Hyper-heuristics Tutorial
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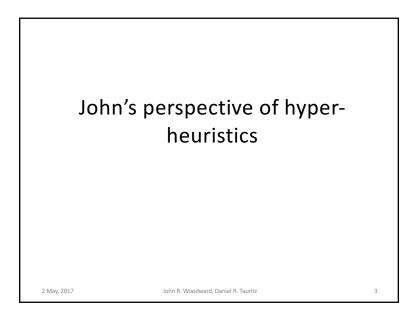
Instructors

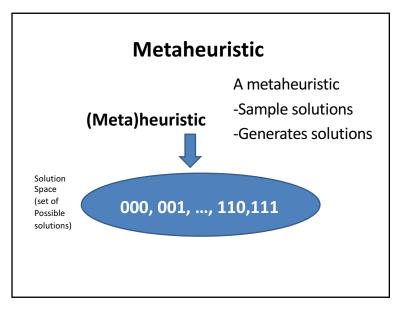
Daniel R. Tauritz is an Associate Professor and Associate Chair for Undergraduate Studies in the <u>Department of Computer Science</u> at the <u>Missouri University of Science and Technology (S&T)</u>, a Contract Scientist for Los Alamos National Laboratory (LANL) and Sandia National Laboratories, the 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.



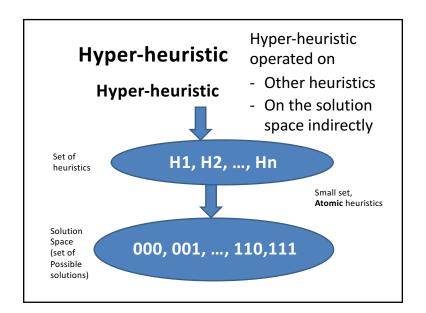
John R. Woodward is a Lecturer at the <u>University of Stirling</u>, within the <u>CHORDS group</u> and is employed on the <u>DAASE project</u>, and for the previous four years was a lecturer with the <u>University of Nottingham</u>. He holds a BSc in Theoretical Physics, an MSc in Cognitive Science 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.

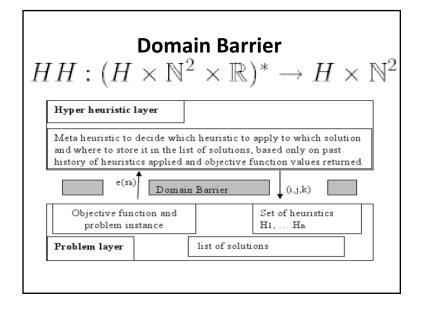
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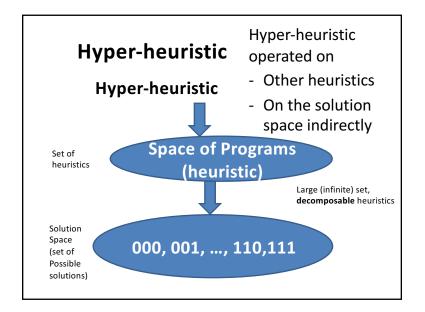


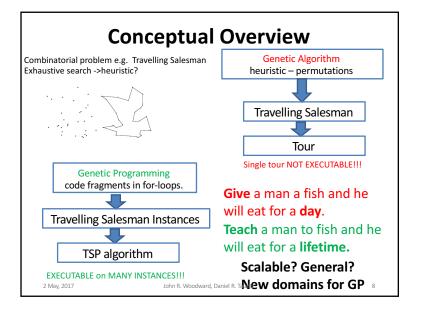


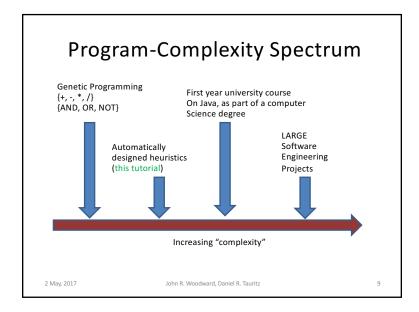
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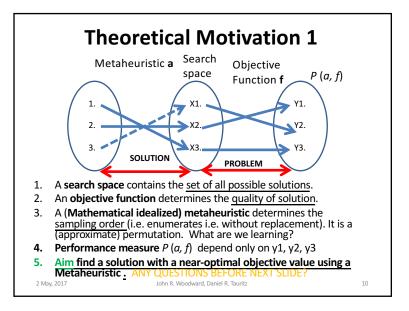


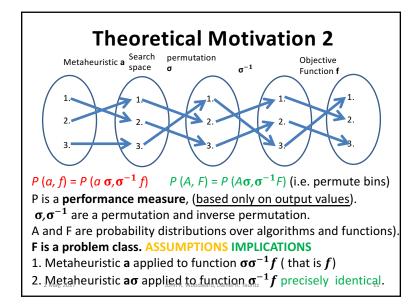


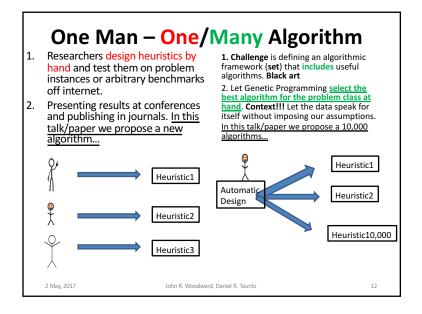


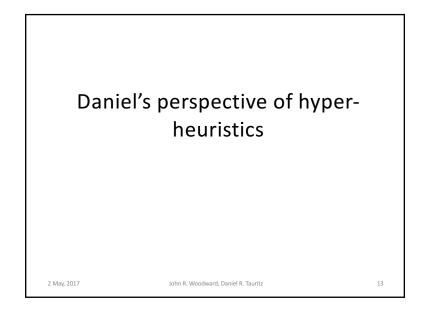












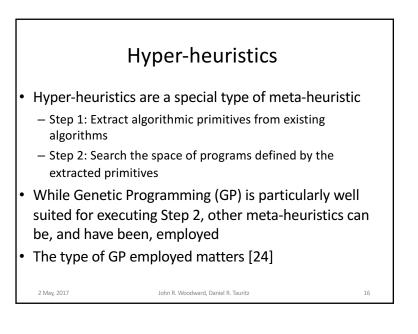
Automated Design of Algorithms

- 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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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 2 May, 2017 John R. Woodward, Daniel R. Tauritz 14



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

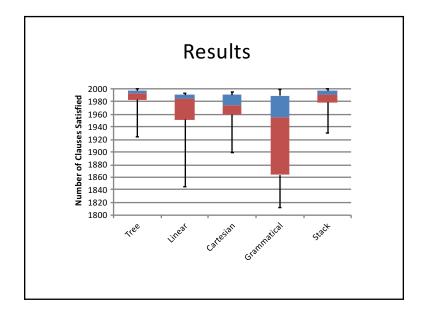
- Search algorithms are represented as an iterative algorithm that passes one or more set of variable assignments to the next iteration
- Genetic program represents a single program iteration
- Algorithm runs starting with a random initial population of solutions for 30 seconds

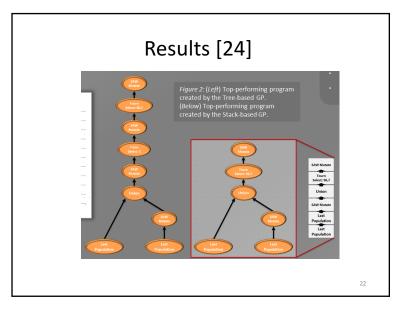
3-SAT Problem

- 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 \lor B \lor C) \land (¬A \lor ¬C \lor D) \land (¬B \lor C V ¬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



