## Next Generation Genetic Algorithms

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With Thanks to: F. Chicano, G. Ochoa, A. Sutton and R. Tinós


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## Next Generation Genetic Algorithms

There is a book chapter that goes with this tutorial.

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SUBJECT: TUTORIAL2018



## Next Generation Genetic Algorithms

What do we mean by "Next Generation?"

1. NOT a Black Box Optimizer.
2. Uses mathematics to characterize problem structure.
3. For many problems: NO MUTATION IS NEEDED



## Next Generation Genetic Algorithms

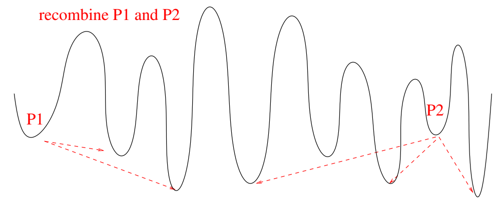
What do we mean by "Next Generation?"

1. NOT cookie cutter.
   Not a blind "population, selection, mutation, crossover" GA.
2. Uses deterministic move operators and crossover operators
3. *Tunnels* between Local Optima.
4. Scales to large problems with millions of variables.
5. Build on our expertise in smart ways.

## Know your Landscape! And Go Downhill!



## What if you could ...



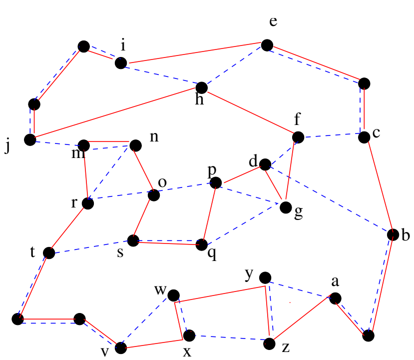

"Tunnel" between local optima on a TSP,
or on an NK Landscape or a MAXSAT problem
and go the BEST reachable local optima!

Tunneling = jump from local optimum to local optimum



## The Partition Crossover Theorem for TSP

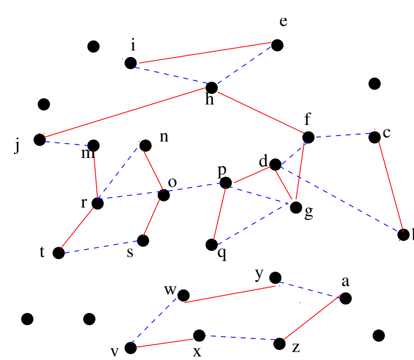
Let G be a graph produced by unioning 2 Hamiltonian Circuits.



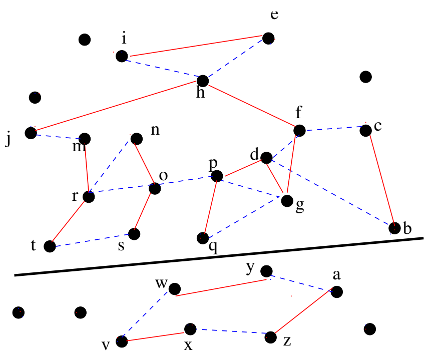



## The Partition Crossover Theorem for TSP

Let G' be a reduced graph so that all common subtours are removed.

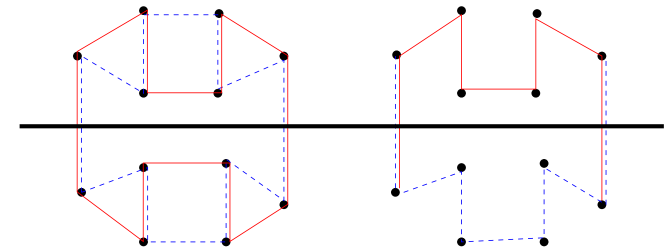


## Partition Crossover in $O(n)$ time






## The Partition Crossover for TSP

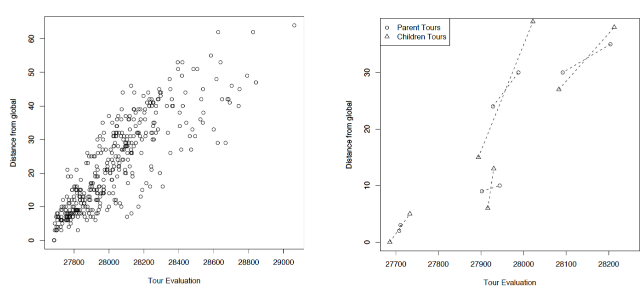


As a side effect: f(P1) + f(P2) = f(C1) + f(C2)



## The Big Valley Hypothesis

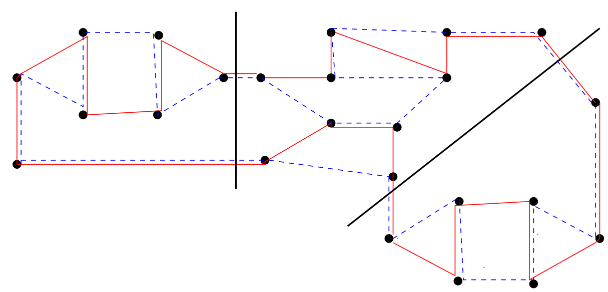
is sometimes used to explain metaheuristic search




Local Optima are “Linked” by Partition Crossover ”Tunnels”



## Generalized Partition Crossover in $O(n)$ time



Generalize Partition Crossover is always feasible if the partitions have 2 exits (same color in and out). If a partition has more than 2 exits, the “colors” must match.

