



Metaheuristic Optimization

11. Difficulties

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- 1 Complexity
- 2 Unsatisfying Convergence
- 3 Ruggedness & Causality
- 4 Deceptiveness
- 5 Neutrality
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website

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- Why?

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- Why?
- What makes optimization difficult?

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- A good summary on this topic given in our recent article *“Evolutionary Optimization: Pitfalls and Booby Traps”* ^[1].

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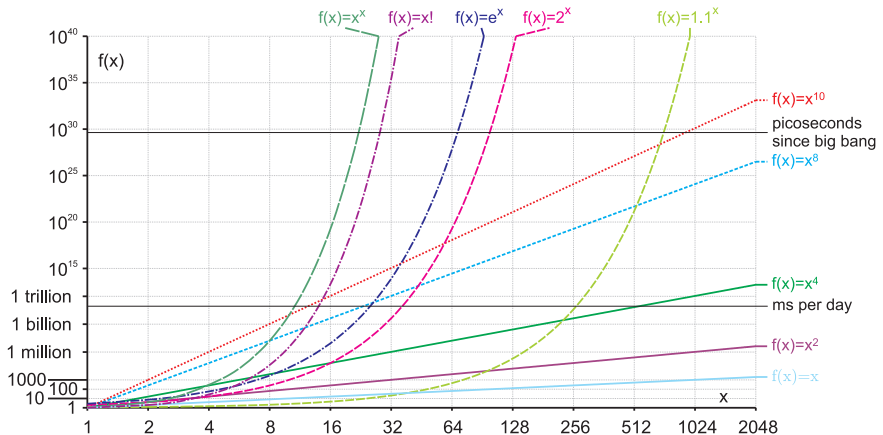
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- For a given input size, there might be a best, worst, and average case scenarios.
- Under algorithmic complexity we can thus understand the average, minimum, or maximum time/space an algorithm needs to finish, as **function** on the input size.

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$$f(x) \in \mathcal{O}(g(x)) \Leftrightarrow \exists x_0 \in \mathbb{R}, m \in \mathbb{R}^+ : |f(x)| \leq m|g(x)| \quad \forall x > x_0 \quad (1)$$

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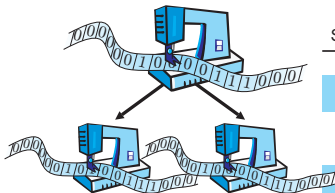
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- If we are conservative, we consider the worst case scenarios, since we cannot really know what problem we will exactly get in practice.
- Can we make this even more general?

- Deterministic Turing Machine (DTM)** ^[5]



State	Tape Symbol	⇒	Print	Motion	Next State
A	0	⇒	1	Right	A
A	1	⇒	0	Right	B
B	0	⇒	1	Right	B
B	1	⇒	1	Left	C
C	1	⇒	0	Left	C
C	0	⇒	1	Right	A

- Non-Deterministic Turing Machine (NTM)**



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B	1	⇒	1	Left	C
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 - ⑤ We need to trade-off runtime vs. solution quality, especially if the problem is not well-researched.

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- When/why can we not get good solutions?

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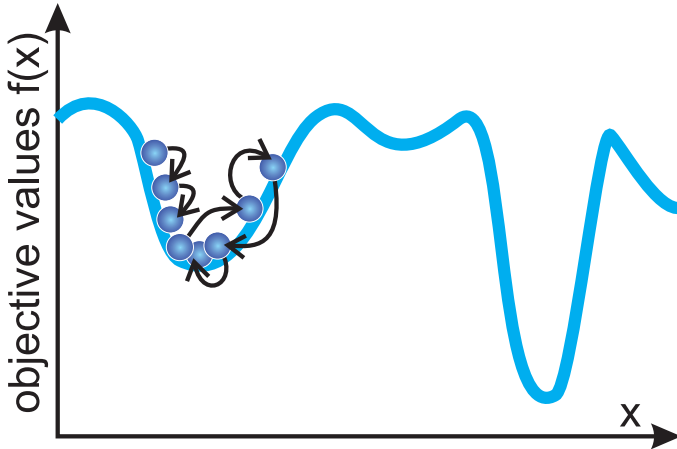
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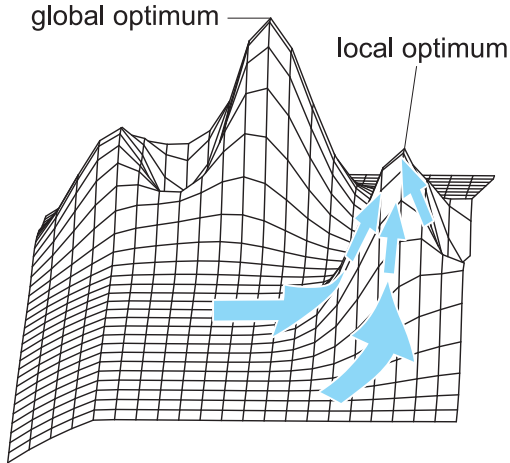
Definition (multi-modality)

