

# Hyper-heuristics

Daniel R. Tauritz ([dtauritz@acm.org](mailto:dtauritz@acm.org))

Natural Computation Laboratory, Missouri University of Science and Technology (<http://web.mst.edu/~tauritzd/nc-lab/>)

John Woodward ([John.Woodward@cs.stir.ac.uk](mailto:John.Woodward@cs.stir.ac.uk))

CHORDS Research Group, Stirling University  
(<http://www.maths.stir.ac.uk/research/groups/chords/>)

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## Instructors

[Daniel R. Tauritz](#) is an Associate Professor in the [Department of Computer Science](#) at the [Missouri University of Science and Technology \(S&T\)](#), a contract scientist for [Sandia National Laboratories](#), a former Guest Scientist at [Los Alamos National Laboratory \(LANL\)](#), the founding director of [S&T's Natural Computation Laboratory](#), and founding academic director of the LANL/S&T Cyber Security Sciences Institute. He received his Ph.D. in 2002 from [Leiden University](#). His research interests include the design of hyper-heuristics and self-configuring evolutionary algorithms and the application of computational intelligence techniques in cyber security, critical infrastructure protection, and program understanding.



[John R. Woodward](#) is a Lecturer at the [University of Stirling](#), within the [CHORDS group](#) and is employed on the [DAASE project](#), and for the previous four years was a lecturer with the [University of Nottingham](#). He holds a BSc in Theoretical Physics, an MSc in Cognitive Science and a PhD in Computer Science, all from the [University of Birmingham](#). His research interests include Automated Software Engineering, particularly Search Based Software Engineering, Artificial Intelligence/Machine Learning and in particular Genetic Programming. He has worked in industrial, military, educational and academic settings, and been employed by EDS, CERN and RAF and three UK Universities.



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## John's perspective of hyper-heuristics

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## Metaheuristic

A metaheuristic

- Sample solutions
- Generates solutions

(Meta)heuristic



Solution Space  
(set of Possible solutions)

000, 001, ..., 110,111

## Hyper-heuristic

### Hyper-heuristic

Set of  
heuristics

H1, H2, ..., Hn

Hyper-heuristic  
operated on

- Other heuristics
- On the solution space indirectly

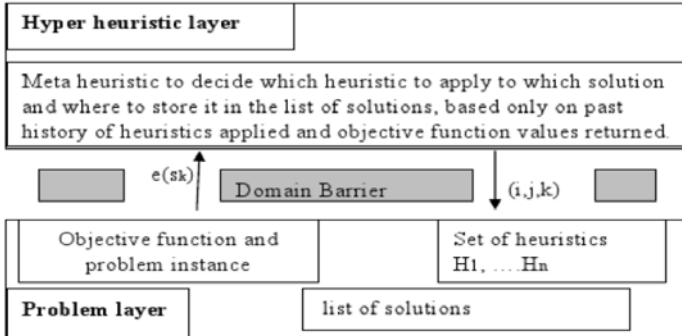
Small set,  
**Atomic** heuristics

Solution  
Space  
(set of  
Possible  
solutions)

000, 001, ..., 110, 111

## Domain Barrier

$$HH : (H \times \mathbb{N}^2 \times \mathbb{R})^* \rightarrow H \times \mathbb{N}^2$$



## Hyper-heuristic

### Hyper-heuristic

Set of  
heuristics

Space of Programs  
(heuristic)

Hyper-heuristic  
operated on

- Other heuristics
- On the solution space indirectly

Large (infinite) set,  
**decomposable** heuristics

Solution  
Space  
(set of  
Possible  
solutions)

000, 001, ..., 110, 111

## Performance table

TABLE I  
A CLASSIFICATION TABLE SHOWING ALGORITHMS IN COLUMNS AND PROBLEMS ROWS, AND THE PERFORMANCE OF THAT ALGORITHM ON THAT PROBLEM IN THE INTERSECTING CELL.

	algorithm-1	algorithm-2	...	algorithm-m
problem-1	1.0	2.3	...	3.6
problem-2	1.6	6.5	...	7.6
...	...	...	...	...
problem-n	3.5	8.6	...	6.5

	$f_{\langle y_1, y_2 \rangle}$	$f_{\langle y_1, y_1 \rangle}$	$f_{\langle y_2, y_2 \rangle}$	$f_{\langle y_2, y_1 \rangle}$
$\langle x_1, x_2 \rangle$	$\langle y_1, y_2 \rangle$	$\langle y_1, y_1 \rangle$	$\langle y_2, y_2 \rangle$	$\langle y_2, y_1 \rangle$
$\langle x_2, x_1 \rangle$	$\langle y_2, y_1 \rangle$	$\langle y_1, y_1 \rangle$	$\langle y_2, y_2 \rangle$	$\langle y_1, y_2 \rangle$

## Conceptual Overview

Combinatorial problem e.g. Travelling Salesman  
Exhaustive search -> heuristic?



Genetic Programming  
code fragments in for-loops.

Travelling Salesman Instances

TSP algorithm

EXECUTABLE on MANY INSTANCES!!!

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Genetic Algorithm  
heuristic – permutations

Travelling Salesman

Tour

Single tour NOT EXECUTABLE!!!

Give a man a fish and he  
will eat for a **day**.  
Teach a man to fish and he  
will eat for a **lifetime**.

Scalable? General?

New domains for GP

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## Program-Complexity Spectrum

Genetic Programming  
{+, -, \*, /}  
{AND, OR, NOT}

First year university course  
On Java, as part of a computer  
Science degree

Automatically  
designed heuristics  
(this tutorial)

LARGE  
Software  
Engineering  
Projects

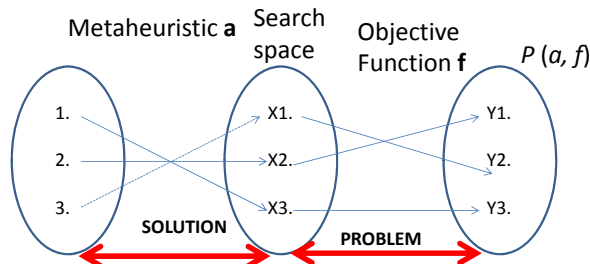
Increasing "complexity"

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## Theoretical Motivation 1



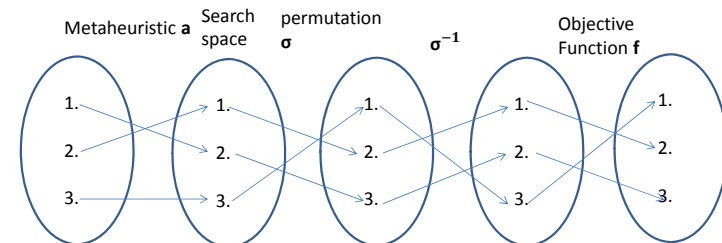
1. A **search space** contains the set of all possible solutions.
2. An **objective function** determines the quality of solution.
3. A (**Mathematical idealized**) **metaheuristic** determines the sampling order (i.e. enumerates i.e. without replacement). It is a (approximate) permutation. What are we learning?
4. **Performance measure**  $P(a, f)$  depend only on  $y_1, y_2, y_3$
5. **Aim** find a solution with a **near-optimal objective value using a Metaheuristic**. **ANY QUESTIONS BEFORE NEXT SLIDE?**

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## Theoretical Motivation 2



- $P(a, f) = P(a, \sigma, \sigma^{-1} f)$   $P(A, F) = P(A, \sigma, \sigma^{-1} F)$  (i.e. permute bins)  
 $P$  is a **performance measure**, (based only on output values).  
 $\sigma, \sigma^{-1}$  are a permutation and inverse permutation.  
 $A$  and  $F$  are probability distributions over algorithms and functions).  
**F is a problem class.** **ASSUMPTIONS IMPLICATIONS**  
 1. Metaheuristic  $a$  applied to function  $\sigma \sigma^{-1} f$  (that is  $f$ )  
 2. Metaheuristic  $a\sigma$  applied to function  $\sigma^{-1} f$  **precisely identical**,

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## Theoretical Motivation 3 [1,14]

- The base-level learns about the function.
- The meta-level learn about the distribution of functions
- The sets do not need to be **finite** (with **infinite sets**, a uniform distribution is not possible)
- The functions do not need to be **computable**.
- We can make claims about the **Kolmogorov Complexity** of the functions and search algorithms.
- $p(f)$  (the probability of sampling a function )is all we can learn in a black-box approach.

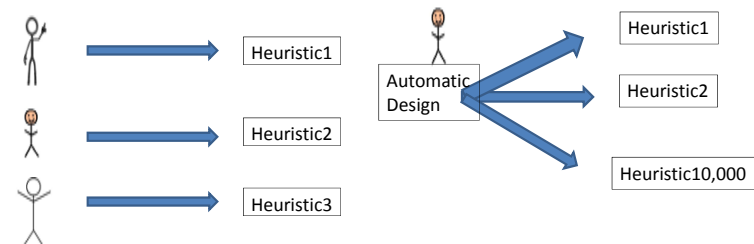
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## One Man – **One/Many** Algorithm

1. Researchers **design heuristics by hand** and test them on problem instances or arbitrary benchmarks off internet.  
**1. Challenge** is defining an algorithmic framework (**set**) that **includes** useful algorithms. **Black art**
2. Let Genetic Programming **select the best algorithm for the problem class at hand**. **Context!!!** Let the data speak for itself without imposing our assumptions.  
**2. Let Genetic Programming select the best algorithm for the problem class at hand. Context!!!** Let the data speak for itself without imposing our assumptions.