## How Many Partitions are Discovered?

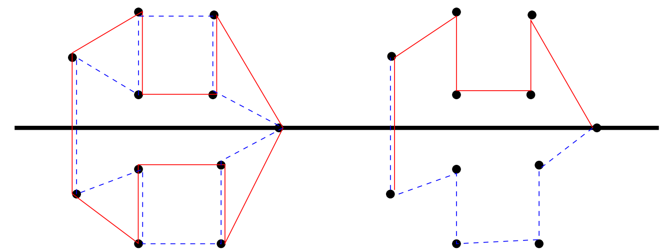
| Instance | att532 | nrw1379 | rand1500 | u1817 |
|---|---|---|---|---|
| 3-opt | $10.5 \pm 0.5$ | $11.3 \pm 0.5$ | $24.9 \pm 0.2$ | $26.2 \pm 0.7$ |

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.

With 1000 components, returns the best of $2^{1000}$ local optima!!!

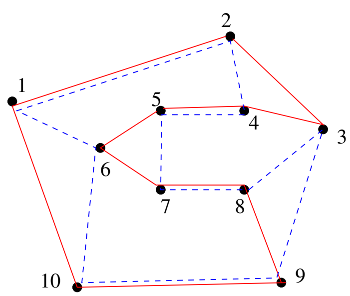




With Thanks to Gabriela Ochoa and Renato Tinós

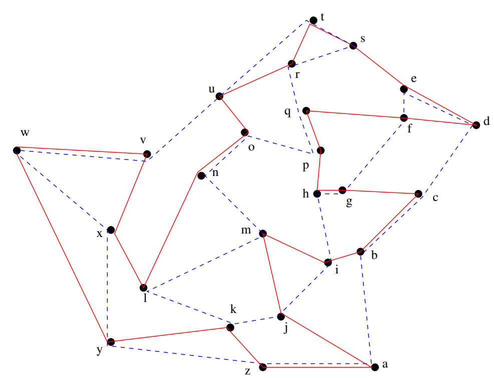


## GPX, Cuts Crossing 4 Edges (IPT fails here)

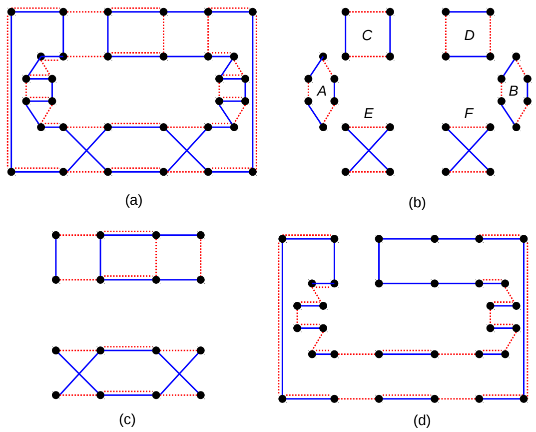





## GPX, Complex Cuts ... Still $O(n)$ time



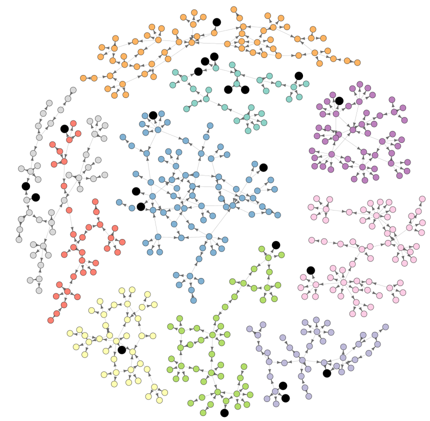
## GPX, Complex Cuts ... Still $O(n)$ time






## Tunneling Between Local Optima

Local Optima are “Linked” by Partition Crossover



Thanks to G. Ochoa and N. Veerapen.



## The Two Best TSP (solo) Heuristics

Lin Kernighan Helsgaun (LKH 2 with Multi-Starts, and IPT Crossover)
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.)

**THE BEST INEXACT “TSP” SOLVERS USE CROSSOVER!**



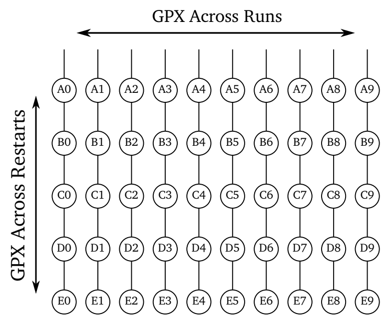
## Lin-Kernighan-Helsgaun-LKH

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.

