Emerging Techniques for Optimisation Heuristics Analysis

– Structural Bias Detection –

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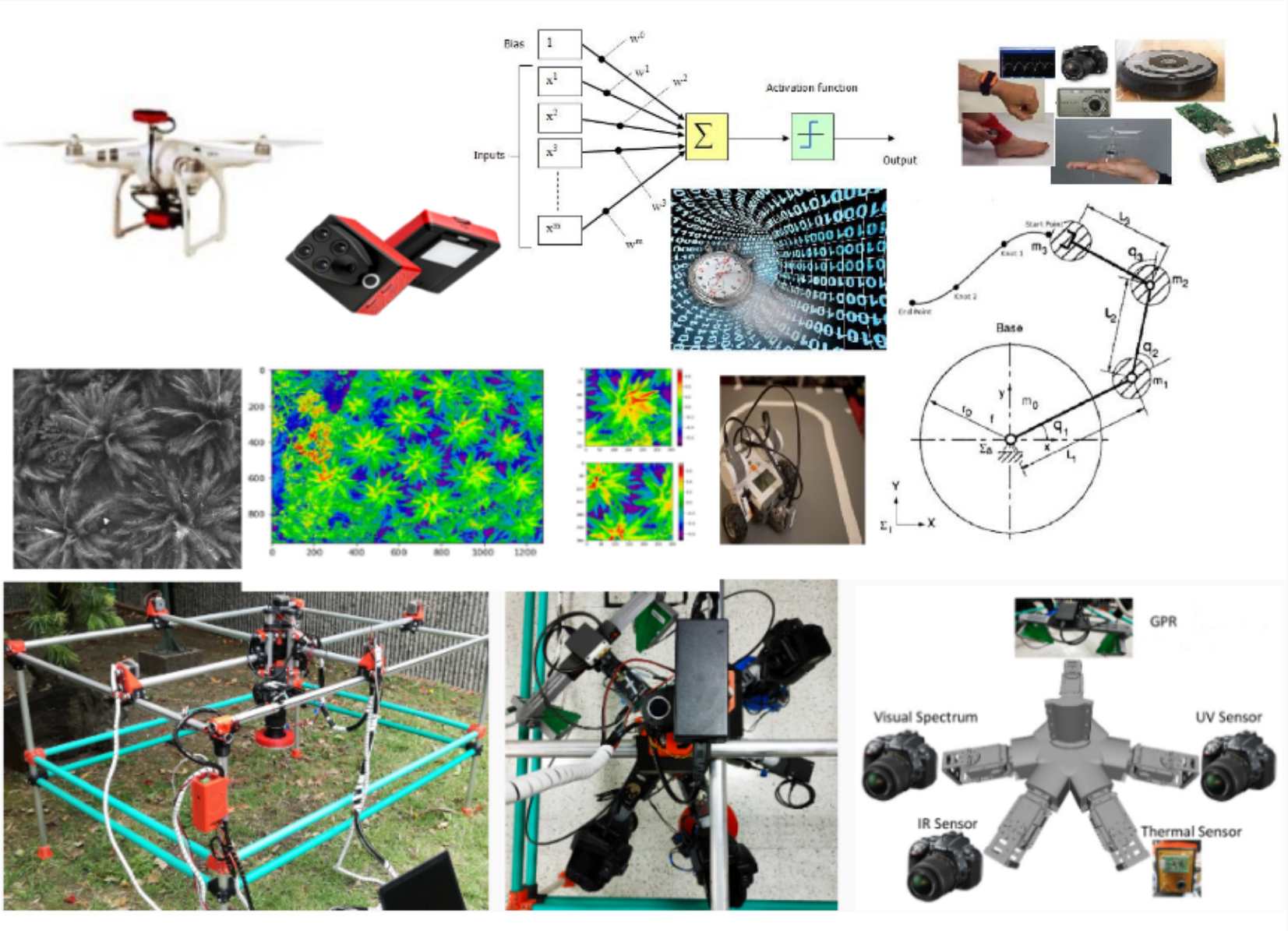



3/08/2023

Heuristcs in the real world

Some of my projects, etc.

[1, 8, 12, 10, 11, 2]



(Meta)heuristic optimisation

No assumptions nor analytical formulation of the problem are required!

A logical choice of such optimisation tools if from the fields:



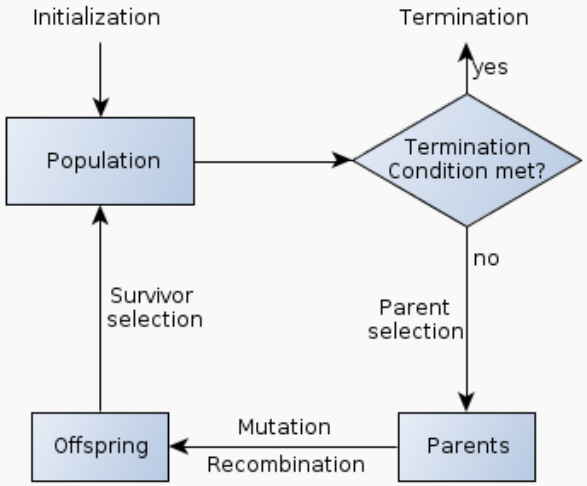


. . . significant EC methods are e.g. those referred to as Evolutionary Algorithms

