### **Next Generation Genetic Algorithms**

Darrell Whitley Computer Science, Colorado State University

With Thanks to: Francisco Chicano, Gabriela Ochoa, Andrew Sutton and Renato Tinós

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### **Next Generation Genetic Algorithms**

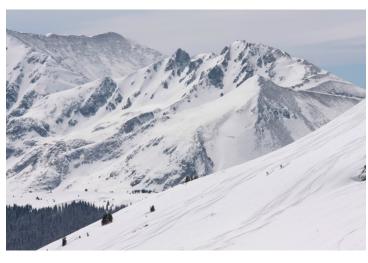
What do we mean by "Next Generation?"

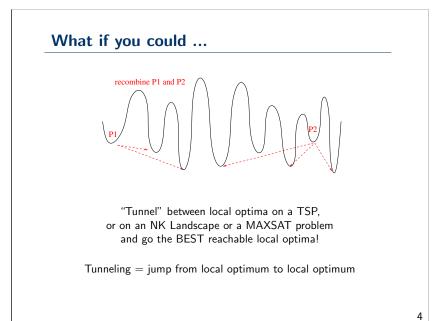
- NOT a Black Box Optimizer.
- 2 Uses mathematics to characterize problem structure.
- ③ NOT cookie cutter.
- Not a blind "population, selection, mutation, crossover" GA.

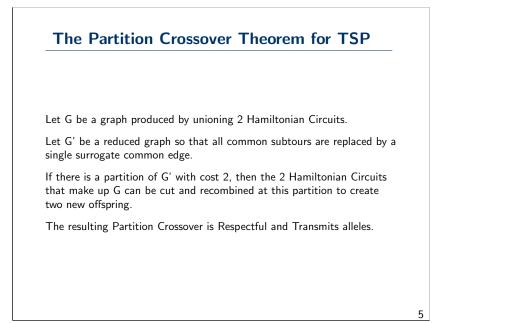
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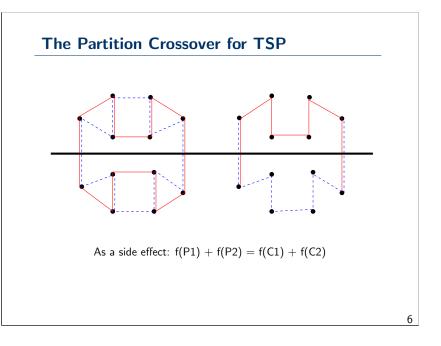
- ④ Uses deterministic move operators and crossover operators
- In Tunnels between Local Optima.
- 6 Scales to large problems with millions of variables.
- Ø Build on our expertise in smart ways.

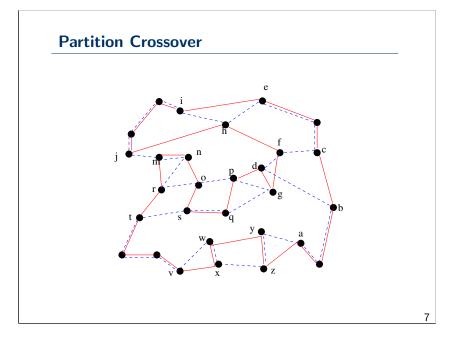
# Know your Landscape! And Go Downhill!

