Hyper-heuristics Tutorial

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John's perspective of hyperheuristics

Instructors

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Domain Barrier

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

Hyper heuristic layer

Meta heuristic to decide which heuristic to apply to which solution and where to store it in the list of solutions, based only on past history of heuristics applied and objective function values returned.

e(sk)	Domain Barrier	(i,j,k)		
Objective functi problem insta	on and ance	Set of heuristics H1,Hn		
Problem layer	list of so	lutions		

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Automated Design of Algorithms Hyper-heuristics Addresses the need for custom algorithms • Hyper-heuristics are a special type of meta-heuristic But due to high computational complexity, only feasible - Step 1: Extract algorithmic primitives from existing for repeated problem solving algorithms Hyper-heuristics accomplish automated design of - Step 2: Search the space of programs defined by the algorithms by searching program space 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] 23 April, 2019 23 April 2019 18 John R. Woodward, Daniel R. Taurita John R. Woodward, Daniel R. Taurit Type of GP Matters: **GP** Individual Description **Experiment Description** Search algorithms are represented as an iterative algorithm that passes one or more set of variable • Implement five types of GP (tree GP, linear GP, canonical Cartesian GP, Stack GP, and Grammatical assignments to the next iteration Evolution) in hyper-heuristics for evolving black-box Genetic program represents a single program iteration search algorithms for solving 3-SAT • Algorithm runs starting with a random initial population of • Base hyper-heuristic fitness on the fitness of the solutions for 30 seconds best search algorithm generated at solving the 3-SAT problem · Compare relative effectiveness of each GP type as a hyper-heuristic

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:
 - $(\mathsf{A} \lor \mathsf{B} \lor \mathsf{C}) \land (\neg \mathsf{A} \lor \neg \mathsf{C} \lor \mathsf{D}) \land (\neg \mathsf{B} \lor \mathsf{C} \lor \neg \mathsf{D})$
 - Satisfied by ¬A, B, C, ¬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 [24]



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Results



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

(Fast) Evolutionary Programming

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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
- A generalization is mutate with a distribution D (generated with genetic programming)
- 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, η_i) $\forall i \in \{1, \dots, \mu\}$, of the population based on the objective function, $f(x_i)$. Each parent (x_i, η_i), i = 1, · · · , μ, creates a single offspring (x_i', η_i') by: for j = 1, · · · , n, $x_i'(j) = x_i(j) + \eta_i(j)N(0, 1),$ $\eta_i'(j) = \eta_i(j) \exp(\tau' N(0, 1) + \tau N_j(0, 1))$ (2) $\eta_1^*(j) = \eta_1(j) \exp\{i^*\lambda(0, 1) + \tau_1\lambda(0, 1))$ (2) where $x_i(j), x_i(j)$, and $\eta_1^*(j)$ denote the *j*-th component of the vectors x_i, x_i^*, η_1 and η_i^* , respec-tively. N(0, 1) denotes a normally distributed one-dimensional random number with mean zero and standard deviation one. $N_i(0, 1)$ indicates that the random number is generated nave for each value of j. The *factors* τ and τ^* have commonly set to j. $\left(\sqrt{2\sqrt{n}}\right)^{-1}$ and $\left(\sqrt{2n}\right)^{-1}$ [9, 8]. Calculate the fitness of each offspring (x_i['], η_i[']), ∀i ∈ $\{1, \dots, \mu\}.$ Conduct pairwise comparison over the union of pa For each individual, q opponents are chosen ran-domly from all the parents and offspring (x_i', η_i') , $\forall i \in \{1, \dots, \mu\}$. equal probability. For each comparison, if the indi-vidual's fitness is no greater than the opponent's, it receives a "win." . Select the μ individuals out of (x_i, η_i) and (x_i', η_i') . $\forall i \in \{1, \dots, \mu\}$, that have the most wins to be par ents of the next generation. 7. Stop if the stopping criterion is satisfied; otherwise, k = k + 1 and go to Step 3.

Designing Mutation Operators for Evolutionary Programming [18]

- **1. Evolutionary programing** 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).
- Not from scratch, but from already well known distributions (Gaussian, Cauchy, Levy). We are "genetically improving probability distributions".
- We are evolving mutation operators for a problem class (probability distributions over functions).
- 6. NO CROSSOVER

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



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

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Optimization & Benchmark Functions

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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 $S \subseteq \mathbb{R}^{n}$.

n	S	f_{min}
30	$[-100, 100]^n$	0
30	$[-10, 10]^n$	0
30	$[-100, 100]^n$	0
30	$[-100, 100]^n$	0
30	$[-30, 30]^n$	0
30	$[-100, 100]^n$	0
30	$[-1.28, 1.28]^n$	0
30	$[-500, 500]^n$	-12569.5
30	$[-5.12, 5.12]^n$	0
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* ~[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.