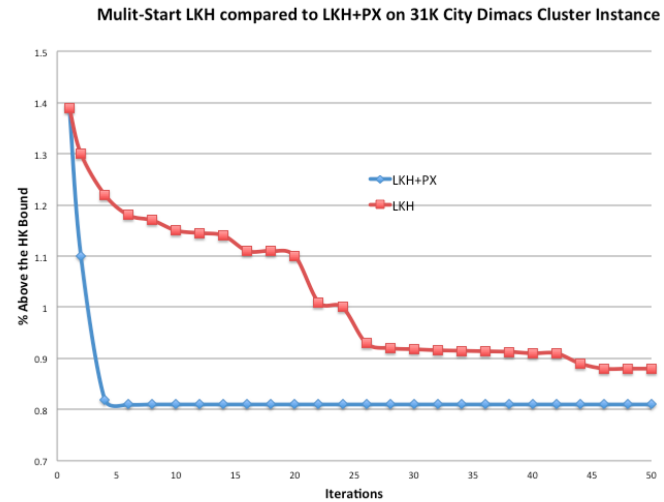
## GPX Across Runs and Restarts




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.

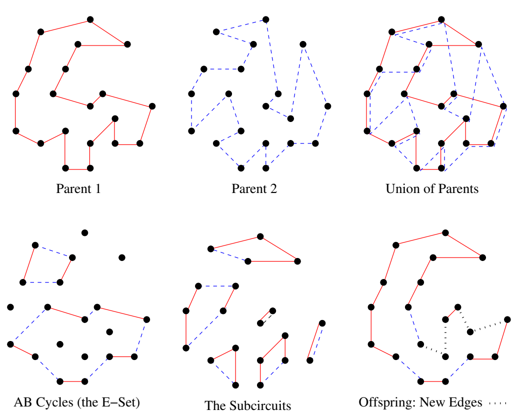


## LKH with Partition Crossover





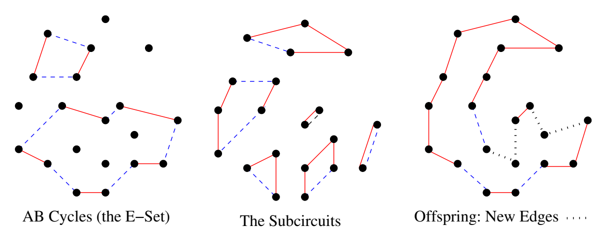

## Edge Assembly Crossover




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.



## 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

1. 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.
4. 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.)

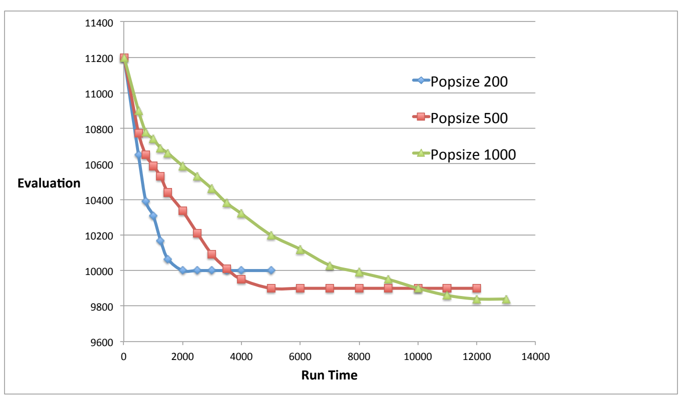


## The EAX Strategy

1. 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

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

# EAX and EAX with Partition Crossover

Standard EAX with restarts

| Dataset | Pop Size | Evaluation Mean | S. D. | Running Time Mean | S. D. | Number 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 |

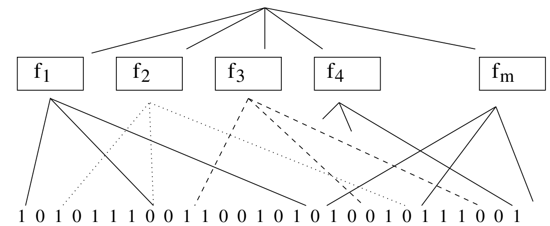
EAX with Partition Crossover

| Dataset | Pop Size | Evaluation Mean | S. D. | Running Time Mean | S. D. | Number 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

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






# 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)

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

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):

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



# k-bounded Pseudo-Boolean functions

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

| | | | |
|---|---|---|---|
| $f_0(x_0, x_1, x_6)$ | $f_1(x_1, x_4, x_8)$ | $f_2(x_2, x_3, x_5)$ | $f_3(x_3, x_2, x_6)$ |
| $f_4(x_4, x_2, x_1)$ | $f_5(x_5, x_7, x_4)$ | $f_6(x_6, x_8, x_1)$ | $f_7(x_7, x_3, x_5)$ |
| | $f_8(x_8, x_7, x_3)$ | $f_9(x_9, x_7, x_8)$ | |

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

$$(\neg x_2 \vee x_1 \vee x_0) \wedge (x_3 \vee \neg x_2 \vee x_1) \wedge (x_3 \vee \neg x_1 \vee \neg x_0)$$