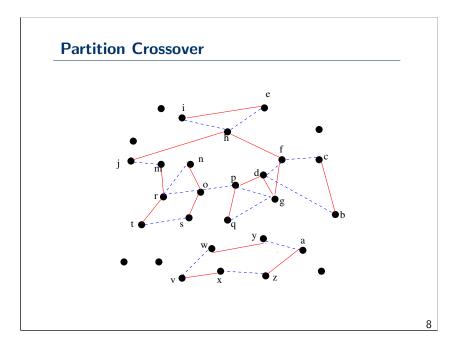


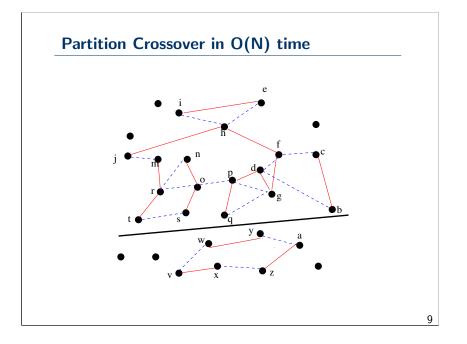


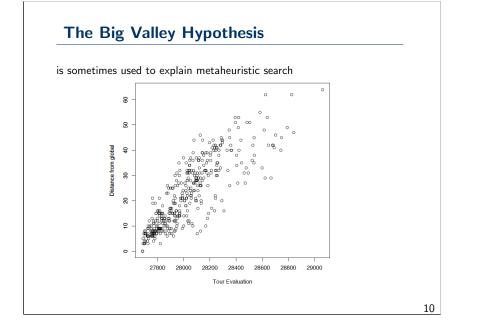


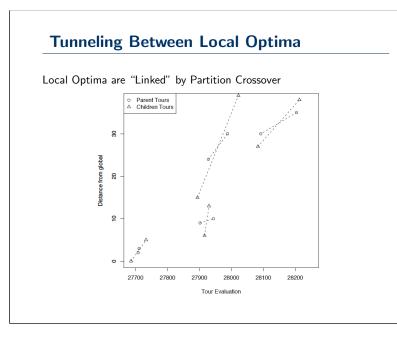


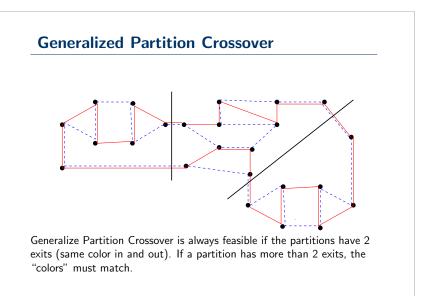












Г	Instance	att532	nrw1379	rand1500	u1817	
	3-opt	$10.5 \pm 0.5$	$11.3 \pm 0.5$	$24.9 \pm 0.2$	$\frac{11017}{26.2 \pm 0.7}$	
able: Average number of <i>partition components</i> used by GPX in 50 ecombinations of random local optima found by 3-opt.						

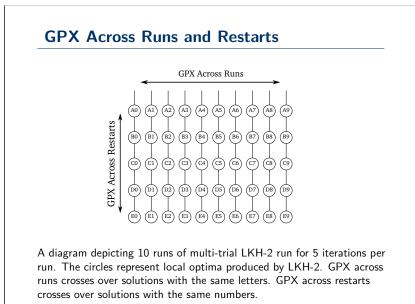
# Lin-Kernighan-Helsgaun-LKH

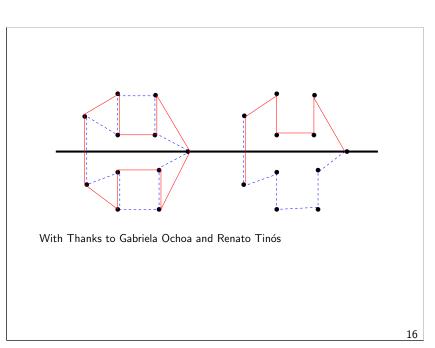
LKH is widely considered the best Local Search algorithm for TSP.

LKH uses deep k-opt moves, clever data structures and a fast implementation.

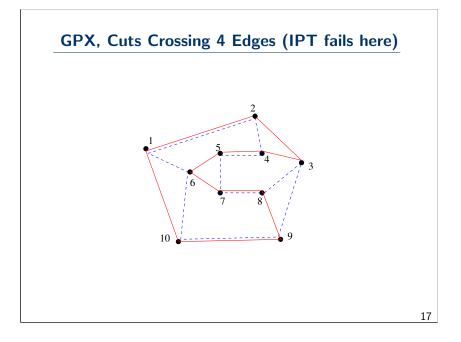
LKH-2 has found the majority of best known solutions on the TSP benchmarks at the Georgia Tech TSP repository that were not solved by complete solvers: http://www.tsp.gatech.edu/data/index.html.

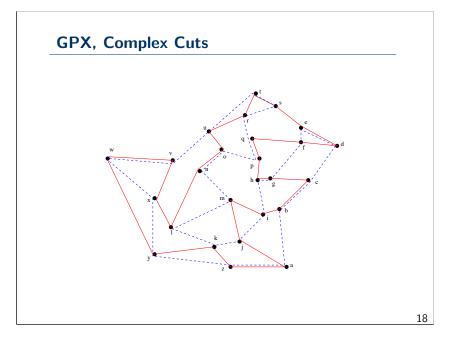


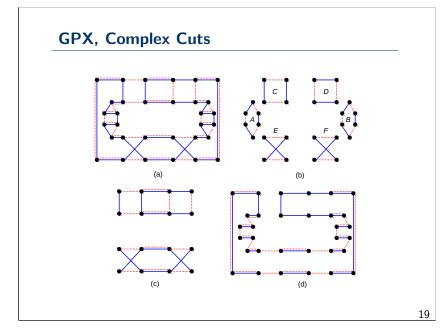


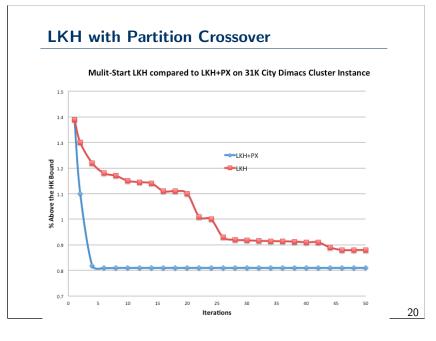


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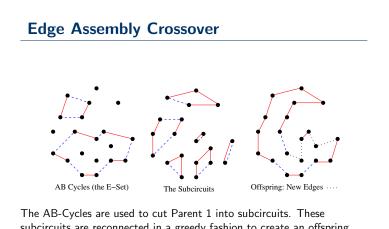
### The Two Best TSP (solo) Heuristics

Lin Kernighan Helsgaun (LKH 2 with Multi-Starts) Iterated Local Search

EAX: Edge Assembly Crossover (Nagata et al.) Genetic Algorithm

Combinations of LKH and EAX using Automated Algorithm Selection Methods (Hoos et al.)