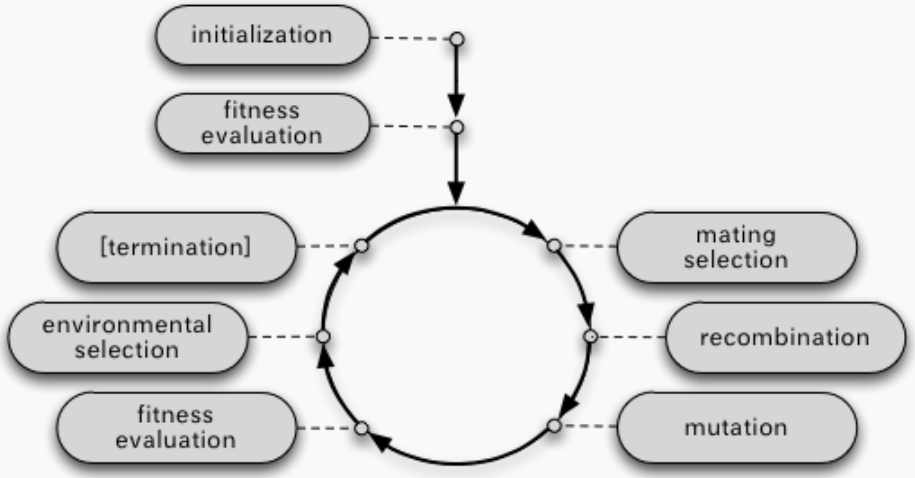
Evolutionary algorithms: general scheme.
[7]

Evolutionary Algorithms pseudo-code

INTITIALISE population with random candidate solutions
EVALUATE each solution
while *condition on budget* **do** ▷ or fitness value!
  SELECT parents ▷ 2 or multiple solutions
  RECOMBINE parents ▷ 2 or some of them
  MUTATE the resulting offspring
  EVALUATE new candidates
  SELECT individual for next generation
end while
Output best individual of the final population



Solutions cycle



Selection and variation operators cycle

Swarm intelligence optimisation: general scheme
(similar iterative frameworks for other classes of heuristic algorithms. . .)

- population-based;
- each individual "move" thanks to a moving operator that makes use of the other individuals;
- One-to-one replacement (one-to-one spawning) right after the move.

Swarm Intelligence optimization

Initialisation ▷ Randomly sample initial swarm
while *Condition on budget* **do**
  for each $x \in$ *Swarm* **do**
    Update moving parameters
    Perform move
    Evaluate $f(x)$ *and eventually perform replacement* ▷ one-to-one spawning
  end for
end while
Output *Best Individual*

A popular
- EA framework is the Genetic Algorithms (GA) [9];
- SI is the Particle Swarm Optimization (PSO) [6];
- while Differential Evolution (DE) [20] is a borderline case.

Where do we stand?

. . . and where do we need to go?

There have been tremendous advancements in the subject field in the last few decades, but. . .

- Algorithmic design is still performed in a partially blind way ✗
  - Due to the lack of theoretical and empirical knowledge of the algorithm!





Methaphore-based algorithm 👎

[3, 19, 27]

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- Parameter tuning is still an open issue and very dependent on the specific problem at hand ✗
  - Is it possible to find fitness-free indicators?

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Performance-driven analysis

- cannot generalise
- premature convergence, diversity loss, etc., still unexplained