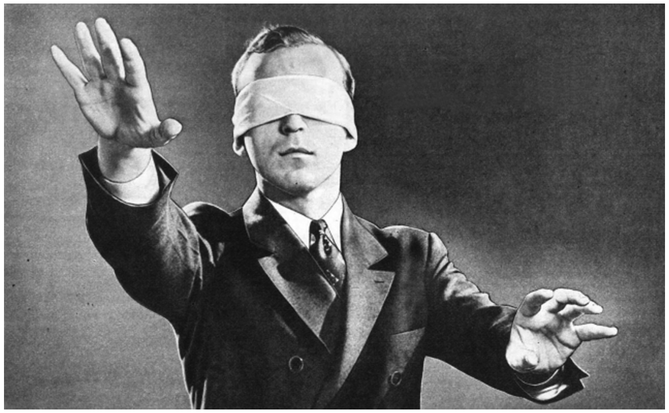
recast as a MAX3SAT Example

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



## BLACK BOX OPTIMIZATION

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





## GRAY BOX OPTIMIZATION

**THEREM: All of the following functions are solved in 1 evaluation in $O(n)$ time.**

**ONEMAX**
**LEADING-ONES** (TRAILING ZEROS)
**TRAP functions**
**Multi-Modal UGLY Deceptive Problems**
**JUMP functions,** $(m << n)$
**UNITATION functions**
**All non-deceptive functions**

Do we want to solve real problem?

Or just pretend to solve toy problems?



## 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

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

## Walsh Example: MAX-3SAT

Walsh Analysis of a Single Clause

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

$$
\begin{array}{lcll}
f(000) & = & 1 & (\neg x_2 T) \\
f(001) & = & 1 & (\neg x_2 T) \\
f(010) & = & 1 & (\neg x_2 T) \\
f(011) & = & 1 & (\neg x_2 T) \\
f(100) & = & 0 & (\neg x_2 F \wedge x_1 F \wedge x_0 F) \\
f(101) & = & 1 & (x_0 T) \\
f(110) & = & 1 & (x_1 T) \\
f(111) & = & 1 & (x_1 T)
\end{array}
$$



## Walsh Example: MAX-3SAT

$$
\frac{1}{8}\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 0 \\ 1 \\ 1 \\ 1 \end{bmatrix}^{\top}
\begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\
1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\
1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\
1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\
1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\
1 & -1 & -1 & 1 & -1 & 1 & 1 & -1
\end{bmatrix}
=
\begin{bmatrix} 0.875 \\ -0.125 \\ -0.125 \\ -0.125 \\ 0.125 \\ 0.125 \\ 0.125 \\ 0.125 \end{bmatrix}
$$

- 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.

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

$$neg(f) = 100$$

Then the Walsh coefficients for $f$ are:

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



## Walsh Example

$$
\begin{aligned}
f_1 &= (\neg x_2 \vee x_1 \vee x_0) \\
f_2 &= (x_3 \vee \neg x_2 \vee x_1) \\
f_3 &= (x_3 \vee \neg x_1 \vee \neg x_0)
\end{aligned}
$$

| $x$ | $w_i$ | $W(f_1)$ | $W(f_2)$ | $W(f_3)$ | $W(f(x))$ |
|---|---|---|---|---|---|
| 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

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 sum of $k$ Eigenvectors:

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



## The Eigenvectors of MAX-3SAT

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

$$\begin{aligned} f1(x) &= f1_a(x) + f1_b(x) + f1_c(x) \\ f2(x) &= f2_a(x) + f2_b(x) + f2_c(x) \\ f3(x) &= f3_a(x) + f3_b(x) + f3_c(x) \\ f4(x) &= f4_a(x) + f4_b(x) + f4_c(x) \end{aligned}$$

$$\begin{aligned} \varphi^{(1)}(x) &= f1_a(x) + f2_a(x) + f3_a(x) + f4_a(x) \\ \varphi^{(2)}(x) &= f1_b(x) + f2_b(x) + f3_b(x) + f4_b(x) \\ \varphi^{(3)}(x) &= f1_c(x) + f2_c(x) + f3_c(x) + f4_c(x) \end{aligned}$$

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



## 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.



## Constant Time Steepest Descent

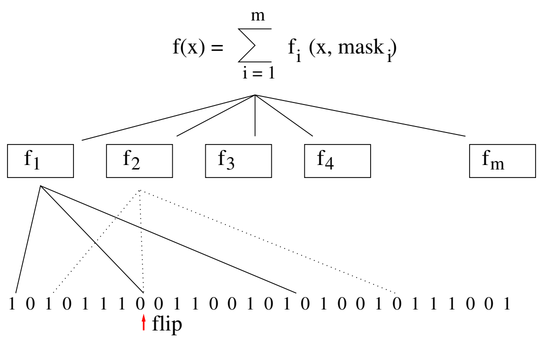
Assume we flip bit $p$ to move from $x$ to $y_p \in N(x)$. Construct a vector $Score$ such that

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

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.

