Exploration and Exploitation in Evolutionary Algorithms: Recent Developments

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University of Catania, April 2, 2025

Overview

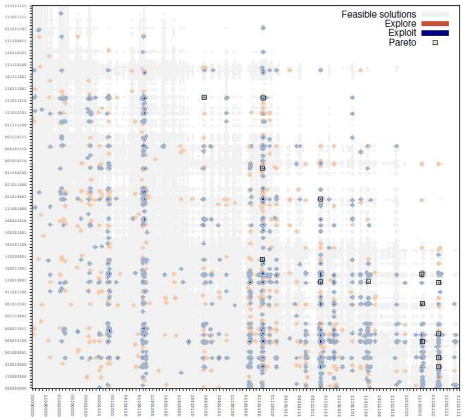
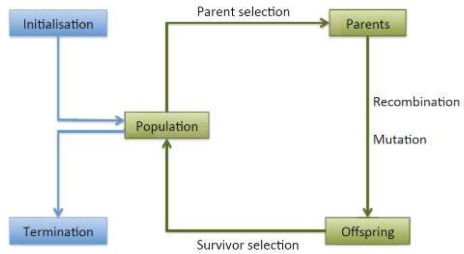


Fig. 7. Search space SPEA2



Short introduction to EAs

Exploration and Exploitation (E & E)

Measuring E & E

Open Problems

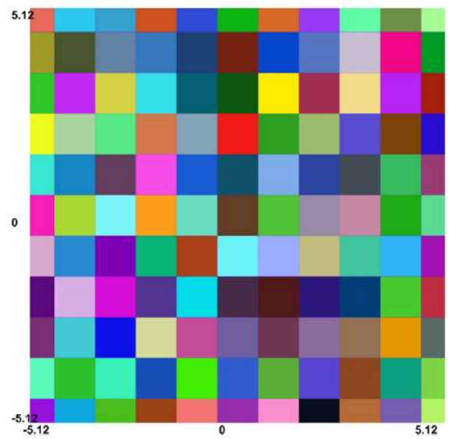
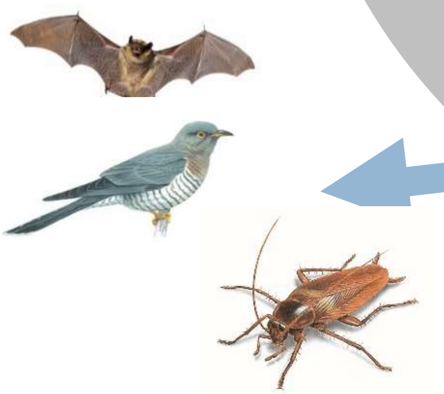


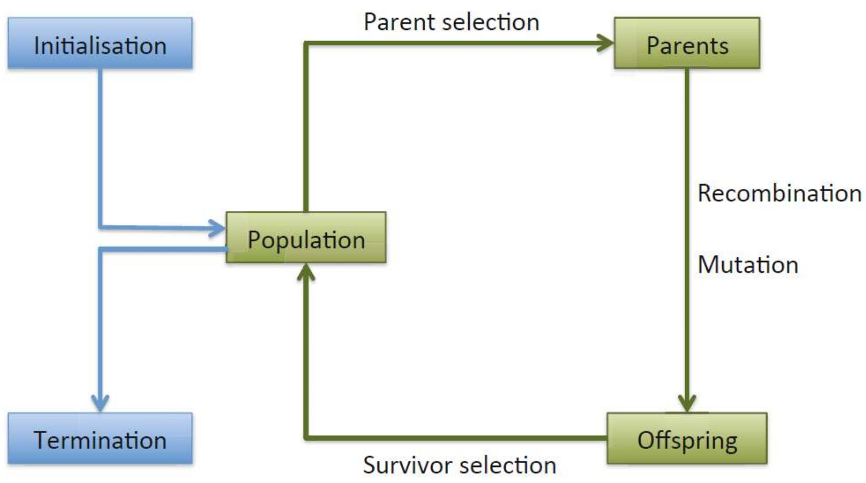
Fig. 4. Attraction basins for the Rastrigin function.



Short introduction to EAs

Basic Evolutionary Algorithm (EA)

```
BEGIN
  INITIALISE population with random candidate solutions;
  EVALUATE each candidate;
  REPEAT UNTIL ( TERMINATION CONDITION is satisfied ) DO
    1 SELECT parents;
    2 RECOMBINE pairs of parents;
    3 MUTATE the resulting offspring;
    4 EVALUATE new candidates;
    5 SELECT individuals for the next generation;
  OD
END
```

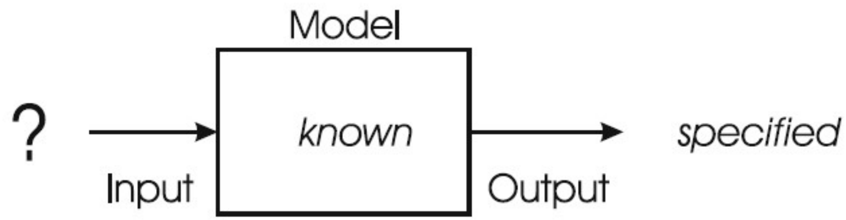


A. E. Eiben, J. E. Smith: *Introduction to Evolutionary Computing*, Springer-Verlag, Berlin, 2003

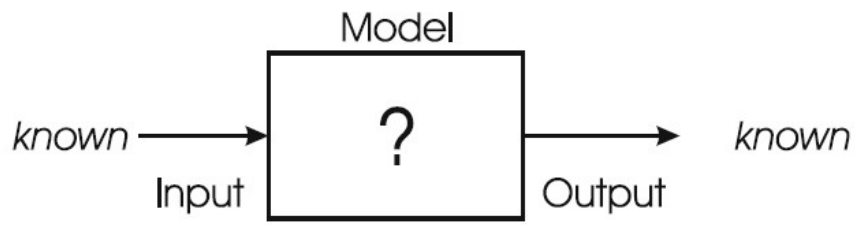
Short introduction to EAs

- Evolutionary Computing: Why?

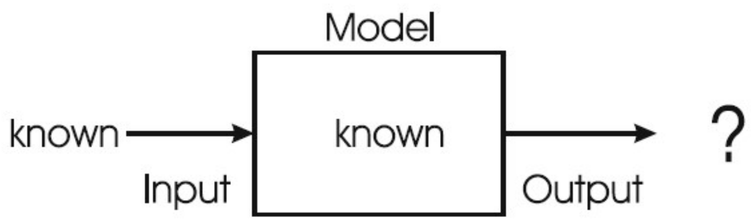
- Optimisation



- Modelling



- Simulation



Exploration and Exploitation

Exploration is a process of visiting entirely new regions of a search space.

Exploitation is a process of visiting regions of a search space based on neighborhood of previously visited points.

M. Črepinšek, S.-H. Liu, M. Mernik. Exploration and Exploitation in Evolutionary Algorithms: A Survey. ACM Computing Surveys, Vol. 45, No. 3, Article 35, 2013.

Exploration and Exploitation

- Many researchers believe that EAs are effective because of a good ratio between exploration and exploitation.
- *„Genetic Algorithms are a class of general purpose (domain independent) search methods which strike a remarkable balance between exploration and exploitation of the search space.“* [Michalewicz 1996]
- *„The genetic algorithm behaviour is determined by the exploitation and exploration relationship kept throughout the run.“* [Herrera and Lozano, 1996]

Exploration and Exploitation

- To be successful a search algorithm needs to find a good balance between exploration and exploitation.

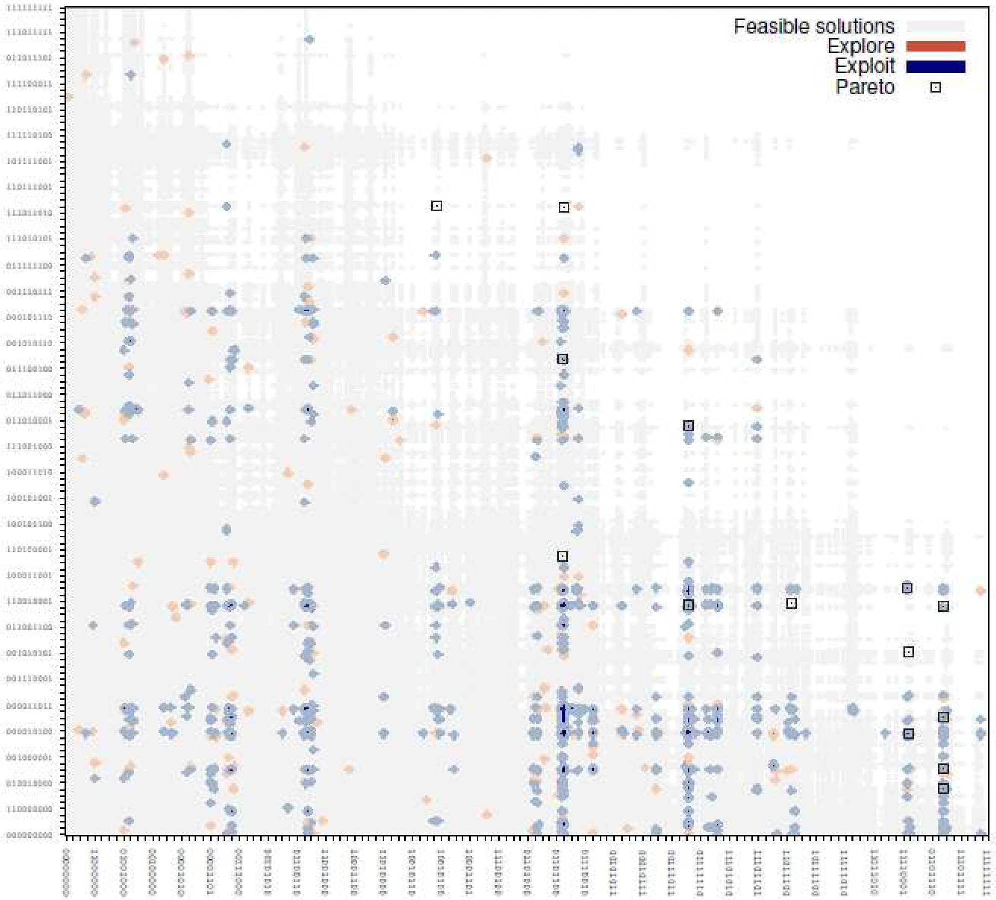


Fig. 6. Search space VEGA

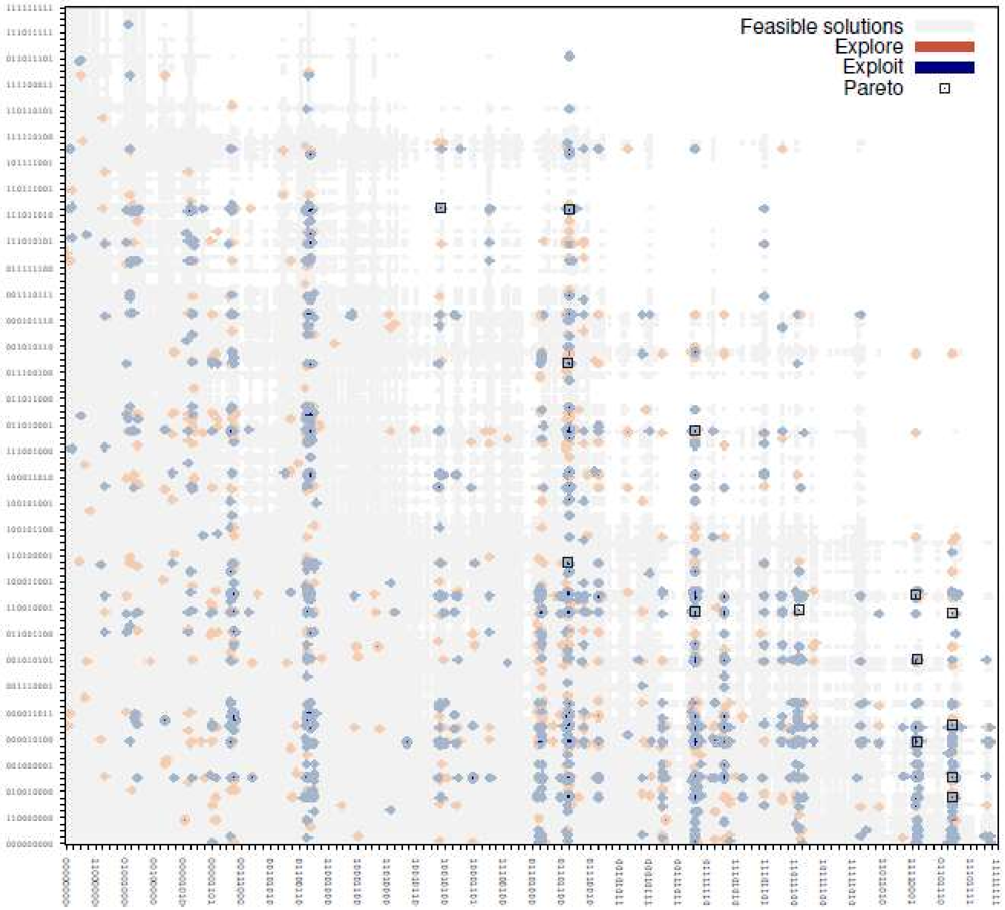


Fig. 7. Search space SPEA2

Exploration and Exploitation

- Common, but wrong, opinion about EAs is that they explore the search space by crossover/mutation operators, while exploitation is done by selection.
- Actually, exploration and exploitation are achieved by selection, mutation and crossover. But it is difficult to delimit exploration from exploitation in these processes.
- If crossover and mutation rates are very high, much of the space will be explored, but there is a high probability of losing good solutions. In such case EA heads towards random search.
- If crossover and mutation rates are low, the search space is not explored, at all. In such case EA is closer to hill climbing algorithms.

Exploration and Exploitation

- To explore or to exploit? This is the question now. *(anonymous EA agent)*

- Up to now, achieving the balance between exploration and exploitation is managed by proper control parameter setting.
- What control parameter settings are most likely to produce the best results is the question that every EA developer/user has to face.
- Parameter tuning and parameter control (deterministic, adaptive, self-adaptive).

Exploration and Exploitation

- With better understanding of Exploration and Exploitation we are able to better understand differences among EAs, and to develop better EAs.
- *„It is a remarkable fact that each algorithm emphasizes different features as being most important for a successful evolution process. … Both ESs and EP concentrate on mutation as the main search operator, while the role of (pure random) mutation in canonical GAs is usually seen to be of secondary (if any) importance. On the other hand, recombination plays a major role in canonical GAs, is missing completely in EP, and is urgently necessary for use in connection to self-adaptation in ESs.“* [Back and Schwefel 1993]

Measuring Exploration and Exploitation

- If we want to control Exploration and Exploitation then we need to know how to measure it.
- However, how to measure exploration and exploitation is an open question in EAs.
- Mostly indirect measures have been used:
  - Diversity based measures,
  - Entropy based measures,
  - Fitness improvement based measures.

Measuring Exploration and Exploitation

- If diversity is high, then individuals in a population are very different from each other. Hence, the algorithm must be in the phase of exploration. Conversely, if diversity is low, then individuals in a population are very similar and the algorithm must be in the phase of exploitation. Although it is simple and intuitive, it is only a rough approximation.

$$Div_j = \frac{1}{n}\sum_{i=1}^{n}\left|median(x^j) - x_i^j\right|$$

$$Div = \frac{1}{m}\sum_{j=1}^{m} Div_j$$

$$XPL\% = \left(\frac{Div}{Div_{max}}\right) \times 100$$

$$XPT\% = \left(\frac{|Div - Div_{max}|}{Div_{max}}\right) \times 100$$

Measuring Exploration and Exploitation

- We proposed a direct measure of exploration and exploitation in 2013:
- Crucial for delimiting exploration from exploitation is a definition of similarity to the closest neighbor *SCN*. However, when a new individual ind_{new} is created, a similarity measurement to the closest neighbor *SCN* can be defined in several ways:
  - As a similarity to its parent(s), ind_{parent}.
  - As a similarity to the most similar individual within the whole population *P*.
  - As a similarity to the most similar individual in the subpopulation $P' \land (P' \subset P)$ (e.g., only to individuals which belong to the same niche).
  - As a similarity to the most similar individual throughout the history of populations.