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subcircuits are reconnected in a greedy fashion to create an offspring. The offspring is composed of edges from Parent 1, edges from Parent 2, and completely new edges not found in either parent.

### The EAX Genetic Algorithm Details

- EAX is used to generate many (e.g. 30) offspring during every recombination. Only the best offspring is retained (Brood Selection).
- ② There is no selection, just "Brood Selection."
- 3 Typical population size: 300.
- **(a)** The order of the population is randomized every generation. Parent i is recombined with Parent i + 1 and the offspring replaces Parent i. (The population is replace every generation.)

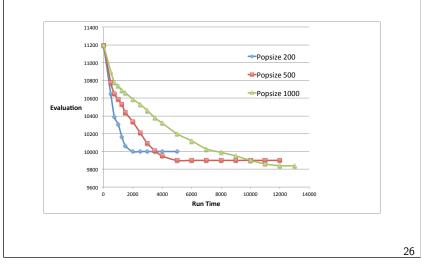
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23

### The EAX Strategy

- EAX can inherit many edges from parents, but also introduces new high quality edges.
- ② EAX disassembles and reassembles, and focuses on finding improvements.
- 3 This gives EAX a "thoroughness" of exploration.
- ④ EAX illustrates the classic trade-off between exploration and exploitation

## Edge Assembly Crossover: Typical Behavior



### **Combining EAX and Partition Crossover**

- Partition Crossover can dramatically speed-up exploitation, but it also impact long term search potential.
- A Strategy: When PAX generates 30 offspring, recombine all of the offspring using Partition Crossover. This can help when EAX gets stuck and cannot find an improvement.

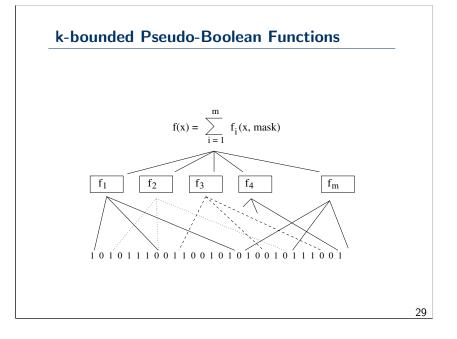
### EAX and EAX with Partition Crossover

	Pop	Evaluation		Running		Number
Dataset	Size	Mean	S. D.	Time Mean	S. D.	Opt. Sol.
rl5934	200	556090.8	50	1433	34	12/30
rl5915	200	565537.57	29	1221	30	23/30
rl11849	200	923297.7	8	8400	130	1/10
ja9847	800	491930.1	2	37906	618	0/10
pla7397	800	23261065.6	552	12627	344	2/10
usa13509	800	19983194.5	411	81689	1355	0/10

EAX with Pa	artition	Crossover				
	Pop	Evaluation		Running		Number
Dataset	Size	Mean	S. D.	Time Mean	S. D.	Opt. Sol.
rl5934	200	556058.63	33	1562	248	21/30
rl5915	200	565537.77	21	1022	73	19/30
rl11849	200	923294.8	8	7484	105	4/10
ja9847	800	491926.33	2	30881	263	4/10
pla7397	800	23260855	222	11647	1235	4/10
usa13509	800	19982987.6	173	66849	818	2/10

28

27



### A General Result over Bit Representations

By Constructive Proof: Every problem with a bit representation and a closed form evaluation function can be expressed as a quadratic (k=2) pseudo-Boolean Optimization problem. (See Boros and Hammer)

$$\begin{aligned} xy &= z \quad iff \quad xy - 2xz - 2yz + 3z = 0 \\ xy &\neq z \quad iff \quad xy - 2xz - 2yz + 3z > 0 \end{aligned}$$

Or we can reduce to k=3 instead:

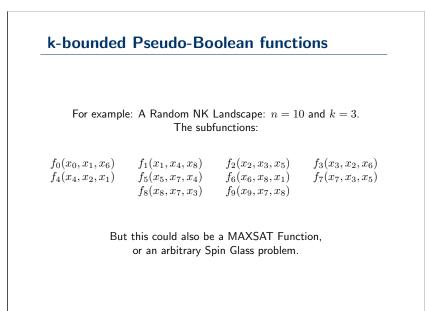
 $f(x_1, x_2, x_3, x_4, x_5, x_6)$ 

becomes (depending on the nonlinearity):

 $f1(z_1, z_2, z_3) + f2(z_1, x_1, x_2) + f3(z_2, x_3, x_4) + f4(z_3, x_5, x_6)$ 

30

32

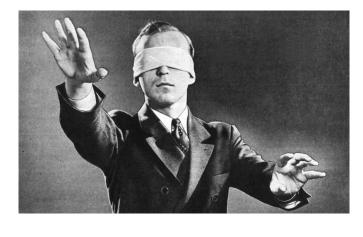


Walsh Example: MAXSATGiven a logical expression consisting of Boolean variables, determine<br/>whether or not there is a setting for the variables that makes the<br/>expression TRUE.Literal: a variable or the negation of a variable<br/>Clause: a disjunct of literalsA 3SAT Example<br/> $(\neg x_2 \lor x_1 \lor x_0) \land (x_3 \lor \neg x_2 \lor x_1) \land (x_3 \lor \neg x_1 \lor \neg x_0)$ <br/>recast as a MAX3SAT Example<br/> $(\neg x_2 \lor x_1 \lor x_0) + (x_3 \lor \neg x_2 \lor x_1) + (x_3 \lor \neg x_1 \lor \neg x_0)$ 

929

### **BLACK BOX OPTIMIZATION**

Don't wear a blind fold during search if you can help it!



