Next Generation Genetic Algorithms

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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?"

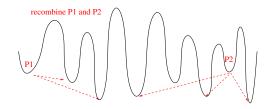
- NOT a Black Box Optimizer.
- 2 Uses mathematics to characterize problem structure.
- NOT cookie cutter.
 Not a blind "population, selection, mutation, crossover" GA.
- Uses deterministic move operators and crossover operators
- ⑤ Tunnels between Local Optima.
- Scales to large problems with millions of variables.
- Build on our expertise in smart ways.

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Know your Landscape! And Go Downhill!



What if you could ...



"Tunnel" between local optima on a TSP, or on an NK Landscape or a MAXSAT problem and go the BEST reachable local optima!

Tunneling = jump from local optimum to local optimum

The Partition Crossover Theorem for TSP

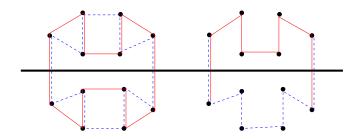
Let G be a graph produced by unioning 2 Hamiltonian Circuits.

Let G' be a reduced graph so that all common subtours are replaced by a single surrogate common edge.

If there is a partition of G' with cost 2, then the 2 Hamiltonian Circuits that make up G can be cut and recombined at this partition to create two new offspring.

The resulting Partition Crossover is Respectful and Transmits alleles.

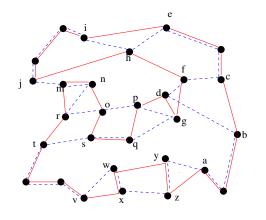
The Partition Crossover for TSP



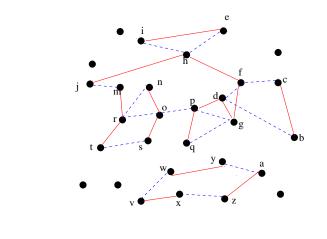
As a side effect: f(P1) + f(P2) = f(C1) + f(C2)

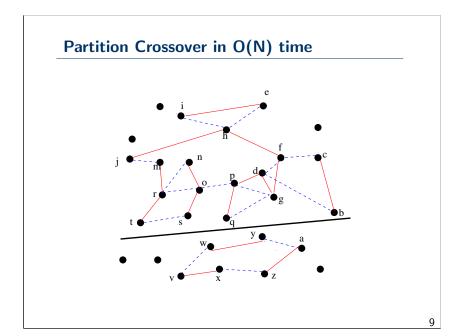
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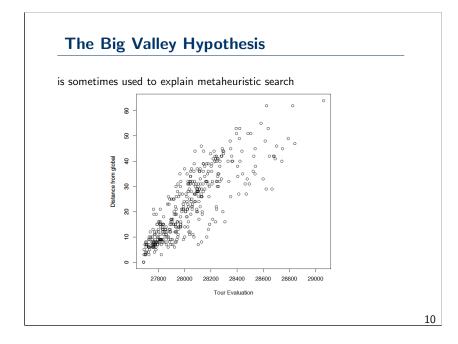
Partition Crossover

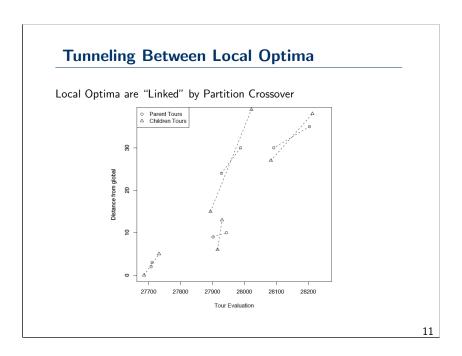


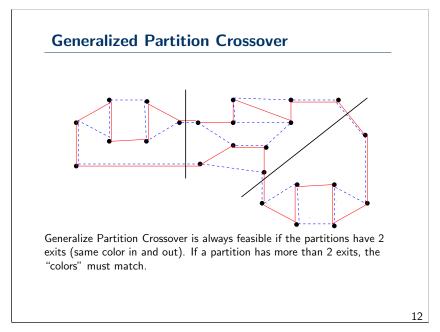
Partition Crossover











How Many Partitions are Discovered?