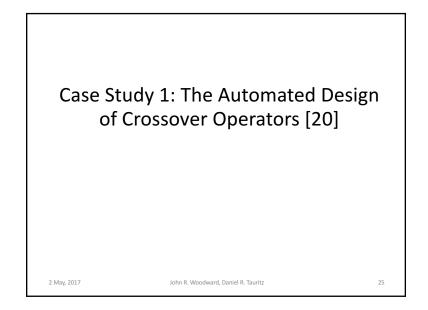


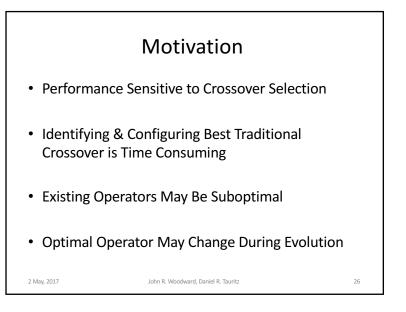
Results

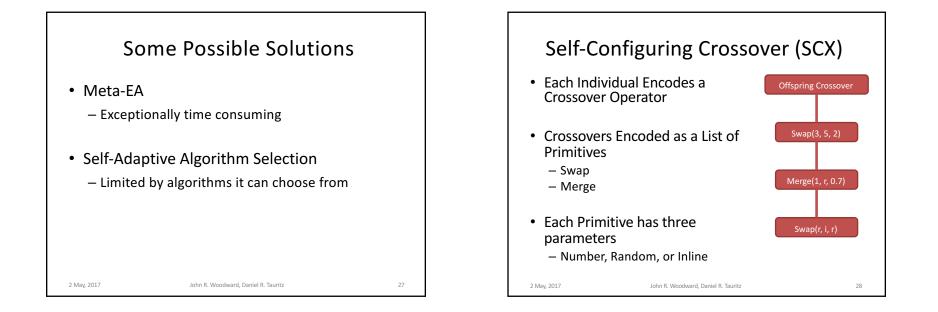
- Generated algorithms mostly performed comparably well on training and test problems
- Tree and stack GP perform similarly well on this problem, as do linear and Cartesian GP
- Tree and stack GP perform significantly better on this problem than linear and Cartesian GP, which perform significantly better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

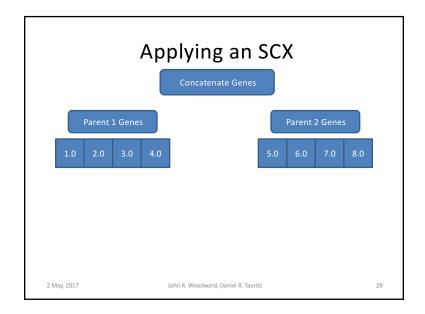
Conclusions

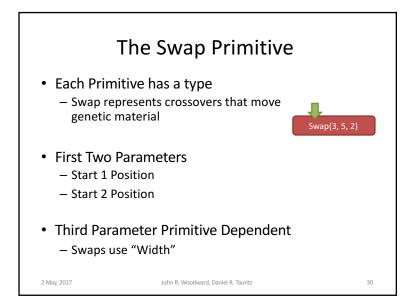
- The choice of GP type makes a significant difference in the performance of the hyper-heuristic
- The size of the search space appears to be a major factor in the performance of the hyper-heuristic