33

### **GRAY BOX OPTIMIZATION**

We can construct "Gray Box" optimization for pseudo-Boolean optimization problems (M subfunctions, k variables per subfunction).

Exploit the general properties of every Mk Landscape:

$$f(x) = \sum_{i=1}^{m} f_i(x)$$

Which can be expressed as a Walsh Polynomial

$$W(f(x)) = \sum_{i=1}^{m} W(f_i(x))$$

Or can be expressed as a sum of k Elementary Landscapes

$$f(x) = \sum_{i=1}^{k} \varphi^{(k)}(W(f(x)))$$

34

36

Walsh Example: MAX-3SAT						
	Walsh Analys	is of a Single Clause				
Consider the $f(x) = \neg x_2$		sisting of a single clause				
	f(000) = 1 f(001) = 1	. ,				
	f(001) = 1 f(010) = 1 f(011) = 1	$(\neg x_2T)$				
	f(100) = 0	$(\neg x_2F \wedge x_1F \wedge x_0F)$				
	f(101) = 1 f(110) = 1 f(111) = 1	$(x_1T)$				

$\frac{1}{8}$	$\begin{bmatrix} 1\\1\\1\\1\\1\\1\\0\\1\\1\\1\\1\\1\\\end{bmatrix}^{T} \begin{bmatrix} 1&1&1&1&1&1&1&1&1\\1&-1&-1&1&1&-1&-1\\1&1&-1&-1&1&1&-1\\1&-1&-1&1&1&-1&-1\\1&1&1&1&$
0	All $\psi_j$ 's except $\psi_0$ have 4 1's and 4 $-1$ 's. $\psi_0$ has all 1's. f for clauses of length 3 will contain one 0

### Walsh Example: MAX-3SAT

Let neg(f) return a K-bit string with 1 bits indicating which variables in the clause are negated.

$$f(100) = 0 \qquad (\neg x_2 F \land x_1 F \land x_0 F)$$

neg(f) = 100

Then the Walsh coefficients for f are:

$$w_j = \begin{cases} \frac{2^{\kappa} - 1}{2^{\kappa}} & \text{if } j = 0\\ -\frac{1}{2^{\kappa}} \psi_j(\operatorname{neg}(f)) & \text{if } j \neq 0 \end{cases}$$

### Walsh Example

$f_1 = (\neg x_2 \lor x_1 \lor x_0)$
$f_2 = (x_3 \vee \neg x_2 \vee x_1)$
$f_3 = (x_3 \vee \neg x_1 \vee \neg x_0)$

$\boldsymbol{x}$	$w_i$	$W(f_1)$	$W(f_2)$	$W(f_3)$	W(f(x))
0000	$w_0$	0.875	0.875	0.875	2.625
0001	$w_1$	-0.125	0	0.125	0
0010	$w_2$	-0.125	-0.125	0.125	-0.125
0011	$w_3$	-0.125	0	-0.125	-0.250
0100	$w_4$	0.125	0.125	0	0.250
0101	$w_5$	0.125	0	0	0.125
0110	$w_6$	0.125	0.125	0	0.250
0111	$w_7$	0.125	0	0	0.125
1000	$w_8$	0	-0.125	-0.125	-0.250
1001	$w_9$	0	0	0.125	0.125
1010	$w_{10}$	0	-0.125	0.125	0
1011	$w_{11}$	0	0	-0.125	-0.125
1100	$w_{12}$	0	0.125	0	0.125
1101	$w_{13}$	0	0	0	0
1110	$w_{14}$	0	0.125	0	0.125
1111	$w_{15}$	0	0	0	0

**GRAY BOX OPTIMIZATION** 

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$$f(x) = \sum_{i=1}^{k} \varphi^{(k)}(W(f(x)))$$

39

The Eigenvectors of MAX-3SAT						
f(x) = f1(x) + f2(x) + f3(x) + f4(x)						
$f1(x) = f1_a(x) + f1_b(x) + f1_c(x)$						
$f2(x) = f2_a(x) + f2_b(x) + f2_c(x)$						
$f3(x) = f3_a(x) + f3_b(x) + f3_c(x)$						
$f4(x) = f4_a(x) + f4_b(x) + f4_c(x)$						
$\varphi^{(1)}(x) = f1_a(x) + f2_a(x) + f3_a(x) + f4_a(x)$						
$\varphi^{(2)}(x) = f1_b(x) + f2_b(x) + f3_b(x) + f4_b(x)$						
$\varphi^{(3)}(x) = f1_c(x) + f2_c(x) + f3_c(x) + f4_c(x)$						
$f(x) = \varphi^{(1)}(x) + \varphi^{(2)}(x) + \varphi^{(3)}(x)$						
	40					

### **Constant Time Steepest Descent**

Assume we flip bit p to move from x to  $y_p \in N(x).$  Construct a vector Score such that

$$Score(x, y_p) = -2\left\{\sum_{\forall b, \ p \subset b} -1^{b^T x} w_b(x)\right\}$$

All Walsh coefficients whose signs will be changed by flipping bit p are collected into a single number  $Score(x, y_p)$ .

