# Gray-Box Optimization for Million <br> Variable Pseudo-Boolean Problems 

Francisco Chicano

Joint work with
Darrell Whitley, Renato Tinós, Gabriela Ochoa and Andrew M. Sutton

## Outline

- Gray-Box (vs. Black-Box) Optimization
- Hamming Ball Hill Climber and Partition Crossover
- Deterministic Recombination and Iterated Local Search
- Experiments
- Conclusions and Future Work


## Gray-Box (vs. Black-Box) Optimization



For most of real problems we know (almost) all the details

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## Gray-Box (vs. Black-Box) Optimization



## OneMax

$\theta(n / \log n)$
$\theta(1)$

Other $\boldsymbol{\theta}(1)$-solvable problems:

- Leading Ones
- Trap Functions
- Jump Functions
- Massively Multimodal Deceptive Problem


## Gray-Box structure: MK Landscapes

$$
f(x)=\sum_{i=1}^{m} f^{(i)}(x) \quad \begin{gathered}
\text { All compresibl } \\
\text { functions can } \\
\text { this in pol }
\end{gathered}
$$

Example ( $k=2$ ):


## Variable Interaction


$x_{i}$ and $x_{j}$ interact when they appear together in the same subfunction*


Variable Interaction Graph (VIG)

If $\mathbf{x}_{\mathrm{i}}$ and $\mathrm{x}_{\mathrm{j}}$ don't interact: $\Delta_{\mathrm{ij}}=\Delta_{\mathrm{i}}+\Delta_{\mathrm{j}}$

## Hamming Ball Hill Climber (HBHC)

Identifying improving moves in a ball of radius $r$ around solution $x$


Based on the concept of Score (delta evaluation): $\Delta_{v}$
GECCO 2014: C., Whitley, Sutton

## Partition Crossover (PX)

## Let us suppose our function has the following VIG...



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## Partition Crossover (PX)

PX creates a graph with only the differing variables (recombination graph)


All the variables in a component are taken from the same parent
The contribution of each component to the fitness value of the offspring is independent of each other

FOGA 2015: Tinós, Whitley, C.

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## Articulation Points Partition Crossover (APX)

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## Articulation Points Partition Crossover (APX)



GECCO 2018: C., Ochoa, Whitley, Tinós

## Articulation Points in a Graph



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## Articulation Points



## Articulation Points Partition Crossover (APX)

APX identifies articulation points in the recombination graph


It implicitly considers all the solutions PX would consider if one or none articulation point is removed from each connected component
GECCO 2018: C., Ochoa, Whitley, Tinós

## Articulation Points Partition Crossover (APX)

## Example for NKQ Landscapes with N=100 000 and K=2 (DRILS+APX)



There are 4339 nodes grouped in 858 components with 1825 articulation points (in red)
GECCO 2018: C., Ochoa, Whitley, Tinós

## Articulation Points Partition Crossover (APX)

The number of implicitly studied solutions is:
Degree of an articulation point in the recominbation graph


## Articulation Points Partition Crossover (APX)

All the analysis can be done using Tarjan's algorithm to find articulation points (DFSlike algorithm) : time complexity is the same as the original PX


GECCO 2018: C., Ochoa, Whitley, Tinós

## Deterministic Recombination and Iterated Local Search (DRILS)



## Experimental Results

- An NK Landscape is a pseudo-Boolean optimization problem with objective function:

$$
f(x)=\sum_{l=1}^{N} f^{(l)}(x)
$$

where each subfunction $f^{\prime \prime}$ depends on variable $x_{I}$ and $K$ other variables