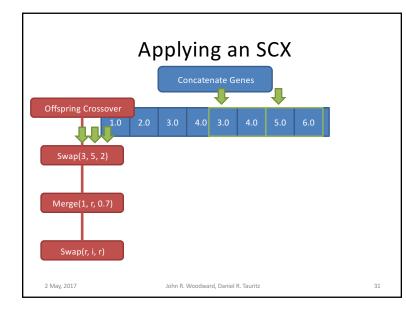


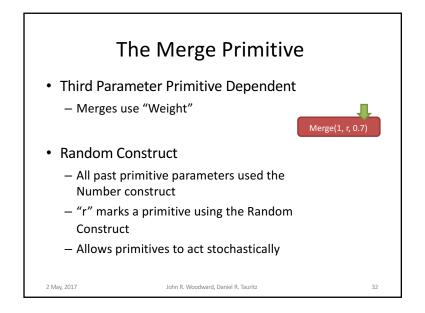


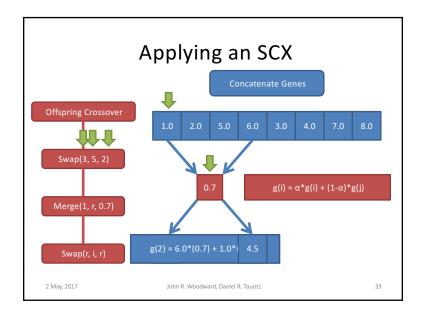


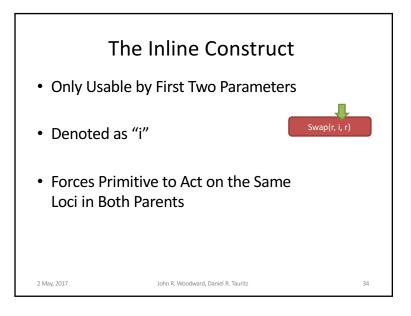


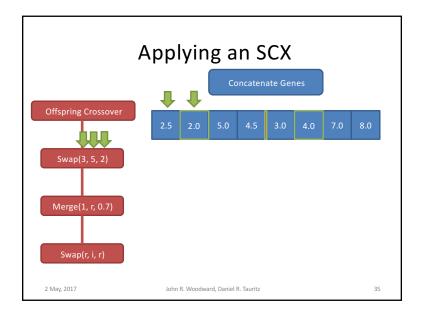


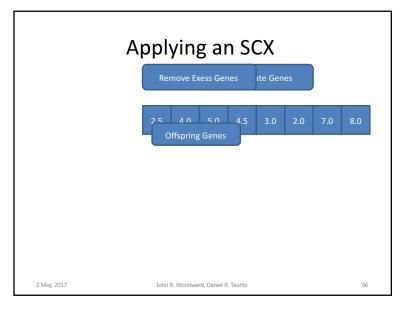


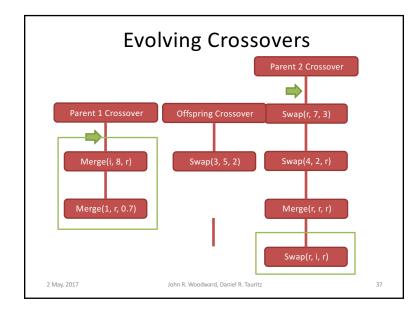


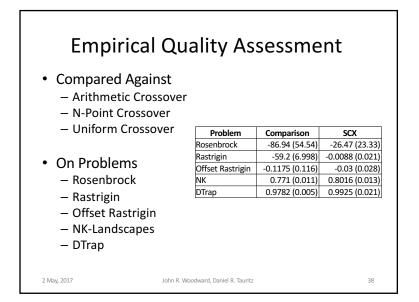


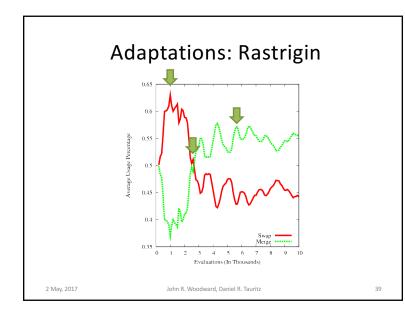


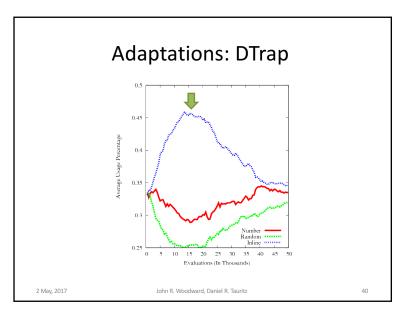


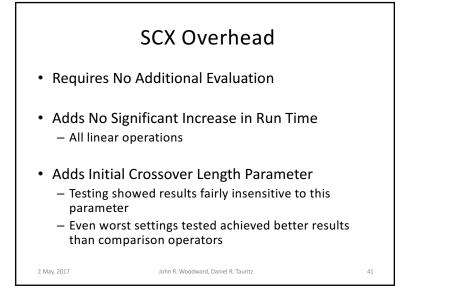


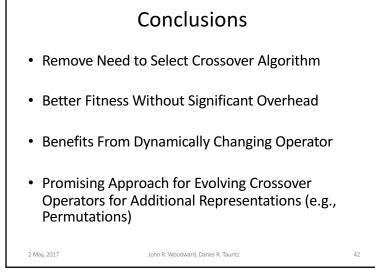


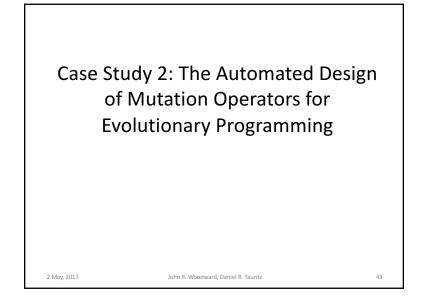


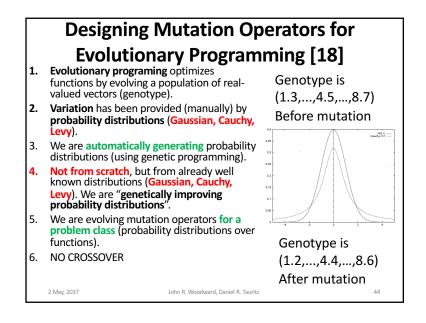


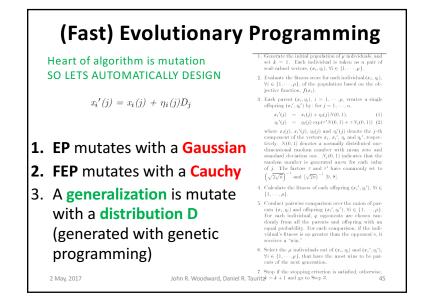












Optimization & Benchmark Functions

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**.

Test function	71	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	
$f_3(x) = \sum_{i=1}^{n} (\sum_{j=1}^{i} x_j)^2$	30	$[-100, 100]^n$	0	
$f_4(x) = \max_i \{ x_i , 1 \le i \le n \}$	30	$[-100, 100]^n$	0	
$f_5(x) = \sum_{i=1}^{n-1} [100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2]$	30	$[-30, 30]^n$	0	
$f_6(x) = \sum_{i=1}^{h} [x_i + 0.5]$	30	$[-100, 100]^n$	0	
$f_7(x) = \sum_{i=1}^{n} ix_i^4 + random[0, 1)$	30	$[-1.28, 1.28]^n$	0	
$f_8(x) = \sum_{i=1}^{n} -x_i \sin(\sqrt{ x_i })$	30	$[-500, 500]^n$	-12569.5	
$f_9(x) = \sum_{i=1}^{n} [x_i^2 - 10 \cos(2\pi x_i) + 10)]$	30	$[-5.12, 5.12]^n$	0	
$f_{10}(x) = -20 \exp \left(-0.2 \sqrt{\frac{1}{n} \sum_{i=1}^{n} x_i^2}\right) - \exp \left(\frac{1}{n} \sum_{i=1}^{n} x_i^2\right)$	$\frac{1}{i} \sum_{i=1}^{n} \cos 2\pi x_i - 30$	$[-32, 32]^n$	0	
$f_{10}(x) = -20 \exp \left(-0.2 \sqrt{\frac{1}{n} \sum_{i=1}^{n} x_i^2}\right) - \exp \left(\frac{1}{n} + 20 + e^{-1}\right)$	$\frac{1}{i}\sum_{i=1}^{n}\cos 2\pi x_i$ = 30	$[-32, 32]^n$	0	

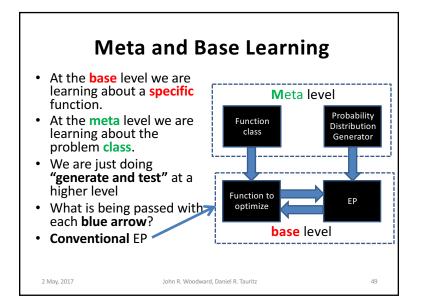
Function	Class	1
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- 1. Machine learning needs to generalize.
- 2. We generalize to function classes.
- 3. $y = x^2$ (a function)
- 4. $y = ax^2$ (parameterised function)
- 5. $y = ax^2$, *a* ~[1,2] (function class)
- 6. We do this for all benchmark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

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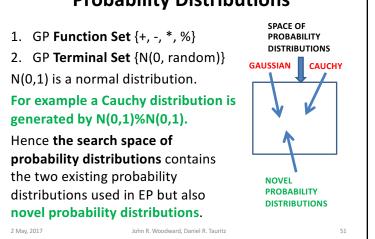
Function Classes 2 Function Classes S \boldsymbol{b} f_{min} $\overline{f_1(x) = a \sum_{i=1}^n x_i^2}$ $f_2(x) = a \sum_{i=1}^n |x_i| + b \prod_{i=1}^n |x_i|$ $f_3(x) = \sum_{i=1}^n (a \sum_{j=1}^i x_j)^2$ $[-100, 100]^n$ N/A 0 $[-10, 10]^n$ $b \in [0, 10^{-5}]$ 0 $[-100, 100]^n$ N/A0 $f_4(x) = \max_i \{ a \mid x_i \mid , 1 \le i \le n \}$ $[-100, 100]^n$ N/A0 $\begin{aligned} f_4(x) &= \max_i \{a \mid x_i \ , 1 \le i \le n\} & [-100, 100] \\ f_5(x) &= \sum_{i=1}^n [a(x_{i+1} - x_i^2)^2 + (x_i - 1)^2] & [-30, 30]^n \\ f_6(x) &= \sum_{i=1}^n [(ax_i + 0.5])^2 & [-100, 100] \\ f_7(x) &= a \sum_{i=1}^n ix_i^4 + random[0, 1) & [-1.28, 1.28] \\ f_8(x) &= \sum_{i=1}^n -(x_i \sin(\sqrt{|x_i|}) + a) & [-500, 500] \end{aligned}$ N/A0 $[-100, 100]^n$ N/A 0 $[-1.28, 1.28]^n N/A$ 0 $[-500, 500]^n$ N/A [-12629.5,-12599.5] $f_9(x) = \sum_{i=1}^{n} [ax_i^2 + b(1 - \cos(2\pi x_i))] \quad [-5.12, 5.12]^n \quad b \in [5, 10]$ 0 $f_{10}(x) = -a \exp(-0.2\sqrt{\frac{1}{n}\sum_{i=1}^{n} x_i^2})$ $[-32, 32]^n$ N/A0 $-\exp(\frac{1}{n}\sum_{i=1}^{n}\cos 2\pi x_i) + a + e$ 2 May, 2017 John R. Woodward, Daniel R. Taurita 48