In almost all cases, Score does not change after a bit flip. Only some Walsh coefficient are affected.

41

### **Constant Time Steepest Descent**

Assume we flip bit p to move from x to  $y_p \in N(x).$  Construct a vector Score such that

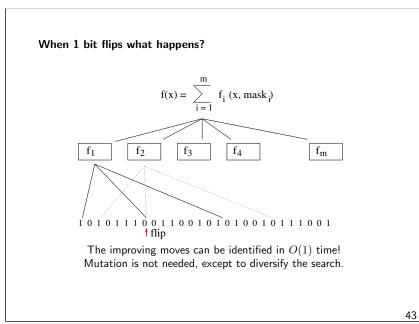
$$Score(x, y_p) = f(y_p) - f(x_p)$$

Thus, are the scores reflect the increase or decrease relative to f(x) associated with flipping bit p.

In almost all cases, Score does not change after a bit flip. Only some subfunctions are affected.

42

44



### The locations of the updates are obvious

### Some Theoretical Results: k-bounded Boolean

- 1) No difference in runtime for BEST First and NEXT First search.
- 2) Constant time improving move selection under all conditions.
- 3) Constant time improving moves in space of statistical moments.
- 4) Auto-correlation computed in closed form.
- 5) Tunneling between local optima.

45

### Best Improving and Next Improving moves

"Best Improving" and "Next Improving" moves cost the same.

### GSAT uses a Buffer of best improving moves

 $Buffer(best.improvement) = \langle M_{10}, M_{1919}, M_{9999} \rangle$ 

But the Buffer does not empty monotonically: this leads to thrashing.

### Instead uses multiple Buckets to hold improving moves

 $Bucket(best.improvement) = < M_{10}, M_{1919}, M_{9999} >$ 

 $Bucket(best.improvement - 1) = < M_{8371}, M_{4321}, M_{847} >$ 

 $Bucket(all.other.improving.moves) = < M_{40}, M_{519}, M_{6799} >$ 

46

48

This improves the runtime of GSAT by a factor of 20X to 30X. The solution for NK Landscapes is only slightly more complicated.

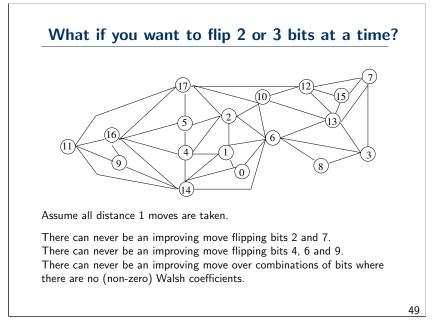
### **Steepest Descent on Moments**

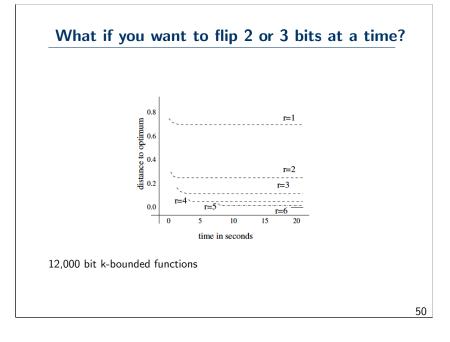
Both f(x) and Avg(N(x)) can be computed with Walsh Spans.

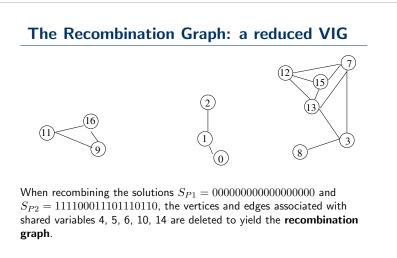
$$f(x) = \sum_{z=0}^{3} \varphi^{(z)}(x)$$
$$Avg(N(x)) = f(x) - 1/d \sum_{z=0}^{3} 2z \varphi^{(p)}(x)$$
$$Avg(N(x)) = \sum_{z=0}^{3} \varphi^{(z)}(x) - 2/N \sum_{z=0}^{3} z \varphi^{(z)}(x)$$

The Variable Interaction Graph

(VIG). There must be fewer than  $2^k M = O(N)$  Walsh coefficients. There is a connection in the VIG between vertex  $v_i$  and  $v_j$  if there is a non-zero Walsh coefficient indexed by i and j, e.g.,  $w_{i,j}$ .