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## Daniel's perspective of hyper-heuristics

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## Real-World Challenges

- Researchers strive to make algorithms increasingly general-purpose
- But practitioners have very specific needs
- Designing custom algorithms tuned to particular problem instance distributions and/or computational architectures can be very time consuming

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## Automated Design of Algorithms

- Addresses the need for custom algorithms
- But due to high computational complexity, only feasible for repeated problem solving
- Hyper-heuristics accomplish automated design of algorithms by searching program space

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## Hyper-heuristics

- Hyper-heuristics are a special type of meta-heuristic
  - Step 1: Extract algorithmic primitives from existing algorithms
  - Step 2: Search the space of programs defined by the extracted primitives
- While Genetic Programming (GP) is particularly well suited for executing Step 2, other meta-heuristics can be, and have been, employed
- The type of GP employed matters [24]

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## Type of GP Matters: Experiment Description

- Implement five types of GP (tree GP, linear GP, canonical Cartesian GP, Stack GP, and Grammatical Evolution) in hyper-heuristics for evolving black-box search algorithms for solving 3-SAT
- Base hyper-heuristic fitness on the fitness of the best search algorithm generated at solving the 3-SAT problem
- Compare relative effectiveness of each GP type as a hyper-heuristic

## GP Individual Description

- Search algorithms are represented as an iterative algorithm that passes one or more set of variable assignments to the next iteration
- Genetic program represents a single program iteration
- Algorithm runs starting with a random initial population of solutions for 30 seconds

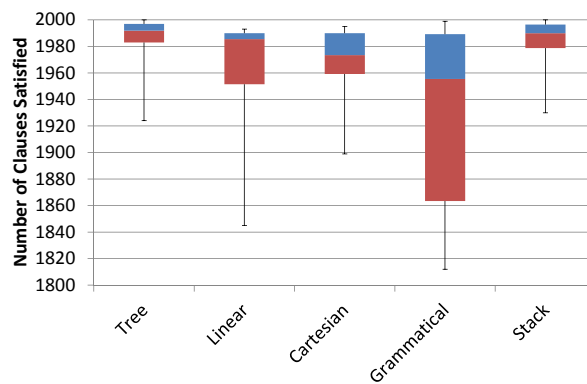
## 3-SAT Problem

- A subset of the Boolean Satisfiability Problem (SAT)
- The goal is to select values for Boolean variables such that a given Boolean equation evaluates as true (is satisfied)
- Boolean equations are in 3-conjunctive normal form
- Example:
  - $(A \vee B \vee C) \wedge (\neg A \vee \neg C \vee D) \wedge (\neg B \vee C \vee \neg D)$
  - Satisfied by  $\neg A, B, C, \neg D$
- Fitness is the number of clauses satisfied by the best solution in the final population

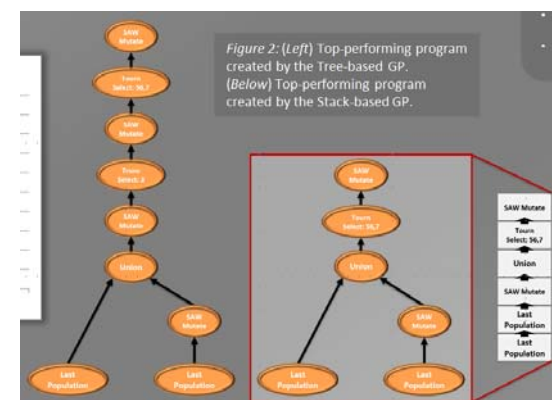
## Genetic Programming Nodes Used

- Last population, Random population
- Tournament selection, Fitness proportional selection, Truncation selection, Random selection
- Bitwise mutation, Greedy flip, Quick greedy flip, Stepwise adaption of weights, Novelty
- Union

## Results



## Results [24]



## Results

- Generated algorithms mostly performed comparably well on training and test problems
- Tree and stack GP perform similarly well on this problem, as do linear and Cartesian GP
- Tree and stack GP perform significantly better on this problem than linear and Cartesian GP, which perform significantly better than grammatical evolution

## Conclusions

- The choice of GP type makes a significant difference in the performance of the hyper-heuristic
- The size of the search space appears to be a major factor in the performance of the hyper-heuristic

## Case Study 1: The Automated Design of Crossover Operators [20]

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## Motivation

- Performance Sensitive to Crossover Selection
- Identifying & Configuring Best Traditional Crossover is Time Consuming
- Existing Operators May Be Suboptimal
- Optimal Operator May Change During Evolution

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## Some Possible Solutions

- Meta-EA
  - Exceptionally time consuming
- Self-Adaptive Algorithm Selection
  - Limited by algorithms it can choose from

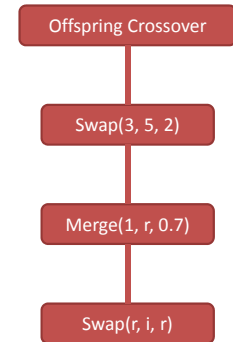
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## Self-Configuring Crossover (SCX)

- Each Individual Encodes a Crossover Operator
- Crossovers Encoded as a List of Primitives
  - Swap
  - Merge
- Each Primitive has three parameters
  - Number, Random, or Inline

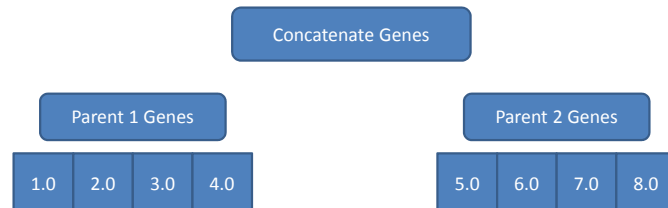


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## Applying an SCX



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## The Swap Primitive

- Each Primitive has a type
  - Swap represents crossovers that move genetic material
- First Two Parameters
  - Start 1 Position
  - Start 2 Position
- Third Parameter Primitive Dependent
  - Swaps use “Width”



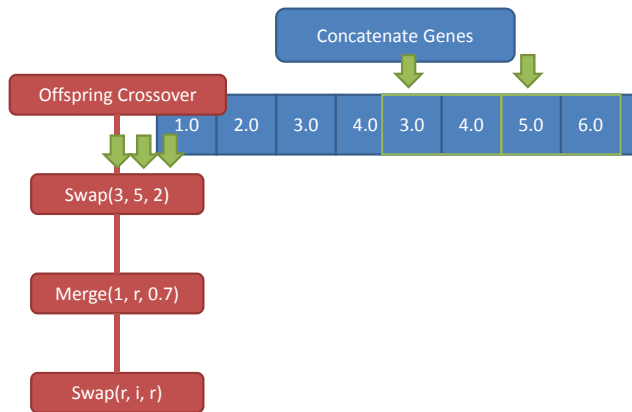
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## Applying an SCX



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## The Merge Primitive

- Third Parameter Primitive Dependent
  - Merges use “Weight”
- Random Construct
  - All past primitive parameters used the Number construct
  - “r” marks a primitive using the Random Construct
  - Allows primitives to act stochastically

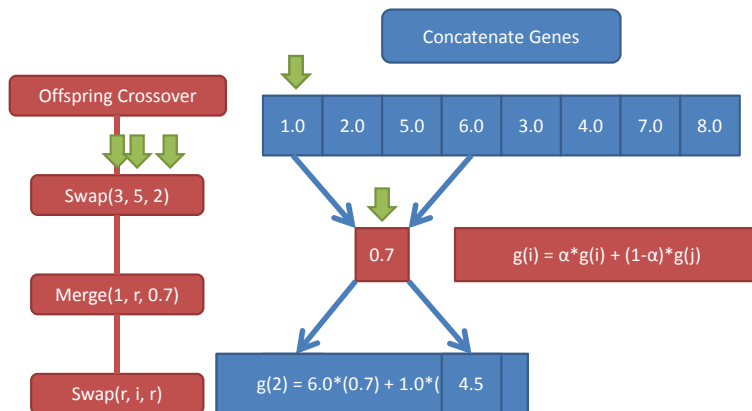


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## Applying an SCX



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## The Inline Construct

- Only Usable by First Two Parameters
- Denoted as “i”
- Forces Primitive to Act on the Same Loci in Both Parents