Compare Signatures (Input-Output)

Evolutionary Programming	Evolutionary Programming								
$(\mathbb{R}^n \rightarrow \mathbb{R}) \rightarrow \mathbb{R}^n$ 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 <u>solution</u> to the problem instance)	<u>Designer</u> [$(R^n \rightarrow R)$] → ($(R^n \rightarrow R) \rightarrow R^n$) Input is a <i>list of</i> 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								
We are raising the level of a	(i.e. the <u>solution method</u> to the problem <u>class</u>). We are raising the level of generality at which we operate.								
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Genetic Programming to Generate Probability Distributions



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	ΞP	GP-disti	ibution
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^{-5}	5.56×10^{-1}
f_2	1.53×10^{-1}				8.14×10^{-4}	
f_3	2.74×10^{-2}	$2.43{ imes}10^{-2}$	$5.15{\times}10^{-2}$	$9.52{\times}10^{-2}$	6.14×10^{-3}	8.78×10^{-10}
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}	$4.96{\times}10^{-4}$	$2.66{ imes}10^{-4}$	$4.65{\times}10^{-5}$	8.39×10^{-7}	1.43×10^{-1}
f_6	3.86×10^{-2}	$3.12{ imes}10^{-2}$	4.40×10	1.42×10^{2}	9.20×10^{-3}	1.34×10^{-3}
f_7	6.49×10^{-2}	$1.04{ imes}10^{-2}$	$6.64{ imes}10^{-2}$	$1.21{\times}10^{-2}$	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}	$1.30{\times}10^{-2}$	1.09×10^{2}	3.58×10	1.74×10^{-3}	4.25×10^{-4}
f_{10}	1.67	$4.26{\times}10^{-1}$	1.45	$2.77{ imes}10^{-1}$	1.38	2.45×10^{-1}
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T-tests

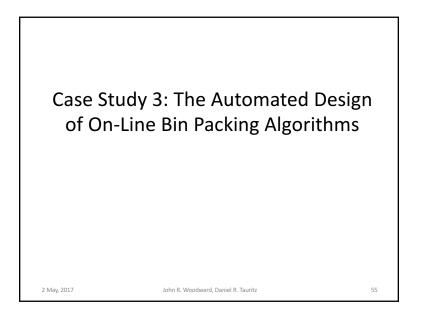
Table 5 2-tailed t-tests comparing EP with GP-distributions, FEP and CEP on $f_1\hbox{-} f_{10}.$

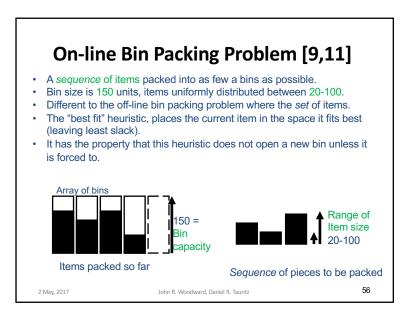
Function	Number of	GP-distribution vs FEP	GP-distribution vs CEP
Class	Generations	t-test	t-test
f_1	1500	2.78×10^{-47}	4.07×10^{-2}
f_2	2000	5.53×10^{-62}	1.59×10^{-54}
f_3	5000	8.03×10^{-8}	1.14×10^{-3}
f_4	5000	1.28×10^{-7}	3.73×10^{-36}
f_5	20000	2.80×10^{-58}	9.29×10^{-63}
f_6	1500	1.85×10^{-8}	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}

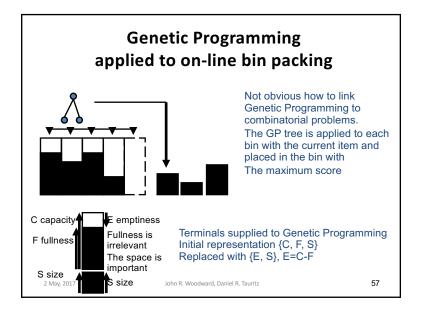
Performance on Other Problem Classes

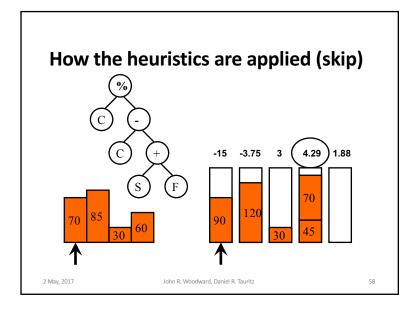
Table 8: This table compares the fitness values (averaged over 20 runs) of each of the 23 ADRs on each of the 23 function classes

	ADRI	ADR2	ADR3	ADR4	ADIO	ADRS	AD87	ADRE	ADR9	ADR:0	ADRI1	ADR12	ADRI3	ADR14	ADR15	ADR16	ADRIT	ADRIS	ADR19	ADR20	AD#21	AD#22	ADR
0	3.7960423	8 3.79679596	88 3.79617249	5 3.80009705	3.79821520	3,79842688	8 379682023	2531,20755	2 3.796057571	3,79999992	3.845998005	3.796386664	3.296277155	3,796649368	3.79612197	1655.307735	16670.6789	8 3.80381910	6 4.26044538	7 379609754	1 44.1875006	3.796066481	3.816
~	(15.533953	59(15.534053	N3)(15.533918	81)(15.5336871	5)(15.5337520	1)(15.533755)	0)(15.5338748	7)(11290.258	97(155338893	4)(15.5339394	5)(15.5298411	5)(15.5339912)	(15.5339230	9)(15.5339252	5)(15.5339908	3)(29)5.67763	5)(7373,98308	09(05.531)743	7)(15.510004)	1) (15.533986	3)(49,9339292	7)(15.5339502	0.055
12	0.0327253	0.01726556	0.06411854	0.243365938	0.227029973	0.24241586	0.14115225	10.8983148	0.013640910	4.01557418	0.878264279	0.048279715	0.068167284	0.10166228	0.03300072	5.652569538	62.0878105	8 0.02963591	0.00305151	9 0.00514776	6 0.26990715	0.033088525	9 0.039
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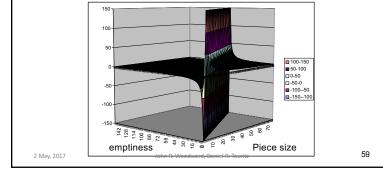


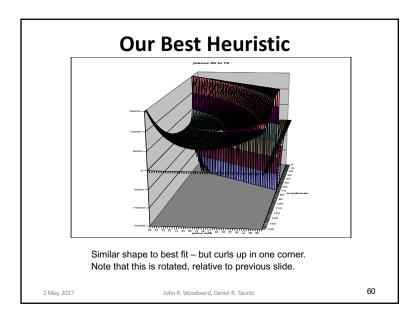
The Best Fit Heuristic

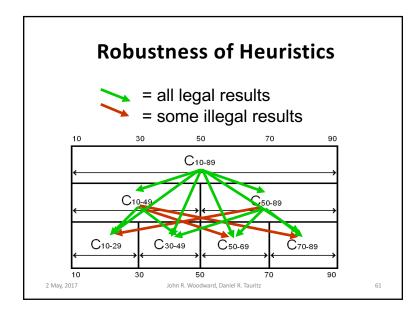
Best fit = 1/(E-S). Point out features.