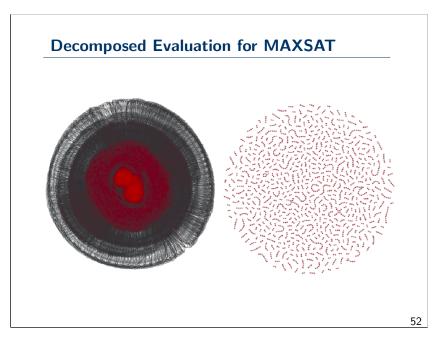






### Tunneling Crossover Theorem:

If the recombination graph of f contains q connected components, then Partition Crossover returns the best of  $2^q$  solutions.



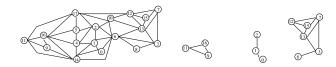
### **MAXSAT** Number of recombining components

N	Min	Median	Max
308,480	7	20	38
37,726	11	1373	1620
991,419	937	1020	1090
182,015	231	371	2084
72,001	34	55	1218
	308,480 37,726 991,419 182,015	308,480 7   37,726 11   991,419 937   182,015 231	308,480 7 20   37,726 11 1373   991,419 937 1020   182,015 231 371

Tunneling "scans"  $2^{1000}$  local optima and returns the best in O(n) time

### 53

### **Decomposed Evaluation**



A new evaluation function can be constructed:

 $g(x) = c + g_1(x_0, x_1, x_2) + g_2(x_9, x_{11}, x_{16}) + g_2(x_3, x_7, x_8, x_{12}, x_{13}, x_{15})$ 

where g(x) evaluates any solution (parents or offspring) that resides in the subspace \*\*\*\*000\*\*\*0\*\*\*0\*\*.

In general:

$$g(x) = c + \sum_{i=1}^{q} g_i(x, mask_i)$$

54

### Partition Crossover and Local Optima

**The Subspace Optimality Theorem:** For any k-bounded pseudo-Boolean function f, if Parition Crossover is used to recombine two parent solutions that are locally optimal, then the offspring must be a local optima in the hyperplane subspace defined by the bits shared in common by the two parents.

Example: if the parents 000000000 and 1100011101 are locally optimal, then the best offspring is locally optimal in the hyperplane subspace \*\*000\*\*\*0\*.

### Percent of Offspring that are Local Optima

### Using a Very Simple (Stupid) Hybrid GA:

N	k	Model	2-point Xover	Uniform Xover	PX
100	2	Adj	74.2 ±3.9	$0.3 \pm 0.3$	$100.0\ \pm0.0$
300	4	Adj	$30.7\ \pm 2.8$	$0.0\ \pm 0.0$	$94.4\ \pm 4.3$
500	2	Adj	78.0 ±2.3	0.0 ±0.0	97.9 ±5.0
500	4	Adj	$31.0\ \pm 2.5$	$0.0\ \pm 0.0$	$93.8~{\pm}4.0$
100	2	Rand	0.8 ±0.9	$0.5 \pm 0.5$	$100.0 \pm 0.0$
300	4	Rand	$0.0\ \pm 0.0$	$0.0\ \pm 0.0$	$86.4\ \pm 17.1$
500	2	Rand	0.0 ±0.0	0.0 ±0.0	98.3 ±4.9
500	4	Rand	$0.0\ \pm 0.0$	$0.0\ \pm 0.0$	$83.6 \ \pm 16.8$

### Number of partition components discovered

$\overline{N}$	k	Model	Paired PX	
			Mean	Max
100	2	Adjacent	3.34 ±0.16	16
300	4	Adjacent	5.24 ±0.10	26
500	2	Adjacent	7.66 ±0.47	55
500	4	Adjacent	$7.52\ \pm0.16$	41
100	2	Random	3.22 ±0.16	15
300	4	Random	$2.41 \pm 0.04$	13
500	2	Random	6.98 ±0.47	47
500	4	Random	$2.46 \pm 0.05$	13

Paired PX uses Tournament Selection. The first parent is selected by fitness. The second parent is selected by Hamming Distance.

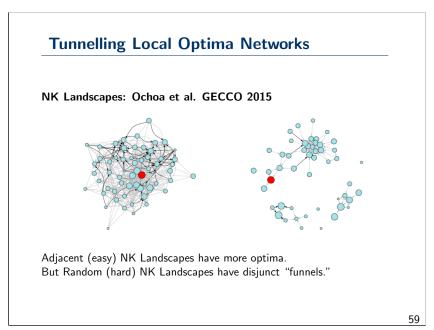
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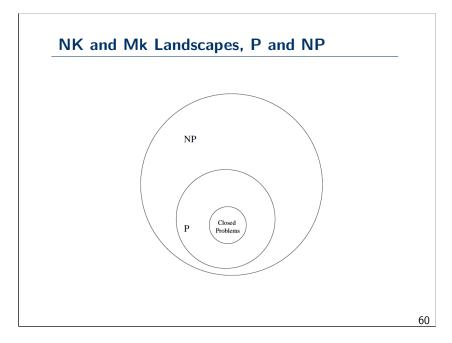


