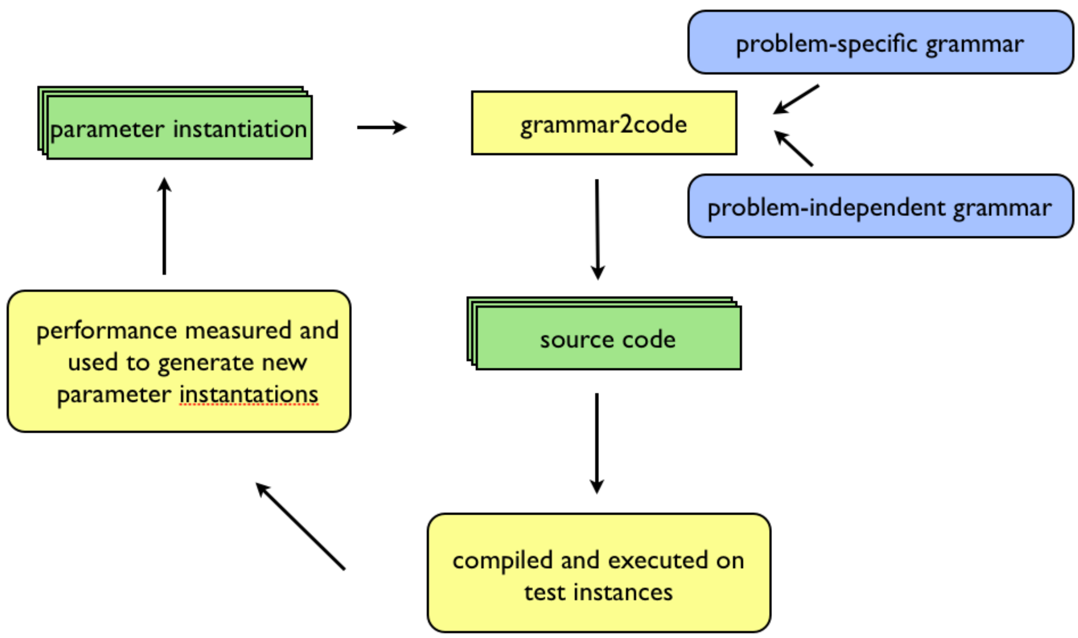
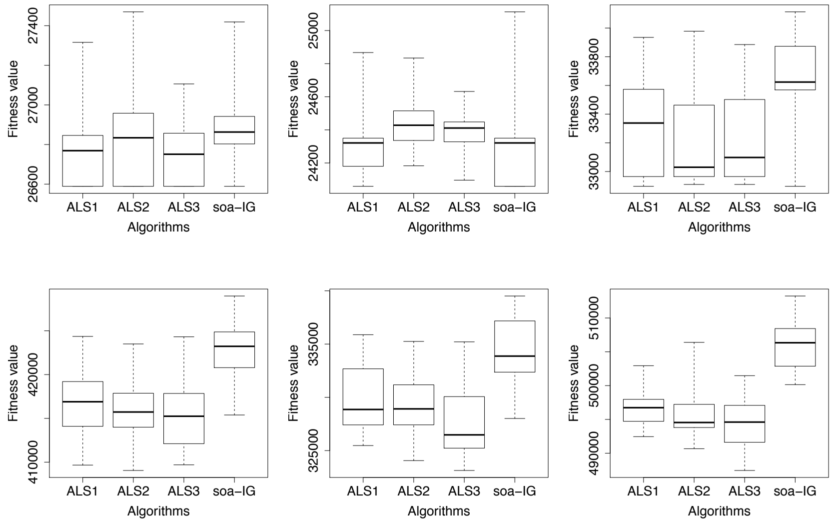
System overview