Measuring Exploration and Exploitation

$$\mathcal{SCN}(ind_{new}, P) = d(ind_{new}, ind_{parent}), \text{ where } ind_{parent} \in P.$$

$$\mathcal{SCN}(ind_{new}, P) = \min_{\substack{ind \in P \\ ind_{new} \neq ind.}} d(ind_{new}, ind).$$

$$\mathcal{SCN}(ind_{new}, P') = \min_{\substack{ind \in P' \wedge (P' \subset P) \\ ind_{new} \neq ind.}} d(ind_{new}, ind).$$

$$\mathcal{SCN}\left(ind_{new}, P^t\right) = \min_{\substack{ind \in P^t, t = 0..current\_gen \\ ind_{new} \neq ind}} d\left(ind_{new}, ind\right).$$

$$\mathcal{SCN}(ind_{new}, P) > X \qquad \text{(exploration)}$$

$$\mathcal{SCN}(ind_{new}, P) \leq X \qquad \text{(exploitation)}$$

Measuring Exploration and Exploitation

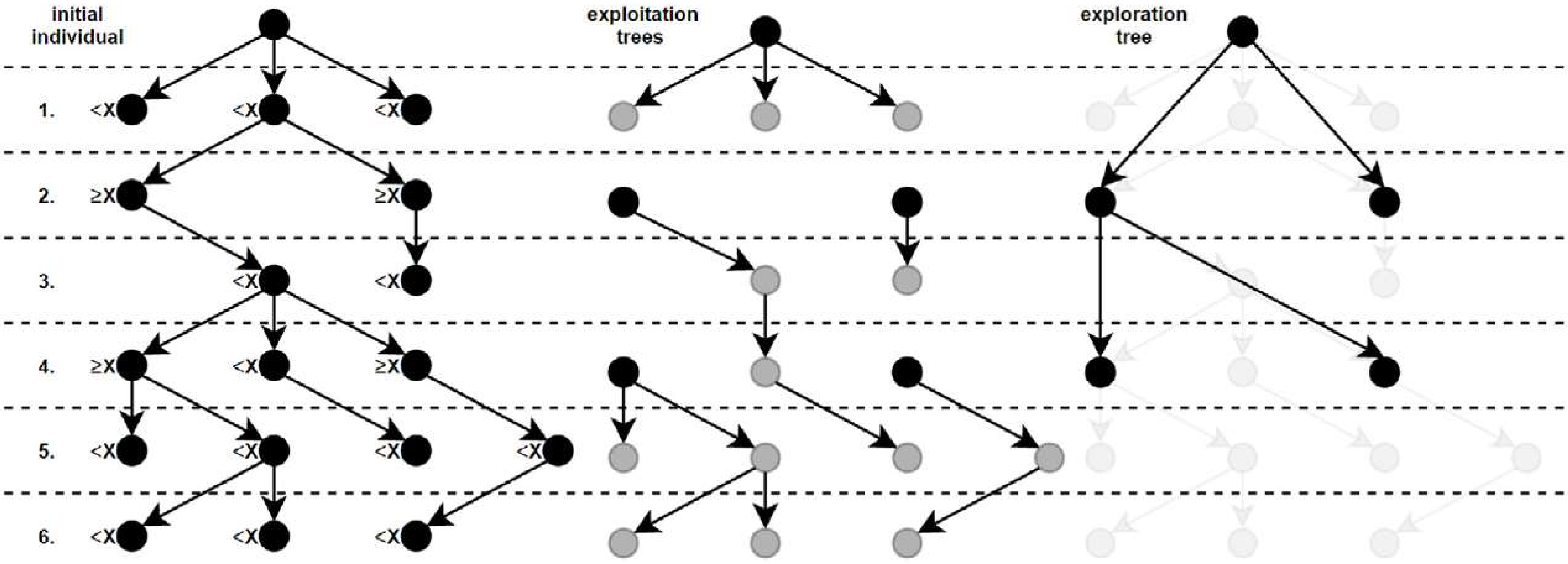


Fig. 6. An ancestry tree after six generations (Left), exploitation trees (Middle), an exploration tree (Right).

Measuring Exploration and Exploitation

- S-H. Liu, M. Mernik, D. Hrnčič, M. Črepinšek. A parameter control method of evolutionary algorithms using exploration and exploitation measures with a practical application for fitting Sovova's mass transfer model. Applied Soft Computing 13 (2013) 3792–3805

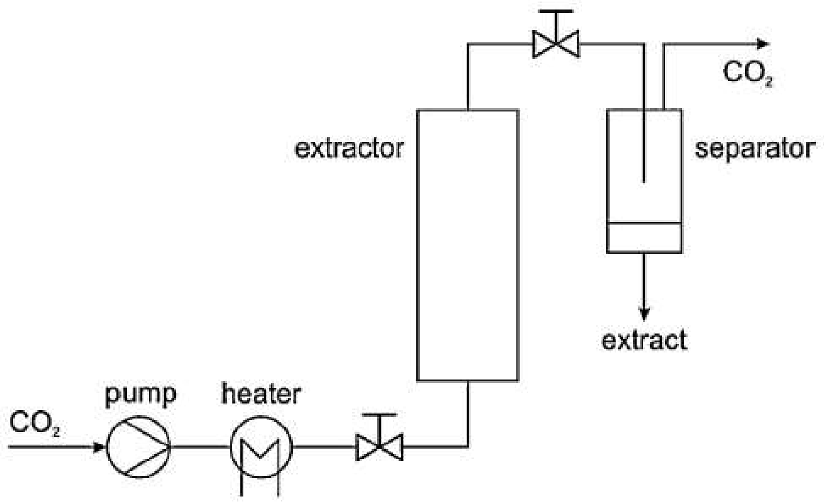


Fig. 2. Simple flow sheet of extraction process.

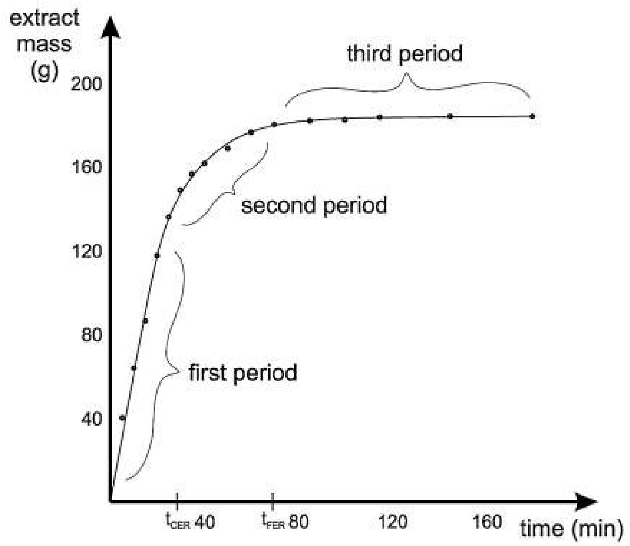


Fig. 3. Extraction curve separated into three periods.

Measuring Exploration and Exploitation

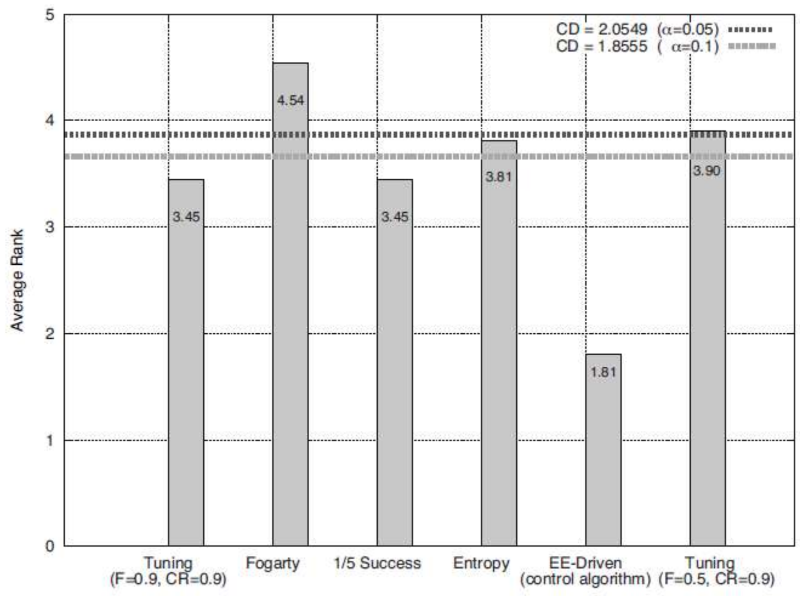


Figure 4: Algorithm comparison with the Bonferroni-Dunn post hoc test with $\alpha = 0.05$ and $\alpha = 0.1$.

The problem is that the threshold value X that defines the boundary of the neighborhood of the closest neighbor needs to be known in advance or to be approximated somehow. Furthermore, neighborhood has been modeled as a hypercube with the same length in all dimensions.

Measuring Exploration and Exploitation

- Y. Gonzalez-Fernandez and S. Chen, "Leaders and followers — A new metaheuristic to avoid the bias of accumulated information," 2015 IEEE Congress on Evolutionary Computation (CEC), 2015, pp. 776-783.

- "… With these definitions, exploration becomes the task of identifying the fittest attraction basin, and exploitation can be expressed as finding the local optimum within a given basin."

Measuring Exploration and Exploitation

- An attraction basin is a part of a search region with a point called an attractor to which a system tends to evolve.
- By using the concept of attraction basins, we can define and measure exploration and exploitation in a natural way.
- Assumption: neighborhood consists of all points that can be accessed with a local search (e.g., gradient method).

- J. Jerebic, M. Mernik, S-H Liu, M. Ravber, M. Baketarić, L. Mernik, M. Črepinšek. A novel direct measure of exploration and exploitation based on attraction basins. Expert Systems with Applications, Volume 167, 1 April 2021, 114353.

Measuring Exploration and Exploitation

- A multi-modal search space can be decomposed into several attraction basins. Each attraction basin has it own single local optimum. Hence, each point in the attraction basin has a monotonic path to the attractor — the local optimum in this attraction basin.

- Whilst a uni-modal search space has only one attraction basin and only one attractor.

Measuring Exploration and Exploitation

- By using the concept of attraction basins, we can defined exploration and exploitation in a more natural way.

- If a newly created individual (solution) belongs to the same attraction basin as its parent, then the search process is in the exploitation phase.
- On the other hand, if a newly created individual belongs to a different attraction basin than its parent, then the search process is in the exploration phase.
- As discussed previously, a parent can be replaced with a whole population, subpopulation, or history.

Measuring Exploration and Exploitation

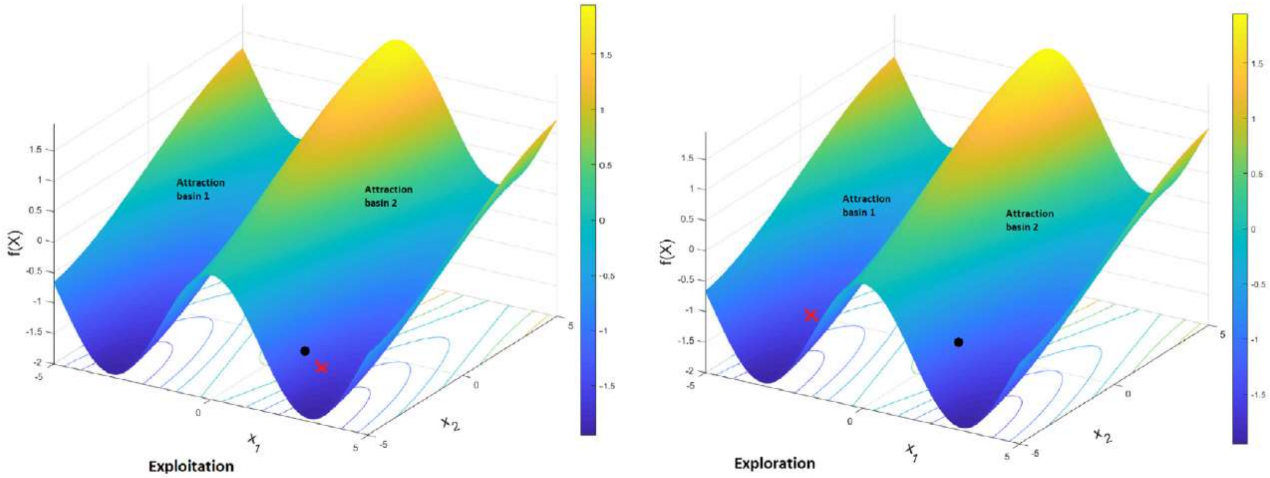


Fig. 1. Exploitation and Exploration based on attraction basins.

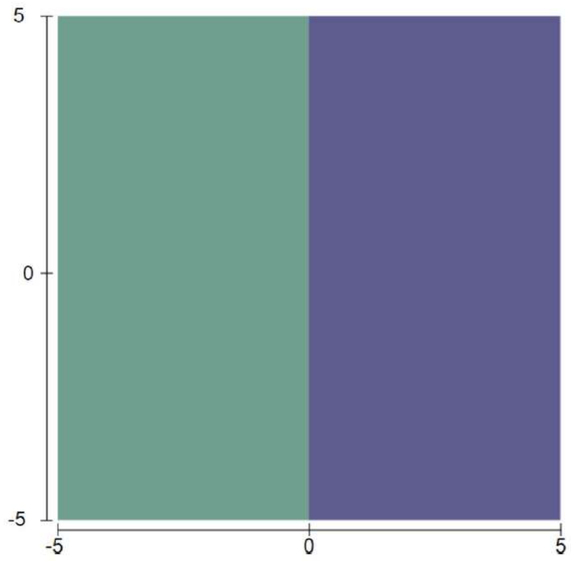


Fig. 2. Attraction basins for the Simple 2D function shown in Fig. 1.

Measuring Exploration and Exploitation

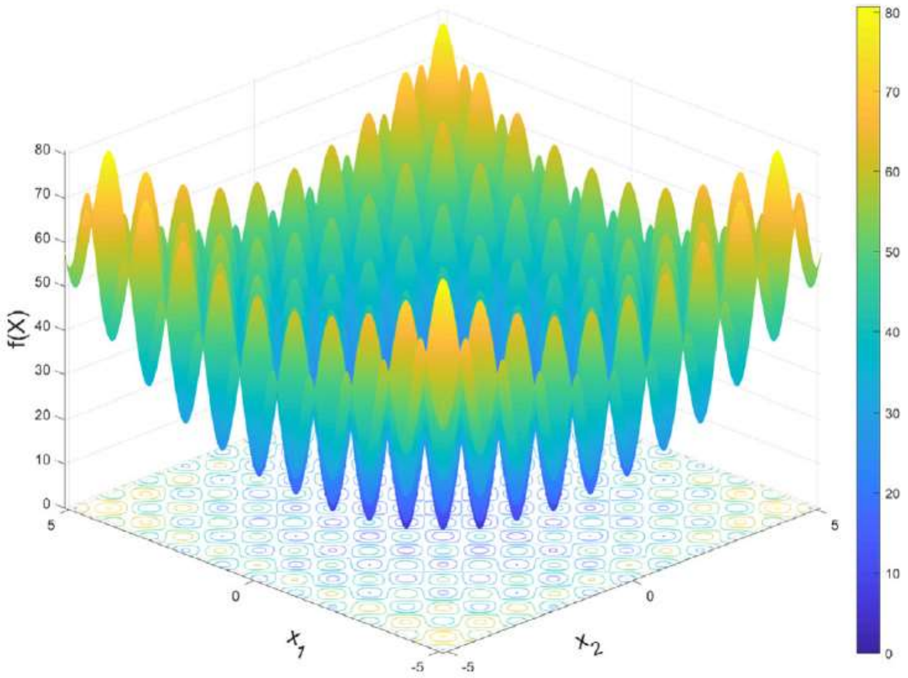


Fig. 3. The Rastrigin function.