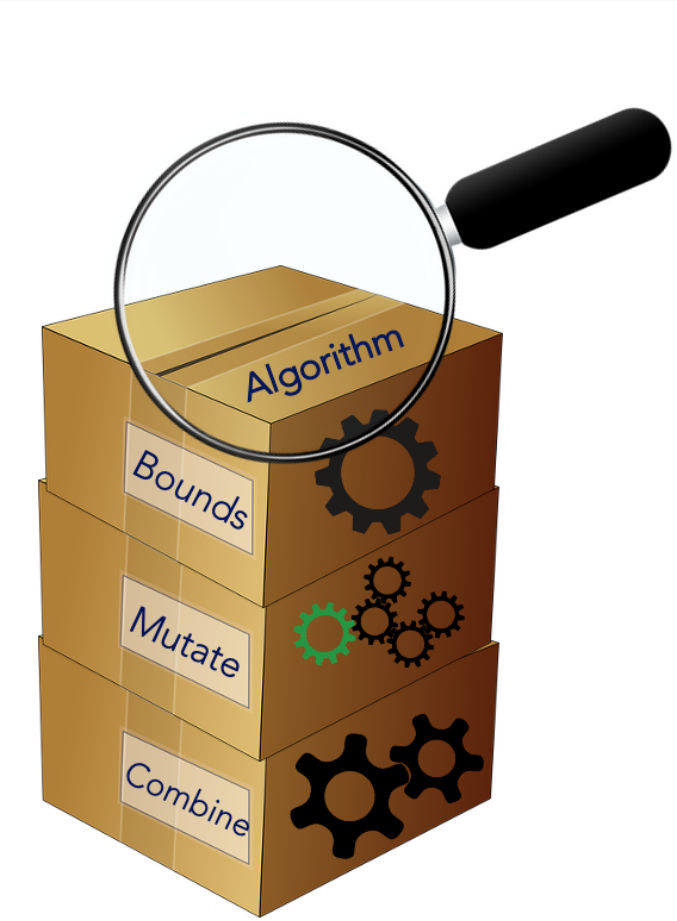
Adding fitness-free analysis 👍

- Algorithm selection and characterisation
- More informed algorithmic design

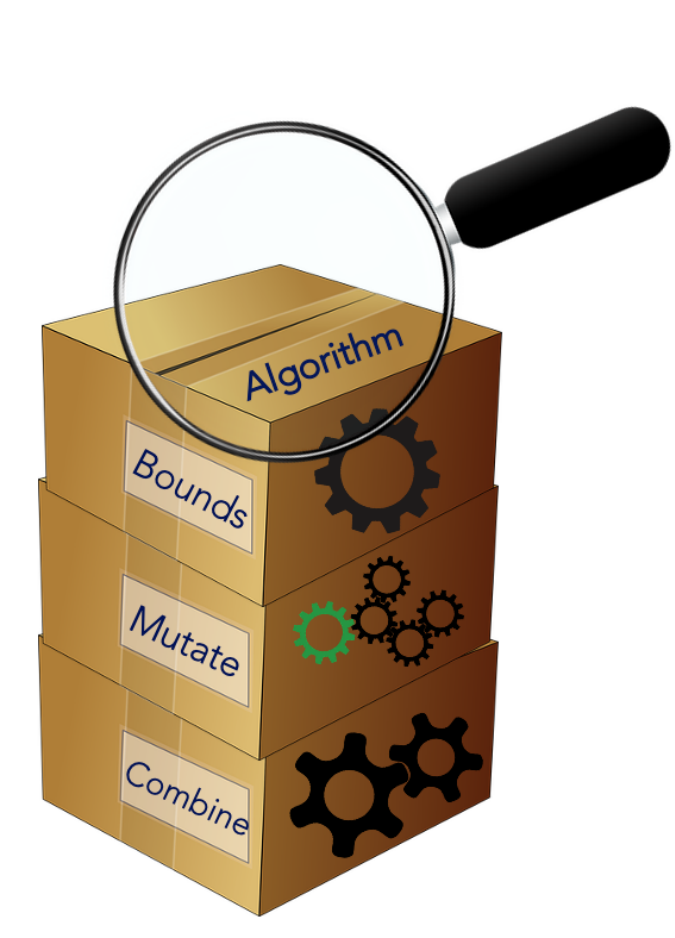
Algorithmich Behaviour

Opening the lid of an optimisation algorithm

- What are the dynamics of the population?
- Are always the problem's features to blame?
- More informed tuning and design approach
- More general knowledge and explainability



Algorithmich Behaviour

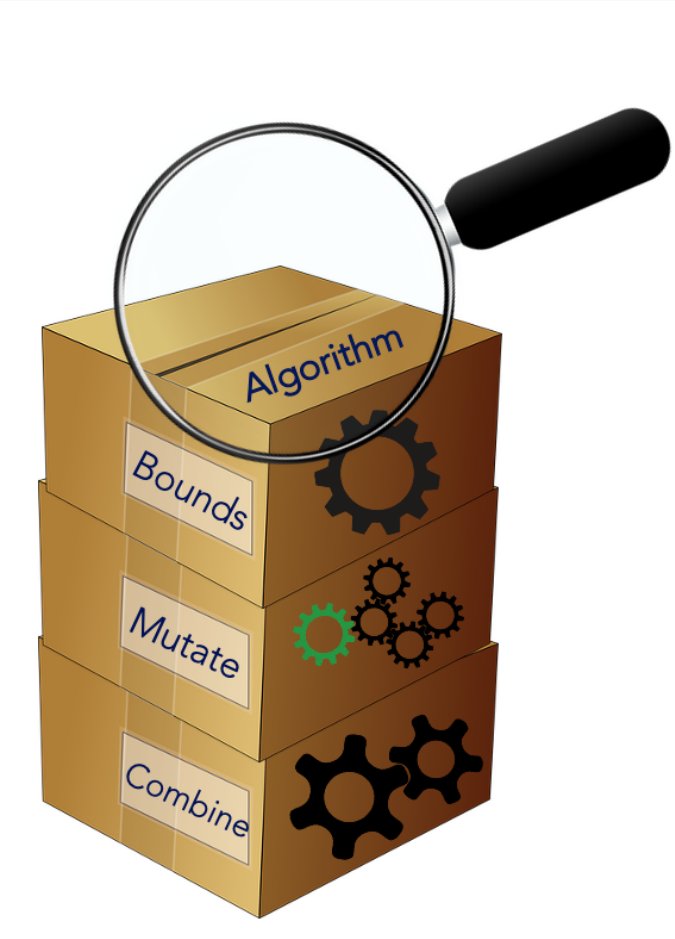


- Network Analysis
- Search direction disruptiveness
- Infeasibility
  (cosine similarity, Euclidean distance,. . .)