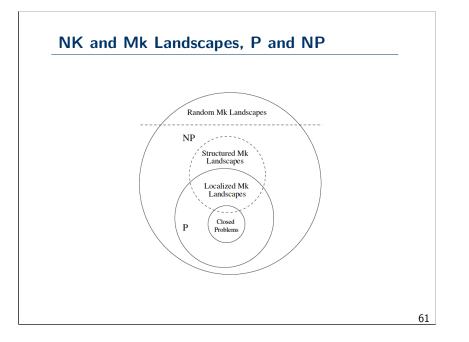
		2-point	Uniform	Paired PX
N	k	Found	Found	Found
300	2	18	0	100
300	3	0	0	100
300	4	0	0	98
500	2	0	0	100
500	3	0	0	98
500	4	0	0	70

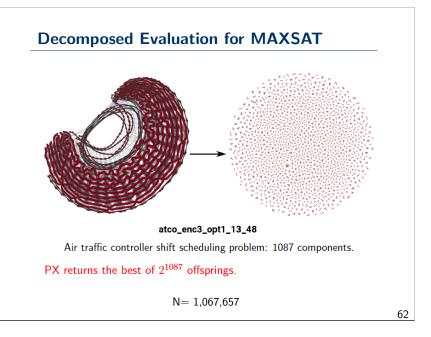
Percentage over 50 runs where the global optimum was Found in the experiments of the hybrid GA with the Adjacent NK Landscape.

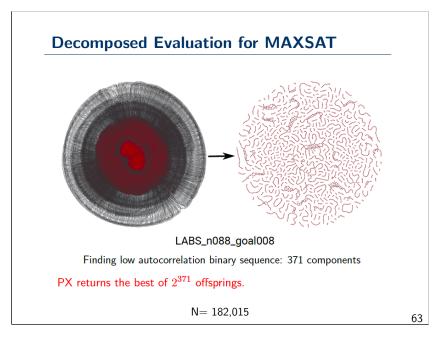


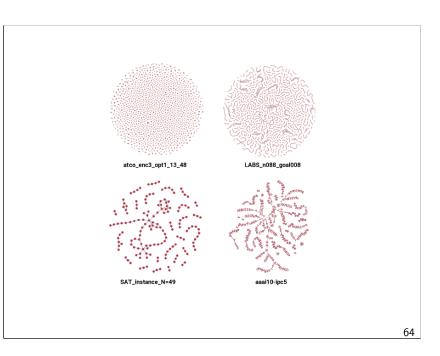












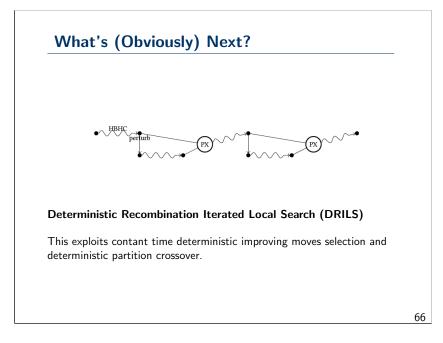
### **MAXSAT** Number of recombining components

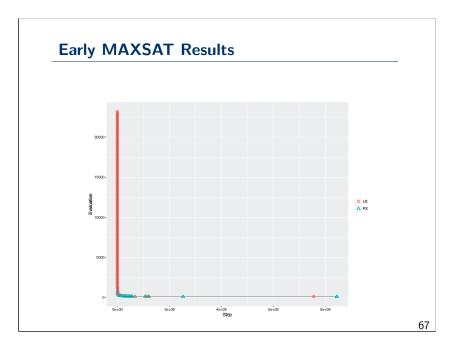
Instance	Ν	Min	Median	Max
aaai10ipc5	308,480	7	20	38
AProVE0906	37,726	11	1373	1620
atcoenc3opt19353	991,419	937	1020	1090
LABSno88goal008	182,015	231	371	2084
SATinstanceN111	72,001	34	55	1218

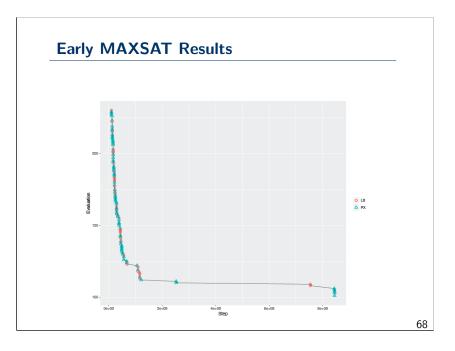
Imagine:

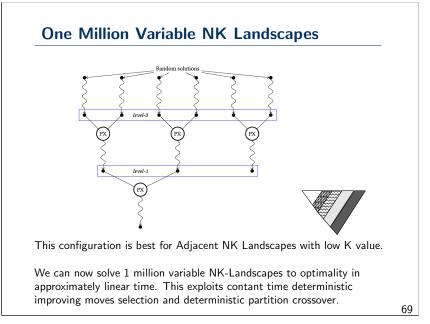
crossover "scans"  $2^{1000}$  local optima and returns the best in O(n) time