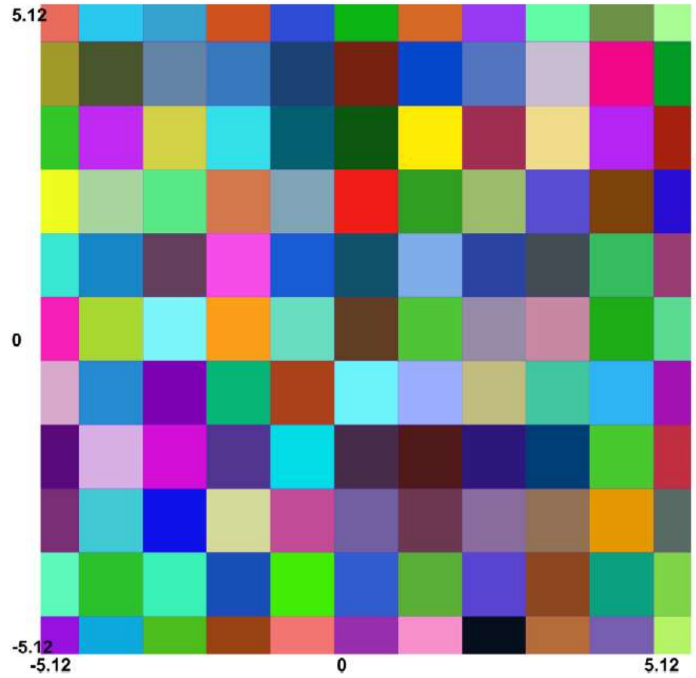


Fig. 4. Attraction basins for the Rastrigin function.

$$f(x) = 10d + \sum_{i=1}^{d} (x_i^2 - 10\cos(2\pi x_i))$$

$$-5.12 \le x_i \le 5.12$$

Measuring Exploration and Exploitation

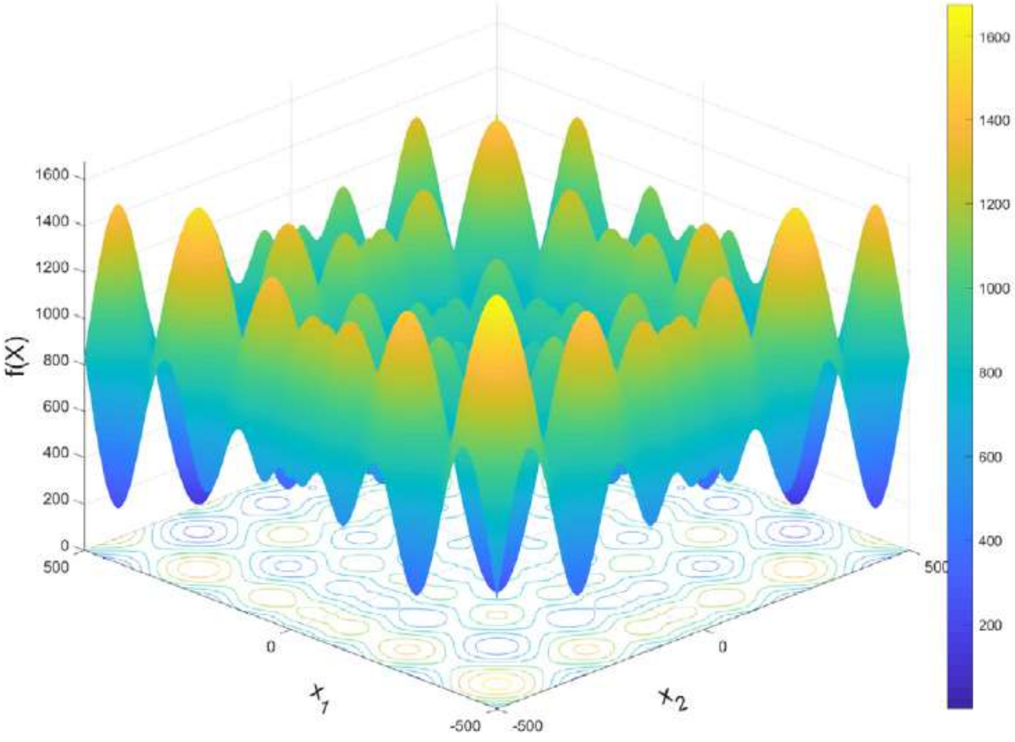


Fig. 9. The Schwefel function.

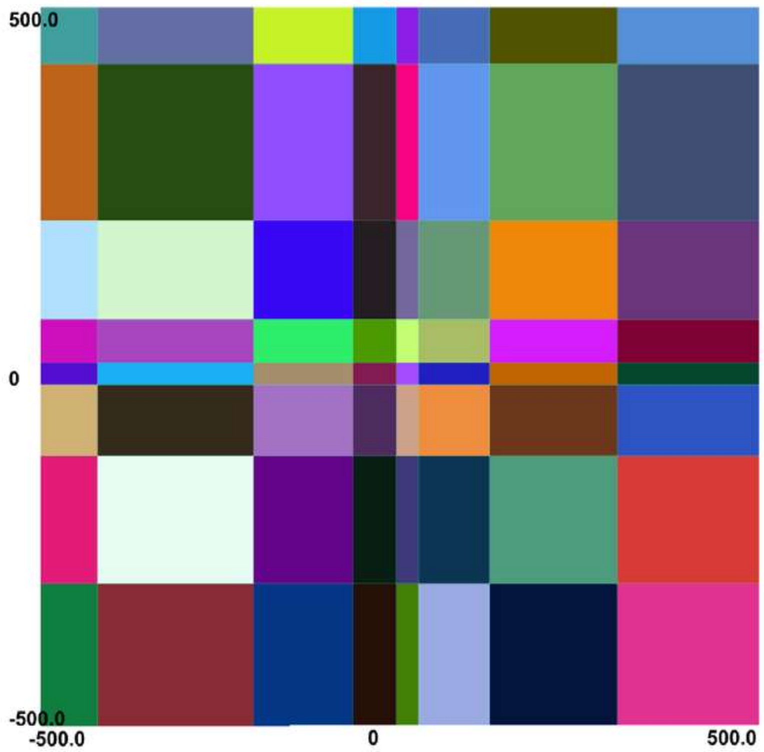


Fig. 11. Attraction basins for the Schwefel function.

$$f(\mathbf{x}) = 418.9829d - \sum_{i=1}^{d} x_i \sin(\sqrt{|x_i|})$$

$$-500 \leq x_i \leq 500$$

Measuring Exploration and Exploitation

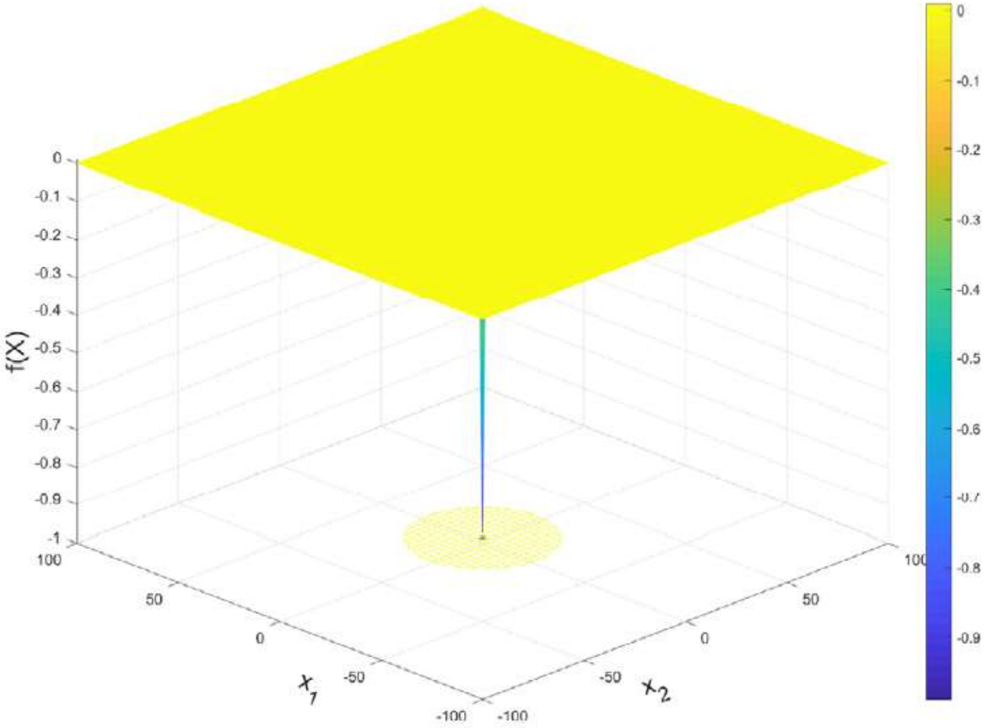


Fig. 14. The Easom function.

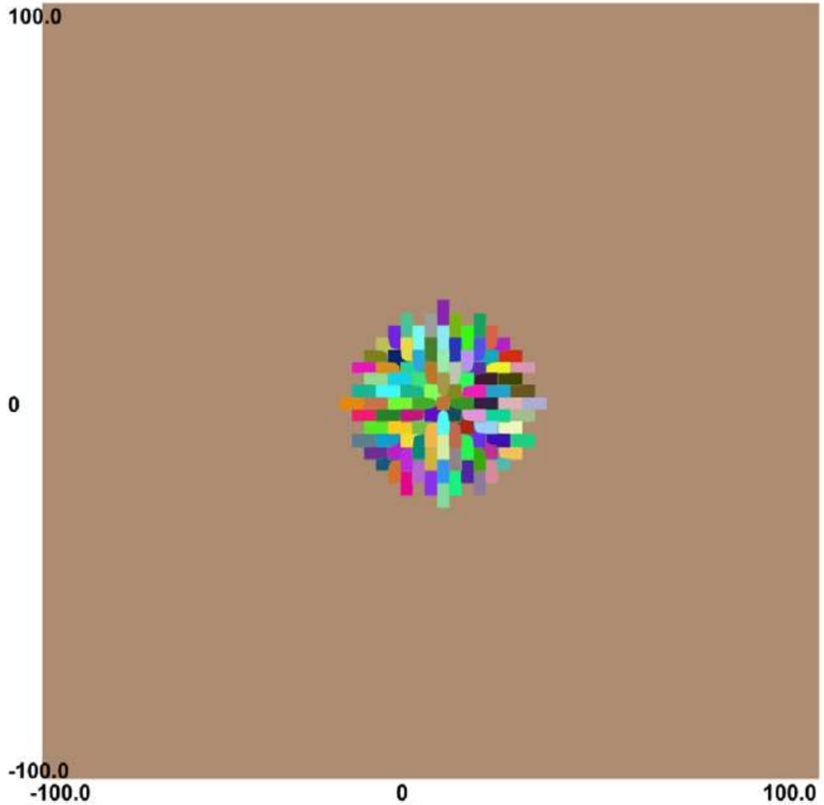


Fig. 16. Attraction basins for the Easom function.

$$f(x) = -\cos(x_1)\cos(x_2)\exp\left(-(x-\pi)^2 - (x_2-\pi)^2\right)$$

$$-100 \le x_i \le 100$$

Measuring Exploration and Exploitation

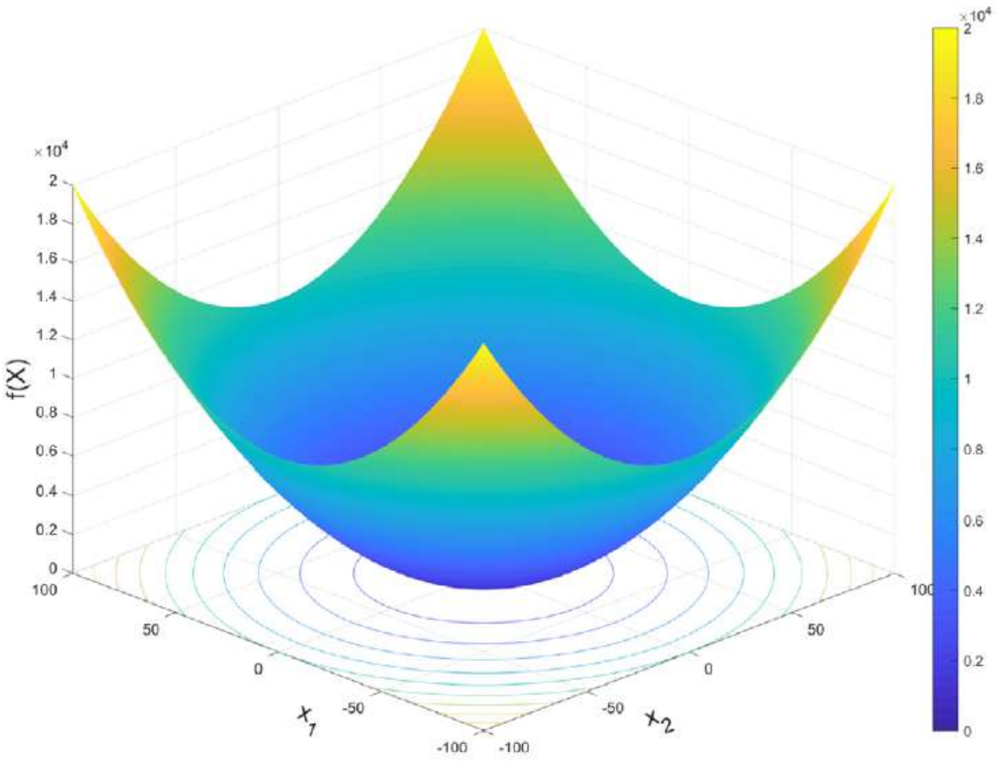


Fig. 19. The Sphere function.

$$f(x) = \sum_{i=1}^{d} x_i^2$$

$$-100 \leq x_i \leq 100$$

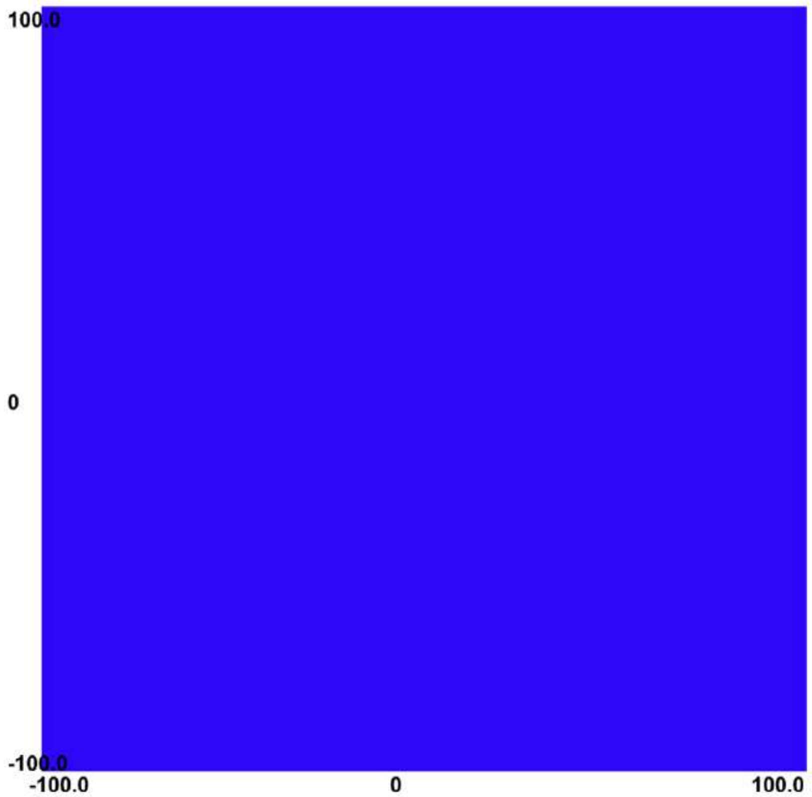


Fig. 21. Attraction basin for the Sphere function.

Measuring Exploration and Exploitation

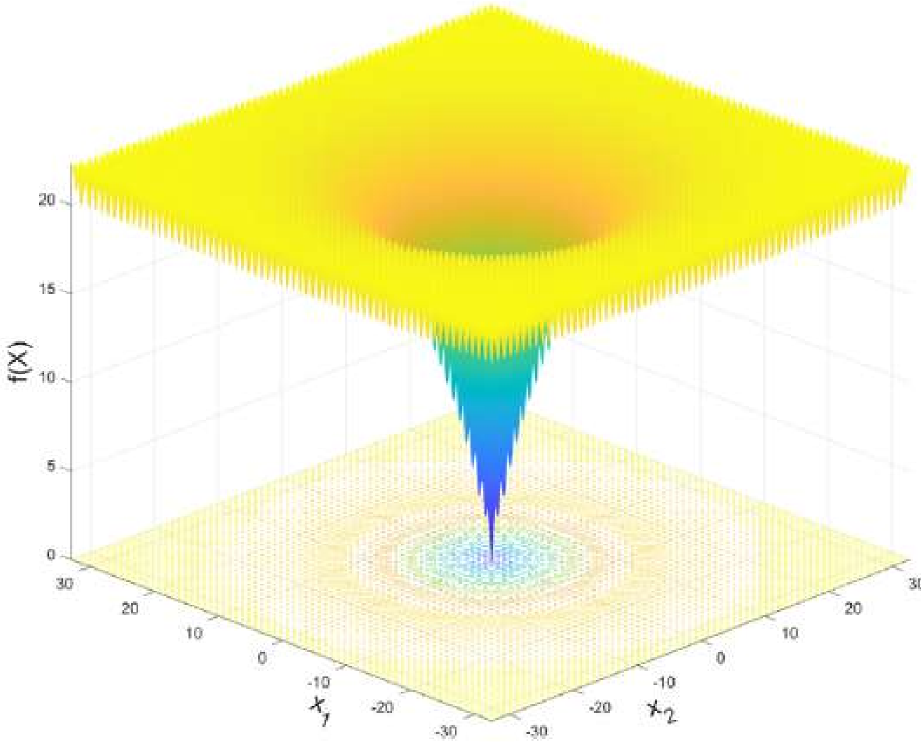


Fig. 22. The Ackley function.