**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

$$
\begin{aligned}
Score(y_p, y_1) &= Score(x, y_1)\\
Score(y_p, y_2) &= Score(x, y_2)\\
Score(y_p, y_3) &= Score(x, y_3) - 2\Big(\sum_{\forall b,\ (p \wedge 3) \subset b} w'_b(x)\Big)\\
Score(y_p, y_4) &= Score(x, y_4)\\
Score(y_p, y_5) &= Score(x, y_5)\\
Score(y_p, y_6) &= Score(x, y_6)\\
Score(y_p, y_7) &= Score(x, y_7)\\
Score(y_p, y_8) &= Score(x, y_8) - 2\Big(\sum_{\forall b,\ (p \wedge 8) \subset b} w'_b(x)\Big)\\
Score(y_p, y_9) &= Score(x, y_9)
\end{aligned}
$$



## Some Theoretical Results: k-bounded Boolean

1) PROOF: Same 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.



## Best Improving and Next Improving moves

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

**GSAT uses a Buffer of best improving moves**

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

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

**Instead uses multiple Buckets to hold improving moves**

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

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

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

This improves the runtime of GSAT by a factor of 20X to 30X.

## Steepest Descent on Moments

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

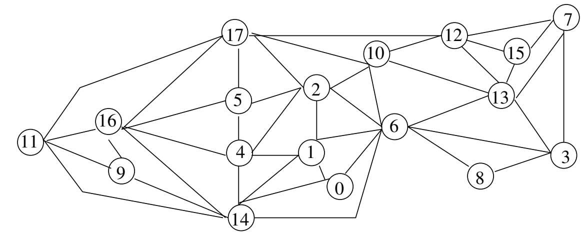
$$f(x) = \sum_{z=0}^{3} \varphi^{(z)}(x)$$

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

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



## The Variable Interaction Graph

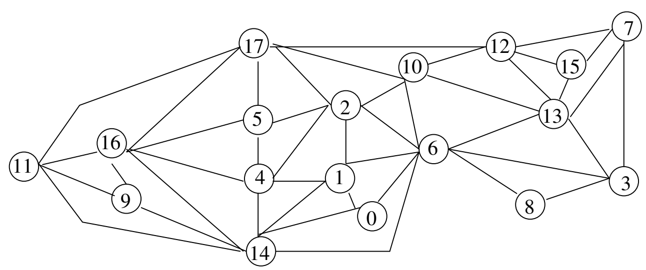



There is a vertex for each variable in the Variable Interaction Graph (VIG). There must be fewer than $2^k$ $M = O(n)$ Walsh coefficients. There is a connection in the VIG between vertex $v_i$ and $v_j$ if there is a

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?

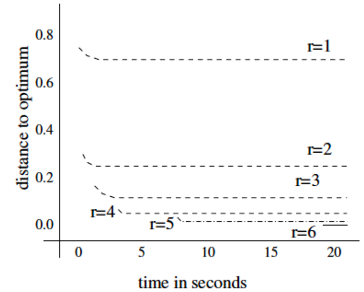



Assume all distance 1 moves are taken.

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.

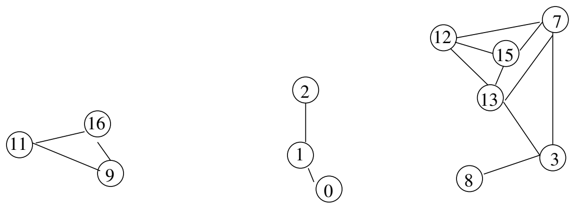


## What if you want to flip 2 or 3 bits at a time?




12,000 bit k-bounded functions

## The Recombination Graph: a reduced VIG



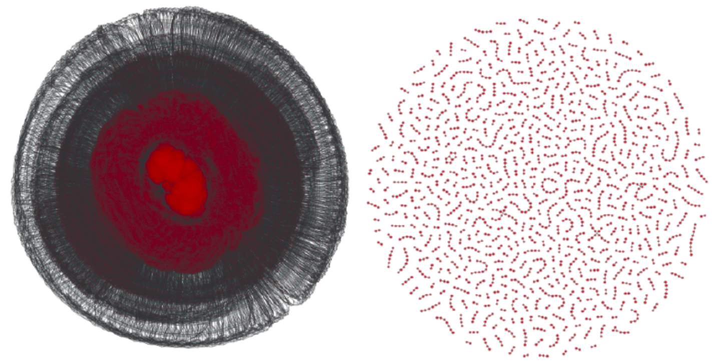

When recombining the solutions $S_{P1} = 000000000000000000$ and $S_{P2} = 111100011101110110$, the vertices and edges associated with shared variables 4, 5, 6, 10, 14 are deleted to yield the **recombination graph**.

**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





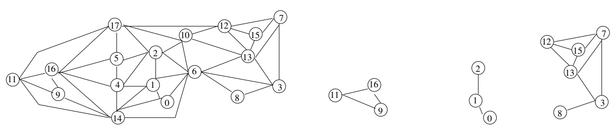
## MAXSAT Number of recombining components

| 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.



## 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:

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

## 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 0000000000 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 ±0.3 | 100.0 ±0.0 |
| 300 | 4 | Adj | 30.7 ±2.8 | 0.0 ±0.0 | 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 ±0.0 | 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 ±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 ±0.0 | 83.6 ±16.8 |



## Number of partition components discovered

| $N$ | $k$ | 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.