Some interesting breakthroughs

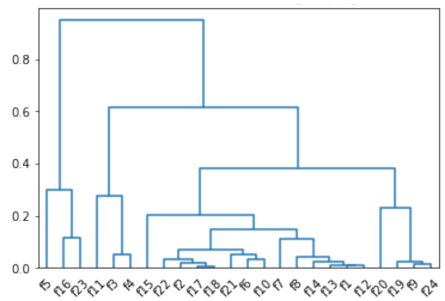
- Differential Evolution Outside the Box [13]
- The Importance of Being Constrained: Dealing with Infeasible Solutions in Differential Evolution and Beyond [17]
- Patterns of convergence and bound constraint violation in differential evolution on sbox-cost benchmarking suite [18]

Algorithmich Behaviour

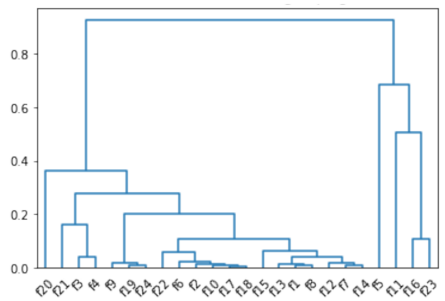


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  (cosine similarity, Euclidean distance,. . .)

Clustering criterion: similarity between functions based on the ratio of infeasible components
Linkage: complete



SBOX

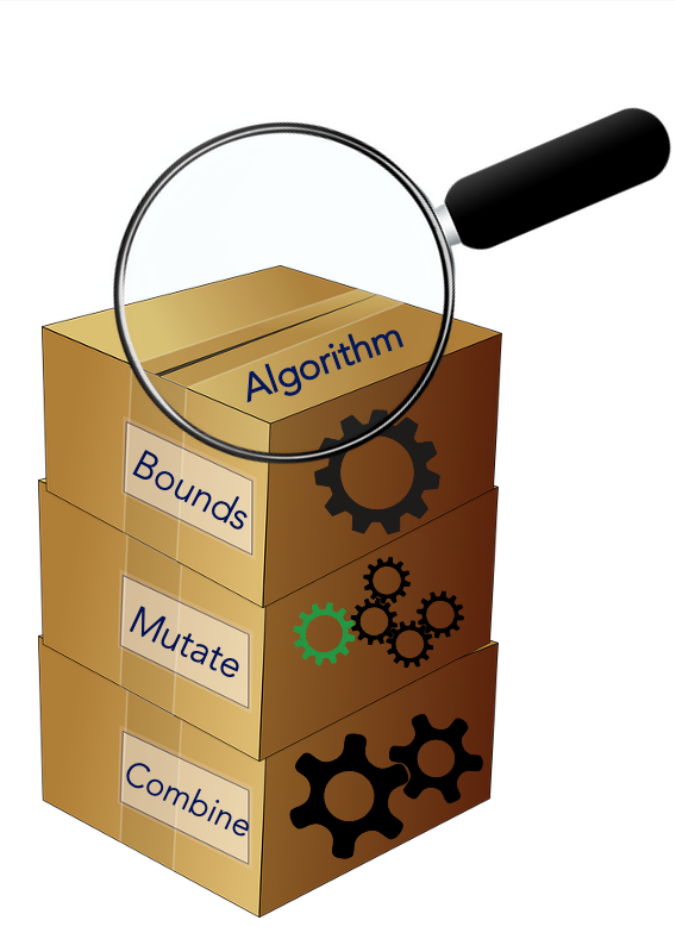


BBOB

$$p_v(g+1) \simeq \frac{p_v(g)}{2} + (1-p_v(g))\left(p_v^2(g)\frac{F}{2} + (1-p_v^2(g))\frac{F}{3}\right)$$

The sequence $p_v(g)$ converges between $F/3$ and $2F/3$ – see [17]

Algorithmich Behaviour
Structural Bias



- Network Analysis
- Search direction disruptiveness
- Infeasibility
  (cosine similarity, Euclidean distance,. . .)
- Distributions of best solutions
  (Structural Bias)

Structural Bias

What is Structural Bias for an optimisation heuristc? An informal definition...

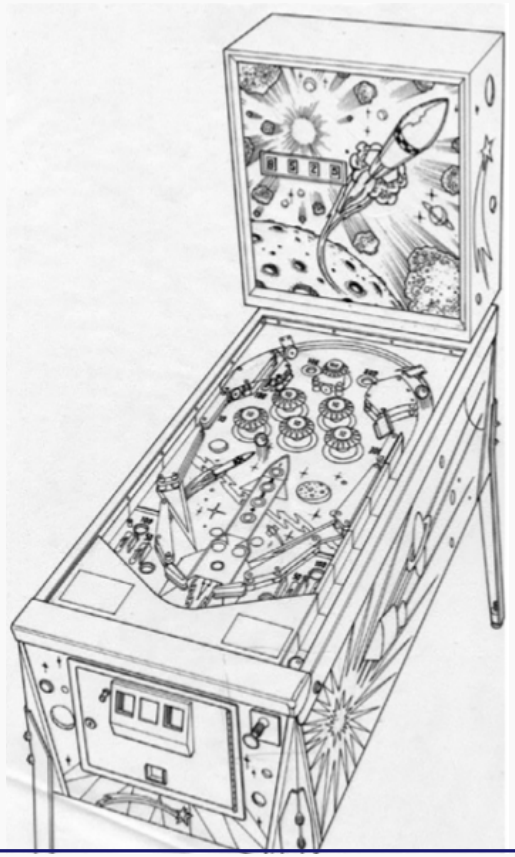
> An optimisation algorithm is said to possess Structural Bias (SB) if it gives preference to some parts of the domain regardless of $f(x)$ [16]

Structural Bias

What is Structural Bias for an optimisation heuristc? An informal definition...