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.







Testing Heuristics on problems of much larger size than in training

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

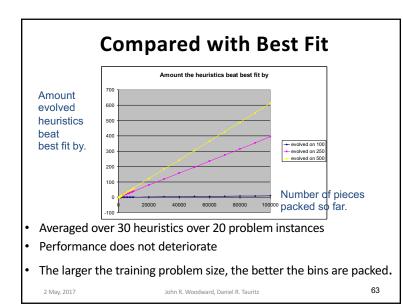
Table shows p-values using the best fit heuristic, for heuristics trained on different size problems, when applied to different sized problems

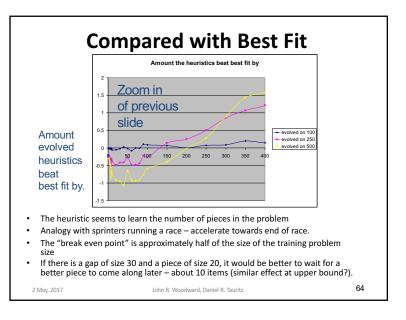
1. As number of items trained on increases, the probability decreases (see next slide).

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

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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

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9. Bug Location – Shin Yoo

2 May, 2017

- 10. Job Shop Scheduling Mengjie Zhang
- 11. Black Box Search Algorithms Daniel Tauritz et al

A Paradigm Shift? Algorithms investigated/unit time One person proposes a One person family of algorithms proposes one algorithm and tests them in the context of and tests it a problem class. in isolation. Human cost (INFLATION) machine cost MOORE'S LAW conventional approach new approach • 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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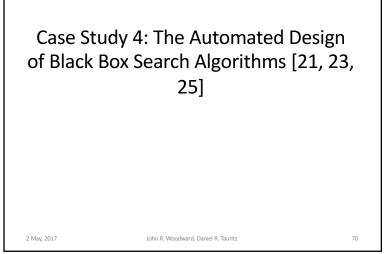
Conclusions
Heuristic are trained to fit a problem class, so are designed in context (like evolution). Let's close the feedback loop! Problem instances live in classes.
We can design algorithms on small problem instances and scale them apply them to large problem instances (TSP, child multiplication).

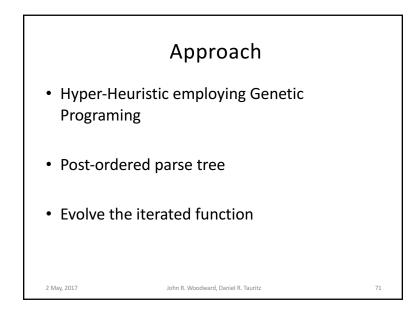
	SUMMARY	
1.	We can automatically design algorithms that consistently outperform human designed algorithms (on various domains).	
2.	The "best" heuristics depends on the set of problem instances. (feedback)	
3.	Resulting algorithm is part man-made part machine- made (synergy)	
4.	not evolving from scratch like Genetic Programming,	
5.	improve existing algorithms and adapt them to the new problem instances.	
6.	Algorithms are reusable , "solutions" aren't. (e.g. tsp algorithm vs route)	

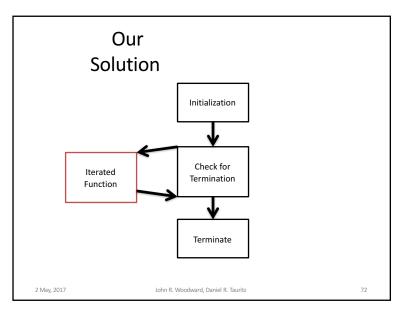
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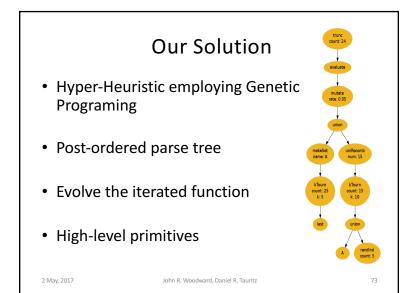
2 May, 2017

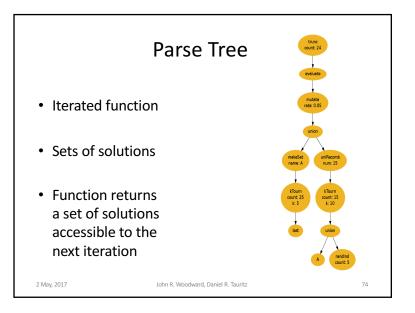
h like Genetic Programming, hms and adapt them to the new , "solutions" aren't. (e.g. tsp