Instance	att532	nrw1379	rand1500	u1817	
3-opt	10.5 ± 0.5	11.3 ± 0.5	24.9 ± 0.2	26.2 ± 0.7	

Table: Average number of *partition components* used by GPX in 50 recombinations of random local optima found by 3-opt.

With 25 components, 2^{25} represents millions of local optima.

Lin-Kernighan-Helsgaun-LKH

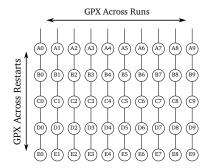
LKH is widely considered the best Local Search algorithm for TSP.

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

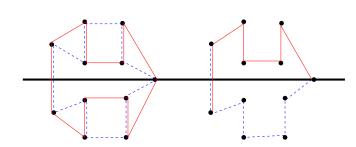
LKH-2 has found the majority of best known solutions on the TSP benchmarks at the Georgia Tech TSP repository that were not solved by complete solvers: http://www.tsp.gatech.edu/data/index.html.

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GPX Across Runs and Restarts



A diagram depicting 10 runs of multi-trial LKH-2 run for 5 iterations per run. The circles represent local optima produced by LKH-2. GPX across runs crosses over solutions with the same letters. GPX across restarts crosses over solutions with the same numbers.

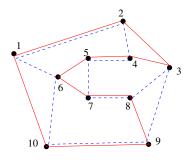


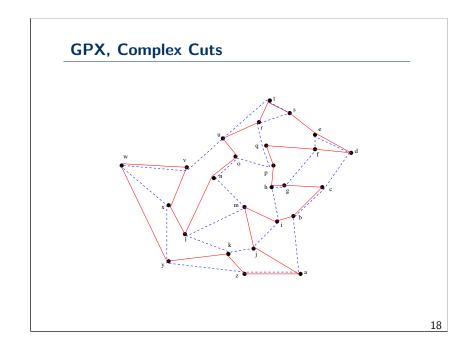
With Thanks to Gabriela Ochoa and Renato Tinós

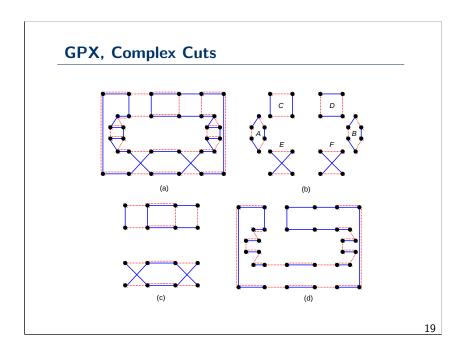
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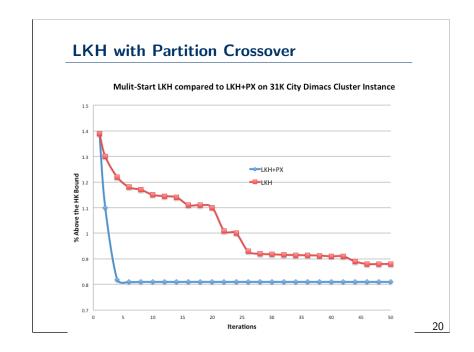
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The Two Best TSP (solo) Heuristics

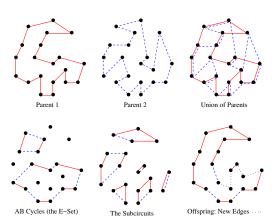
Lin Kernighan Helsgaun (LKH 2 with Multi-Starts) Iterated Local Search

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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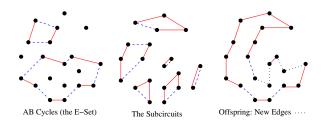
Edge Assembly Crossover



AB-Cycles are extracted from the graph which is the Union of the Parents. The AB-Cycles are used to cut Parent 1 into subcircuits.