A function/optimization problem is multi-modal if it has more than one minimum / maximum / optimum. [10–14]

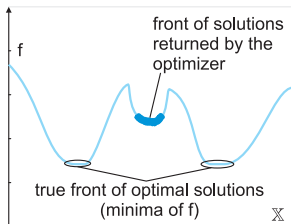
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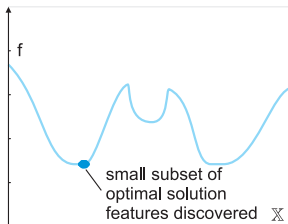
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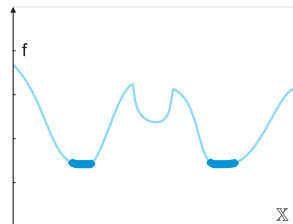
- Uniformity of convergence: We want a good scan of the potentially optimal features



Bad convergence, good spread (uniformity)

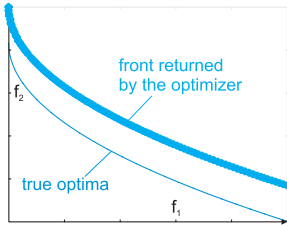


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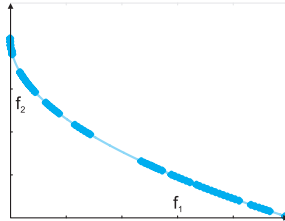


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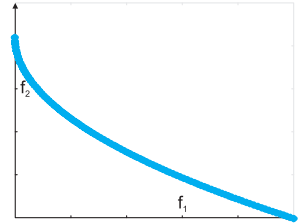
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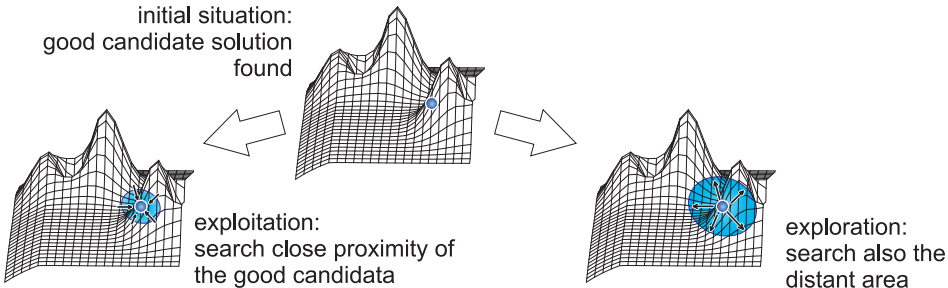
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- This is called the **Exploration versus Exploitation Dilemma** ^[16–23]

initial situation:
good candidate
solution
found



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 - ② Design complete search operators ^[24–26]:
 - it should be possible to reach all other points in the search space from the current one
 - ideally within one search step

- Countermeasures against Premature Convergence
 - ① Delay convergence by balancing exploration and exploitation and remembering diverse candidate solutions ^[16, 17, 21]
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 - ③ Restarting ^[27, 28]:
 - if no improvement for some time, restart algorithm

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 - slows down search

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 - slows down search
 - only sometimes ^[31, 68]

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 - Give solutions that are very similar to each other a worse fitness

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 - Here: cluster population, treat every cluster separately
 - Allows the population to trace different optima at once

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 - 7 Self-Adaptation ^[58, 59]

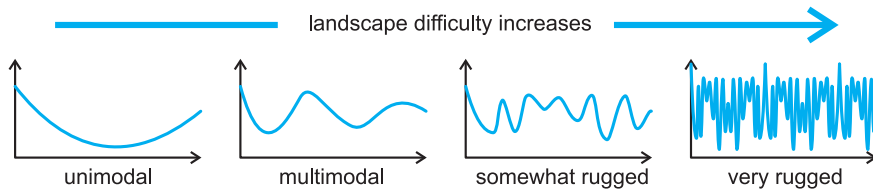
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 - change parameters of optimization algorithm in order to prevent (or speed-up) convergence

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 - ⑧ Multi-Objectivization [60–67]:
 - turn a single-objective problem into an multi-objective one by creating an artificial objective function targeting one specific aspect of the solutions
 - Pareto-based optimization (see Lesson 15: *Multi-Objective Optimization*) then increases diversity

- 1 Complexity
- 2 Unsatisfying Convergence
- 3 Ruggedness & Causality
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- Why??