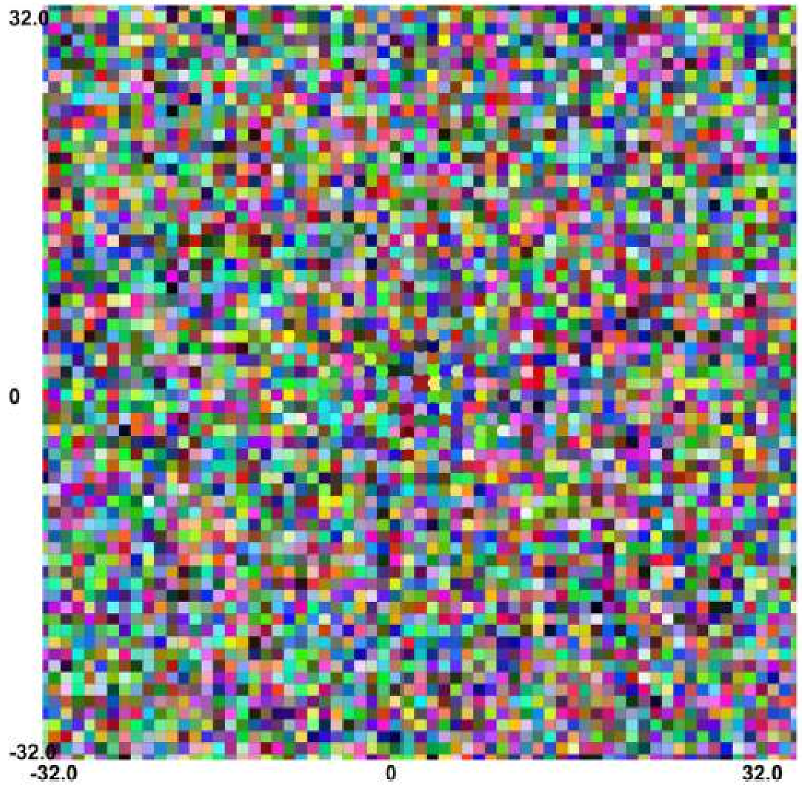


Fig. 24. Attraction basins for the Ackley function.

$$f(x) = -20\exp\left(-0.2\sqrt{\frac{1}{d}\sum_{i=1}^{d} x_i^2}\right) - \exp\left(\frac{1}{d}\sum_{i=1}^{d}\cos(2\pi x_i)\right) + 20 + e$$

$$-32 \le x_i \le 32$$

Measuring Exploration and Exploitation

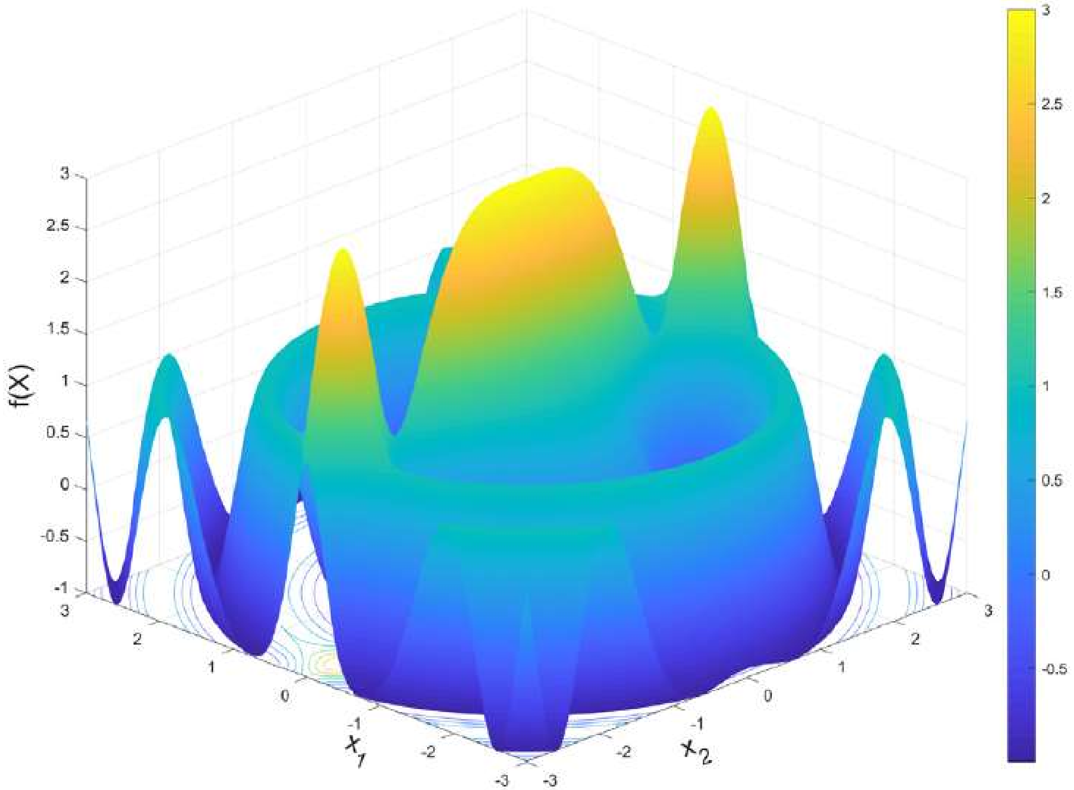


Fig. 40. Split Drop Wave function.

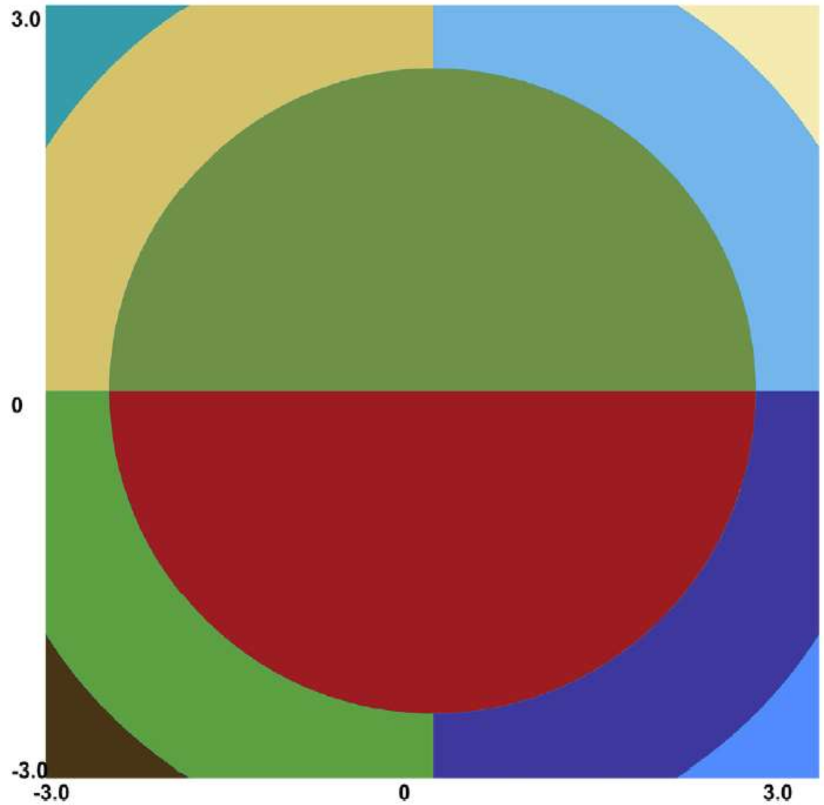


Fig. 42. Attraction basins for the Split Drop Wave function.

$$f(x) = cos(x^2 + y^2) + 2 * e^{-10*y^2}$$

$$-3 \leq x_i \leq 3$$

Measuring Exploration and Exploitation

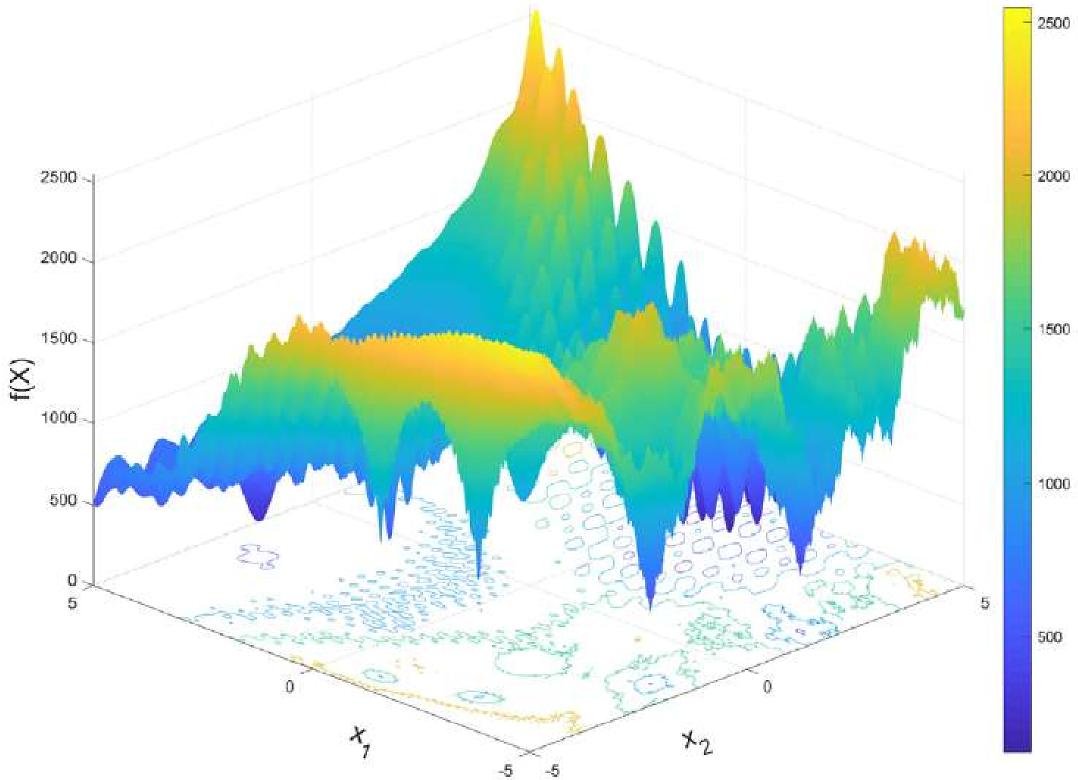


Fig. 45. Rotated Hybrid Composition function 1.

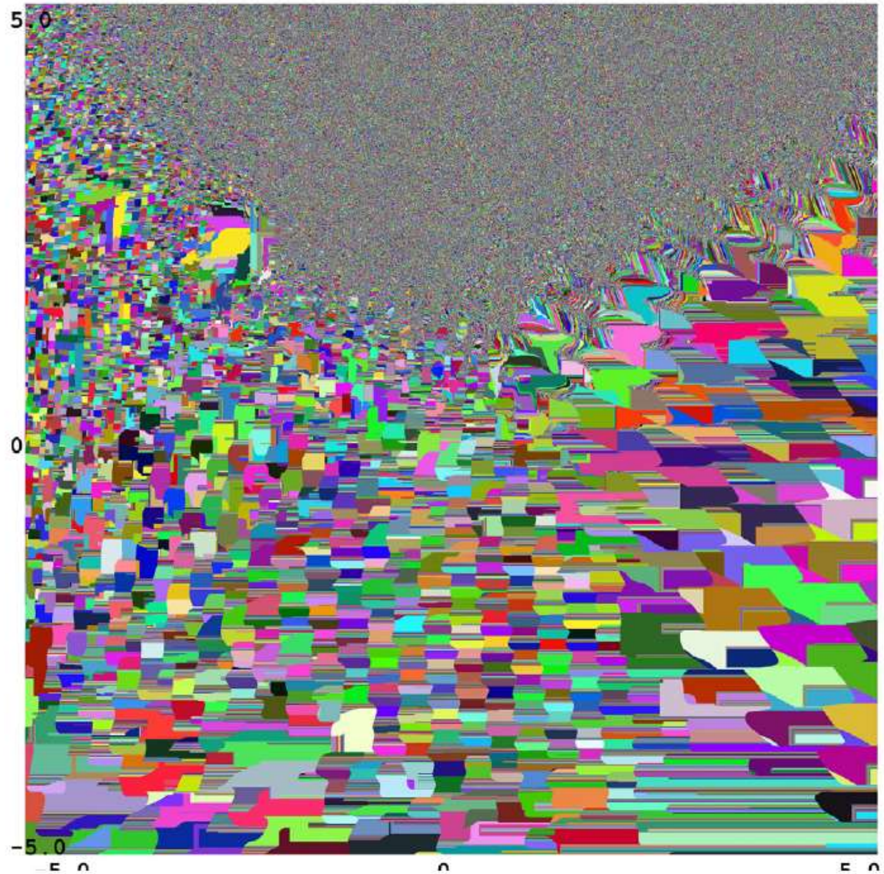


Fig. 47. Attraction basins for the Rotated Hybrid Composition function 1.

Measuring Exploration and Exploitation

Table 2
The results of the Rastrigin function.

Algorithm	Fitness	ExpBas	ExpDist	Diversity
RWSi	0.8517 ±0.5041	1.0000 ±0.0000	1.0000 ±0.0000	5.1173 ±0.0291
Hill Climbing	5.9112 ±3.3128	0.0041 ±0.0060	0.0020 ±0.0000	4.9672 ±0.3875
JADE	0.0000 ±0.0000	0.0575 ±0.0084	0.0601 ±0.0090	0.2259 ±0.0448
DE-best-1-bin	0.4776 ±0.7033	0.0183 ±0.0043	0.0204 ±0.0049	0.0728 ±0.0256
jDElscop	0.0199 ±0.1407	0.0572 ±0.0117	0.0598 ±0.0120	0.2294 ±0.0514
TLBO	0.0199 ±0.1407	0.0663 ±0.0197	0.0716 ±0.0217	0.3982 ±0.1056

Table 3
Pearson correlation coefficient for the Rastrigin function.

Algorithm	ExpBas vs. ExpDist	ExpBas vs. Diversity	ExpDist vs. Diversity
Hill Climbing	−1.0000	−0.1297	0.0000
JADE	−0.9831	0.7587	0.8237
DE-best-1-bin	−0.9810	0.7361	0.7453
jDElscop	−0.8970	0.8693	0.9016
TLBO	−0.9885	0.8905	0.8775

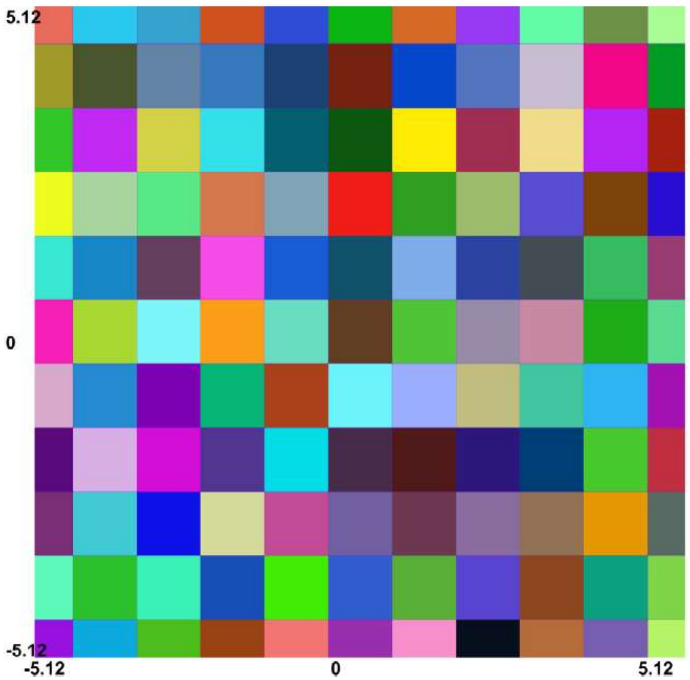


Fig. 4. Attraction basins for the Rastrigin function.

Measuring Exploration and Exploitation

Table 6
The results of the Easom function.