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Edge Assembly Crossover



The AB-Cycles are used to cut Parent 1 into subcircuits. These 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

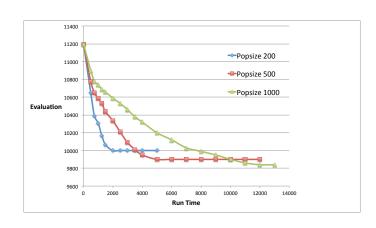
- ② EAX is used to generate many (e.g. 30) offspring during every recombination. Only the best offspring is retained (Brood Selection).
- 2 There is no selection, just "Brood Selection."
- Typical population size: 300.
- 3 The order of the population is randomized every generation. Parent i is recombined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

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.
- EAX illustrates the classic trade-off between exploration and exploitation

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Edge Assembly Crossover: Typical Behavior



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Combining EAX and Partition Crossover

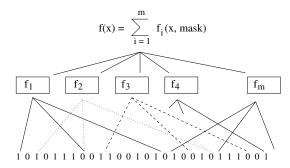
- Partition Crossover can dramatically speed-up exploitation, but it also impact long term search potential.
- ② A Strategy: When PAX generates 30 offspring, recombine all of the offspring using Partition Crossover. This can help when EAX gets stuck and cannot find an improvement.

EAX and **EAX** with Partition Crossover

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

EAX with Pa	rtition Pop	Crossover 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

k-bounded Pseudo-Boolean Functions



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)

$$xy = z \quad iff \quad xy - 2xz - 2yz + 3z = 0$$

$$xy \neq z$$
 iff $xy - 2xz - 2yz + 3z > 0$

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):

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

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k-bounded Pseudo-Boolean functions

For example: A Random NK Landscape: n=10 and k=3. The subfunctions:

$$\begin{array}{llll} f_0(x_0,x_1,x_6) & f_1(x_1,x_4,x_8) & f_2(x_2,x_3,x_5) & f_3(x_3,x_2,x_6) \\ f_4(x_4,x_2,x_1) & f_5(x_5,x_7,x_4) & f_6(x_6,x_8,x_1) & f_7(x_7,x_3,x_5) \\ f_8(x_8,x_7,x_3) & f_9(x_9,x_7,x_8) \end{array}$$

But this could also be a MAXSAT Function, or an arbitrary Spin Glass problem.

Walsh Example: MAXSAT

Given a logical expression consisting of Boolean variables, determine whether or not there is a setting for the variables that makes the expression TRUE.

Literal: a variable or the negation of a variable

Clause: a disjunct of literals

A 3SAT Example $(\neg x_2 \lor x_1 \lor x_0) \land (x_3 \lor \neg x_2 \lor x_1) \land (x_3 \lor \neg x_1 \lor \neg x_0)$

recast as a MAX3SAT Example

 $(\neg x_2 \lor x_1 \lor x_0) + (x_3 \lor \neg x_2 \lor x_1) + (x_3 \lor \neg x_1 \lor \neg x_0)$

BLACK BOX OPTIMIZATION

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



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

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

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Walsh Example: MAX-3SAT

Walsh Analysis of a Single Clause

Consider the example function consisting of a single clause $f(x) = \neg x_2 \vee x_1 \vee x_0$

 $f(000) = 1 \quad (\neg x_2 T)$

 $f(001) = 1 \quad (\neg x_2 T)$

 $f(010) = 1 \quad (\neg x_2 T)$

 $f(011) = 1 (\neg x_2 T)$

 $f(100) = 0 \quad (\neg x_2 F \wedge x_1 F \wedge x_0 F)$

 $f(101) = 1 (x_0T)$

 $f(110) = 1 (x_1T)$

 $f(111) = 1 \quad (x_1T)$

Walsh Example: MAX-3SAT

• All ψ_j 's except ψ_0 have 4 1's and 4 -1's.