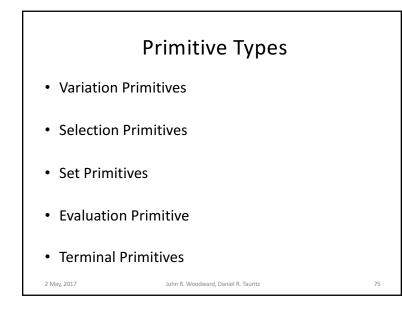


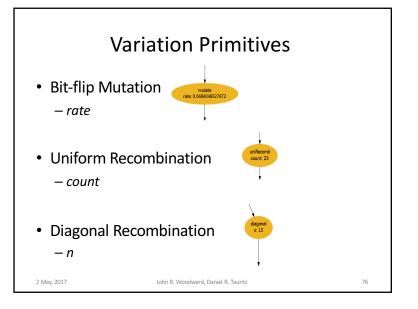


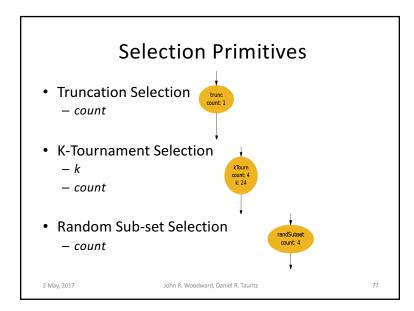


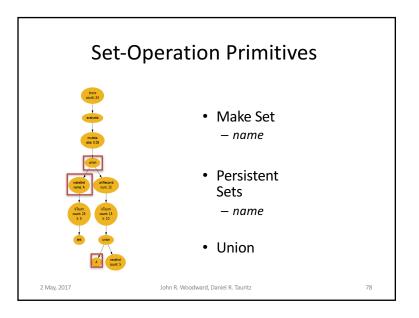


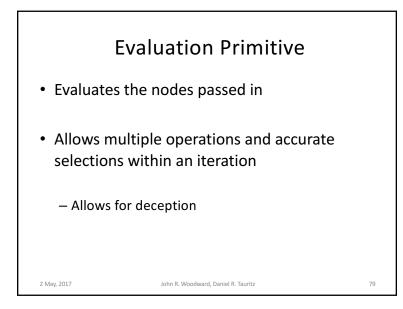


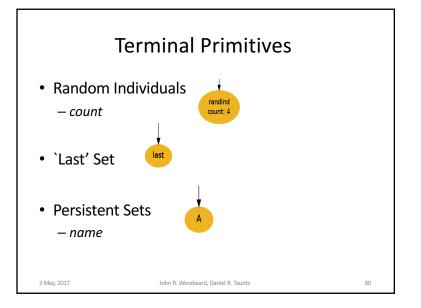


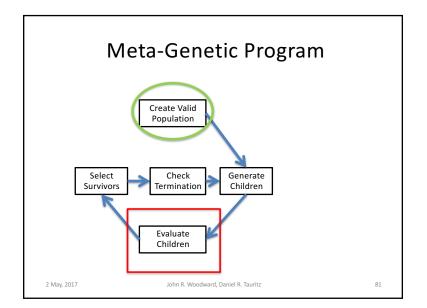


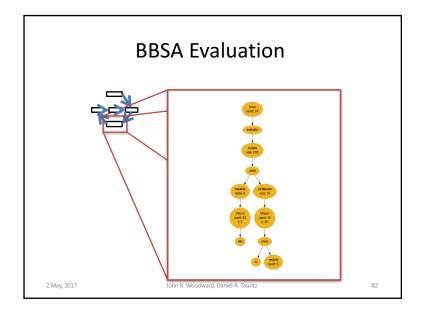


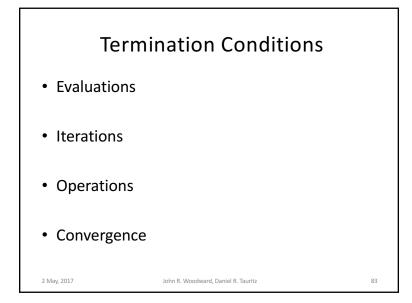


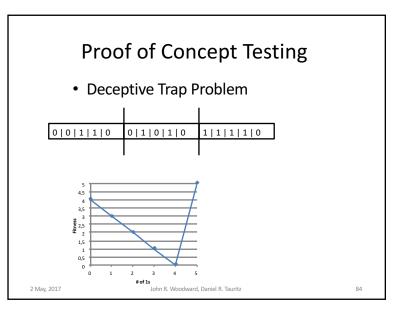


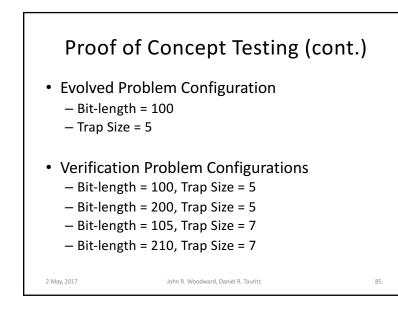


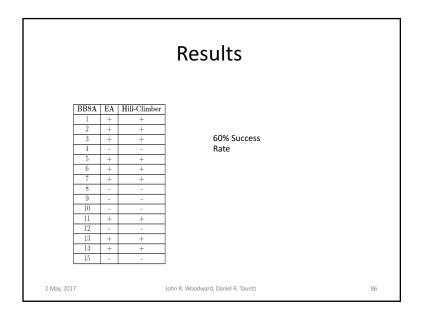


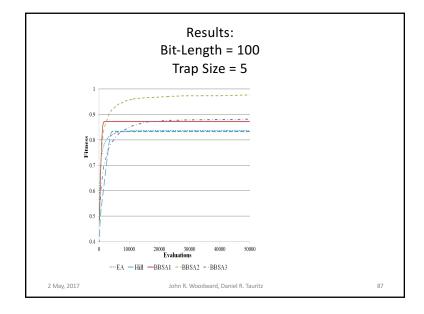


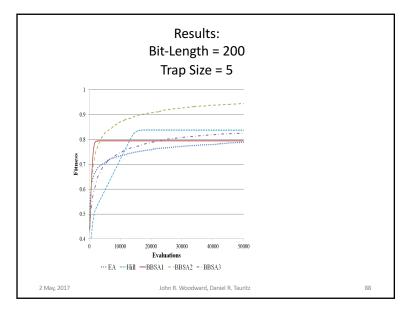


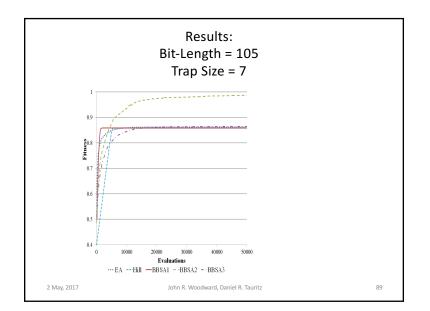


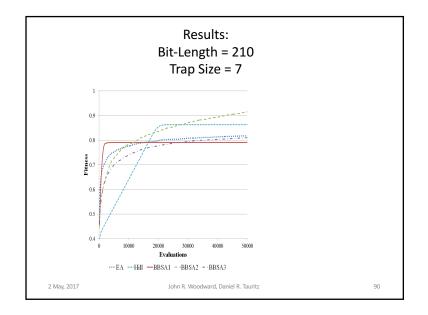


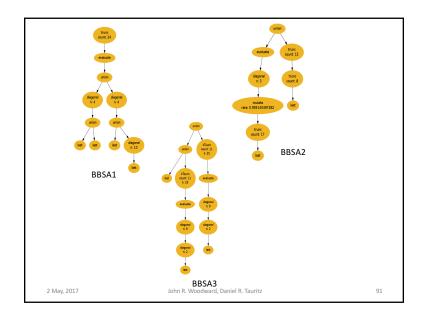


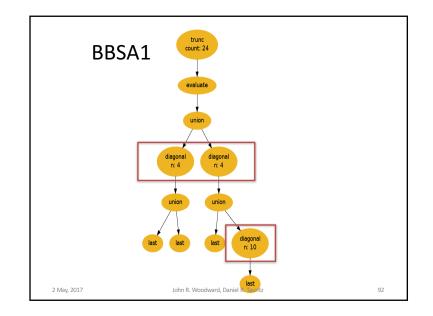


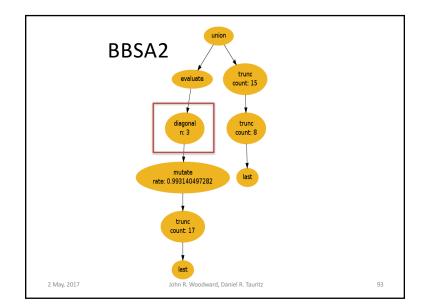


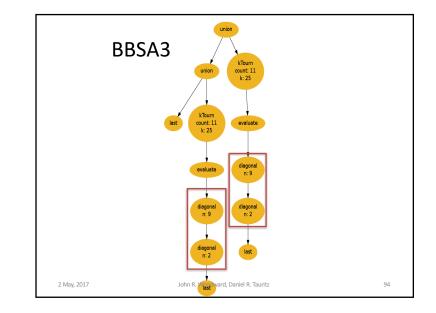


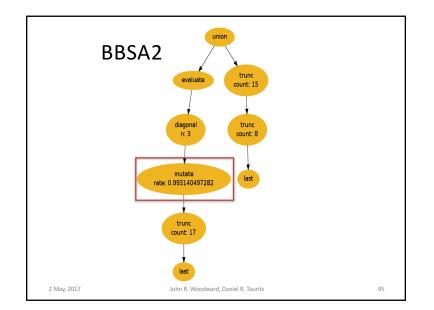


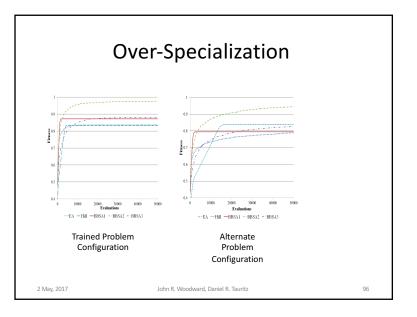


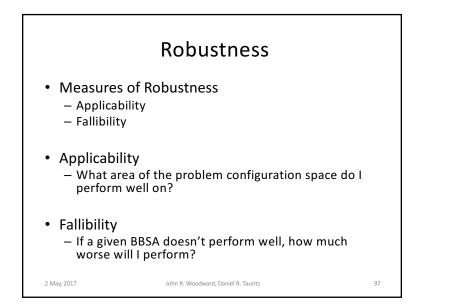


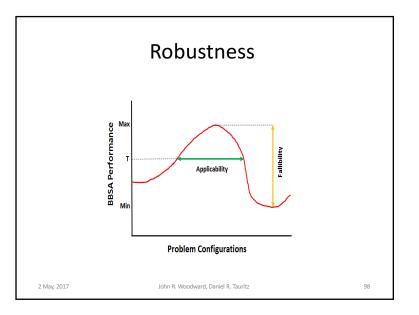


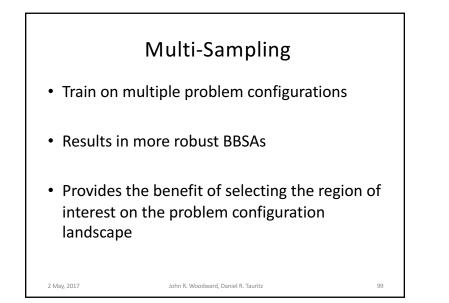


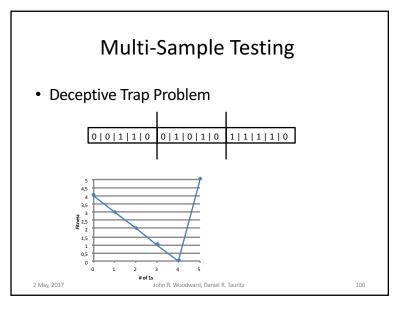


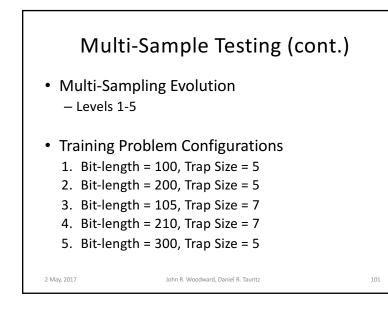


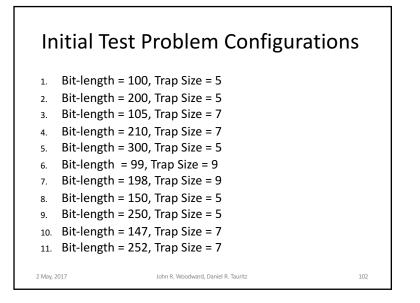


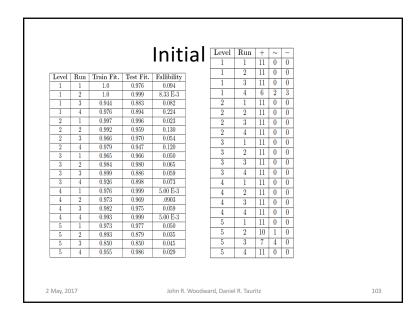