Algorithm	Fitness	ExpBas	ExpDist	Diversity
RWSi	−0.1809 ±0.2687	1.0000 ±0.0000	1.0000 ±0.0000	99.8960 ±0.5404
Hill Climbing	−0.0200 ±0.1414	0.0025 ±0.0025	0.0057 ±0.0049	96.0517 ±9.1713
JADE	−1.0000 ±0.0000	0.0398 ±0.0063	0.1271 ±0.0207	7.9450 ±2.7384
DE-best-1-bin	−1.0000 ±0.0000	0.0153 ±0.0024	0.0421 ±0.0136	2.7841 ±3.1682
jDElscop	−1.0000 ±0.0000	0.0797 ±0.0059	0.1523 ±0.0201	6.9160 ±2.4821
TLBO	−1.0000 ±0.0000	0.2090 ±0.0180	0.4049 ±0.0180	6.6957 ±1.4661

Table 7
Pearson correlation coefficients for the Easom function.

Algorithm	ExpBas vs. ExpDist	ExpBas vs. Diversity	ExpDist vs. Diversity
Hill Climbing	−0.4017	0.0561	0.0318
JADE	−0.0588	−0.3148	0.8825
DE-best-1-bin	−0.2367	0.1016	0.9638
jDElscop	−0.5542	0.2155	0.9148
TLBO	−0.4354	−0.0276	0.5722

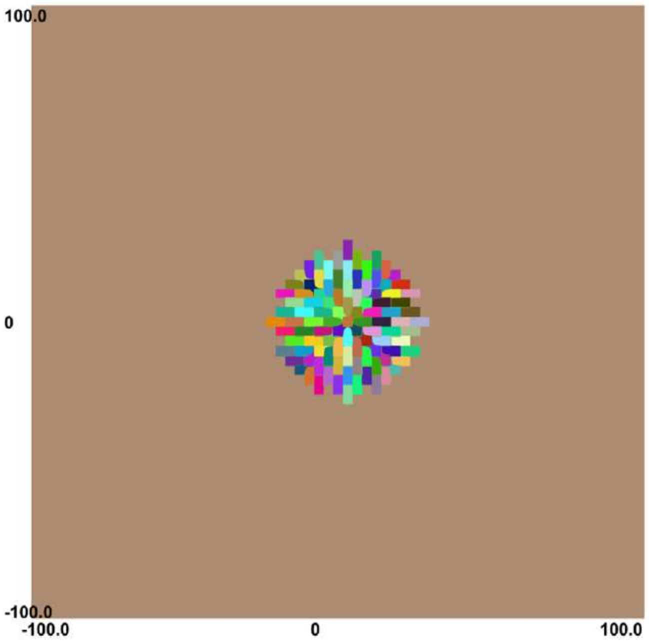


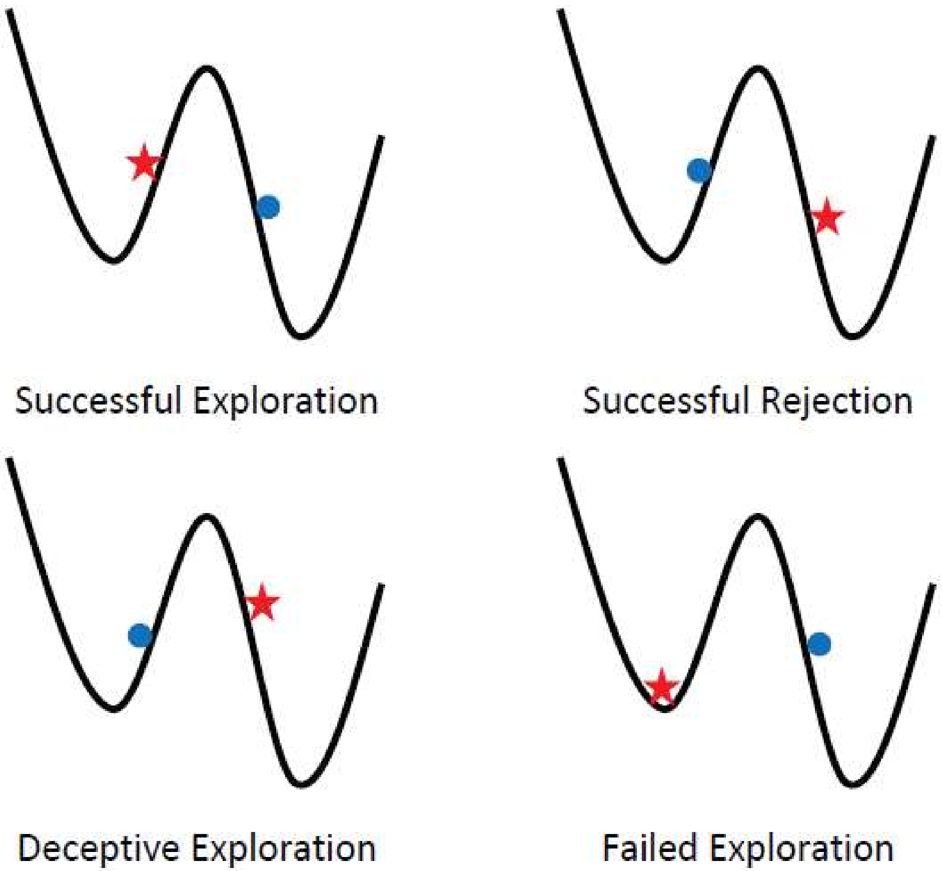
Fig. 16. Attraction basins for the Easom function.

Measuring Exploration and Exploitation

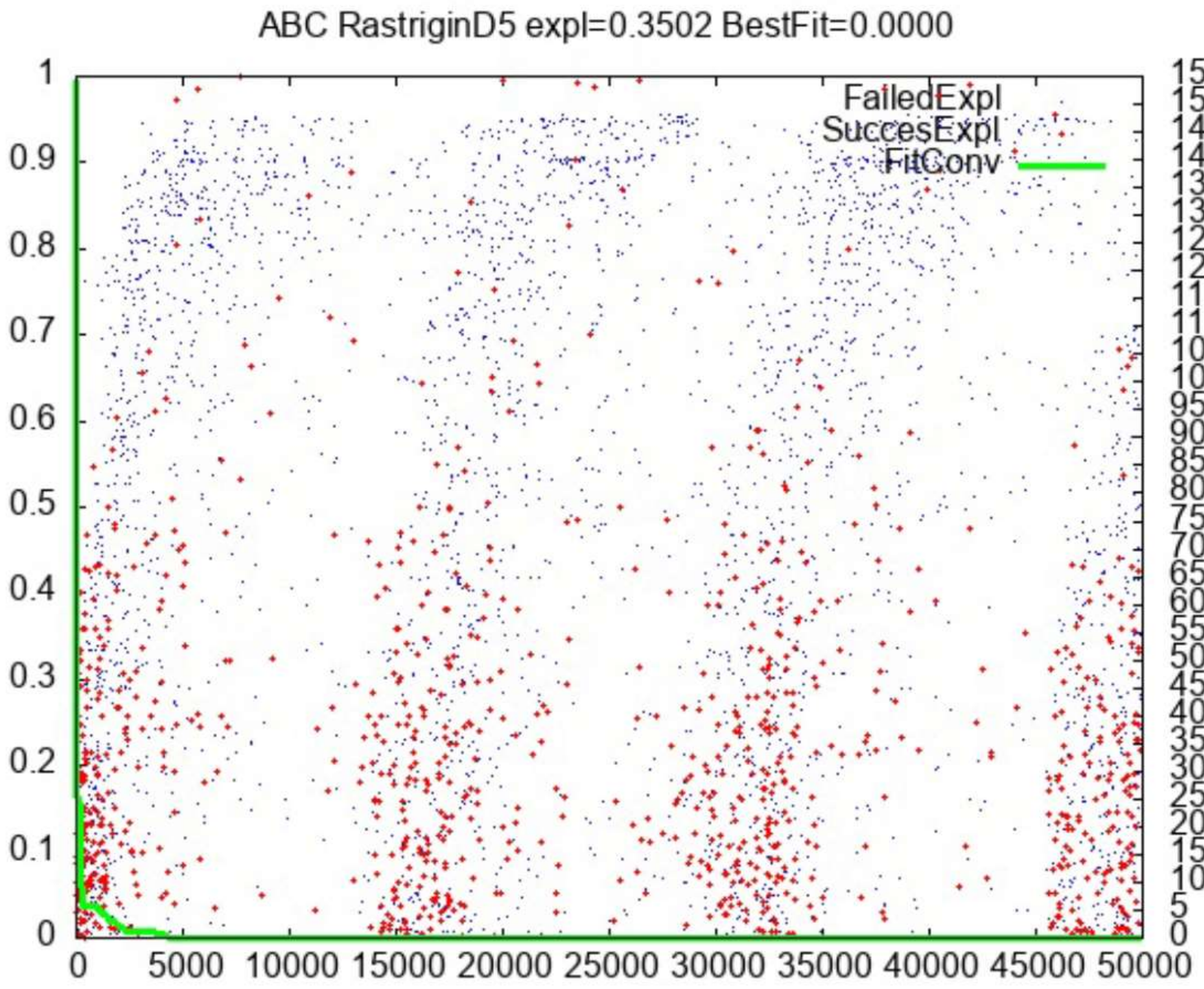
- Different types of exploration can be identified:
  - successful exploration,
  - successful rejection,
  - deceptive exploration, and
  - failed exploration.