 \bullet ψ_0 has all 1's.

• f for clauses of length 3 will contain one 0

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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:

$$w_j = \left\{ \begin{array}{ll} \frac{2^K-1}{2^K} & \text{if } j=0 \\ -\frac{1}{2^K} \psi_j(\operatorname{neg}(f)) & \text{if } j \neq 0 \end{array} \right.$$

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Walsh Example

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

\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

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Or can be expressed as a sum of k Elementary Landscapes

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

The Eigenvectors of MAX-3SAT

$$f(x) = f1(x) + f2(x) + f3(x) + f4(x)$$

$$f1(x) = f1_a(x) + f1_b(x) + f1_c(x)$$

$$f2(x) = f2_a(x) + f2_b(x) + f2_c(x)$$

$$f3(x) = f3_a(x) + f3_b(x) + f3_c(x)$$

$$f4(x) = f4_a(x) + f4_b(x) + f4_c(x)$$

$$\varphi^{(1)}(x) = f1_a(x) + f2_a(x) + f3_a(x) + f4_a(x)$$

$$\varphi^{(2)}(x) = f1_b(x) + f2_b(x) + f3_b(x) + f4_b(x)$$

$$\varphi^{(3)}(x) = f1_c(x) + f2_c(x) + f3_c(x) + f4_c(x)$$

$$f(x) = \varphi^{(1)}(x) + \varphi^{(2)}(x) + \varphi^{(3)}(x)$$

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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.

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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

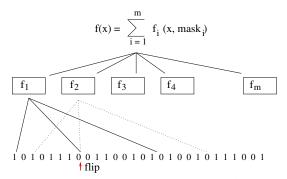
$$Score(x, y_p) = f(y_p) - f(x)$$

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.

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When 1 bit flips what happens?



The improving moves can be identified in O(1) time! Mutation is not needed, except to diversify the search.

The locations of the updates are obvious

$$\begin{array}{lclcrcl} Score(y_{p},y_{1}) & = & Score(x,y_{1}) \\ Score(y_{p},y_{2}) & = & Score(x,y_{2}) \\ Score(y_{p},y_{3}) & = & Score(x,y_{3}) - 2(\sum\limits_{\forall b,\ (p\wedge3)\subset b}w'_{b}(x)) \\ Score(y_{p},y_{4}) & = & Score(x,y_{4}) \\ Score(y_{p},y_{5}) & = & Score(x,y_{5}) \\ Score(y_{p},y_{6}) & = & Score(x,y_{6}) \\ Score(y_{p},y_{7}) & = & Score(x,y_{7}) \\ Score(y_{p},y_{8}) & = & Score(x,y_{8}) - 2(\sum\limits_{\forall b,\ (p\wedge8)\subset b}w'_{b}(x)) \\ Score(y_{p},y_{9}) & = & Score(x,y_{9}) \end{array}$$

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.

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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

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

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

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

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

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Steepest Descent on Moments

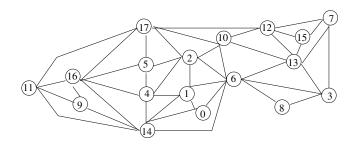
Both f(x) and Avg(N(x)) can be computed with Walsh Spans.

$$f(x) = \sum_{z=0}^{3} \varphi^{(z)}(x)$$

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

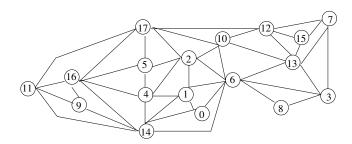
$$Avg(N(x)) = \sum_{z=0}^{3} \varphi^{(z)}(x) - 2/N \sum_{z=0}^{3} z \varphi^{(z)}(x)$$

The Variable Interaction Graph



There is a vertex for each variable in 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., $w_{i,j}$.

What if you want to flip 2 or 3 bits at a time?



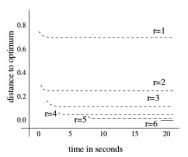
Assume all distance 1 moves are taken.