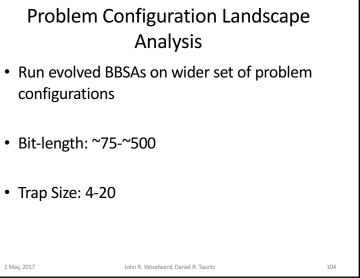


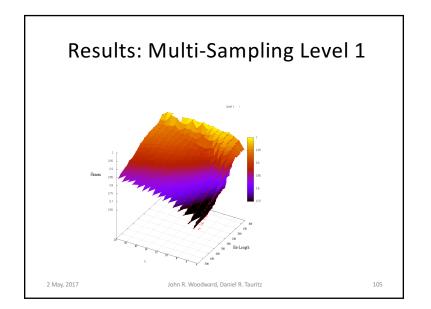


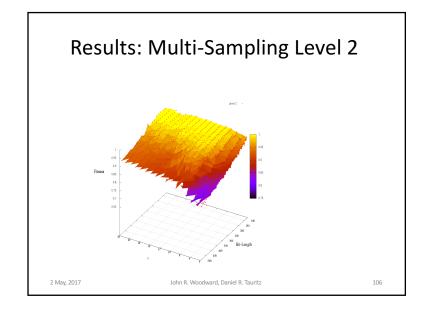


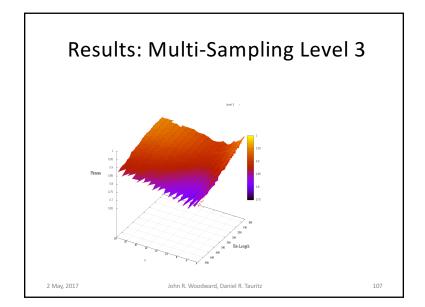


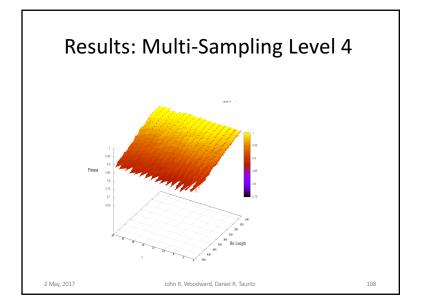


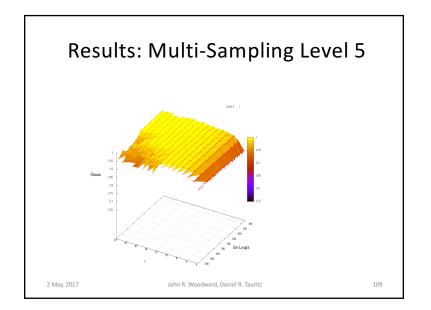


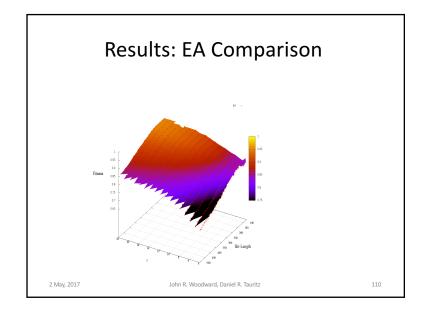


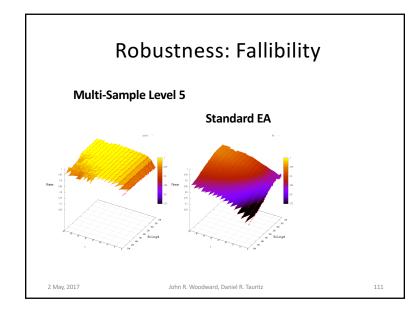


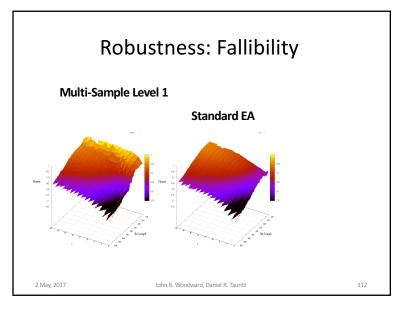


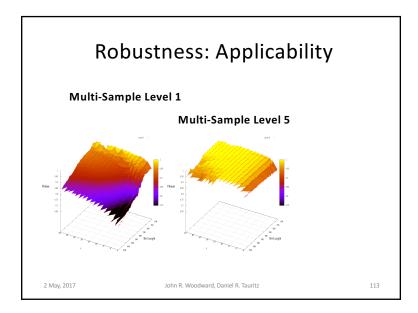




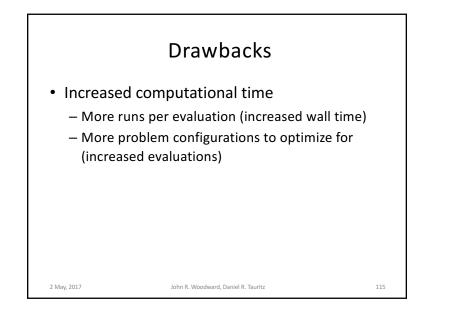


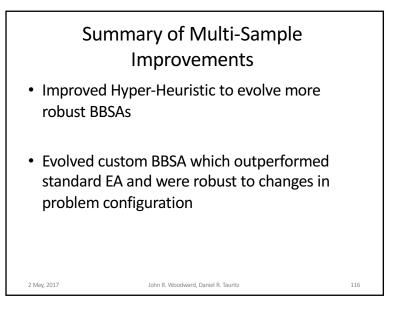


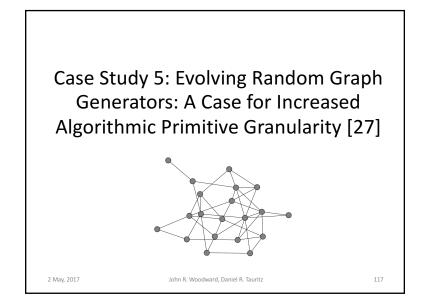


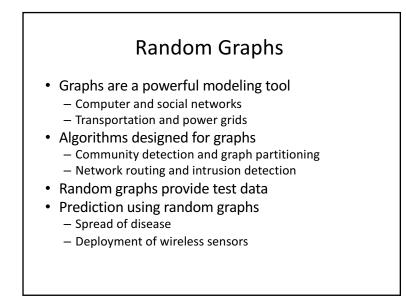


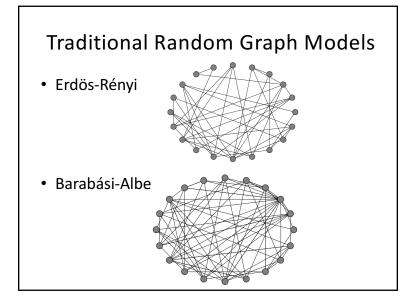
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	5	2	0.893	0.879	0.035		
	5	3	0.850	0.850	0.045		
	5	4	0.955	0.986	0.029		
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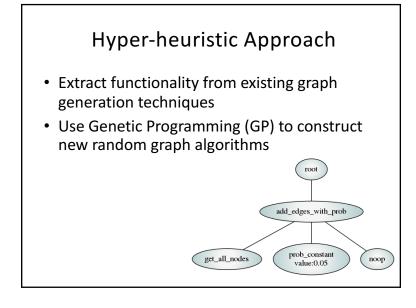




Automated Random Graph Model Design

- Random graph model needs to accurately reflect intended concept
- Model selection can be automated, but relies on having a good solution available
- 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?



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

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