- Basic assumption behind metaheuristic optimization:

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Definition (Strong Causality)

Small changes to an object should lead to small changes in its behavior / objective values. ^[69–71]

- What happens if the causality in a problem is weak?

- ① Hybridization of EAs with local search:

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 - Lamarckian evolution ^[72, 73]

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- other hybrid approaches ^[87–94]:
 - Combinations of Evolutionary Algorithms with local search, or combinations of Evolutionary Algorithms with other concepts from Machine Learning

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- Try to adjust the parameters of a (simple) model M or function so that it behaves similar to the (points so-far seen from the) objective function f

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- After a few steps, go back to original f and test solutions
- Update M , then repeat

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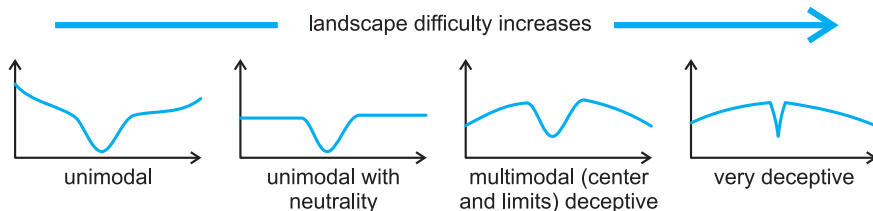
2 Landscape approximation [95]

3 (2-, n-) Staged optimization [96]:

- First, apply an optimization algorithm with slow convergence, which is good in exploring the search space and finding the region where the optimum may reside
- Then, apply an optimization algorithm which is very good at exploitation in that region only

- 1 Complexity
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- Gradient and information lead optimizer away from optimum [88, 97, 98]



- Why??

- Countermeasures

- Countermeasures
 - ① Choose appropriate representation, maybe combine representations ^[99]

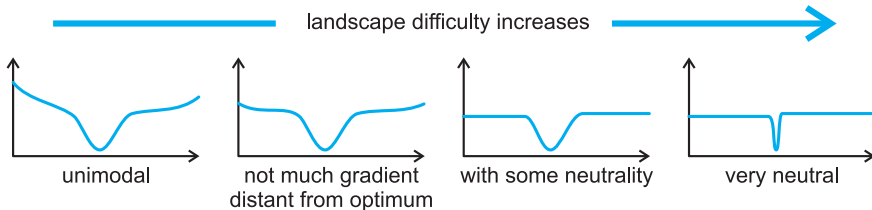
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- Neutrality: Many candidate solutions have same objective values
- Little or no information gained from sampling the solution space



- Why??

Definition (Evolvability)

The evolvability of an optimization process in its current state defines how likely the search operations will lead to candidate solutions with new (and eventually, better) objectives values. ^[107–111]

Definition (Evolvability)

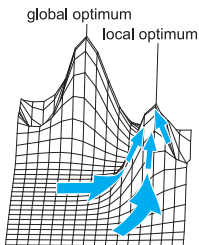
The evolvability of an optimization process in its current state defines how likely the search operations will lead to candidate solutions with new (and eventually, better) objectives values. ^[107–111]

- Neutral networks can connect different places in the search space

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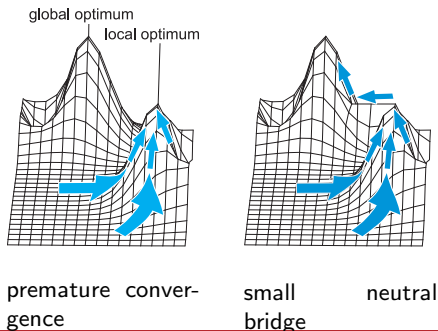


premature conver-
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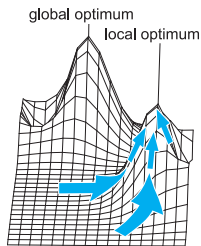
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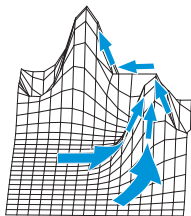
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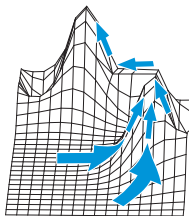


premature convergence



small bridge

neutral

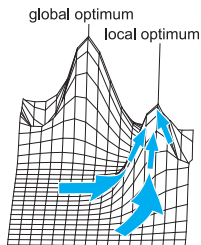


wide neutral bridge

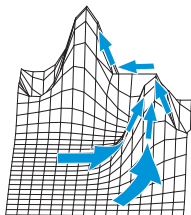
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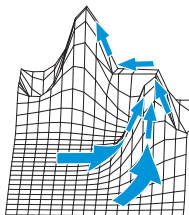