Measuring Exploration and Exploitation

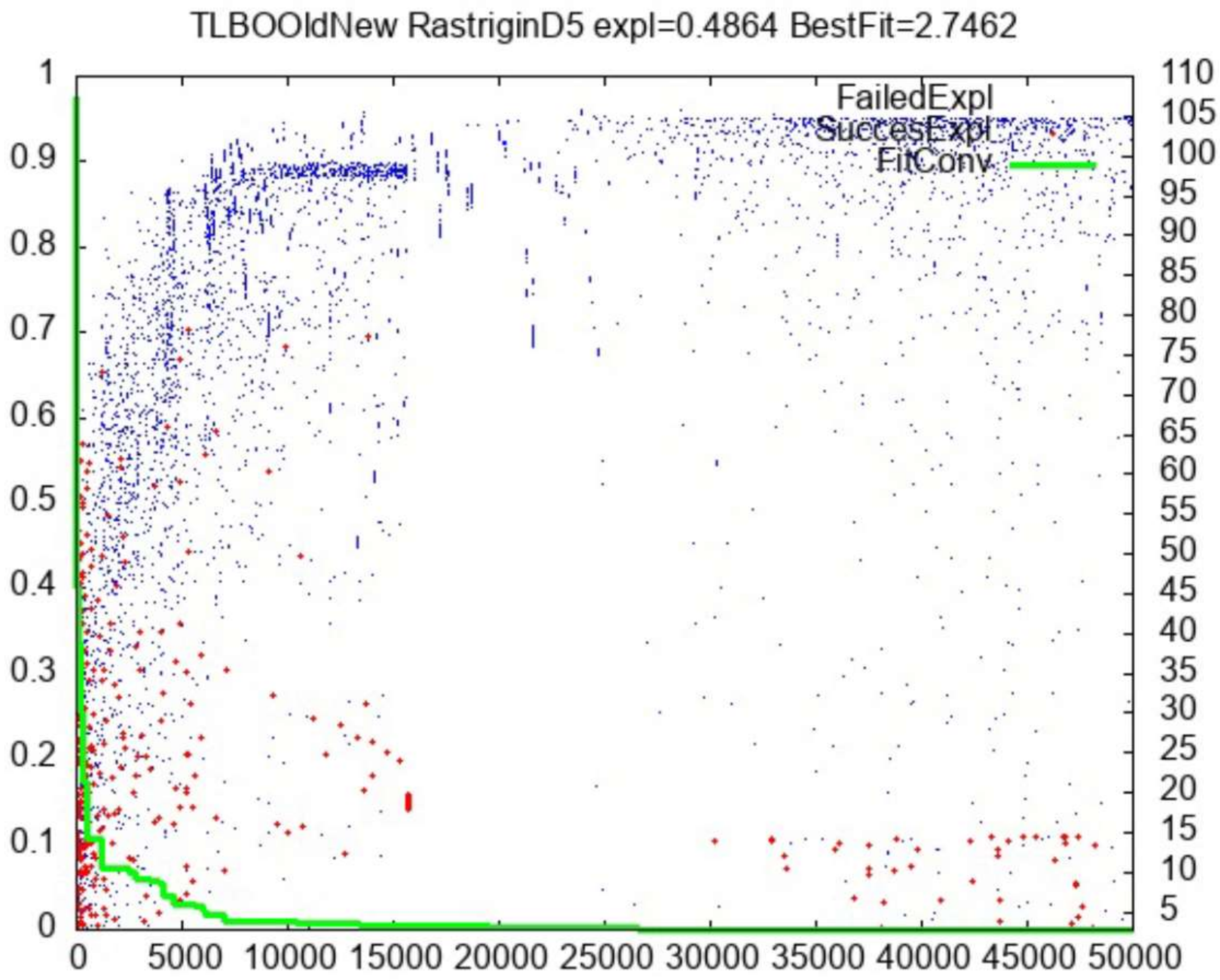
- Different types of exploration



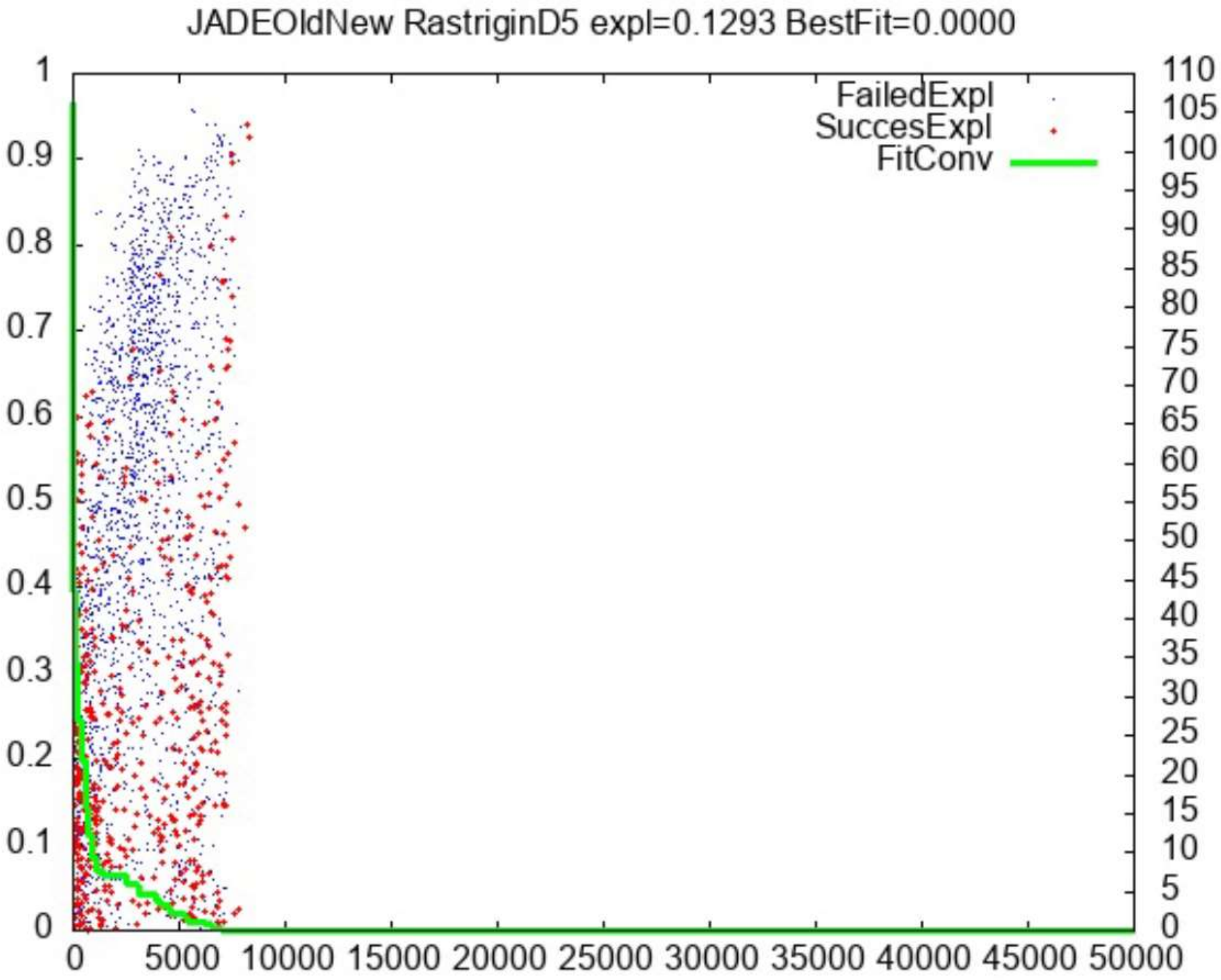
Measuring Exploration and Exploitation



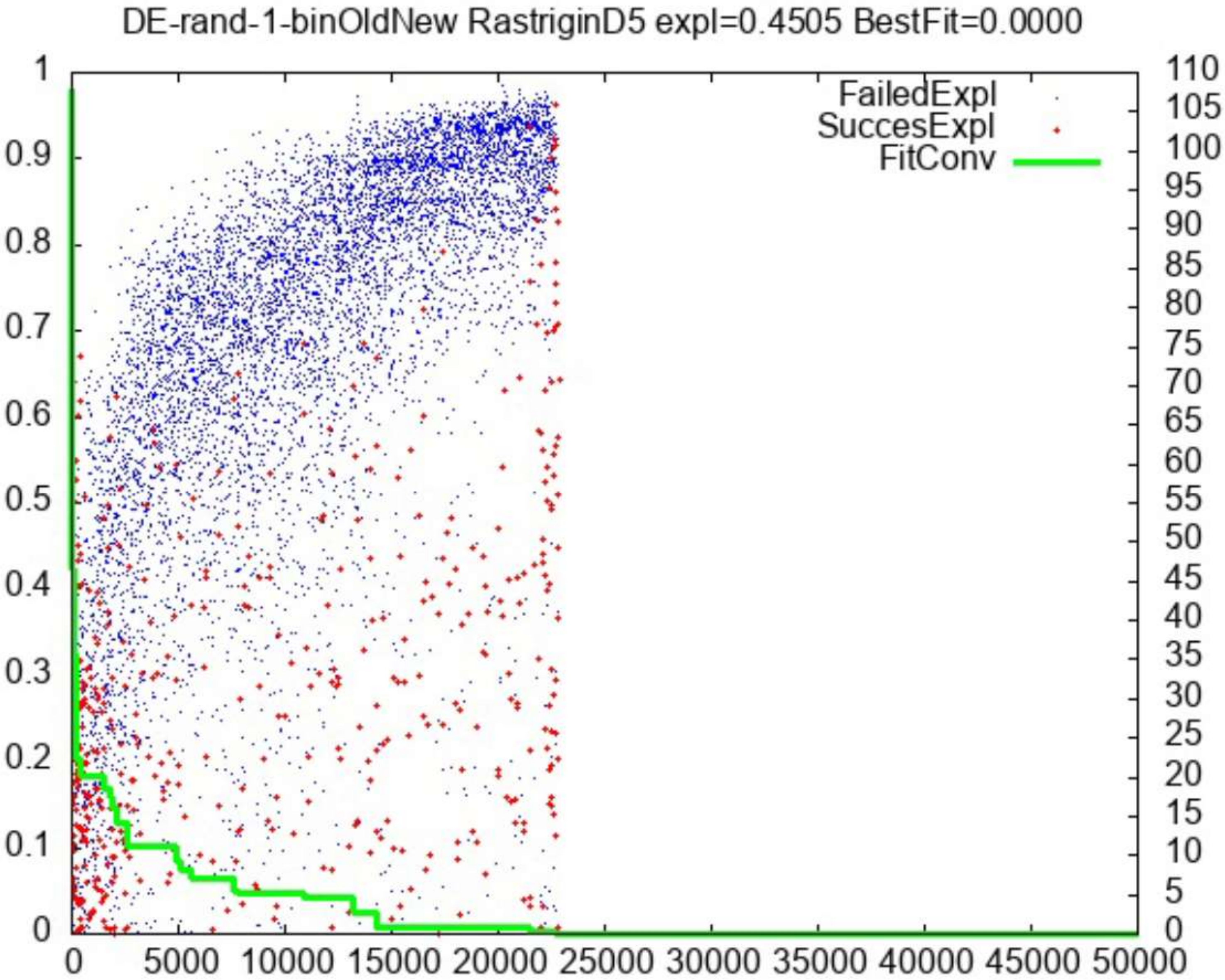
Measuring Exploration and Exploitation



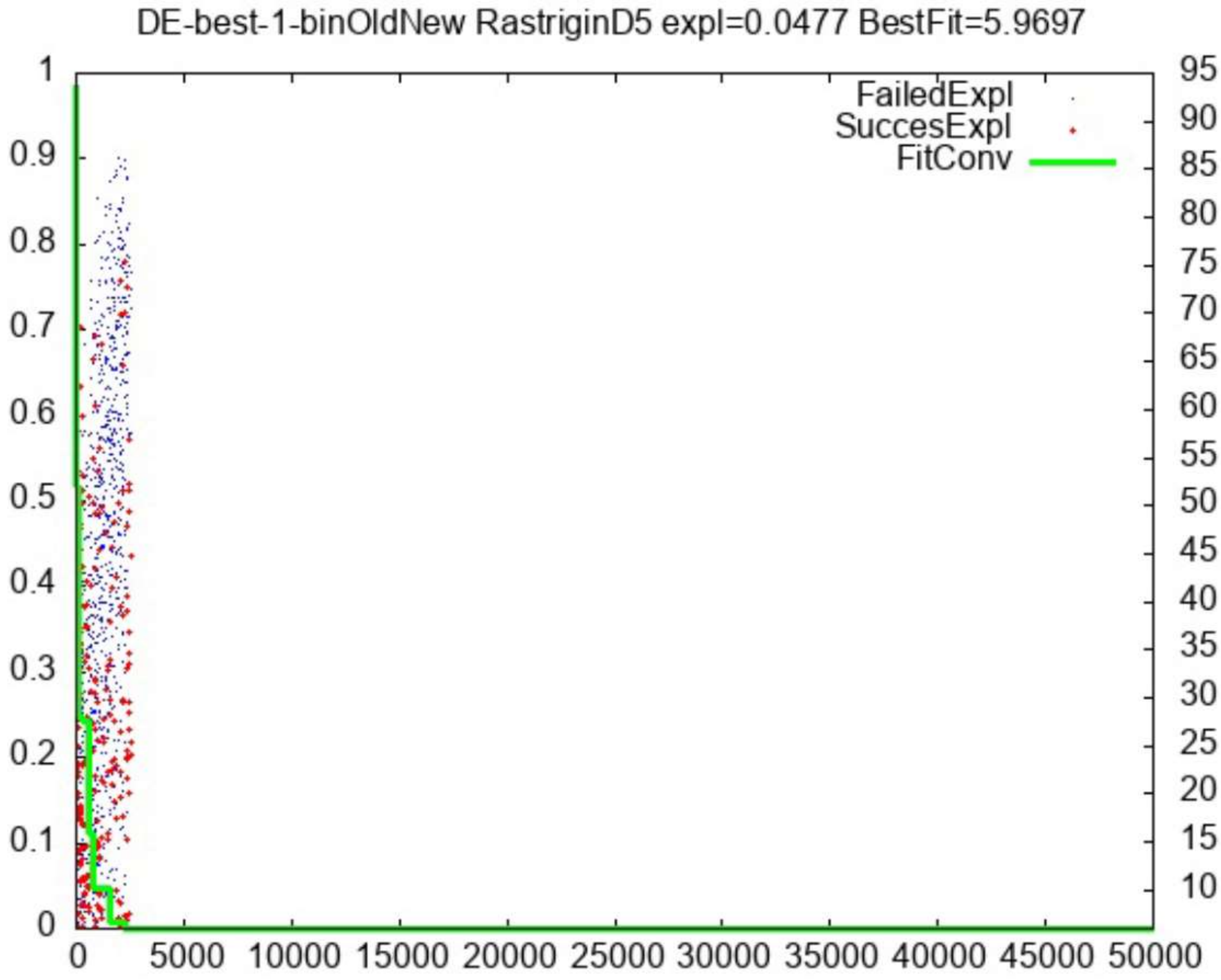
Measuring Exploration and Exploitation



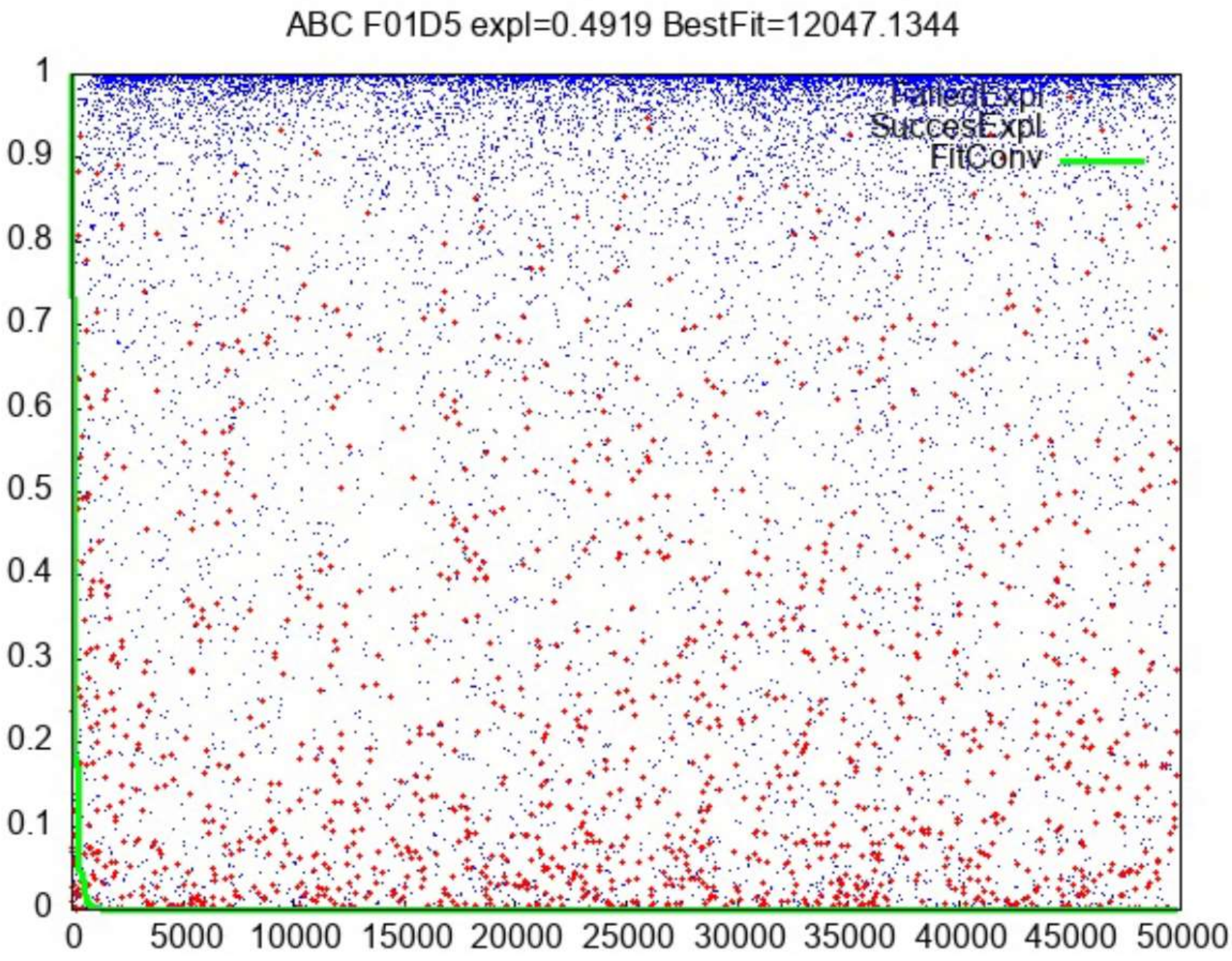
Measuring Exploration and Exploitation



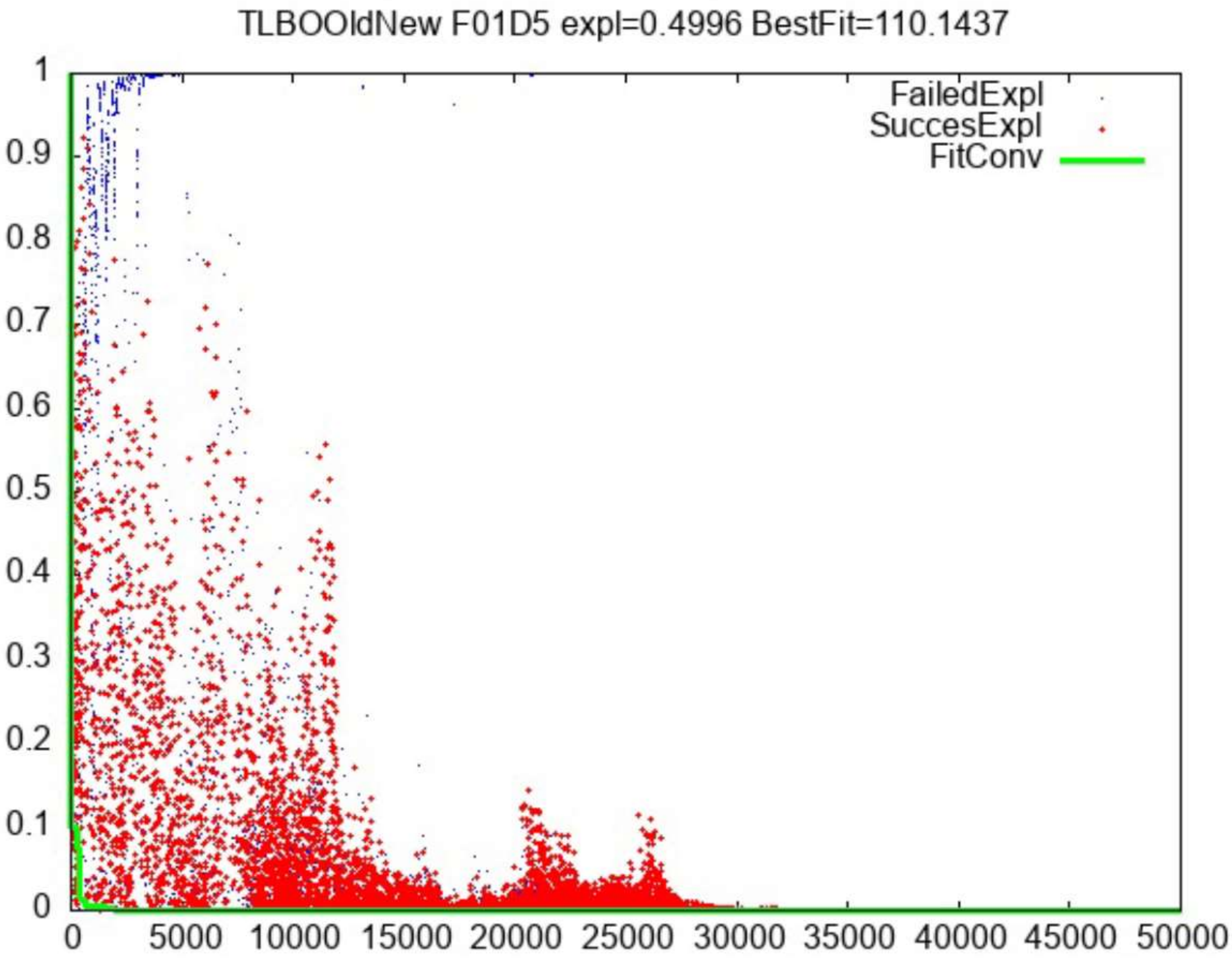
Measuring Exploration and Exploitation



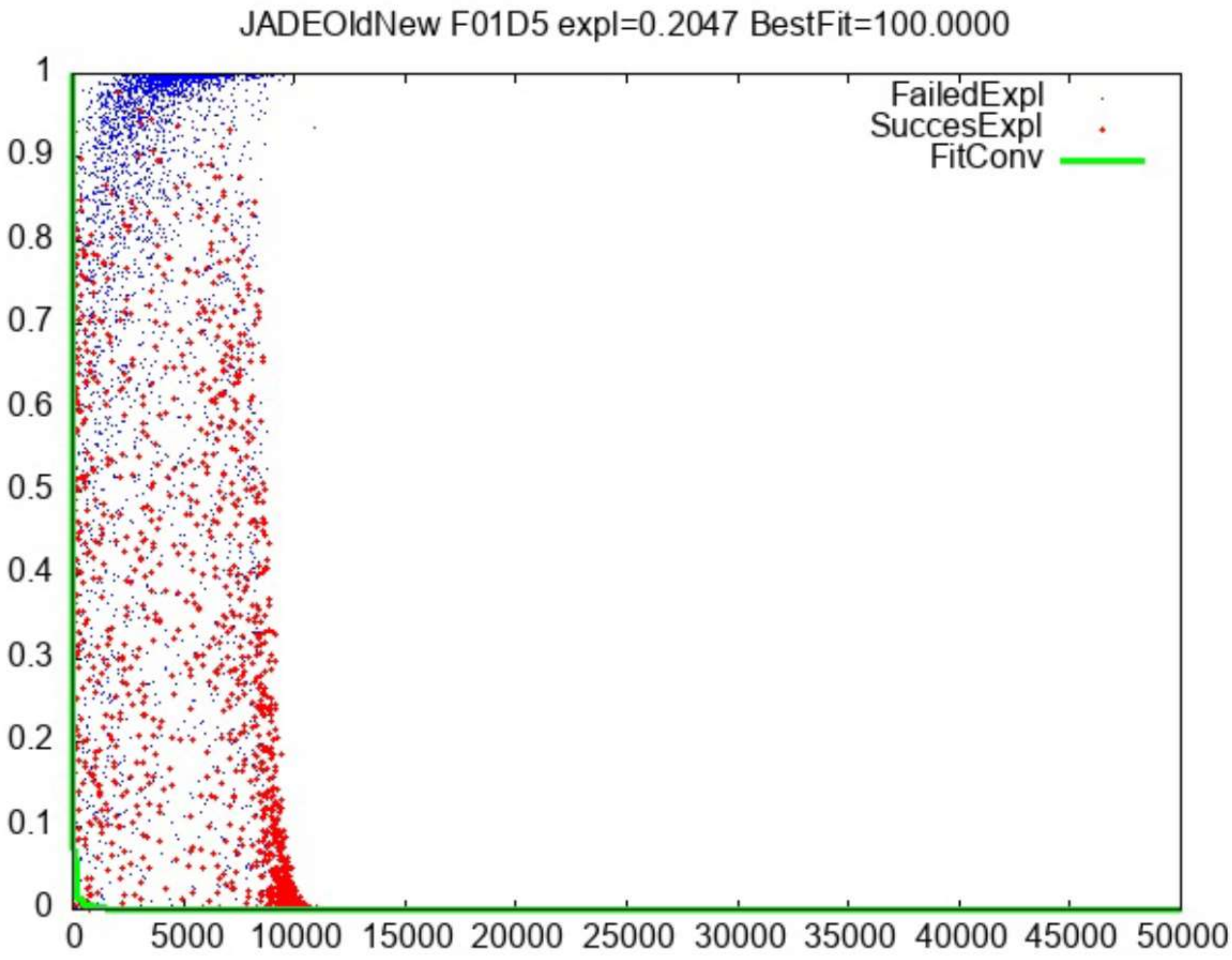
Measuring Exploration and Exploitation



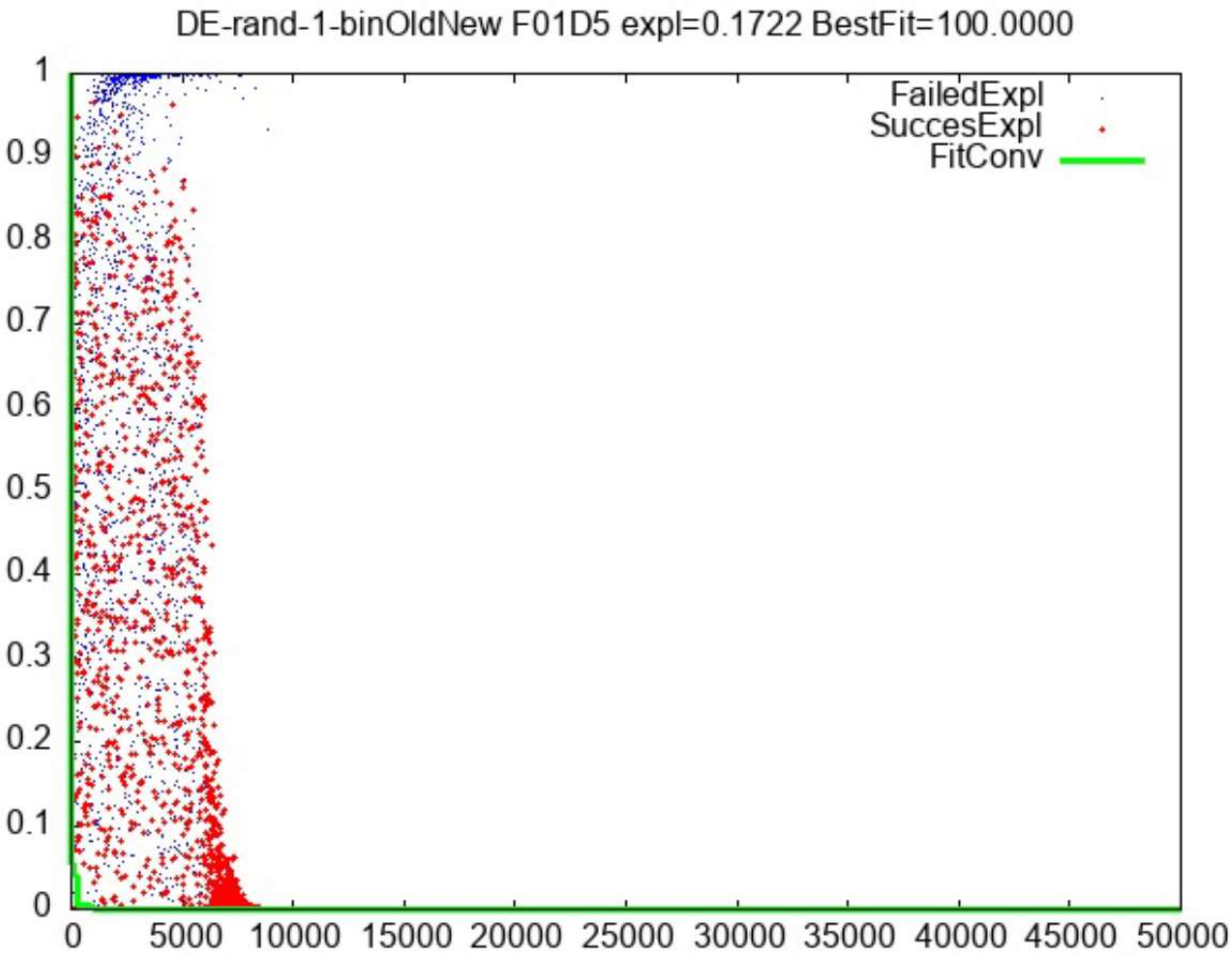
Measuring Exploration and Exploitation



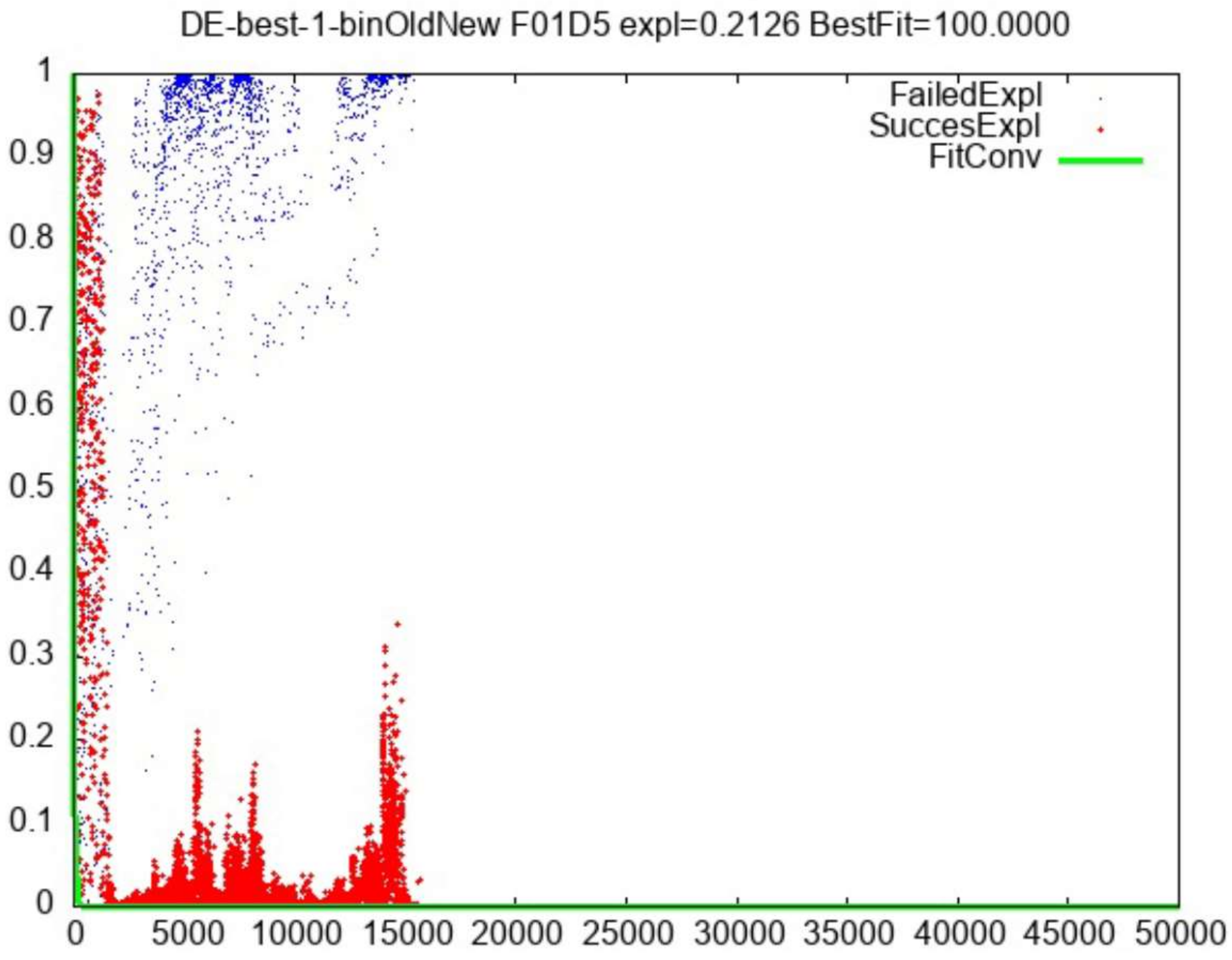
Measuring Exploration and Exploitation



Measuring Exploration and Exploitation



Measuring Exploration and Exploitation

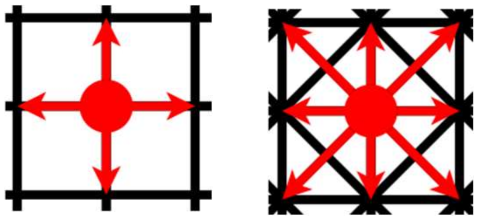


Measuring Exploration and Exploitation

Algorithm	Success Expl	Failed Expl	Deceptive Expl	Success Reject	Exploration	Diver	Best Fit
ABClim50 AckleyD5	0.1527 0.0074	0.1126 0.0050	0.0305 0.0022	0.7042 0.0075	0.1906 0.0092	6.1776 0.5472	0.0000 0.0000
ABClim50 GriewankD5	0.0716 0.0042	0.1562 0.0054	0.0207 0.0016	0.7515 0.0104	0.5918 0.0225	114.5098 8.2840	0.0000 0.0001
ABClim50 RastriginD5	0.0597 0.0025	0.1671 0.0044	0.0151 0.0008	0.7581 0.0034	0.3237 0.0075	2.2418 0.0967	0.0000 0.0000
ABClim125 AckleyD5	0.1492 0.0045	0.1076 0.0037	0.0301 0.0013	0.7131 0.0054	0.1888 0.0067	6.0351 0.6523	0.0000 0.0000
ABClim125 GriewankD5	0.0436 0.0017	0.1266 0.0085	0.0121 0.0006	0.8176 0.0095	0.4914 0.0170	64.9442 2.3475	0.0000 0.0000