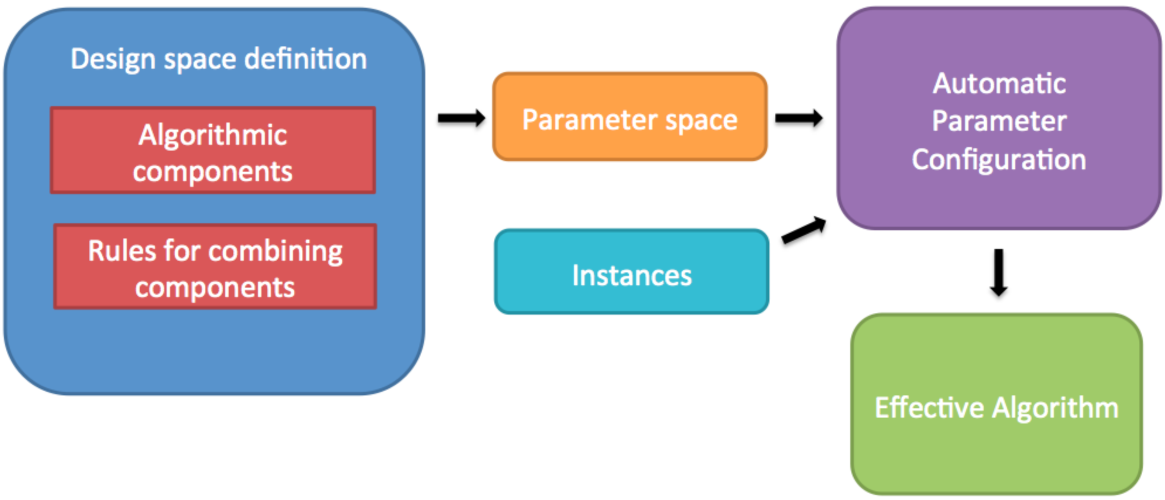


Flow-shop problem with weighted tardiness

- Automatic configuration:
  - 1, 2 or 3 levels of recursion (r)
  - 80, 127, and 174 parameters, respectively
  - budget: r $\times$ 10 000 trials each of 30 seconds



General approach



Main approaches

Top-down approaches

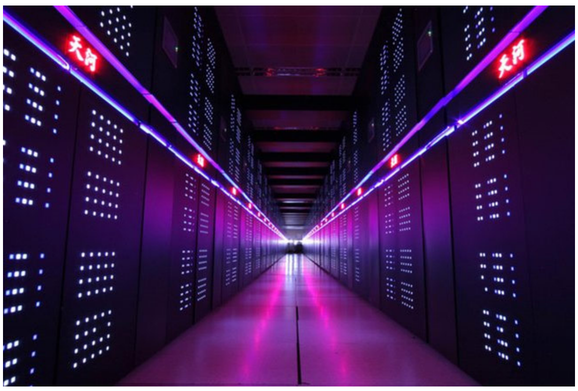
- develop flexible framework following a fixed algorithm template with alternatives
- apply high-performing configurators
- Examples: Satenstein, MOACO, MOEA, MIP Solvers?(!)

Bottom-up approaches

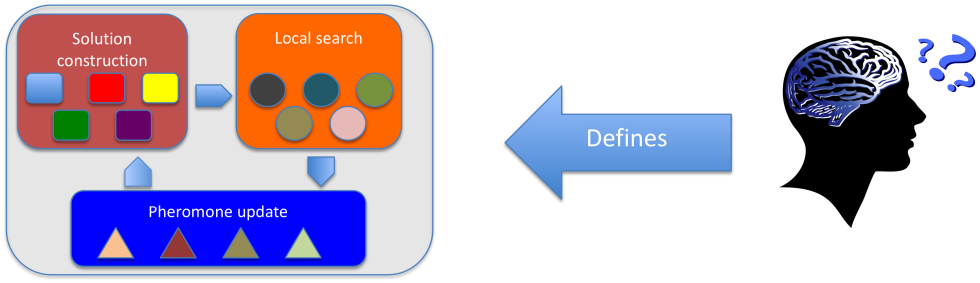
- flexible framework implementing algorithm components
- define rules for composing algorithms from components e.g. through grammars
- frequently usage of genetic programming, grammatical evolution etc.

Why automatic algorithm configuration?

- improvement over manual, ad-hoc methods for tuning
- reduction of development time and human intervention
- increase number of considerable degrees of freedom
- empirical studies, comparisons of algorithms
- support for end users of algorithms