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- imagine an algorithm (**general purpose and thus unbiased**) as a pinball machine where a player aims at keeping the ball on the game surface as long as possible:



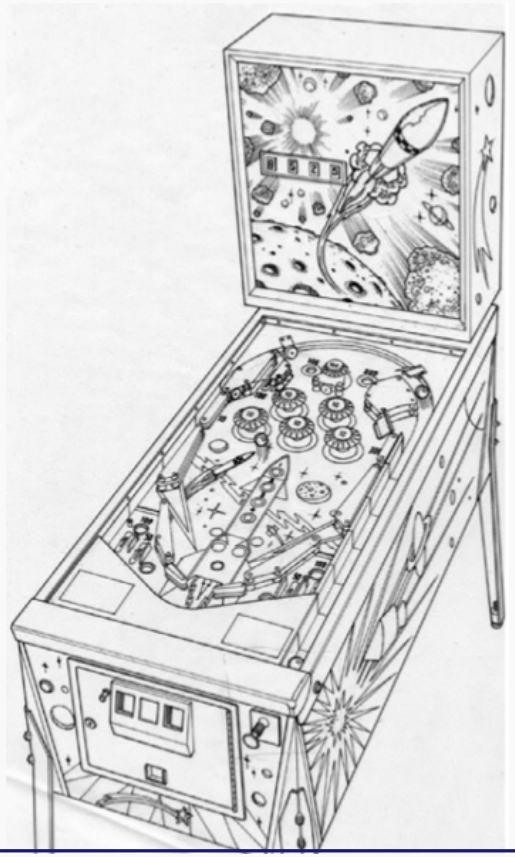
- if the ball is the candidate solution;
  - and multiple games are happening to conceptualise population-based frameworks;
- then trajectories drawn by the balls should access the entire game surface...

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However, this is not the case:

no matter how trained the player is and the precise mechanical structure of the pinball, due to gravity, the balls will eventually roll to its lower side!

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Similarly, metaheuristics algorithms intrinsically tend to privilege regions of the search space, ending up with:

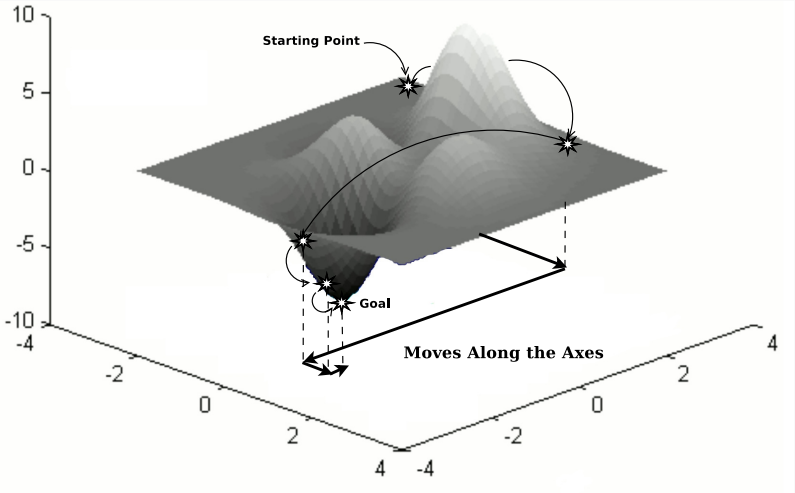
- premature convergence;
- unsatisfactory solutions;
- low exploration of the search space, etc.

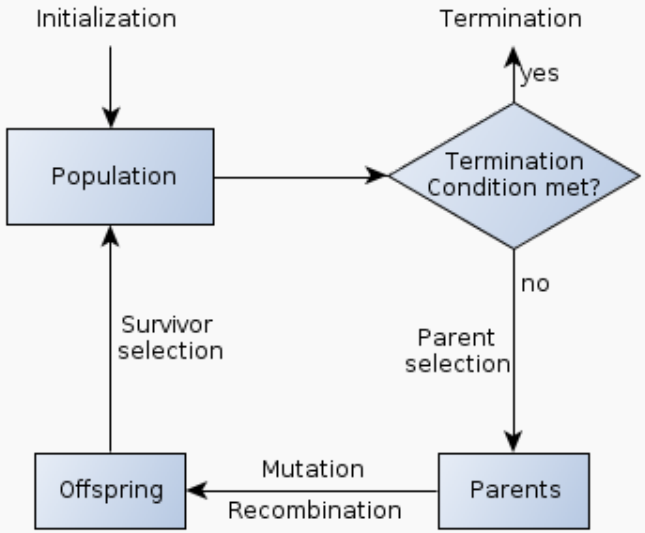


Looking for Structural Bias

For a general objective function, the movement of a solution or population of solutions is dictated by a superposition of two forces of:

1. the "gradient" formed by the values of objective function in the current population
2. SB that originates from the structure of the iteratively operating algorithm.





These are not necessarily in agreement in terms of direction and strength!

To detect 1, one must nullify 2!