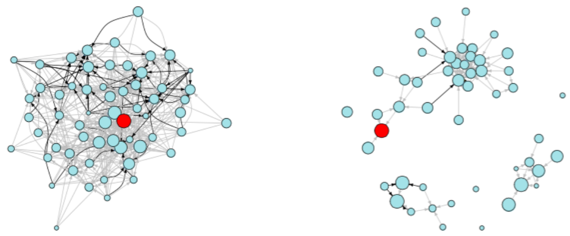
## Optimal Solutions for Adjacent NK

| | | 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.

## Tunneling Local Optima Networks

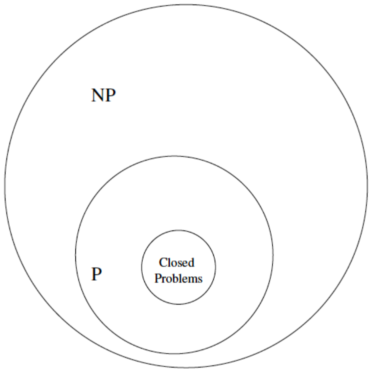
**Multimodal problems are not always difficult**
**NK Landscapes: Ochoa et al. GECCO 2015**



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

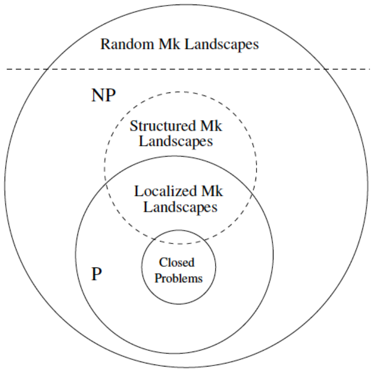


## NK and Mk Landscapes, P and NP



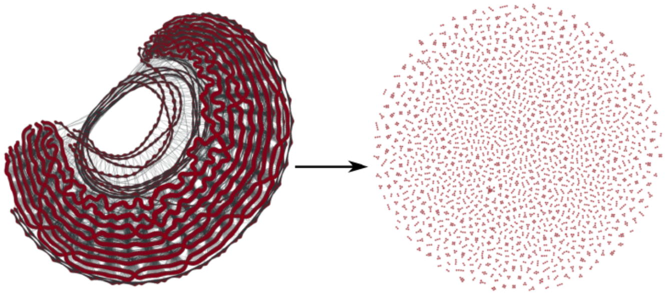



## NK and Mk Landscapes, P and NP






## Decomposed Evaluation for MAXSAT



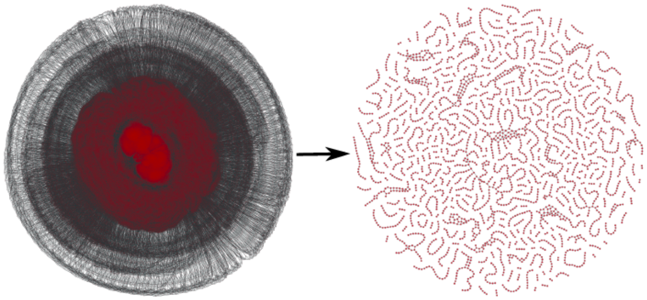
**atco_enc3_opt1_13_48**

Air traffic controller shift scheduling problem: 1087 components.

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

N= 1,067,657

## Decomposed Evaluation for MAXSAT



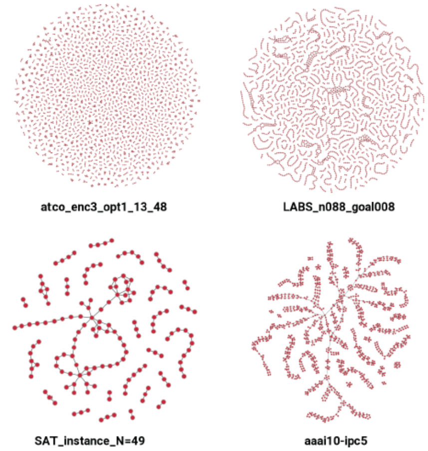
LABS_n088_goal008

Finding low autocorrelation binary sequence: 371 components

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

N= 182,015








## MAXSAT Number of recombining components

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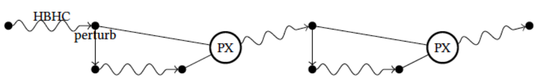
| atcoenc3opt19353 | 991,419 | 937 | 1020 | 1090 |
| LABSno88goal008 | 182,015 | 231 | 371 | 2084 |
| SATinstanceN111 | 72,001 | 34 | 55 | 1218 |

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



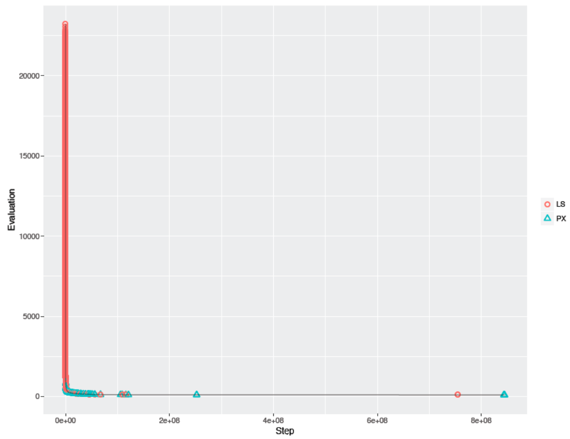
## What's (Obviously) Next?