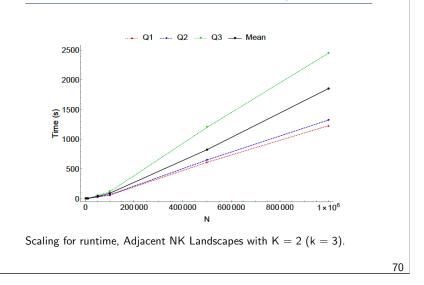


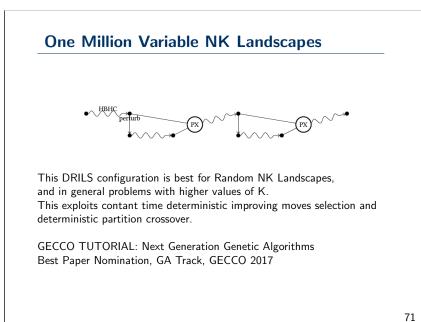






### **One Million Variable NK Landscapes**





### Cast Scheduling: K. Deb and C. Myburgh.

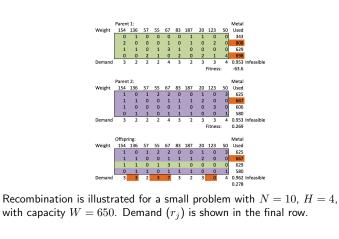
A foundry casts objects of various sizes and numbers by melting metal on a crucible of capacity *W*. Each melt is called a *heat*.

Assume there N total objects to be cast, with  $r_j$  copies of the  $j^{th}$  object. Each object has a fixed weight  $w_i$ , thereby requiring  $M = \sum_{j=1}^N r_j w_j$  units of metal.

DEMAND: Number of copies of the  $j^{th}$  object. CAPACITY of the crucible, W.

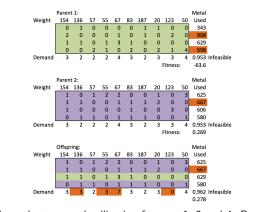


### **Cast Scheduling: Deterministic Recombination**



### **Cast Scheduling: Deterministic Recombination** 154 136 57 55 67 83 187 20 123 50 Used Weight 343 0 0 0 0 1 0 0 1 0 0 808 1 0 0 629 0 3 0 0 2 1 0 2 0 2 1 4 698 3 2 2 2 4 3 2 3 3 4 0.953 Infeasible Demand Fitness: -63.6 Parent 2: Metal Weight 154 136 57 55 67 83 187 20 123 50 Used 1 2 2 0 0 1 0 625 1 1 1 2 0 667 606 1 0 0 1 0 0 3 580 1 0 0 0 1 1 3 2 2 2 4 3 2 3 3 4 0.953 Infeasible Demand Fitness: 0.269 Offspring: Metal 154 136 57 55 67 83 187 20 123 50 Used Weight 2 2 0 0 1 625 0 1 1 1 2 667 629 0 1 3 1 580 4 0.962 Infeasible Demand 0.278 Columns indicate objects and rows indicate heats. The last column prints $\sum_{i=1}^{N} w_i x_{ij}$ for each heat. Offspring are constructed using the best rows.

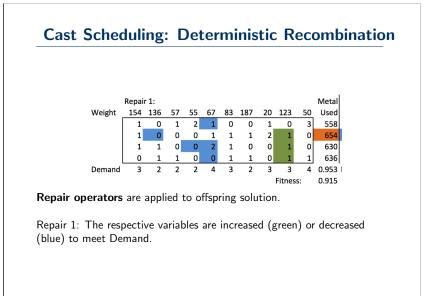
Cast Scheduling: Deterministic Recombination



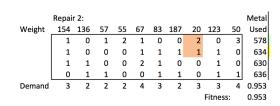
Parent 2 has a better metal utilization for rows 1, 2 and 4. Row 3 is taken from Parent 1. Recombination is greedy.

940

75



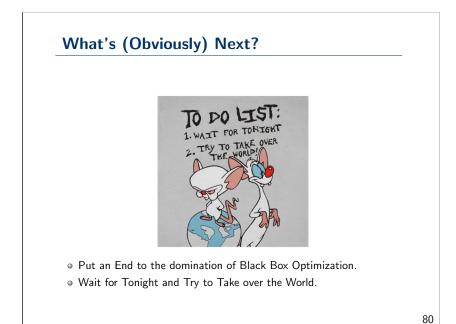
### **Cast Scheduling: Deterministic Recombination**



Repair operators are applied to offspring solution.

Repair 2: Objects are moved to different heats within the individual columns to reduce or minimize infeasibility.

**One Billion Variables** Computational Time (sec) 10 Not 10 Computational Time (sec) 10 Utime (sec) 1M6.2d 1.6d 2.8h 16.7m Slope=1.11 100 1.7m 10s 1s50k 500k 5M 50M 500M 1M 10M 100M 100k 1BNumber of Variables Breaking the Billion-Variable Barrier in Real World Optimization Using a Customized Genetic Algorithm. K. Deb and C. Myburgh. GECCO 2016.



77