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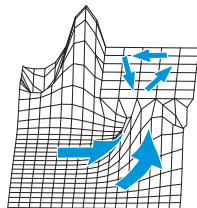


small bridge

neutral



wide neutral bridge



neutral area too large

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A function of n variables is separable if it can be rewritten as a sum of n functions of just one variable ^[120–123]

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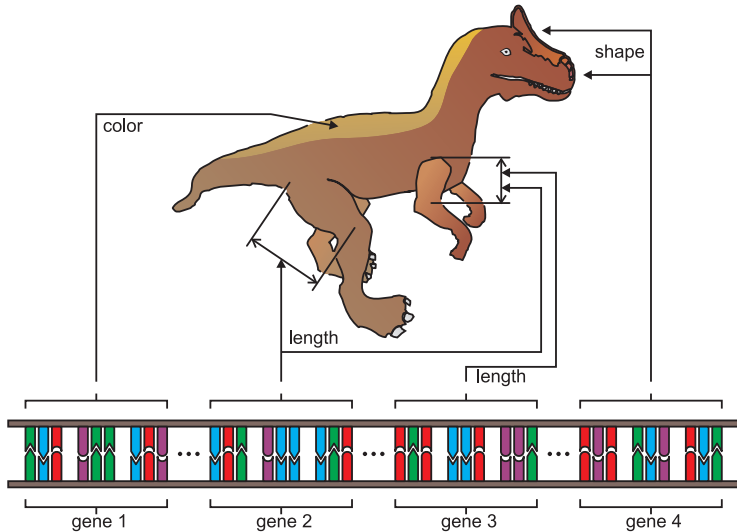
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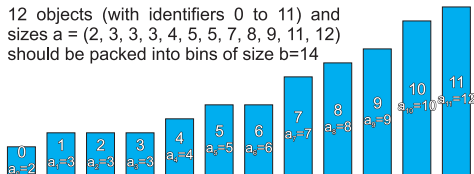
A function of n variables is separable if it can be rewritten as a sum of n functions of just one variable ^[120–123]

- non-epistatic (separable) problems can be solved efficiently by decomposition



Epistasis in Bin Packing with a pure permutation representation

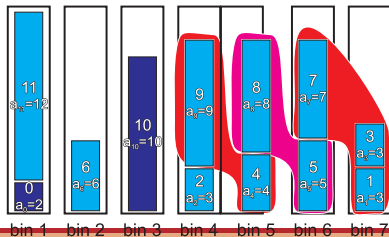
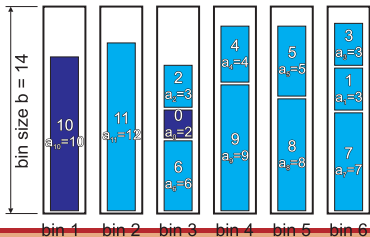
12 objects (with identifiers 0 to 11) and sizes $a = (2, 3, 3, 3, 4, 5, 5, 7, 8, 9, 11, 12)$ should be packed into bins of size $b=14$

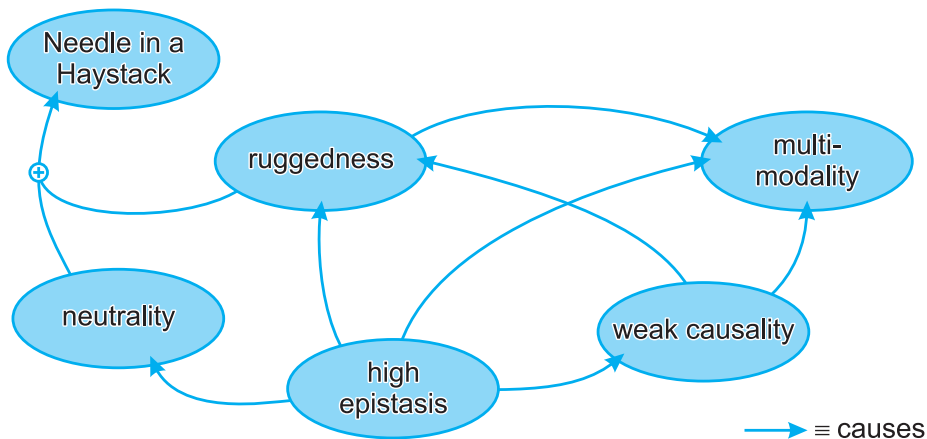


swap the first and fourth element of the permutation

$g_1 = x_1 = (10, 11, 6, 0, 2, 9, 4, 8, 5, 7, 1, 3)$

$g_1 = x_2 = (0, 11, 6, 10, 2, 9, 4, 8, 5, 7, 1, 3)$





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 - Try to find out which genes (components of the genotype) are (epistatically) linked together
 - Try to change these genes only together, consider them as a unit
 - For example: In crossover, try to always pass such genes together to the offspring and to not separate them

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- 5 If epistasis is limited: cooperative-coevolution approach ^[136–138] (see later)

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- **any** algorithm (for non-trivial problems) takes longer for larger inputs. . .