ABClim125 RastriginD5	0.0536 0.0034	0.1686 0.0057	0.0133 0.0012	0.7645 0.0046	0.2834 0.0115	1.9084 0.1090	0.0000 0.0000
ABClim200 AckleyD5	0.1490 0.0089	0.1111 0.0098	0.0318 0.0025	0.7081 0.0075	0.1635 0.0094	5.7410 0.5323	0.0000 0.0000
ABClim200 GriewankD5	0.0402 0.0020	0.1111 0.0100	0.0113 0.0011	0.8374 0.0113	0.4816 0.0095	63.5088 3.7401	0.0000 0.0000
ABClim200 RastriginD5	0.0557 0.0033	0.1714 0.0069	0.0144 0.0015	0.7586 0.0082	0.2641 0.0099	1.7897 0.0698	0.0000 0.0000
ABClim500 AckleyD5	0.1522 0.0105	0.1110 0.0081	0.0301 0.0024	0.7067 0.0079	0.1271 0.0105	4.3485 0.6025	0.0000 0.0000
ABClim500 GriewankD5	0.0319 0.0015	0.0916 0.0086	0.0084 0.0006	0.8682 0.0092	0.4322 0.0141	48.5713 3.4319	0.0032 0.0037
ABClim500 RastriginD5	0.0531 0.0030	0.1741 0.0070	0.0135 0.0011	0.7593 0.0061	0.1977 0.0112	1.3314 0.0903	0.0000 0.0000
ABClim1000 AckleyD5	0.1494 0.0107	0.1107 0.0079	0.0300 0.0024	0.7099 0.0139	0.1228 0.0076	4.1982 0.5293	0.0000 0.0000
ABClim1000 GriewankD5	0.0268 0.0019	0.0899 0.0102	0.0068 0.0007	0.8765 0.0104	0.4171 0.0166	42.8147 1.7521	0.0022 0.0036

Attraction basins

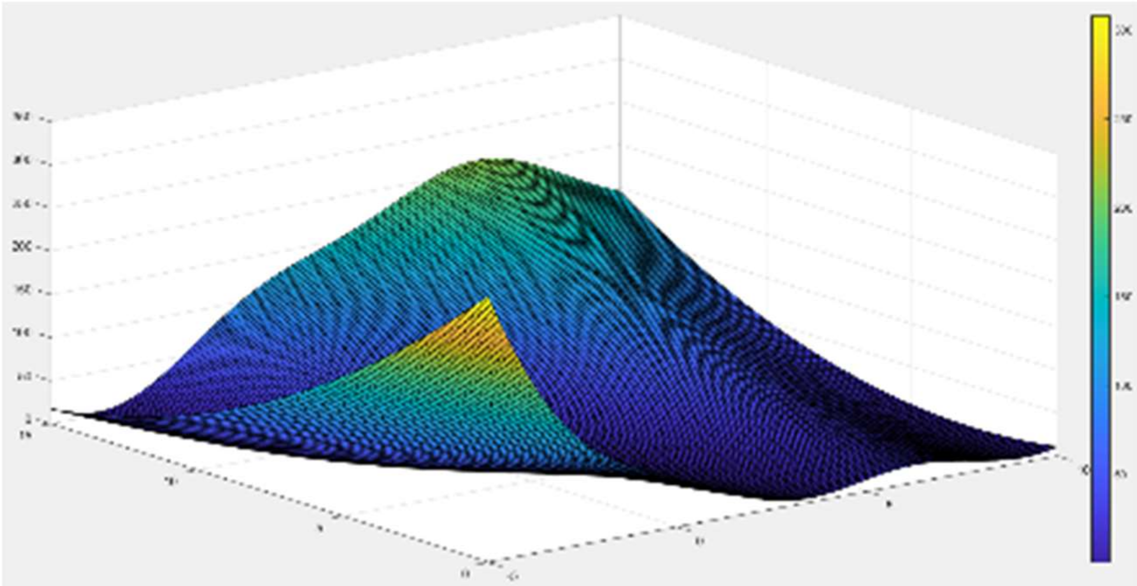
- An attraction basin $A(x*)$ is a part of a search space S with a local optimum $x*$ called an attractor, which can be accessed from any other point $y \in A(x*)$ in this attraction basin simply by performing a local search.
- Problems:
  - Different local searches (First Improvement vs Best Improvement)
  - Definition of a neighbourhood (Sparse vs Dense)



  - Order of neighbouring points
  - Plateaus and boundary points
  - Discretization of the continuous search space, where optima might be missed.