Looking for Structural Bias
The testbed

- For the purpose of identifying SB, we make use of an optimisation problem defined as:

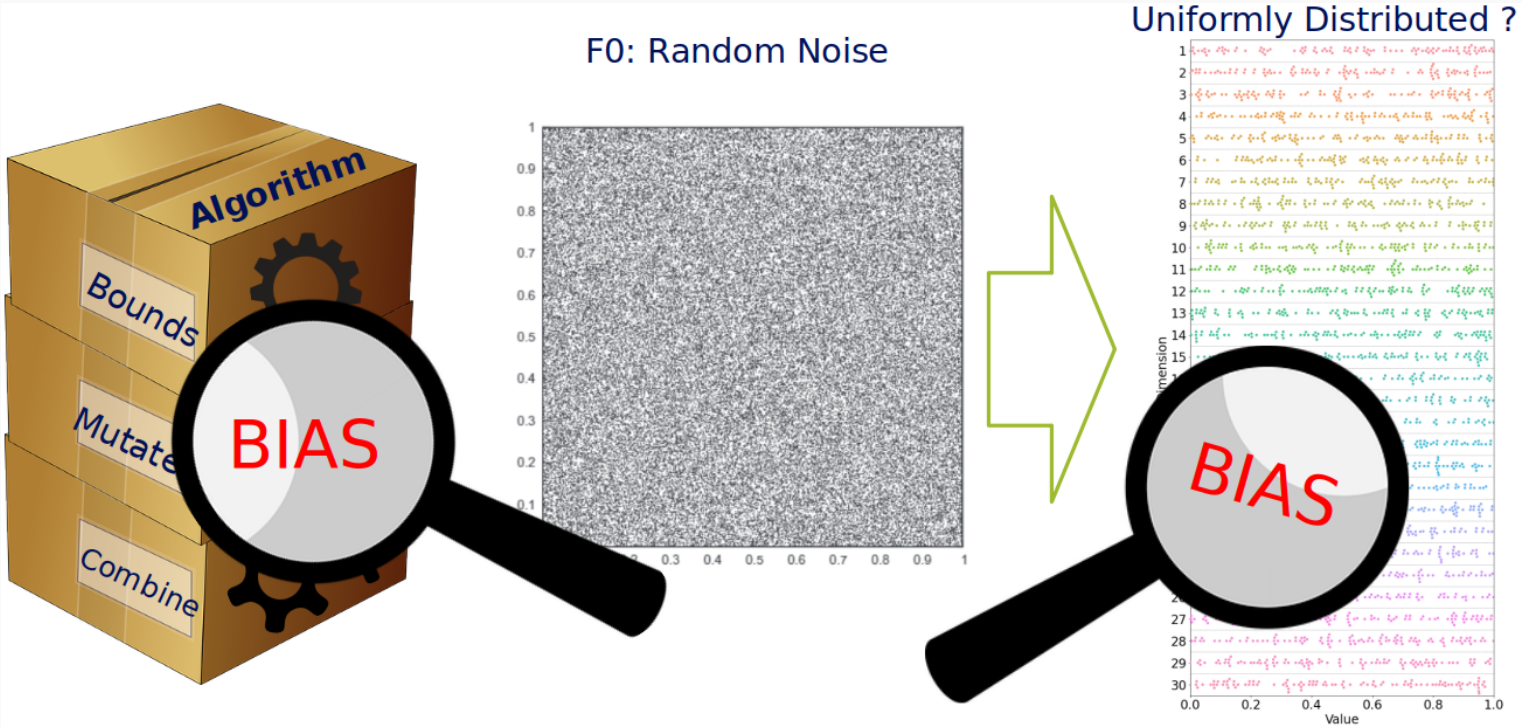
$$f_0 \rightarrow min, \quad f_0 : [0,1]^n \subset \mathbb{R}^n \rightarrow [0,1], \quad f_0(x) = Uniform[0,1]$$

- An ideal unbiased algorithm should return a uniform distribution of the best final solutions, over a series of independent runs [16].

Looking for Structural Bias

A formal (operative) definition

An optimisation algorithm is structurally biased if the distribution of the best solutions obtained with multiple runs on $f_0(x)$ is not uniform.

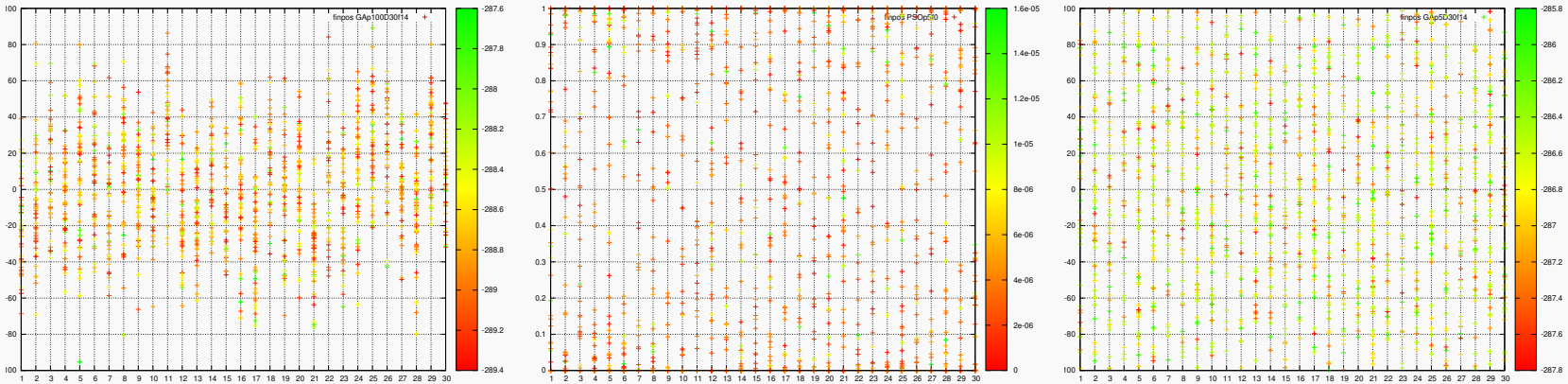


Looking for Structural Bias
A visual approach

- Final populations (obtained in different runs) were displayed in parallel coordinates,
  - i.e. coordinates of a vector in an n-dimensional space are marked on n equally spaced parallel lines.