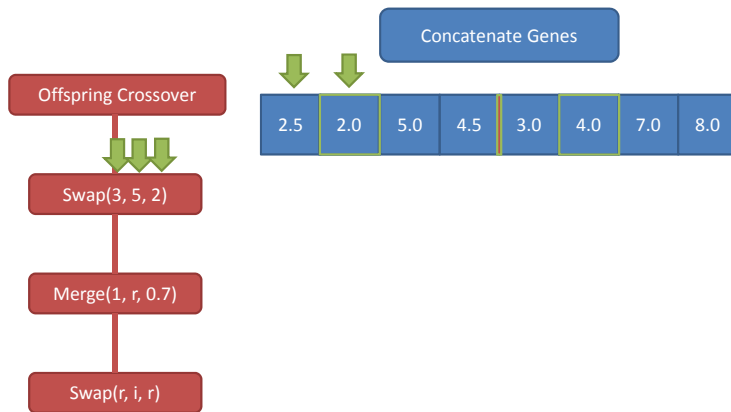


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## Applying an SCX



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## Applying an SCX

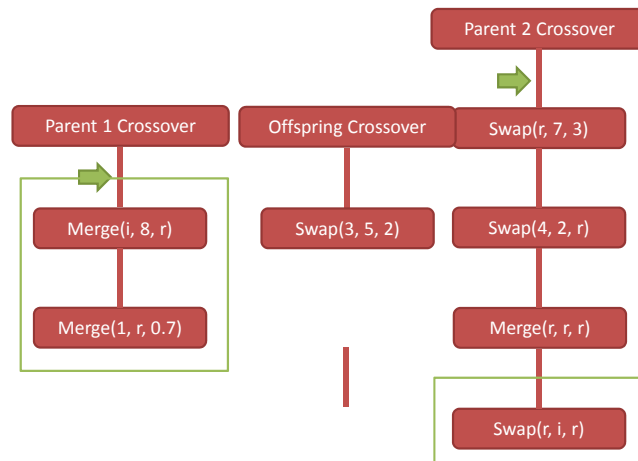


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## Evolving Crossovers



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## Empirical Quality Assessment

- Compared Against
  - Arithmetic Crossover
  - N-Point Crossover
  - Uniform Crossover
- On Problems
  - Rosenbrock
  - Rastrigin
  - Offset Rastrigin
  - NK-Landscapes
  - DTrap

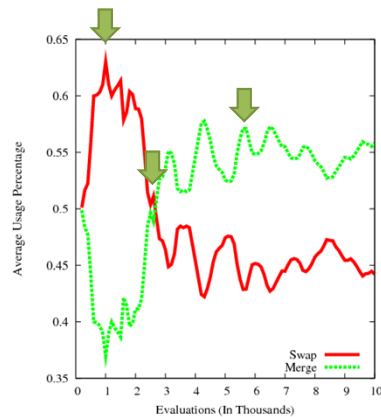
Problem	Comparison	SCX
Rosenbrock	-86.94 (54.54)	-26.47 (23.33)
Rastrigin	-59.2 (6.998)	-0.0088 (0.021)
Offset Rastrigin	-0.1175 (0.116)	-0.03 (0.028)
NK	0.771 (0.011)	0.8016 (0.013)
DTrap	0.9782 (0.005)	0.9925 (0.021)

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## Adaptations: Rastrigin

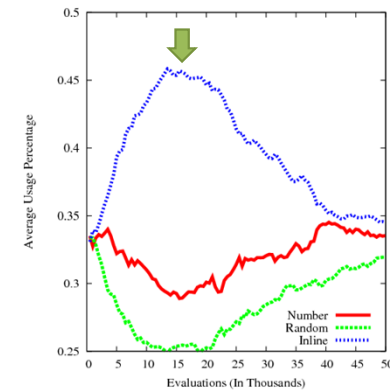


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## Adaptations: DTrap



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## SCX Overhead

- Requires No Additional Evaluation
- Adds No Significant Increase in Run Time
  - All linear operations
- Adds Initial Crossover Length Parameter
  - Testing showed results fairly insensitive to this parameter
  - Even worst settings tested achieved better results than comparison operators

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## Conclusions

- Remove Need to Select Crossover Algorithm
- Better Fitness Without Significant Overhead
- Benefits From Dynamically Changing Operator
- Promising Approach for Evolving Crossover Operators for Additional Representations (e.g., Permutations)

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## Case Study 2: The Automated Design of Mutation Operators for Evolutionary Programming

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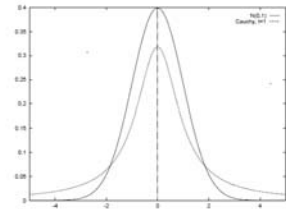
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## Designing Mutation Operators for Evolutionary Programming [18]

1. **Evolutionary programming** optimizes functions by evolving a population of real-valued vectors (genotype).
2. **Variation** has been provided (manually) by **probability distributions (Gaussian, Cauchy, Levy)**.
3. We are **automatically generating** probability distributions (using genetic programming).
4. **Not from scratch**, but from already well known distributions (**Gaussian, Cauchy, Levy**). We are “**genetically improving probability distributions**”.
5. We are evolving mutation operators **for a problem class** (probability distributions over functions).
6. **NO CROSSOVER**

Genotype is  
(1.3,...,4.5,...,8.7)  
Before mutation



Genotype is  
(1.2,...,4.4,...,8.6)  
After mutation

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## (Fast) Evolutionary Programming

Heart of algorithm is mutation  
SO LETS AUTOMATICALLY DESIGN

$$x_i'(j) = x_i(j) + \eta_i(j)D_j$$

1. **EP** mutates with a **Gaussian**
2. **FEP** mutates with a **Cauchy**
3. A **generalization** is mutate with a **distribution D** (generated with genetic programming)

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1. Generate the initial population of  $\mu$  individuals, and set  $k = 1$ . Each individual is taken as a pair of real-valued vectors,  $(x_i, \eta_i)$ ,  $\forall i \in \{1, \dots, \mu\}$ .
2. Evaluate the fitness score for each individual  $(x_i, \eta_i)$ ,  $\forall i \in \{1, \dots, \mu\}$ , of the population based on the objective function,  $f(x_i)$ .
3. Each parent  $(x_i, \eta_i)$ ,  $i = 1, \dots, \mu$ , creates a single offspring  $(x_i', \eta_i')$  by: for  $j = 1, \dots, n$ ,  

$$x_i'(j) = x_i(j) + \eta_i(j)N(0, 1), \quad (1)$$

$$\eta_i'(j) = \eta_i(j) \exp(r'N(0, 1) + \tau N_j(0, 1)) \quad (2)$$
 where  $x_i(j)$ ,  $x_i'(j)$ ,  $\eta_i(j)$  and  $\eta_i'(j)$  denote the  $j$ -th component of the vectors  $x_i$ ,  $x_i'$ ,  $\eta_i$  and  $\eta_i'$ , respectively.  $N(0, 1)$  denotes a normally distributed one-dimensional random number with mean zero and standard deviation one.  $N_j(0, 1)$  indicates that the random number is generated anew for each value of  $j$ . The factors  $\tau$  and  $r'$  have commonly set to  $(\sqrt{2/n})^{-1}$  and  $(\sqrt{2n})^{-1}$  [9, 8].
4. Calculate the fitness of each offspring  $(x_i', \eta_i')$ ,  $\forall i \in \{1, \dots, \mu\}$ .
5. Conduct pairwise comparison over the union of parents  $(x_i, \eta_i)$  and offspring  $(x_i', \eta_i')$ ,  $\forall i \in \{1, \dots, \mu\}$ . For each individual,  $q$  opponents are chosen randomly from all the parents and offspring with an equal probability. For each comparison, if the individual's fitness is no greater than the opponent's, it receives a "win".
6. Select the  $\mu$  individuals out of  $(x_i, \eta_i)$  and  $(x_i', \eta_i')$ ,  $\forall i \in \{1, \dots, \mu\}$ , that have the most wins to be parents of the next generation.
7. Stop if the stopping criterion is satisfied; otherwise,  $k = k + 1$  and go to Step 2.

## Optimization & Benchmark Functions

A set of 23 benchmark functions is typically used in the literature. **Minimization**  $\forall x \in S : f(x_{min}) \leq f(x)$   
We use them as **problem classes**.

Table 1: The 23 test functions used in our experimental studies, where  $n$  is the dimension of the function,  $f_{min}$  the minimum value of the function, and  $S \subseteq R^n$ .