There can never be an improving move flipping bits 2 and 7.

There can never be an improving move flipping bits 4, 6 and 9.

There can never be an improving move over combinations of bits where there are no (non-zero) Walsh coefficients.

What if you want to flip 2 or 3 bits at a time?

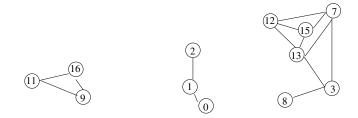


12,000 bit k-bounded functions

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The Recombination Graph: a reduced VIG

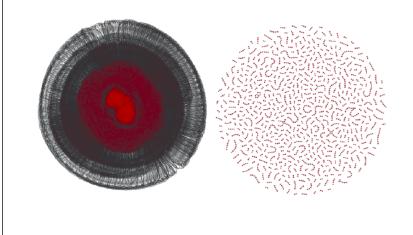


When recombining the solutions $S_{P1}=000000000000000000000$ and $S_{P2}=111100011101110110$, the vertices and edges associated with shared variables 4, 5, 6, 10, 14 are deleted to yield the **recombination graph**.

Tunneling Crossover Theorem:

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

Decomposed Evaluation for MAXSAT



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MAXSAT Number of recombining components

	Instance	N	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

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

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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***.

In general:

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

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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:

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

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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 ± 0.16	41	
100	2	Random	3.22 ± 0.16	15	
300	4	Random	2.41 ± 0.04	13	
500	2	Random	6.98 ± 0.47	47	
500	4	Random	2.46 ± 0.05	13	

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

Optimal Solutions for Adjacent NK $\,$

		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		

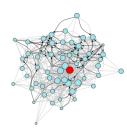
Percentage over 50 runs where the global optimum was Found in the experiments of the hybrid GA with the Adjacent NK Landscape.

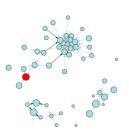
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Tunnelling Local Optima Networks

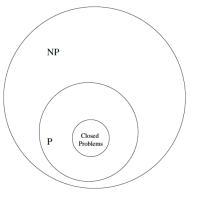
NK Landscapes: Ochoa et al. GECCO 2015





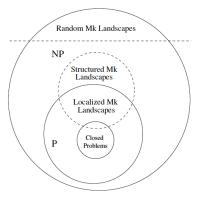
Adjacent (easy) NK Landscapes have more optima. But Random (hard) NK Landscapes have disjunct "funnels."

NK and Mk Landscapes, P and NP



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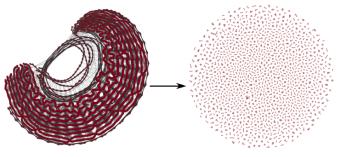
NK and Mk Landscapes, P and NP



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Decomposed Evaluation for MAXSAT



atco_enc3_opt1_13_48

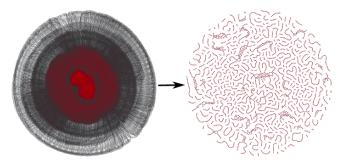
Air traffic controller shift scheduling problem: 1087 components.

PX returns the best of 2^{1087} offsprings.

N = 1,067,657

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Decomposed Evaluation for MAXSAT

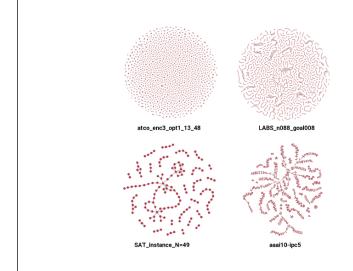


LABS_n088_goal008

Finding low autocorrelation binary sequence: 371 components

PX returns the best of 2^{371} offsprings.

N = 182,015



MAXSAT Number of recombining components

Instance	N	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

What's (Obviously) Next?