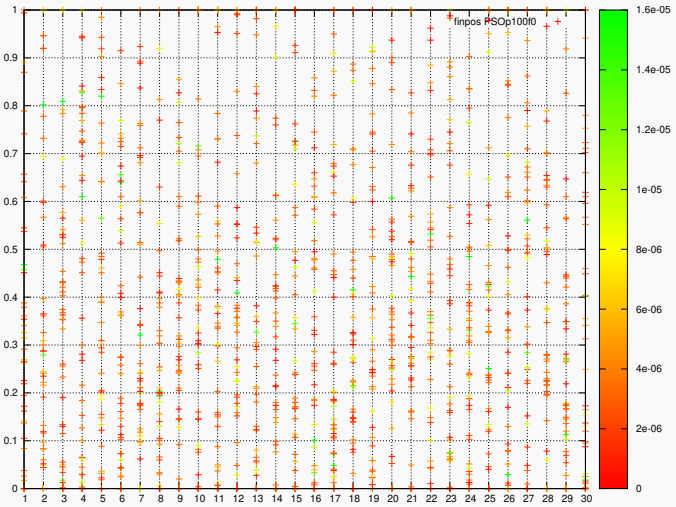
An unbiased structure should return points homogeneously filling the entire interval in each dimension.

Conversely, a biased one, should show clusters of best solutions accumulated in one or more segments of parallel lines.



Looking for Structural Bias
A visual approach

- Easy to produce and intuitive 👍 (in the presence of clear SB)
- Subjective and time-onerous to inspect in large-scale experiments 👎



- We visualised SB for hundreds and hundreds of algorithm configurations [16, 4, 5, 14, 15, 26]
- and found multiple bias types and interesting patterns and correlations to performance, parameters, bound constraint handling methods,. . . [24, 21, 23]

Want to see more?

Look at the online repositories 🔗🔗🔗 (also referenced in the articles).

Looking for Structural Bias
A statistical approach

Testing for uniformity

- Staistic is an established field ✓
- Tests are easily automatised and displayed even in large-scale settings ✓
  - Degree (strength) of SB computed as # of rejected dimensions ✓

Kind of SB test:	visual					statistical				
Configuration:	CUTN	dismiss	mirror	saturation	toroidal	CUTN	dismiss	mirror	saturation	toroidal
cDE/rand/1/bin	=	=	•	•	=	0.00	0.00	0.02	∞	0.13
cDE/rand/1/exp	=	•	=	•	=	0.00	0.00	0.00	∞	0.02
cDE/rand/2/bin	•	=	•	•	•	0.02	0.00	0.02	∞	0.21
cDE/rand/2/exp	=	=	=	•	=	0.00	0.00	0.00	∞	0.06
cDE/current-to-rand/1	=	=	=	•	•	0.00	0.02	0.00	∞	0.00
cDE/best/1/bin	=	•	•	•	=	0.01	0.00	0.00	∞	0.00
cDE/best/1/exp	•	=	=	•	•	0.00	0.00	0.00	∞	0.00
cDE/best/2/bin	=	=	=	•	•	0.01	0.00	0.00	∞	0.01
cDE/best/2/exp	=	=	=	•	•	0.00	0.00	0.00	∞	0.01
cDE/current-to-best/1/bin	•	=	=	•	•	0.00	0.00	0.01	∞	0.02
cDE/current-to-best/1/exp	•	=	=	•	•	0.00	0.00	0.00	1.00	0.01
cDE/rand-to-best/2/bin	•	=	=	•	=	0.00	0.00	0.00	∞	0.01
cDE/rand-to-best/2/exp	•	•	•	•	•	0.02	0.00	0.00	∞	0.02
cDE-Light	•	•	•	•	•	0.00	0.00	0.00	0.01	0.00
cPSO	=	•	=	•	=	0.03	0.00	0.44	∞	0.01
cBFO	=	=	=	=	=	1.00	0.92	1.00	0.96	0.93
cGA (no SDIS, shown as dismiss)	×	•	×	×	×	×	0.01	×	×	×
Found strong SB/total cases:	1/16	1/17	2/16	1/16	1/16	1/16	1/17	2/16	15/16	2/16
Found mild SB/total cases:	8/16	6/17	4/16	13/16	9/16	5/16	2/17	3/16	1/16	10/16
Strong/mild/no SB cases:	6/40/35					21/26/59				
Agreement between	56	65	69	6	44	all cases				
visual and statistical	100	100	100	100	100	cases with strong SB only*				
tests (in %, calculated	38	17	25	0	55	cases with mild SB only				
'post factum'):	71	90	80	0	17	cases with no SB only				