Test function	$n$	$S$	$f_{min}$
$f_1(x) = \sum_{i=1}^n x_i^2$	30	$[-100, 100]^n$	0
$f_2(x) = \sum_{i=1}^n x_i + \prod_{i=1}^n  x_i $	30	$[-10, 10]^n$	0
$f_3(x) = \sum_{i=1}^n (\sum_{j=1}^n x_j)^2$	30	$[-100, 100]^n$	0
$f_4(x) = \max_i \{x_i\}, 1 \leq i \leq n$	30	$[-100, 100]^n$	0
$f_5(x) = \sum_{i=1}^n [100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2]$	30	$[-30, 30]^n$	0
$f_6(x) = \sum_{i=1}^n [x_i + 0.5]$	30	$[-100, 100]^n$	0
$f_7(x) = \sum_{i=1}^n [x_i^2 + \text{random}[0, 1)]$	30	$[-1.28, 1.28]^n$	0
$f_8(x) = \sum_{i=1}^n -x_i \sin(\sqrt{x_i})$	30	$[-500, 500]^n$	12599.5
$f_9(x) = \sum_{i=1}^n [x_i^2 - 10 \cos(2\pi x_i) + 10]$	30	$[-5.12, 5.12]^n$	0
$f_{10}(x) = -20 \exp\left(-0.2 \sqrt{\frac{1}{n} \sum_{i=1}^n x_i^2}\right) - \exp\left(\frac{1}{n} \sum_{i=1}^n \cos 2\pi x_i\right) + 20 + \epsilon$	30	$[-32, 32]^n$	0

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## Function Class 1

1. Machine learning needs to generalize.
2. We generalize to function classes.
3.  $y = x^2$  (**a function**)
4.  $y = ax^2$  (parameterised function)
5.  $y = ax^2, a \sim [1,2]$  (**function class**)
6. We do this for all benchmark functions.
7. The mutation operators is evolved to fit the probability distribution of functions.

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## Function Classes 2

Function Classes	$S$	$b$	$f_{min}$
$f_1(x) = a \sum_{i=1}^n x_i^2$	$[-100, 100]^n$	N/A	0
$f_2(x) = a \sum_{i=1}^n  x_i  + b \prod_{i=1}^n  x_i $	$[-10, 10]^n$	$b \in [0, 10^{-5}]$	0
$f_3(x) = \sum_{i=1}^n (a \sum_{j=1}^i x_j)^2$	$[-100, 100]^n$	N/A	0
$f_4(x) = \max_i \{a  x_i , 1 \leq i \leq n\}$	$[-100, 100]^n$	N/A	0
$f_5(x) = \sum_{i=1}^n [a(x_{i+1} - x_i^2)^2 + (x_i - 1)^2]$	$[-30, 30]^n$	N/A	0
$f_6(x) = \sum_{i=1}^n [(ax_i + 0.5)]^2$	$[-100, 100]^n$	N/A	0
$f_7(x) = a \sum_{i=1}^n ix_i^4 + \text{random}[0, 1)$	$[-1.28, 1.28]^n$	N/A	0
$f_8(x) = \sum_{i=1}^n -(x_i \sin(\sqrt{ x_i }) + a)$	$[-500, 500]^n$	N/A	$[-12629.5, -12599.5]$
$f_9(x) = \sum_{i=1}^n [ax_i^2 + b(1 - \cos(2\pi x_i))]$	$[-5.12, 5.12]^n$	$b \in [5, 10]$	0
$f_{10}(x) = -a \exp(-0.2 \sqrt{\frac{1}{n} \sum_{i=1}^n x_i^2}) - \exp(\frac{1}{n} \sum_{i=1}^n \cos 2\pi x_i) + a + e$	$[-32, 32]^n$	N/A	0

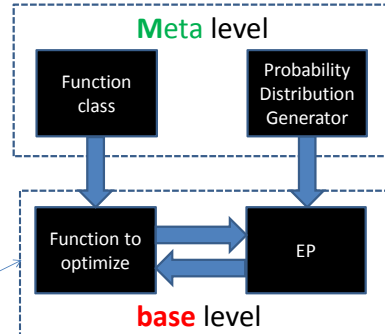
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## Meta and Base Learning

- At the **base** level we are learning about a **specific** function.
- At the **meta** level we are learning about the problem **class**.
- We are just doing “**generate and test**” at a higher level
- What is being passed with each **blue arrow**?
- **Conventional EP**



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## Compare Signatures (Input-Output)

### Evolutionary Programming

$(R^n \rightarrow R) \rightarrow R^n$

**Input** is a function mapping real-valued vectors of length  $n$  to a real-value.

**Output** is a (near optimal) real-valued vector (i.e. the solution to the problem instance)

### Evolutionary Programming Designer

$[(R^n \rightarrow R)] \rightarrow ((R^n \rightarrow R) \rightarrow R^n)$

**Input** is a *list of* functions mapping real-valued vectors of length  $n$  to a real-value (i.e. sample problem instances from the problem class).

**Output** is a (near optimal) (mutation operator for) Evolutionary Programming (i.e. the solution method to the problem class)

We are **raising the level of generality** at which we operate.

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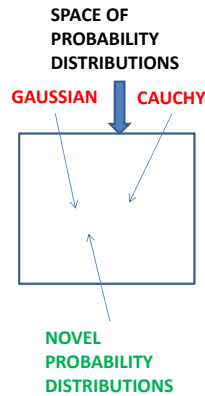
# Genetic Programming to Generate Probability Distributions

1. GP Function Set  $\{+, -, *, \%\}$
2. GP Terminal Set  $\{N(0, \text{random})\}$

$N(0,1)$  is a normal distribution.

For example a Cauchy distribution is generated by  $N(0,1)\%N(0,1)$ .

Hence the search space of probability distributions contains the two existing probability distributions used in EP but also novel probability distributions.



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# Means and Standard Deviations

These results are good for two reasons.

1. starting with a manually designed distributions (Gaussian).
2. evolving distributions for each function class.

Function Class	FEP			CEP			GP-distribution		
	Mean	Best	Std Dev	Mean	Best	Std Dev	Mean	Best	Std Dev
$f_1$	$1.24 \times 10^{-3}$	$2.69 \times 10^{-4}$	$1.45 \times 10^{-4}$	$9.95 \times 10^{-5}$	$6.37 \times 10^{-5}$	$5.56 \times 10^{-5}$	$6.37 \times 10^{-5}$	$5.56 \times 10^{-5}$	
$f_2$	$1.53 \times 10^{-1}$	$2.72 \times 10^{-2}$	$4.30 \times 10^{-2}$	$9.08 \times 10^{-3}$	$8.14 \times 10^{-4}$	$8.50 \times 10^{-4}$	$8.14 \times 10^{-4}$	$8.50 \times 10^{-4}$	
$f_3$	$2.74 \times 10^{-2}$	$2.43 \times 10^{-2}$	$5.15 \times 10^{-2}$	$9.52 \times 10^{-2}$	$6.14 \times 10^{-3}$	$8.78 \times 10^{-3}$	$6.14 \times 10^{-3}$	$8.78 \times 10^{-3}$	
$f_4$	1.79	1.84	$1.75 \times 10$	6.10	$2.16 \times 10^{-1}$	$6.54 \times 10^{-1}$	$2.16 \times 10^{-1}$	$6.54 \times 10^{-1}$	
$f_5$	$2.52 \times 10^{-3}$	$4.96 \times 10^{-4}$	$2.66 \times 10^{-4}$	$4.65 \times 10^{-5}$	$8.39 \times 10^{-7}$	$1.43 \times 10^{-7}$	$8.39 \times 10^{-7}$	$1.43 \times 10^{-7}$	
$f_6$	$3.86 \times 10^{-2}$	$3.12 \times 10^{-2}$	$4.40 \times 10$	$1.42 \times 10^2$	$9.20 \times 10^{-3}$	$1.34 \times 10^{-2}$	$9.20 \times 10^{-3}$	$1.34 \times 10^{-2}$	
$f_7$	$6.49 \times 10^{-2}$	$1.04 \times 10^{-2}$	$6.64 \times 10^{-2}$	$1.21 \times 10^{-2}$	$5.25 \times 10^{-2}$	$8.46 \times 10^{-3}$	$5.25 \times 10^{-2}$	$8.46 \times 10^{-3}$	
$f_8$	-11342.0	$3.26 \times 10^2$	-7894.6	$6.14 \times 10^2$	-12611.6	$2.30 \times 10$	-12611.6	$2.30 \times 10$	
$f_9$	$6.24 \times 10^{-2}$	$1.30 \times 10^{-2}$	$1.09 \times 10^2$	$3.58 \times 10$	$1.74 \times 10^{-3}$	$4.25 \times 10^{-4}$	$1.74 \times 10^{-3}$	$4.25 \times 10^{-4}$	
$f_{10}$	1.67	$4.26 \times 10^{-1}$	1.45	$2.77 \times 10^{-1}$	1.38	$2.45 \times 10^{-1}$	1.38	$2.45 \times 10^{-1}$	

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# T-tests

Table 5 2-tailed t-tests comparing EP with GP-distributions, FEP and CEP on  $f_1$ - $f_{10}$ .