Towards a shift of paradigm in algorithm design



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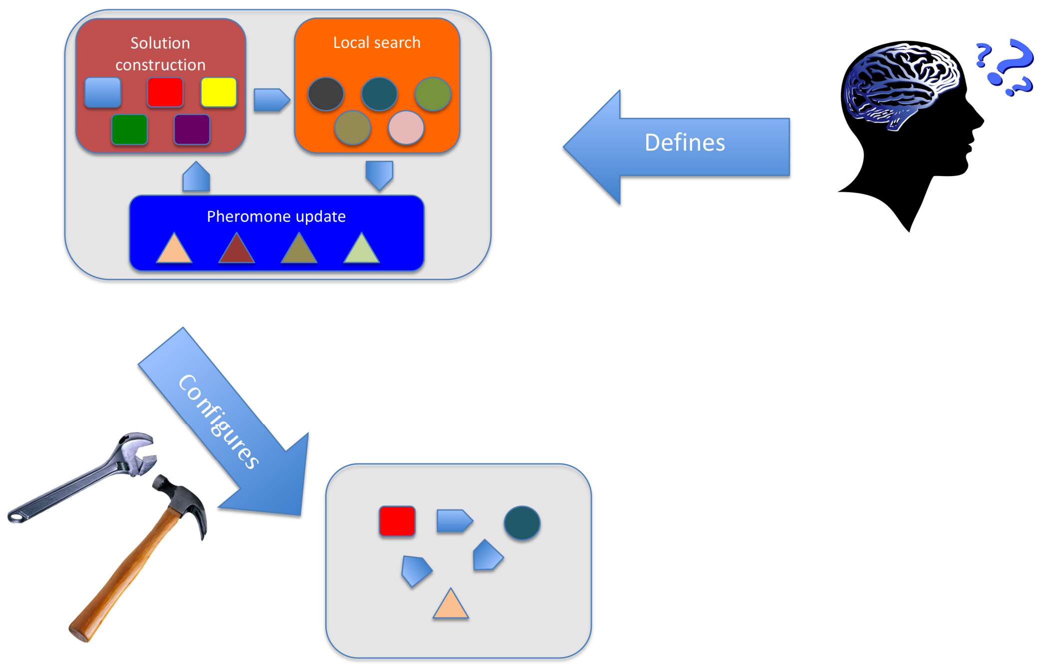

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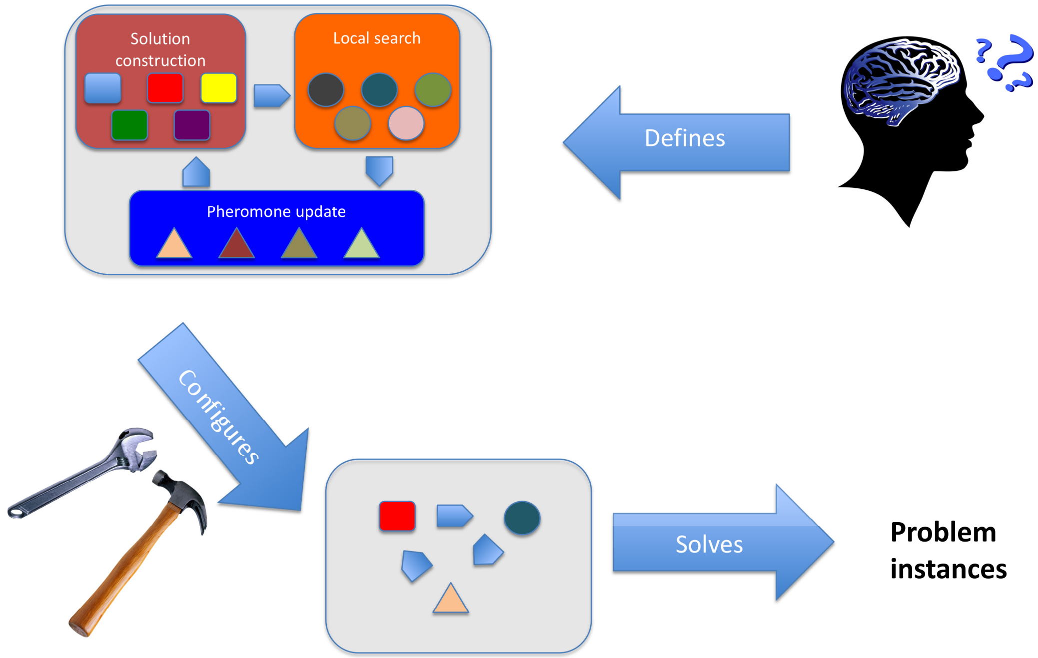

Conclusions

Automatic Configuration

- leverages computing power for software design
- is rewarding w.r.t. development time and algorithm performance
- leads ultimately to a shift in algorithm design

Future work

- more powerful configurators
- pushing the borders
- best practice