**Deterministic Recombination Iterated Local Search (DRILS)**

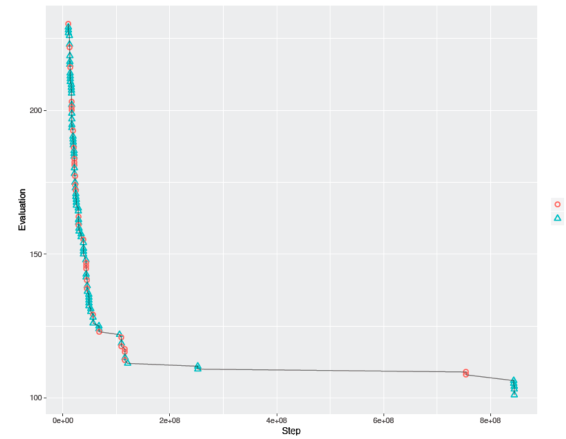
This exploits contant time deterministic improving moves selection and deterministic partition crossover.

## Early MAXSAT Results



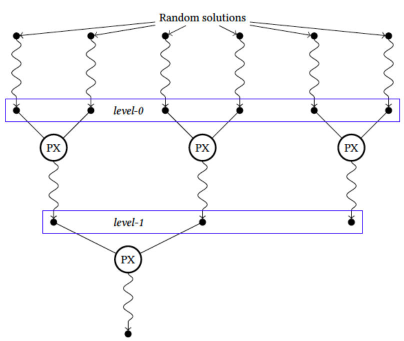


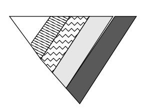

## Early MAXSAT Results






## One Million Variable NK Landscapes



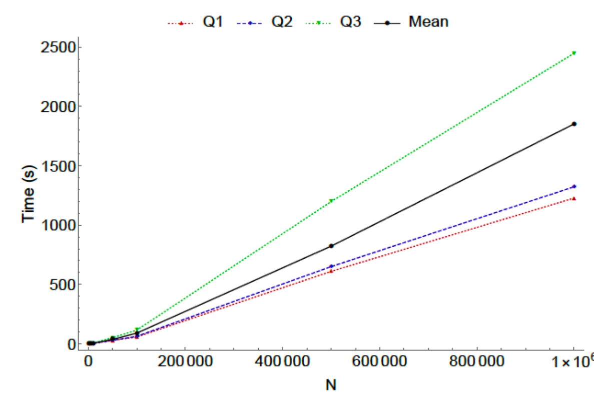



This configuration is best for Adjacent NK Landscapes with low K value.

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.



## One Million Variable NK Landscapes




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

## 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 constant time deterministic improving moves selection and deterministic partition crossover.



## NK Landscapes and MAXSAT

**Black Box Optimization is HOPELESSLY inefficient.**

In expectation, for N= 1,000,000, with 1 improving move available:

In the worst case,
for the 1 improving move made by a Black Box Optimizer
a Gray Box Optimizer can make 1,000,000 improving moves.



## 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*.

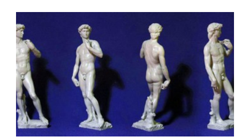
Assume there $N$ total objects to be cast, with $r_j$ copies of the $j^{th}$ object.
Each object has a fixed weight $w_i$, thereby requiring $M = \sum_{j=1}^{N} r_j w_j$ units of metal.

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



## Casts: Multiple Objects, Multiple Copies





## Cast Scheduling: Deterministic Recombination

Parent 1:

| Weight | 154 | 136 | 57 | 55 | 67 | 83 | 187 | 20 | 123 | 50 | Metal Used | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 0 | 1 | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 343 | |
| | 2 | 0 | 0 | 0 | 1 | 0 | 1 | 0 | 2 | 0 | 808 | |
| | 1 | 1 | 0 | 1 | 3 | 1 | 0 | 0 | 0 | 0 | 629 | |
| | 0 | 0 | 2 | 1 | 0 | 2 | 0 | 2 | 1 | 4 | 698 | |
| Demand | 3 | 2 | 2 | 2 | 4 | 3 | 2 | 3 | 3 | 4 | 0.953 | Infeasible |
| | | | | | | | | | | Fitness: | -63.6 | |

Parent 2:

| Weight | 154 | 136 | 57 | 55 | 67 | 83 | 187 | 20 | 123 | 50 | Metal Used | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 1 | 0 | 1 | 2 | 2 | 0 | 0 | 1 | 0 | 3 | 625 | |
| | 1 | 1 | 0 | 0 | 1 | 1 | 1 | 2 | 0 | 0 | 667 | |
| | 1 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 3 | 0 | 606 | |
| | 0 | 1 | 1 | 0 | 1 | 1 | 1 | 0 | 0 | 1 | 580 | |
| Demand | 3 | 2 | 2 | 2 | 4 | 3 | 2 | 3 | 3 | 4 | 0.953 | Infeasible |
| | | | | | | | | | | Fitness: | 0.269 | |