Function Class	Number of Generations	GP-distribution vs FEP $t$ -test	GP-distribution vs CEP $t$ -test
$f_1$	1500	$2.78 \times 10^{-47}$	$4.07 \times 10^{-2}$
$f_2$	2000	$5.53 \times 10^{-62}$	$1.59 \times 10^{-54}$
$f_3$	5000	$8.03 \times 10^{-8}$	$1.14 \times 10^{-3}$
$f_4$	5000	$1.28 \times 10^{-7}$	$3.73 \times 10^{-36}$
$f_5$	20000	$2.80 \times 10^{-58}$	$9.29 \times 10^{-63}$
$f_6$	1500	$1.85 \times 10^{-8}$	$3.11 \times 10^{-2}$
$f_7$	3000	$3.27 \times 10^{-9}$	$2.00 \times 10^{-9}$
$f_8$	9000	$7.99 \times 10^{-48}$	$5.82 \times 10^{-75}$
$f_9$	5000	$6.37 \times 10^{-55}$	$6.54 \times 10^{-39}$
$f_{10}$	1500	$9.23 \times 10^{-5}$	$1.93 \times 10^{-1}$

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# Performance on Other Problem Classes

Table 8: This table compares the fitness values (averaged over 20 runs) of each of the 23 ADRs on each of the 23 function classes. Standard deviations are in parentheses.

ADR	ADR1	ADR2	ADR3	ADR4	ADR5	ADR6	ADR7	ADR8	ADR9	ADR10	ADR11	ADR12	ADR13	ADR14	ADR15	ADR16	ADR17	ADR18	ADR19	ADR20	ADR21	ADR22	ADR23
$f_1$	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
$f_2$	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
$f_3$	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
$f_4$	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
$f_5$	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
$f_6$	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
$f_7$	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
$f_8$	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
$f_9$	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
$f_{10}$	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...

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## Case Study 3: The Automated Design of On-Line Bin Packing Algorithms

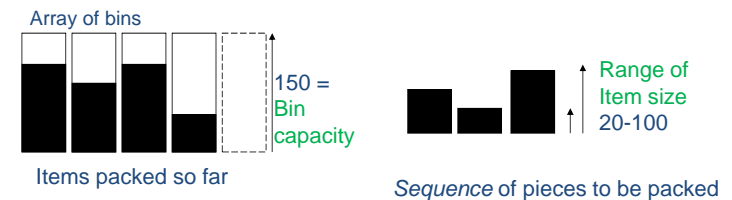
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## On-line Bin Packing Problem [9,11]

- A **sequence of items** packed into as few a bins as possible.
- Bin size is **150 units**, items uniformly distributed between **20-100**.
- Different to the off-line bin packing problem where the **set** of items.
- The "best fit" heuristic, places the current item in the space it fits best (leaving least slack).
- It has the property that this heuristic does not open a new bin unless it is forced to.

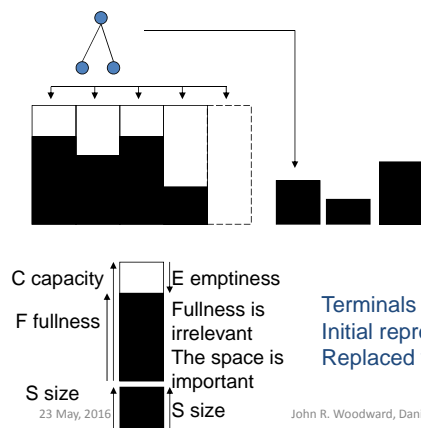


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## Genetic Programming applied to on-line bin packing



Not obvious how to link Genetic Programming to combinatorial problems. The GP tree is applied to each bin with the current item and placed in the bin with The maximum score

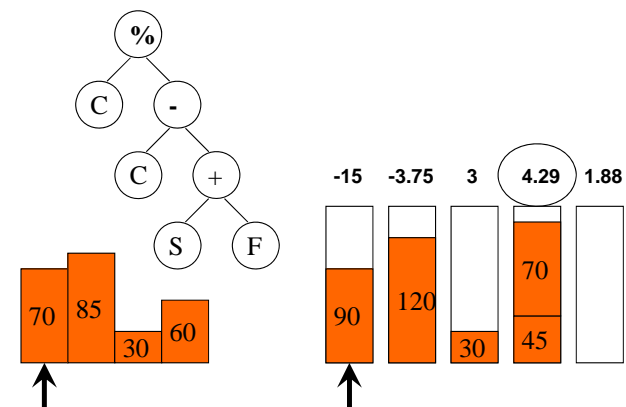
Terminals supplied to Genetic Programming  
Initial representation {C, F, S}  
Replaced with {E, S},  $E = C - F$

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## How the heuristics are applied (skip)



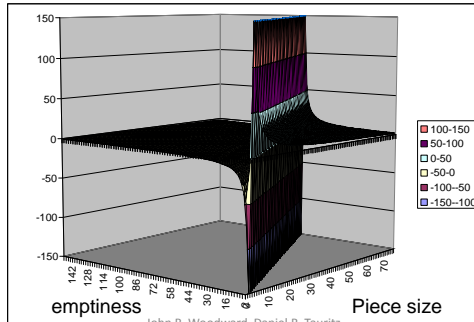
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## The Best Fit Heuristic

Best fit =  $1/(E-S)$ . Point out features.  
 Pieces of size  $S$ , which fit well into the space remaining  $E$ , score well.  
 Best fit applied produces a set of points on the surface,  
 The bin corresponding to the maximum score is picked.

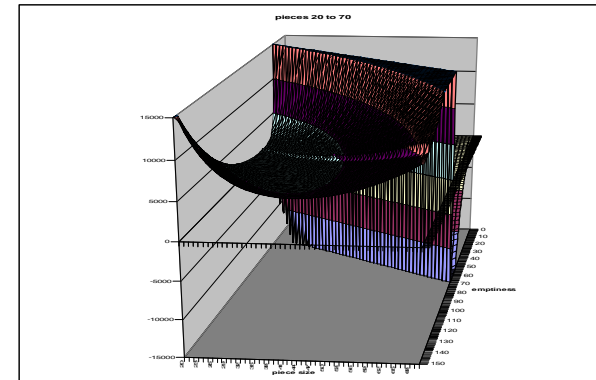


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## Our Best Heuristic



Similar shape to best fit – but curls up in one corner.  
 Note that this is rotated, relative to previous slide.

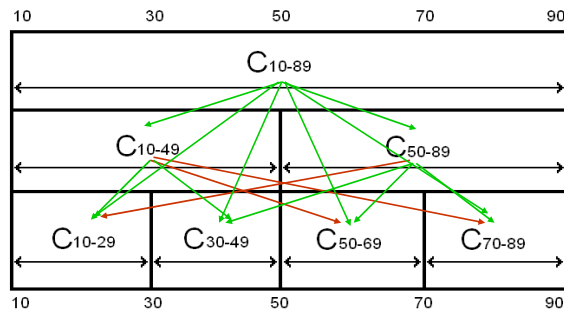
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## Robustness of Heuristics

→ = all legal results  
 → = some illegal results



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## Testing Heuristics on problems of much larger size than in training

Table I	$H$ trained 100	$H$ trained 250	$H$ trained 500
100	0.427768358	0.298749035	0.140986023
1000	0.406790534	0.010006408	0.000350265
10000	0.454063071	2.58E-07	9.65E-12
100000	0.271828318	1.38E-25	2.78E-32

Table shows p-values using the best fit heuristic, for heuristics trained on different size problems, when applied to different sized problems

1. As number of items trained on increases, the probability decreases (see next slide).
2. As the number of items packed increases, the probability decreases (see next slide).

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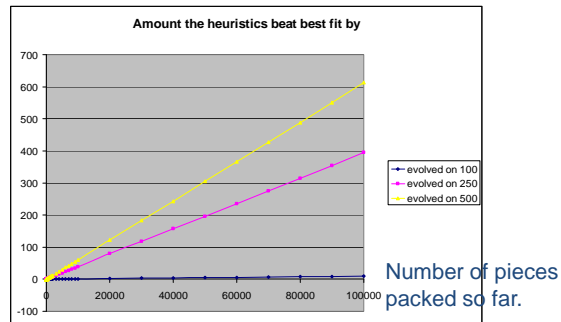
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## Compared with Best Fit

Amount evolved heuristics beat best fit by.



- Averaged over 30 heuristics over 20 problem instances
- Performance does not deteriorate
- The larger the training problem size, the better the bins are packed.

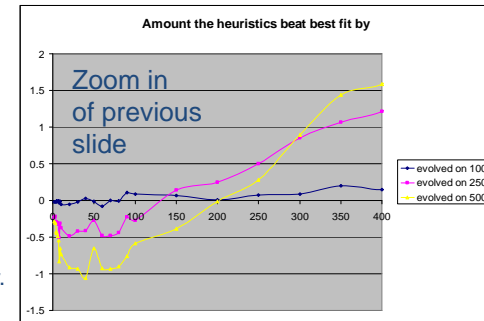
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## Compared with Best Fit

Amount evolved heuristics beat best fit by.



- The heuristic seems to learn the number of pieces in the problem
- Analogy with sprinters running a race – accelerate towards end of race.
- The “break even point” is approximately half of the size of the training problem size
- If there is a gap of size 30 and a piece of size 20, it would be better to wait for a better piece to come along later – about 10 items (similar effect at upper bound?).