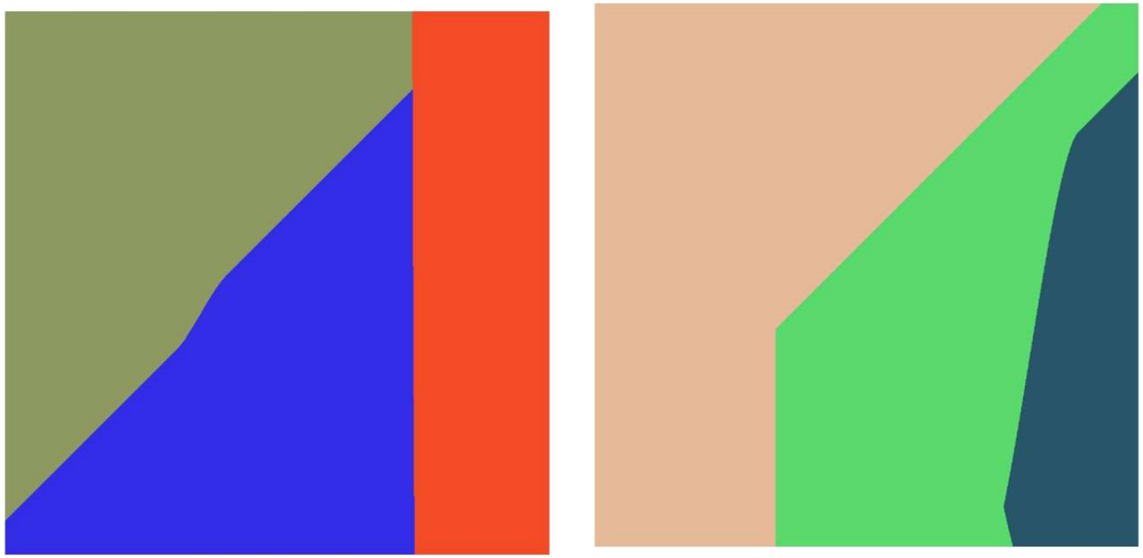
Attraction basins

Branin function



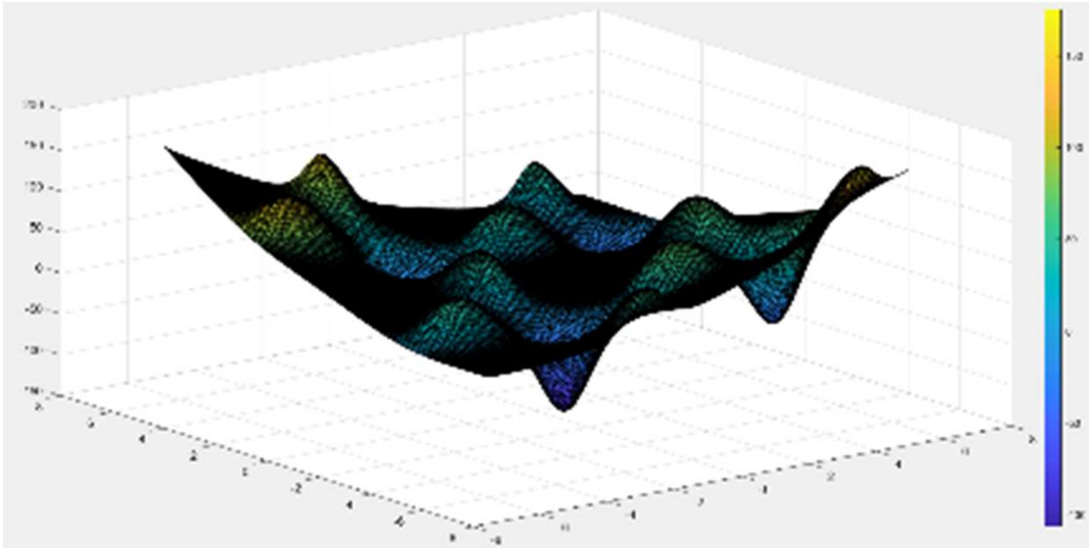
a) Best Improvement

b) First Improvement



a) b)

Attraction basins



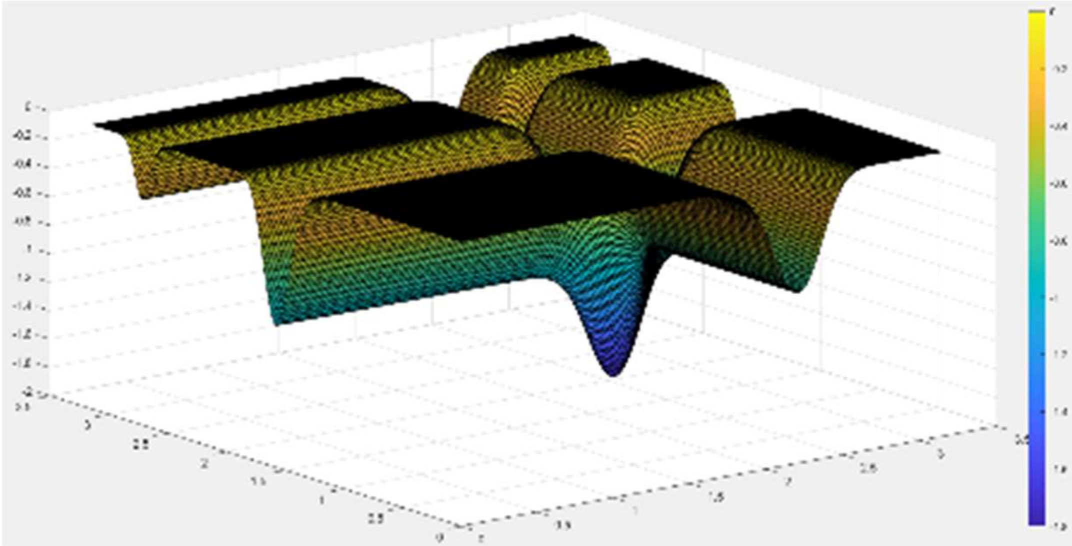
Bird function - Best Improvement

a) Dense neighbourhood

b) Sparse neighbourhood

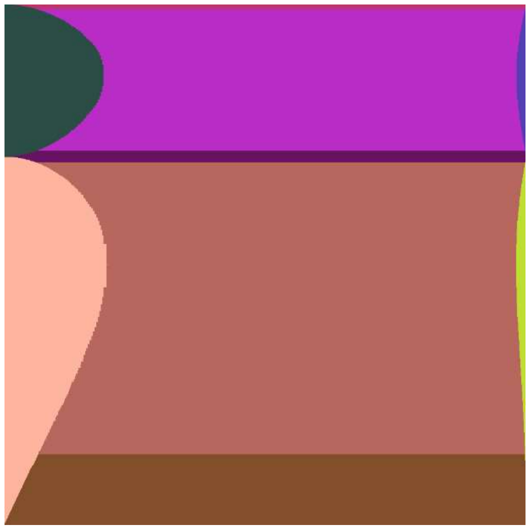
a) b)

Attraction basins

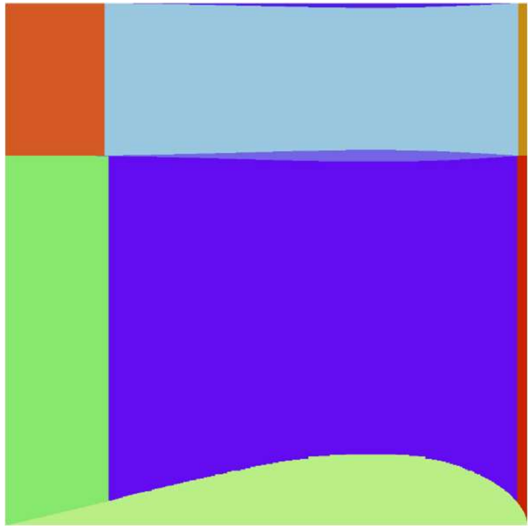


Michalewicz function - First Improvement & Sparse neighbourhood

a) Non-reversed order
b) Reversed order



a)



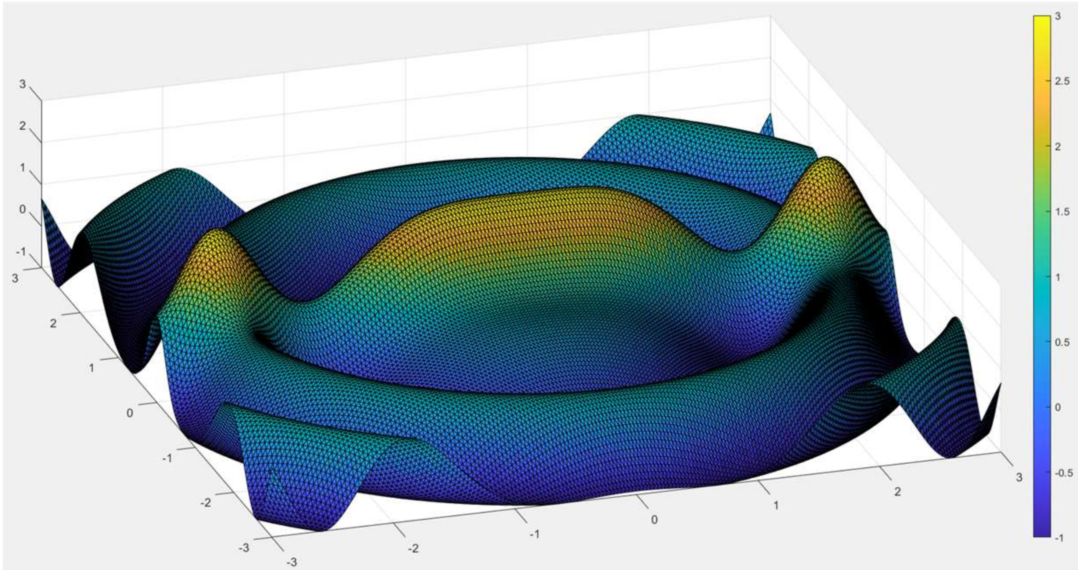
b)

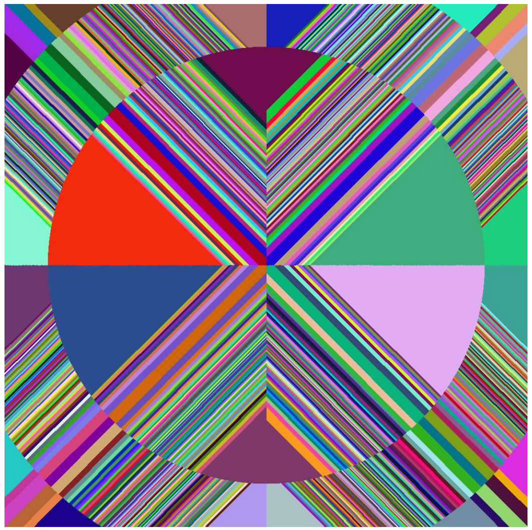
Attraction basins

SplitDropWave function

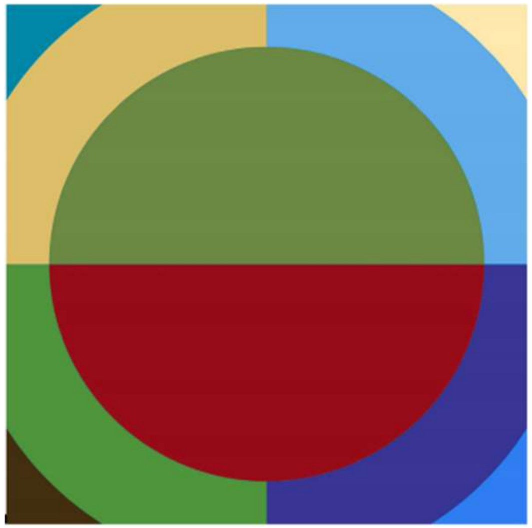
a) Best Improvement & Dense neighbourhood

b) Correct solution





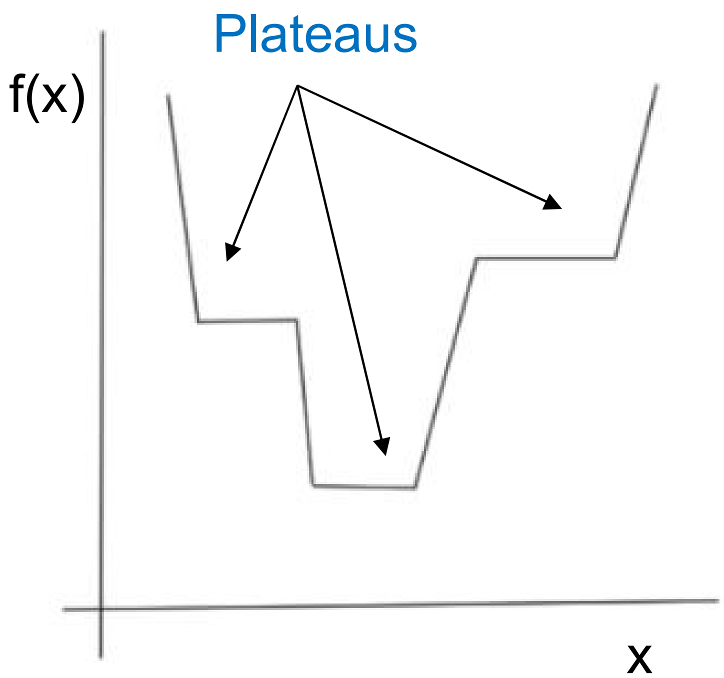
a)

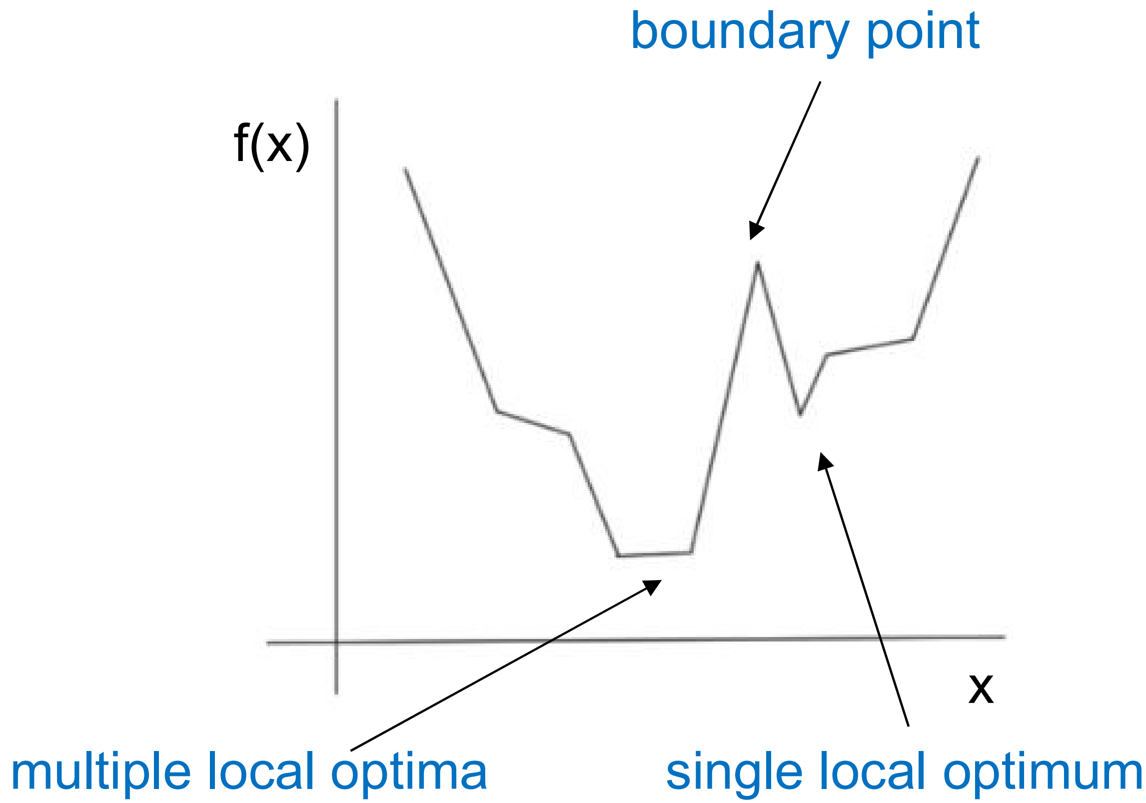


b)

Attraction basins

- Plateaus and boundary points





EAs Open Problems

- Many EAs are the same in terms of the updating operators, but with different mimicking scenarios and names. It would be possible to distinguish metaheuristics based on how they perform exploration and exploitation. The novelty of the proposed metaheuristics would be easier to identify.
- Many authors tried to propose new genetic operators that influence exploration and exploitation. With the proposed new direct exploration and exploitation measure, the authors can verify more easily if their newly proposed genetic operators indeed improve the balance between exploration and exploitation.

EAs Open Problems

- Based on the shape and number of attraction basins, we anticipate it would be possible to identify a family of metaheuristics that perform well on such shape of attraction basins.
- Until now, achieving a balance between exploration and exploitation has been controlled implicitly by proper parameter settings, off-the-fly or on-the-fly. With the newly proposed direct measure of exploration and exploitation, the effect of different settings of parameters can be quantified better.

Collaborators

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- Shih-Hsi Liu (California State University Fresno, USA)
- Stephen Chen (York University, Toronto, Canada)

Conclusion & Questions

- Exploration and exploitation are fundamental concepts of any search algorithm, and it is surprisingly that these concepts are not better understand in EAs.