Methodology

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

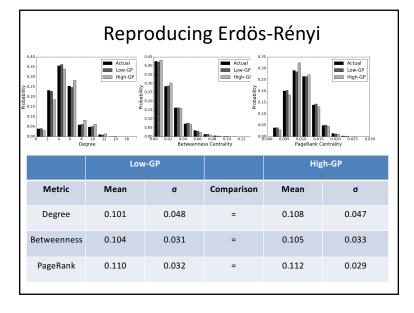
Primitive Operations

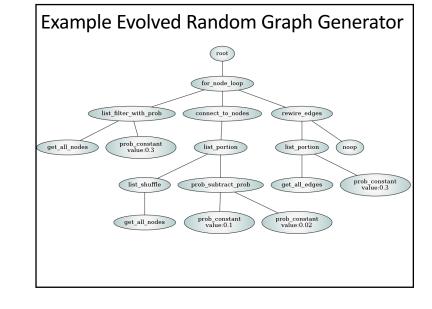
Terminals

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

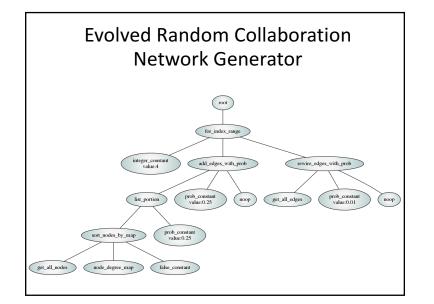
Functions

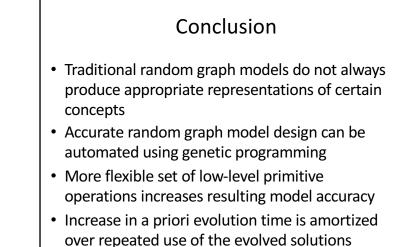
- Basic programming constructs: for, while, if-else
- Data structures: lists of values, nodes, or edges, list
- combining/selection/sorting
- Math and logic operators: add, multiply, <, ==, AND, OR
- Graph operators: add edges, add subgraph, rewire edges

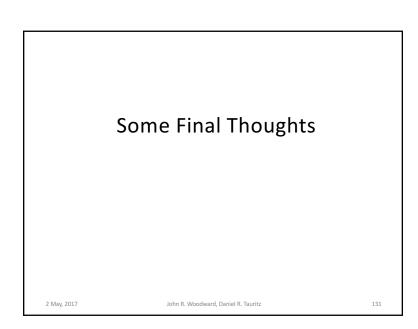




Reproducing Random Community Graphs											
	Low	r-GP		Hig	h-GP						
Metric	Mean	σ	Comparison	Mean	σ						
Degree	0.436	0.075	<	0.458	0.055						
Betweenness	0.209	0.105	<	0.320	0.126						
PageRank	0.127	0.029	<	0.150	0.036						
Actual G	iraph	Low	v-GP	Hig	h-GP						

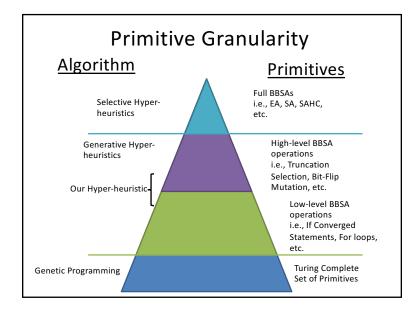


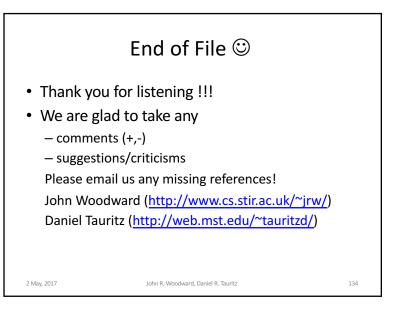




Challenges in Hyper-heuristics

- Hyper-heuristics are very computationally expensive (use Asynchronous Parallel GP [26,30])
- 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 [25,27])





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