## Experimental Results

1M variable adjacent NK Landscape with $\mathrm{K}=3$


## Experimental Results

100,000 variable adjacent NK Landscape

$K=1$

$K=5$

GB-P3: Gray-Box Parameter-less Population Pyramid
GECCO 2015: Goldman, Punch

## Experimental Results

100,000 variable random NK Landscape

$K=1$

$K=5$

## Experimental Results

## Average number of components found by Partition Crossover

|  | Perturbation Factor $(\alpha)$ |  |  |  |  |  |
| :---: | ---: | ---: | ---: | ---: | ---: | :---: |
| $K$ | 0.005 | 0.01 | 0.05 | 0.10 | 0.15 |  |
| 1 | 683 | 1,314 | 6,059 | 11,442 | 16,259 |  |
| 2 | 967 | 1,772 | 6,938 | 11,426 | 13,428 |  |
| 3 | 1,041 | 1,810 | 4,970 | 3,639 | 2,367 |  |
| 4 | 993 | 1,657 | 1,780 | 661 | 301 |  |
| 5 | 903 | 1,344 | 517 | 100 | 38 |  |

## 24,970 solutions considered in each PX ( $10^{1,485}$ solutions per nanosecond)

1M variable random NK Landscapes

## Experimental Results

APX runtime is in the same order of magnitude than that of PX

| $N$ | $K$ | \#Comp. | \#APs | $d_{a}$ | $\log _{2} E(x, y)$ |
| ---: | ---: | ---: | ---: | ---: | ---: |
| $10^{5}$ | 2 | 662 | 687 | 2.25 | 1311 |
|  | 4 | 503 | 1151 | 2.37 | 1105 |
|  | 5 | 138 | 196 | 2.33 | 286 |
|  | 3 | 7774 | 10836 | 2.28 | 15987 |
|  | 3 | 4515 | 21793 | 2.35 | 9454 |
|  | 4 | 1748 | 6281 | 2.38 | 3907 |
|  | 5 | 1105 | 7207 | 2.34 | 2341 |


| Runtime (ms) |  |
| ---: | ---: |
| APX | PX |
| 55 | 46 |
| 67 | 73 |
| 55 | 52 |
| 63 | 52 |
| 1383 | 970 |
| 1785 | 2485 |
| 1360 | 1439 |
| 1633 | 1559 |

## Experimental Results

APX runtime is in the same order of magnitude than that of $P X$ and the number of solutions explored is squared!

$|A P X| \approx|P X|^{2}$


| $N$ | $K$ | \#Comp. | \#APs | $d_{a}$ | $\log _{2} E(x, y)$ |
| ---: | ---: | ---: | ---: | ---: | ---: |
| $10^{5}$ | 2 | 662 | 687 | 2.25 | 1311 |
|  | 4 | 503 | 1151 | 2.37 | 1105 |
|  | 5 | 138 | 196 | 2.33 | 286 |
|  | 2 | 7774 | 218 | 2.36 | 254 |
|  | 3 | 4515 | 21793 | 2.35 | 9454 |
|  | 4 | 1748 | 6281 | 2.38 | 3907 |
|  | 5 | 1105 | 7207 | 2.34 | 2341 |

## Experimental Results

## DRILS and DRILS+APX solving NKQ Landscapes with $\mathbf{N}=1$ Million and $\mathrm{K}=3$



## Experimental Results

DRILS and DRILS+APX solving MAX-SAT (instances from MAX-SAT Evaluation 2017)

| Instances | $\alpha$ | DRILS performance |  |  | Runtime ( $\mu \mathrm{s}$ ) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | APX | PX | Sim. | APX | PX |
| Unweighted | 0.10 | 78 | 1 | 81 | 463 | 454 |
|  | 0.20 | 82 | 2 | 75 | 684 | 729 |
|  | 0.30 | 85 | 2 | 73 | 849 | 1060 |
| Weighted | 0.10 | 26 | 19 | 87 | 1425 | 882 |
|  | 0.20 | 49 | 14 | 69 | 1859 | 1416 |
|  | 0.30 | 77 | 5 | 50 | 2365 | 1713 |

## Conclusions

- The Variable Interaction Graph provides useful information to improve the search
- Articulation Points Partition Crossover squares the number of solutions considered by $P X$ in around the same time
- APX is specially good in Unweighted MAX-SAT instances (many plateaus)
- Take home message: use Gray-Box Optimization if you can


## Future Work

- Plateaus exploration in MAX-SAT guided by APX
- New ways of perturbing the solution to maximize the components in (A)PX
- Look at the Variable Interaction Graph of industrial problems


## Enhancing Partition Crossover with Articulation Points Analysis



## Acknowledgements