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## Step by Step Guide to Automatic Design of Algorithms [8, 12]

1. Study the literature for **existing heuristics** for your chosen domain (manually designed heuristics).
2. Build an **algorithmic framework or template** which expresses the known heuristics.
3. Let metaheuristics (e.g. **Genetic Programming search for variations on the theme**).
4. **Train and test** on problem instances drawn from the same probability distribution (like machine learning). Constructing an optimizer is machine learning (**this approach prevents “cheating”**).

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## A Brief History (Example Applications) [5]

1. **Image Recognition** – Roberts Mark
2. **Travelling Salesman Problem** – Keller Robert
3. **Boolean Satisfiability** – Holger Hoos, Fukunaga, Bader-El-Den, Alex Bertels & Daniel Tauritz
4. **Data Mining** – Gisele L. Pappa, Alex A. Freitas
5. **Decision Tree** - Gisele L. Pappa et al
6. **Crossover Operators** – Oltean et al, Brian Goldman and Daniel Tauritz
7. **Selection Heuristics** – Woodward & Swan, Matthew Martin & Daniel Tauritz
8. **Bin Packing 1,2,3 dimension** (on and off line) Edmund Burke et. al. & Riccardo Poli et al
9. **Bug Location** – Shin Yoo
10. **Job Shop Scheduling** – Mengjie Zhang
11. **Black Box Search Algorithms** – Daniel Tauritz et al

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## Comparison of Search Spaces

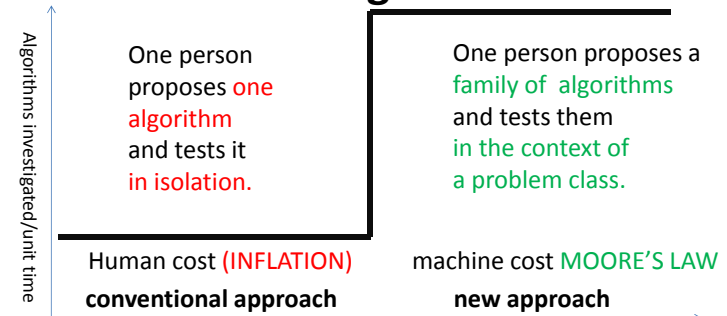
- If **we tackle a problem instance directly**, e.g. Travelling Salesman Problem, we get a **combinatorial explosion**. The search space consists of *solutions*, and therefore explodes as we tackle larger problems.
- If we tackle a generalization of the problem, **we do not get an explosion** as the distribution of functions expressed in the search space tends to a limiting distribution. The search space consists of *algorithms to produce solutions* to a problem instance of any size.
- The algorithm to tackle TSP of size 100-cities, is the same size as The algorithm to tackle TSP of size 10,000-cities

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## A Paradigm Shift?



- Previously **one** person proposes **one** algorithm
- Now **one** person proposes a **set of** algorithms
- Analogous to “**industrial revolution**” from hand made to machine made. Automatic Design.

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## Conclusions

1. Heuristic are **trained to fit a problem class**, so are designed in context (like evolution). Let's close the feedback loop! **Problem instances live in classes.**
2. We can design algorithms on **small** problem instances and **scale** them apply them to **large** problem instances (TSP, child multiplication).

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## SUMMARY

1. We can automatically design algorithms that **consistently outperform human designed algorithms (on various domains)**.
2. **Humans should not provide variations— genetic programing can do that.**
3. We are altering the heuristic to suit the set of problem instances presented to it, in the hope that it will generalize to new problem instances (**same distribution - central assumption in machine learning**).
4. The “best” heuristics **depends on the set of problem instances. (feedback)**
5. Resulting algorithm is **part man-made part machine-made** (synergy)
6. **not evolving from scratch like Genetic Programming,**
7. improve existing algorithms and adapt them to the new problem instances.
8. Humans are working at a **higher level of abstraction** and more creative. Creating search spaces for GP to sample.
9. **Algorithms are reusable, “solutions” aren't.** (e.g. tsp algorithm vs route)
10. **Opens up new problem domains.** E.g. bin-packing.

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## Case Study 4: The Automated Design of Black Box Search Algorithms [21, 23, 25]

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## Approach

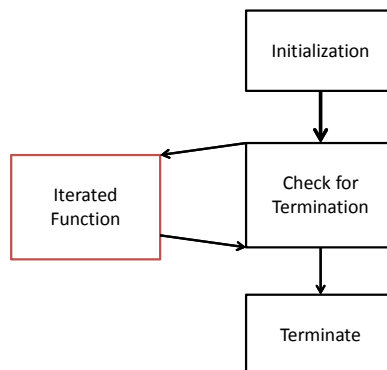
- Hyper-Heuristic employing Genetic Programming
- Post-ordered parse tree
- Evolve the iterated function

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## Our Solution



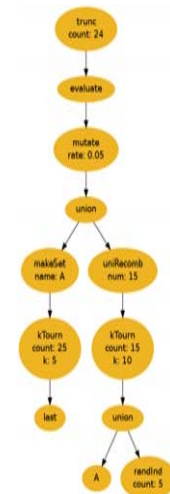
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## Our Solution

- Hyper-Heuristic employing Genetic Programming
- Post-ordered parse tree
- Evolve the iterated function
- High-level primitives



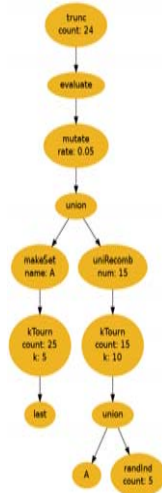
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## Parse Tree

- Iterated function
- Sets of solutions
- Function returns a set of solutions accessible to the next iteration



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## Primitive Types

- Variation Primitives
- Selection Primitives
- Set Primitives
- Evaluation Primitive
- Terminal Primitives

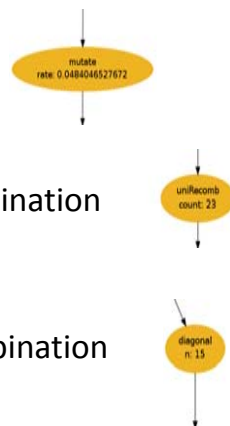
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## Variation Primitives

- Bit-flip Mutation  
– *rate*
- Uniform Recombination  
– *count*
- Diagonal Recombination  
– *n*



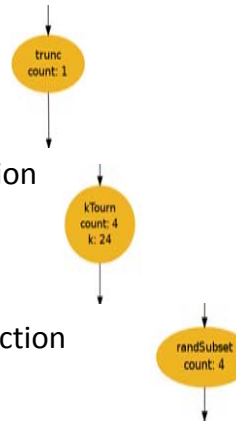
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## Selection Primitives

- Truncation Selection  
– *count*
- K-Tournament Selection  
– *k*  
– *count*
- Random Sub-set Selection  
– *count*

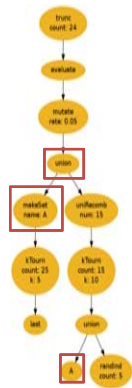


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## Set-Operation Primitives



- Make Set  
– *name*
- Persistent Sets  
– *name*
- Union

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## Evaluation Primitive

- Evaluates the nodes passed in
- Allows multiple operations and accurate selections within an iteration  
– Allows for deception

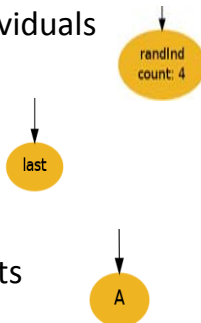
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## Terminal Primitives

- Random Individuals  
– *count*
- 'Last' Set
- Persistent Sets  
– *name*

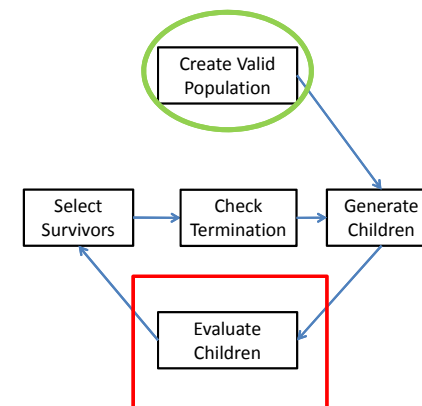


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## Meta-Genetic Program

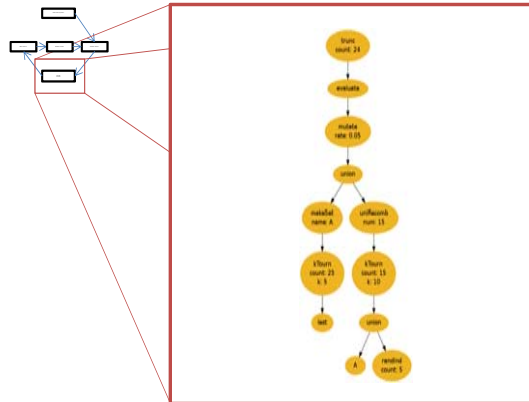


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## BBSA Evaluation



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## Termination Conditions

- Evaluations
- Iterations
- Operations
- Convergence

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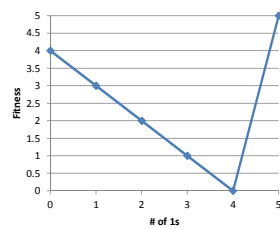
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## Proof of Concept Testing

- Deceptive Trap Problem

0	0	1	1	0	0	1	0	1	0	1	1	1	1	0
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---



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## Proof of Concept Testing (cont.)