Function Classes 2

Function Classes	\boldsymbol{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
$f_4(x) = \max_i \{ a \mid x_i \mid , 1 \le i \le n \}$	$[-100, 100]^n$	N/A	0
$f_5(x) = \sum_{i=1}^{n} \left[a(x_{i+1} - x_i^2)^2 + (x_i - 1)^2 \right]$	$[-30, 30]^n$	N/A	0
$f_6(x) = \sum_{i=1}^{n} (\lfloor ax_i + 0.5 \rfloor)^2$	$[-100, 100]^n$	N/A	0
$f_7(x) = a \sum_{i=1}^{n} ix_i^4 + random[0, 1)$	$[-1.28, 1.28]^n$	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
$f_{10}(x) = -a \exp(-0.2\sqrt{\frac{1}{n}\sum_{i=1}^{n} x_i^2})$	$[-32, 32]^n$	N/A	0
$-\exp(\frac{1}{n}\sum_{i=1}^n\cos 2\pi x_i) + a + e$			

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Meta and Base Learning

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- 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



Compare Signatures (Input-Output)

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Evolutionary Programming	Evolutionary Programming
$(R^n \rightarrow R) \rightarrow R^n$	Designer
Input is a function	$[(R^n \to R)] \to ((R^n \to R) \to R^n)$
mapping real-valued vectors of length n to a real-value.	Input is a <i>list of</i> functions mapping real-valued vectors of length n to a real-value (i.e. sample problem
Output is a (near optimal)	instances from the problem class).
real-valued vector	Output is a (near optimal)
(i.e. the <u>solution to</u> the	Evolutionary Programming
problem i <u>nstance</u>)	(i.e. the <u>solution</u> <u>method</u> 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

GP Function Set {+, -, *, %}
 GP Terminal Set {N(0, 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	FF	P	C	EP	GP-dist:	ribution
Class	Mean Best	$Std \ Dev$	Mean Best	$Std \ Dev$	Mean Best	Std Dev
f_1	1.24×10^{-3}	$2.69{ imes}10^{-4}$	$1.45{ imes}10^{-4}$	9.95×10^{-5}	6.37×10^{-8}	5.56×10^{-5}
f_2	1.53×10^{-1}	2.72×10^{-2}	4.30×10^{-2}	9.08×10^{-3}	8.14×10^{-4}	8.50×10^{-4}
f_3	2.74×10^{-2}	2.43×10^{-2}	5.15×10^{-2}	9.52×10^{-2}	6.14×10^{-3}	8.78×10^{-3}
f_4	1.79	1.84	1.75×10	6.10	2.16×10^{-1}	6.54×10^{-1}
f_5	2.52×10^{-3}	4.96×10^{-4}	2.66×10^{-4}	4.65×10^{-5}	8.39×10^{-7}	1.43×10^{-7}
f_6	$3.86{ imes}10^{-2}$	$3.12{ imes}10^{-2}$	4.40×10	1.42×10^{2}	9.20×10^{-3}	1.34×10^{-2}
f_7	6.49×10^{-2}	1.04×10^{-2}	$6.64{ imes}10^{-2}$	1.21×10^{-2}	5.25×10^{-2}	8.46×10^{-3}
f_8	-11342.0	3.26×10^{2}	-7894.6	6.14×10^{2}	-12611.6	2.30×10
f_9	6.24×10^{-2}	1.30×10^{-2}	1.09×10^{2}	3.58×10	1.74×10^{-3}	4.25×10^{-4}
f_{10}	1.67	4.26×10^{-1}	1.45	2.77×10^{-1}	1.38	2.45×10^{-1}

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T-tests

Table 5 2-tailed t-tests comparing EP with GP-distributions, FEP and CEP on $f_{\rm 1}\text{-}f_{\rm 10}.$

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

Performance on Other Problem Classes

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 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.

 Stardard deviations are in parentheses.

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Table I	H trained100	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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10

C10-29

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C50-69

= all legal results = some illegal results

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C10-89

C30-49

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C70-89

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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").

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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Traditional Random Graph Models

• Erdös-Rényi



• Barabási-Albert



Random graph model needs to accurately reflect intended concept

• Model selection can be automated, but relies on having a good solution available

Automated Random Graph Model Design

• Developing an accurate model for a new application can be difficult

Can the model design process be automated to produce an accurate graph model given examples?

Hyper-heuristic Approach

- Extract functionality from existing graph generation techniques
- Use Genetic Programming (GP) to construct new random graph algorithms



Previous Attempts at Evolving Random Graph Generators

- Assumes "growth" model, adding one node at a time
- Does well at reproducing traditional models
- Not demonstrated to do well at generating real complex networks
- Limits the search space of possible solutions

Increased Algorithmic Primitive Granularity

- Remove the assumed "growth" structure
- More flexible lower-level primitive set
- Benefit: Can represent a larger variety of algorithms
- Drawback: Larger search space, increasing complexity

Methodology

- NSGA-II evolves population of random graph models
- Strongly typed parse tree representation
- · Centrality distributions used to evaluate solution
- quality (degree, betweenness, PageRank)

Primitive Operations

Terminals

- Graph elements: nodes, edges
- Graph properties: average degree, size, order
- Constants: integers, probabilities, Booleans, user inputs
- No-op terminators

Functions

- Basic programming constructs: for, while, if-else
- Data structures: lists of values, nodes, or edges, list
- combining/selection/sorting
- Math and logic operators: add, multiply, <, ==, AND, OR
- Graph operators: add edges, add subgraph, rewire edges

Example Evolved Random Graph Generator







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