Offspring:

| Weight | 154 | 136 | 57 | 55 | 67 | 83 | 187 | 20 | 123 | 50 | Metal Used | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 1 | 0 | 1 | 2 | 2 | 0 | 0 | 1 | 0 | 3 | 625 | |
| | 1 | 1 | 0 | 0 | 1 | 1 | 1 | 2 | 0 | 0 | 667 | |
| | 1 | 1 | 0 | 1 | 3 | 1 | 0 | 0 | 0 | 0 | 629 | |
| | 0 | 1 | 1 | 0 | 1 | 1 | 1 | 0 | 0 | 1 | 580 | |
| Demand | 3 | 3 | 2 | 3 | 7 | 3 | 2 | 3 | 0 | 4 | 0.962 | Infeasible |
| | | | | | | | | | | | 0.278 | |

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



## Cast Scheduling: Deterministic Recombination

Parent 1:

| Weight | 154 | 136 | 57 | 55 | 67 | 83 | 187 | 20 | 123 | 50 | Metal Used | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 0 | 1 | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 343 | |
| | 2 | 0 | 0 | 0 | 1 | 0 | 1 | 0 | 2 | 0 | 808 | |
| | 1 | 1 | 0 | 1 | 3 | 1 | 0 | 0 | 0 | 0 | 629 | |
| | 0 | 0 | 2 | 1 | 0 | 2 | 0 | 2 | 1 | 4 | 698 | |
| Demand | 3 | 2 | 2 | 2 | 4 | 3 | 2 | 3 | 3 | 4 | 0.953 | Infeasible |
| | | | | | | | | | | Fitness: | -63.6 | |

Parent 2:

| Weight | 154 | 136 | 57 | 55 | 67 | 83 | 187 | 20 | 123 | 50 | Metal Used | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 1 | 0 | 1 | 2 | 2 | 0 | 0 | 1 | 0 | 3 | 625 | |
| | 1 | 1 | 0 | 0 | 1 | 1 | 1 | 2 | 0 | 0 | 667 | |
| | 1 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 3 | 0 | 606 | |
| | 0 | 1 | 1 | 0 | 1 | 1 | 1 | 0 | 0 | 1 | 580 | |
| Demand | 3 | 2 | 2 | 2 | 4 | 3 | 2 | 3 | 3 | 4 | 0.953 | Infeasible |
| | | | | | | | | | | Fitness: | 0.269 | |

Offspring:

| Weight | 154 | 136 | 57 | 55 | 67 | 83 | 187 | 20 | 123 | 50 | Metal Used | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 1 | 0 | 1 | 2 | 2 | 0 | 0 | 1 | 0 | 3 | 625 | |
| | 1 | 1 | 0 | 0 | 1 | 1 | 1 | 2 | 0 | 0 | 667 | |
| | 1 | 1 | 0 | 1 | 3 | 1 | 0 | 0 | 0 | 0 | 629 | |
| | 0 | 1 | 1 | 0 | 1 | 1 | 1 | 0 | 0 | 1 | 580 | |
| Demand | 3 | 3 | 2 | 3 | 7 | 3 | 2 | 3 | 0 | 4 | 0.962 | Infeasible |
| | | | | | | | | | | | 0.278 | |

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 1:

| Weight | 154 | 136 | 57 | 55 | 67 | 83 | 187 | 20 | 123 | 50 | Metal Used |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | 1 | 0 | 1 | 2 | 1 | 0 | 0 | 1 | 0 | 3 | 558 |
| | 1 | 0 | 0 | 0 | 1 | 1 | 1 | 2 | 1 | 0 | 654 |
| | 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: | 0.915 |

**Repair operators** are applied to offspring solution.

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



## Cast Scheduling: Deterministic Recombination

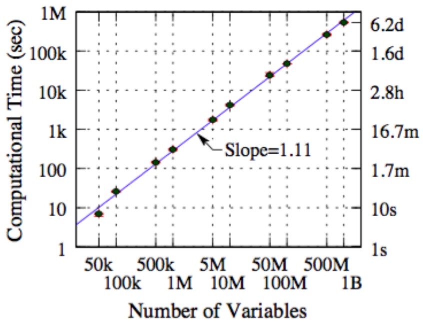
Repair 2:

| Weight | 154 | 136 | 57 | 55 | 67 | 83 | 187 | 20 | 123 | 50 | Metal 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.

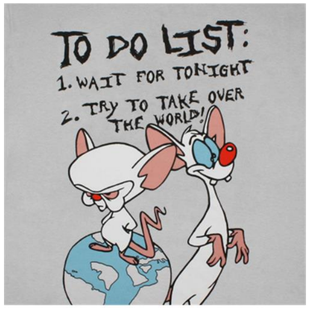
## One Billion Variables




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.