- Evolved Problem Configuration
  - Bit-length = 100
  - Trap Size = 5
- Verification Problem Configurations
  - Bit-length = 100, Trap Size = 5
  - Bit-length = 200, Trap Size = 5
  - Bit-length = 105, Trap Size = 7
  - Bit-length = 210, Trap Size = 7

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## Results

BBSA	EA	Hill-Climber
1	+	+
2	+	+
3	+	+
4	-	-
5	+	+
6	+	+
7	+	+
8	-	-
9	-	-
10	-	-
11	+	+
12	-	-
13	+	+
14	+	+
15	-	-

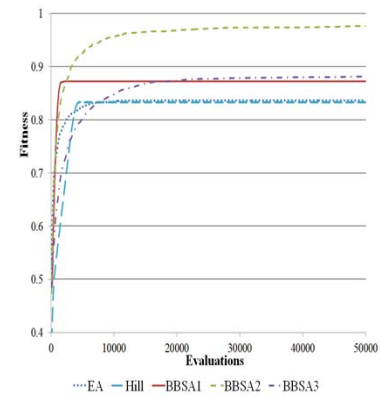
60% Success Rate

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Results:  
Bit-Length = 100  
Trap Size = 5

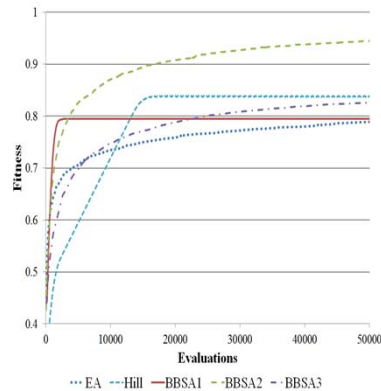


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Results:  
Bit-Length = 200  
Trap Size = 5

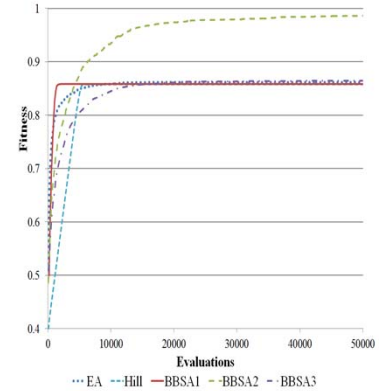


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Results:  
Bit-Length = 105  
Trap Size = 7

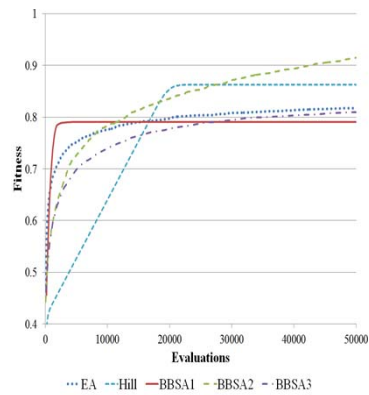


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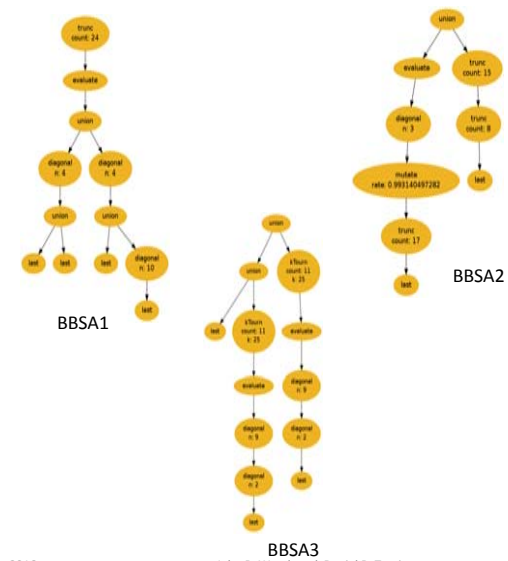
Results:  
Bit-Length = 210  
Trap Size = 7



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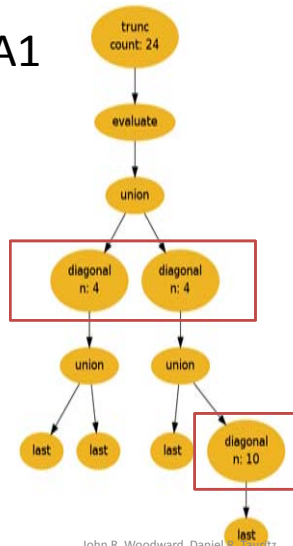


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**BBSA1**

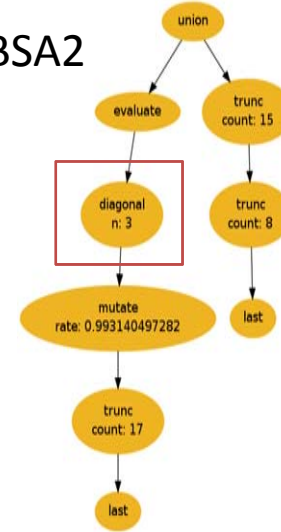


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**BBSA2**



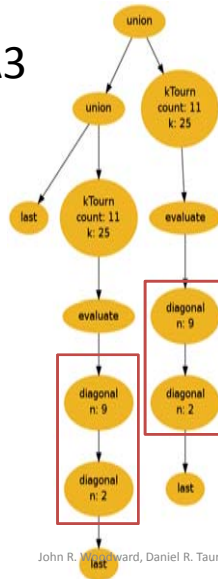
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## BBSA3

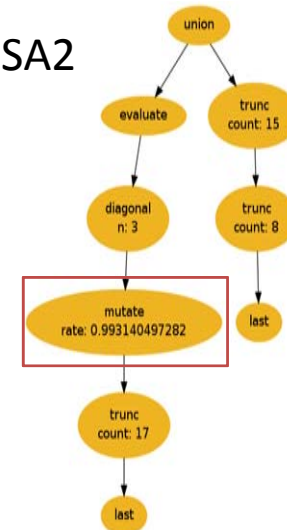


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## BBSA2

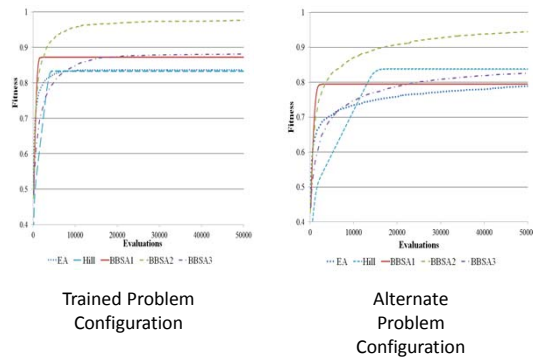


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## Over-Specialization



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## Robustness

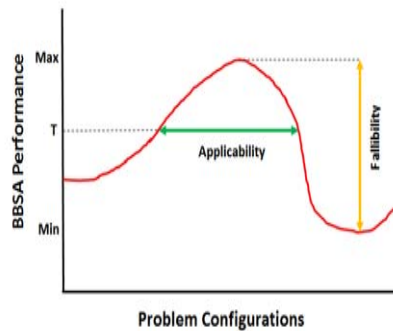
- Measures of Robustness
  - Applicability
  - Fallibility
- Applicability
  - What area of the problem configuration space do I perform well on?
- Fallibility
  - If a given BBSA doesn't perform well, how much worse will I perform?

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## Robustness



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## Multi-Sampling

- Train on multiple problem configurations
- Results in more robust BBSAs
- Provides the benefit of selecting the region of interest on the problem configuration landscape

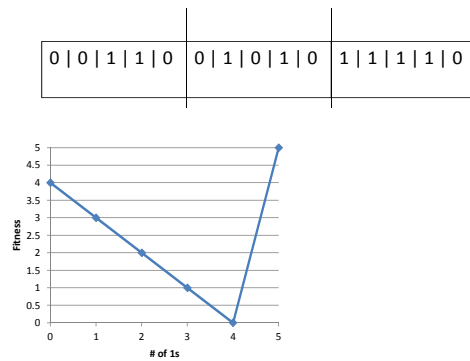
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## Multi-Sample Testing

- Deceptive Trap Problem



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## Multi-Sample Testing (cont.)