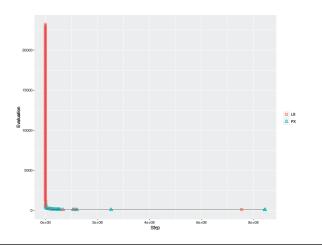
Deterministic Recombination Iterated Local Search (DRILS)

This exploits contant time deterministic improving moves selection and deterministic partition crossover.

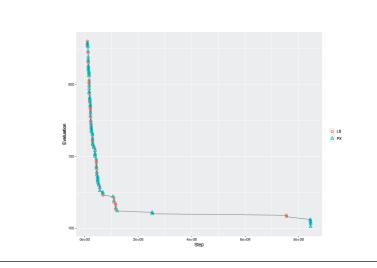
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Early MAXSAT Results

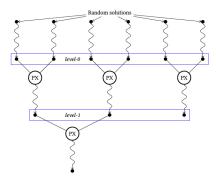


Early MAXSAT Results



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One Million Variable NK Landscapes



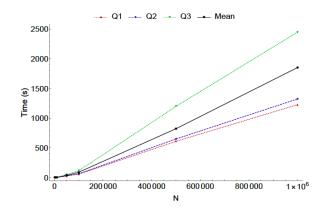


This configuration is best for Adjacent NK Landscapes with low K value.

We can now solve 1 million variable NK-Landscapes to optimality in approximately linear time. This exploits contant time deterministic improving moves selection and deterministic partition crossover.

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One Million Variable NK Landscapes



Scaling for runtime, Adjacent NK Landscapes with K = 2 (k = 3).

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One Million Variable NK Landscapes



This DRILS configuration is best for Random NK Landscapes, and in general problems with higher values of K. This exploits contant time deterministic improving moves selection and deterministic partition crossover.

GECCO TUTORIAL: Next Generation Genetic Algorithms Best Paper Nomination, GA Track, GECCO 2017

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.

Casts: Multiple Objects, Multiple Copies



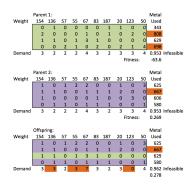






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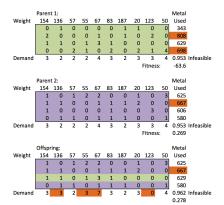
Cast Scheduling: Deterministic Recombination



Recombination is illustrated for a small problem with $N=10,\,H=4,$ with capacity W=650. Demand (r_i) is shown in the final row.

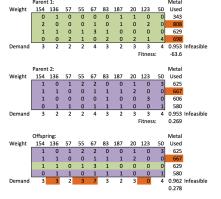
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Cast Scheduling: Deterministic Recombination



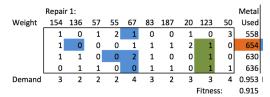
Columns indicate objects and rows indicate heats. The last column prints $\sum_{i=1}^N w_j x_{ij}$ for each heat. Offspring are constructed using the best rows.

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.

Cast Scheduling: Deterministic Recombination



Repair operators are applied to offspring solution.

Repair 1: The respective variables are increased (green) or decreased (blue) to meet Demand.

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Cast Scheduling: Deterministic Recombination

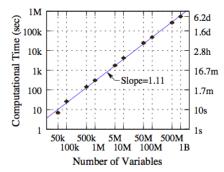
	Repai	r 2:									Metal
Weight	154	136	57	55	67	83	187	20	123	50	Used
	1	0	1	2	1	0	0	2	0	3	578
	1	0	0	0	1	1	1	1	1	0	634
	1	1	0	0	2	1	0	0	1	0	630
	0	1	1	0	0	1	1	0	1	1	636
Demand	3	2	2	2	4	3	2	3	3	4	0.953
									Fitness	:	0.953

Repair operators are applied to offspring solution.

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

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One Billion Variables



Breaking the Billion-Variable Barrier in Real World Optimization Using a Customized Genetic Algorithm. K. Deb and C. Myburgh. GECCO 2016.

What's (Obviously) Next?



- Put an End to the domination of Black Box Optimization.
- Wait for Tonight and Try to Take over the World.