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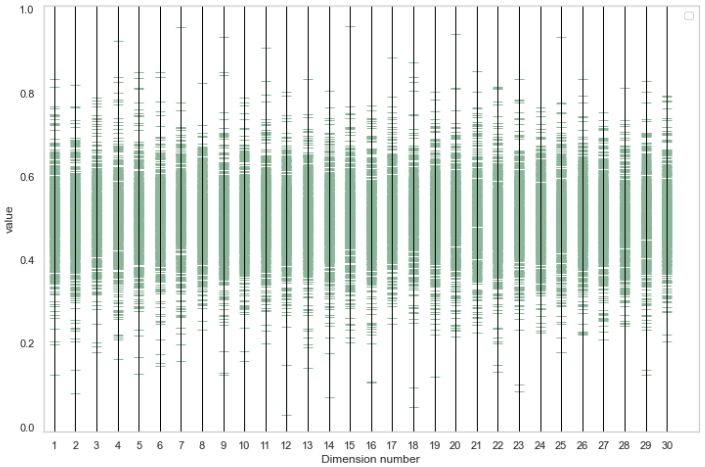
Challenges **[16, 15, 14, 21]**

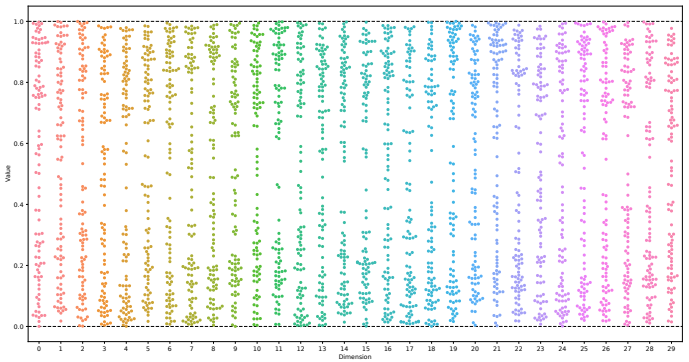
- Sensitivity, etc. depends on the sample size N! ✗
- different test might disagree with low/high sample sizes ✗
- Kolmogorov–Smirnov→Cramér-Von Mises→Anderson–Darling + Benjamini–Hochberg correction ($N = 100$, detect Strong SB)
- To detect mild SB with good results $N = 600$ is needed (unpractical 👎)

Looking for Structural Bias
A statistical approach

BIAS TOOLBOX [25]
(also available on)

- 36 per-dimension statistical tests
- 32 across-dimension statistical tests
  - + Random Forest
- Comes with data and plot generator! 👍
- Detects/predicts bias 👍
- Classifies its kind 👍
- Measure SB strength 👍
- $N = 30 - 50$ 👍



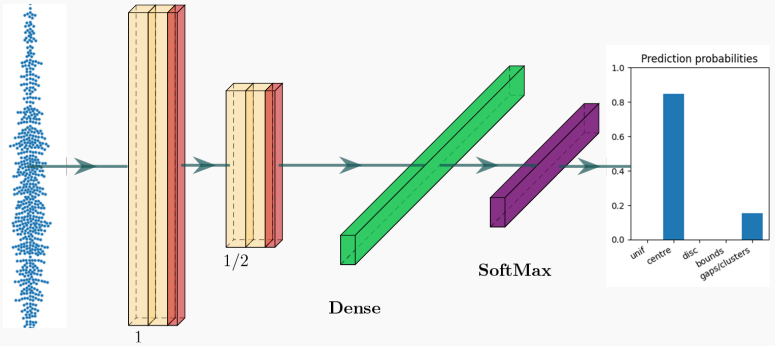


Looking for Structural Bias

A Deep Learning approach

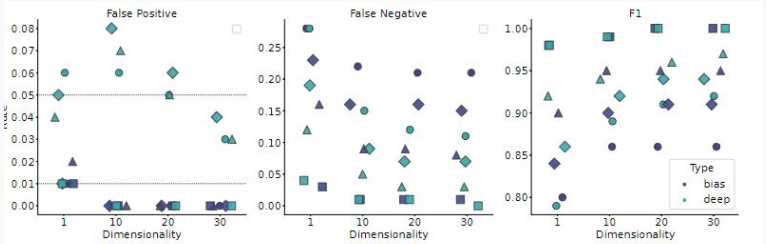
[code also available on GitHub]

Deep-BIAS extends the BIAS toolbox with a one-dimensional CNN to detect and classify SB [22].



Compared to BIAS, Deep-BIAS displays interesting and advantageous features:

- It outperforms the statistical test-based approach in classifying the type of SB.
- It gives a better measure of the strength of the SB by using the class probabilities.
- It provides additional insight by using XAI, where regions of interest in distributions can be further analysed to understand the mechanism behind the classifications



igure 1. Comparison (with $\alpha = 0.01$) of the original BIAS toolbox (blue) and the Deep-BIAS eal) in terms of false positives (left), false negatives (middle) and F1-score (right). On all gures, markers identify the used sample size: ○, ◇, △ and □ are 30, 50, 100 and 600, espectively.

Strucutral Bias
Why bother?

- to improve upon performances of "general purpose" algorithms;
- to achieve a more informed algorithm design, which is currently done in a partially blind manner by researchers;
- to help practitioners pick the right "off-the-shelf" optimiser and produce solutions of satisfactory quality for their real-world scenarios.


Thanks for Listening

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