- Multi-Sampling Evolution
  - Levels 1-5
- Training Problem Configurations
  1. Bit-length = 100, Trap Size = 5
  2. Bit-length = 200, Trap Size = 5
  3. Bit-length = 105, Trap Size = 7
  4. Bit-length = 210, Trap Size = 7
  5. Bit-length = 300, Trap Size = 5

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## Initial Test Problem Configurations

1. Bit-length = 100, Trap Size = 5
2. Bit-length = 200, Trap Size = 5
3. Bit-length = 105, Trap Size = 7
4. Bit-length = 210, Trap Size = 7
5. Bit-length = 300, Trap Size = 5
6. Bit-length = 99, Trap Size = 9
7. Bit-length = 198, Trap Size = 9
8. Bit-length = 150, Trap Size = 5
9. Bit-length = 250, Trap Size = 5
10. Bit-length = 147, Trap Size = 7
11. Bit-length = 252, Trap Size = 7

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## Initial

Level	Run	Train Fit.	Test Fit.	Fallibility
1	1	1.0	0.976	0.094
1	2	1.0	0.999	8.33 E-3
1	3	0.944	0.883	0.082
1	4	0.976	0.894	0.224
2	1	0.997	0.996	0.023
2	2	0.992	0.959	0.130
2	3	0.966	0.970	0.054
2	4	0.979	0.947	0.120
3	1	0.965	0.966	0.050
3	2	0.984	0.980	0.065
3	3	0.899	0.886	0.059
3	4	0.926	0.898	0.073
4	1	0.976	0.999	5.00 E-3
4	2	0.973	0.969	.0903
4	3	0.982	0.975	0.059
4	4	0.993	0.999	5.00 E-3
5	1	0.973	0.977	0.050
5	2	0.893	0.879	0.035
5	3	0.850	0.850	0.045
5	4	0.955	0.986	0.029

Level	Run	+	~	-
1	1	11	0	0
1	2	11	0	0
1	3	11	0	0
1	4	6	2	3
2	1	11	0	0
2	2	11	0	0
2	3	11	0	0
2	4	11	0	0
3	1	11	0	0
3	2	11	0	0
3	3	11	0	0
3	4	11	0	0
4	1	11	0	0
4	2	11	0	0
4	3	11	0	0
4	4	11	0	0
5	1	11	0	0
5	2	10	1	0
5	3	7	4	0
5	4	11	0	0

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## Problem Configuration Landscape Analysis

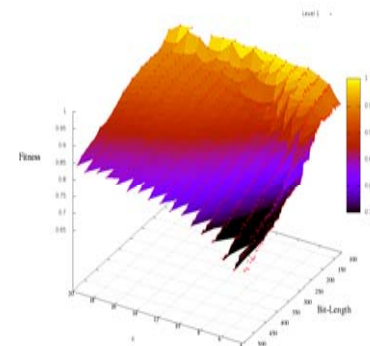
- Run evolved BBSAs on wider set of problem configurations
- Bit-length: ~75-~500
- Trap Size: 4-20

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## Results: Multi-Sampling Level 1

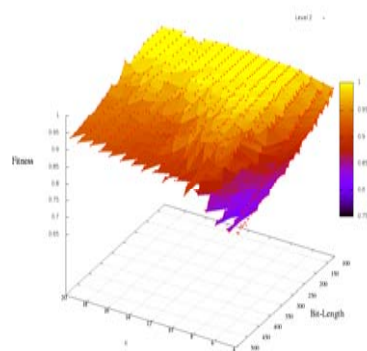


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## Results: Multi-Sampling Level 2

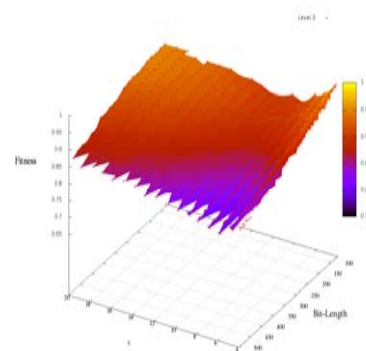


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## Results: Multi-Sampling Level 3

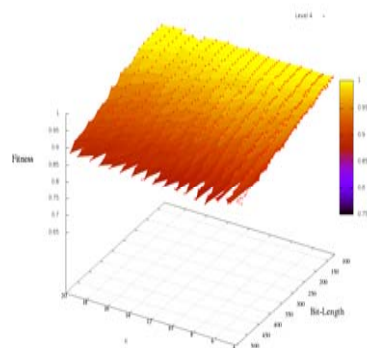


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## Results: Multi-Sampling Level 4

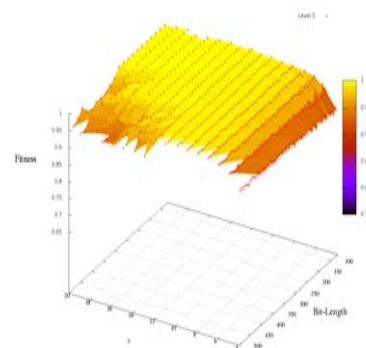


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## Results: Multi-Sampling Level 5

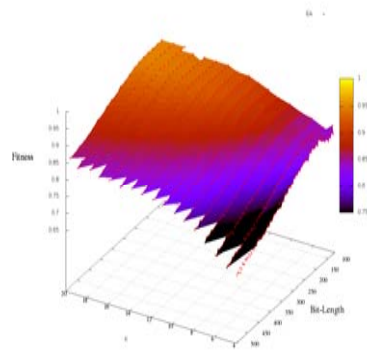


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## Results: EA Comparison



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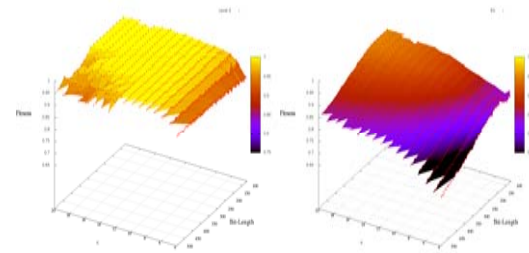
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## Robustness: Fallibility

Multi-Sample Level 5

Standard EA



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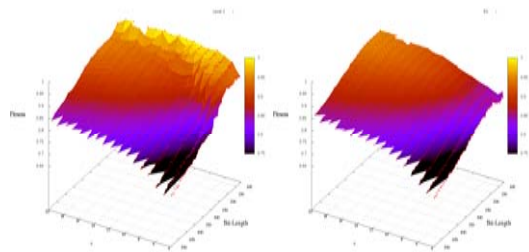
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## Robustness: Fallibility

Multi-Sample Level 1

Standard EA



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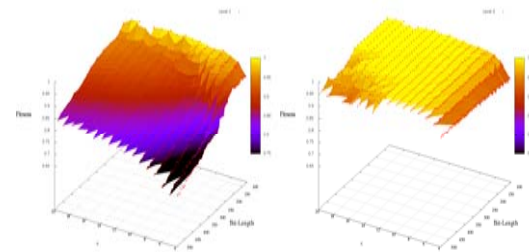
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## Robustness: Applicability

Multi-Sample Level 1

Multi-Sample Level 5



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## Robustness: Fallibility

Level	Run	Train Fit.	Test Fit.	Fallibility
5	1	0.973	0.977	0.050
5	2	0.893	0.879	0.035
5	3	0.850	0.850	0.045
5	4	0.955	0.986	0.029

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## Drawbacks

- Increased computational time
  - More runs per evaluation (increased wall time)
  - More problem configurations to optimize for (increased evaluations)

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## Summary of Multi-Sample Improvements

- Improved Hyper-Heuristic to evolve more robust BBSAs
- Evolved custom BBSA which outperformed standard EA and were robust to changes in problem configuration

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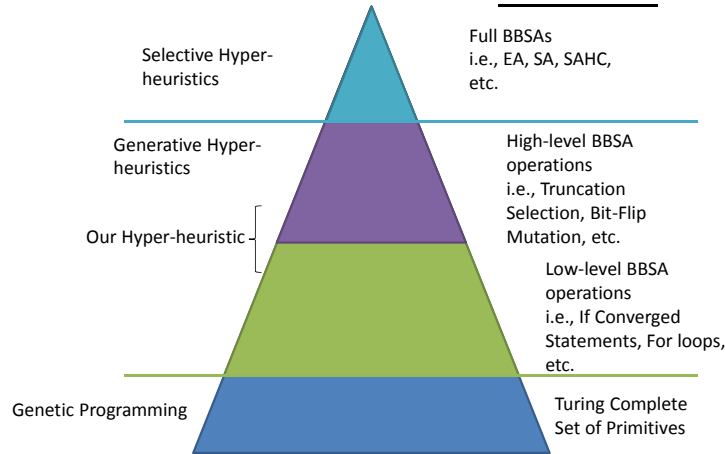
## Challenges in Hyper-heuristics

- Hyper-heuristics are very computationally expensive (use Asynchronous Parallel GP [26])
- What is the best primitive granularity? (see next slide)
- How to automate decomposition and recomposition of primitives?
- How to automate primitive extraction?
- How does hyper-heuristic performance scale for increasing primitive space size? (see [25])

## Primitive Granularity

### Algorithm

### Primitives



## End of File ☺

- Thank you for listening !!!
- We are glad to take any

- comments (+,-)
- suggestions/criticisms

Please email us any missing references!

John Woodward (<http://www.cs.stir.ac.uk/~jrw/>)

Daniel Tauritz (<http://web.mst.edu/~tauritzd/>)

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