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 - ① Parallelization and distribution

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 - Parallelization: Use multi-core CPU + multiple threads or GPUs ^[150–155]

- Countermeasures

- ① Parallelization and distribution:

- sub-linear speed-up can be achieved ^[149]
 - Parallelization: Use multi-core CPU + multiple threads or GPUs ^[150–155]
 - Distribution: Use multiple computers in a network ^[156, 157], a cluster, or a grid

- Countermeasures
 - ① Parallelization and distribution
 - ② Indirect Representation 1: Generative ^[141, 142]

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 - ② Indirect Representation 1: Generative ^[141, 142]:
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 - ① Parallelization and distribution
 - ② Indirect Representation 1: Generative ^[141, 142]:
 - Genotypes are small, search space is smaller, can be explored more easily
 - They are mapped to larger, more complex phenotypes by a simple functional GPM
 - Utilizes/assumes symmetries in the phenotypes

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 - ② Indirect Representation 1: Generative ^[141, 142]
 - ③ Indirect Representation 2: Development ^[143, 144]

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 - ② Indirect Representation 1: Generative ^[141, 142]
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 - ① Parallelization and distribution
 - ② Indirect Representation 1: Generative ^[141, 142]
 - ③ Indirect Representation 2: Development ^[143, 144]:
 - Similar to generative mapping, the search space is smaller
 - But: GPM is more complex, a simulation which incorporates feedback from an environment or the objective function
 - Better behavior than generative mappings

- Countermeasures
 - ① Parallelization and distribution
 - ② Indirect Representation 1: Generative ^[141, 142]
 - ③ Indirect Representation 2: Development ^[143, 144]
 - ④ Exploiting Separability, e.g., with coevolution ^[136–138, 145, 146]

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 - Try to divide the problem into (almost) unrelated problems with smaller search spaces

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 - Try to divide the problem into (almost) unrelated problems with smaller search spaces
 - Solve them more or less separately, combine solutions to get overall solution, and repeat
 - Cooperative Coevolution ^[136, 138]: Use an EA that can find out how to divide the problem by itself and then applies the above

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 - ③ Indirect Representation 2: Development ^[143, 144]
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 - ⑤ Using multiple algorithms at once ^[147] or portfolios ^[148]

- 1 Complexity
- 2 Unsatisfying Convergence
- 3 Ruggedness & Causality
- 4 Deceptiveness
- 5 Neutrality
- 6 Epistasis
- 7 Scalability
- 8 No Free Lunch Theorem**

- Question: Can an optimization algorithm A be better than algorithm B ?

- Question: Can an optimization algorithm A be better than algorithm B ?
- Question: Can an optimization algorithm A be better than a Random Walk?

- Question: Can an optimization algorithm A be better than algorithm B ?
- Question: Can an optimization algorithm A be better than a Random Walk?
- Wolpert and Macready ^[158] – No Free Lunch Theorem: Over all optimization problems ϕ over finite domains, the sum of the probabilities to reach a certain objective value y after m steps with algorithm A is the same as with algorithm B

$$\sum_{\forall \phi} P(y|\phi, m, A) = \sum_{\forall \phi} P(y|\phi, m, B) \quad (2)$$

- According to the No Free Lunch Theorem, the answers are:

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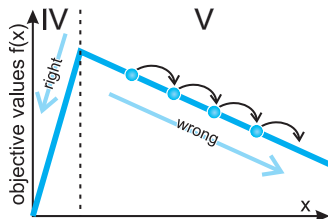
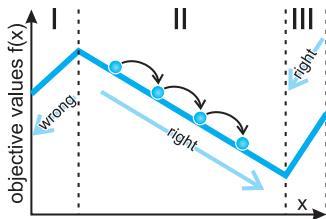
- According to the No Free Lunch Theorem, the answers are:
- Question: Can an optimization algorithm A be better than algorithm B ? **Not for all problems!**

- According to the No Free Lunch Theorem, the answers are:
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- Question: Can an optimization algorithm A be better than a Random Walk?

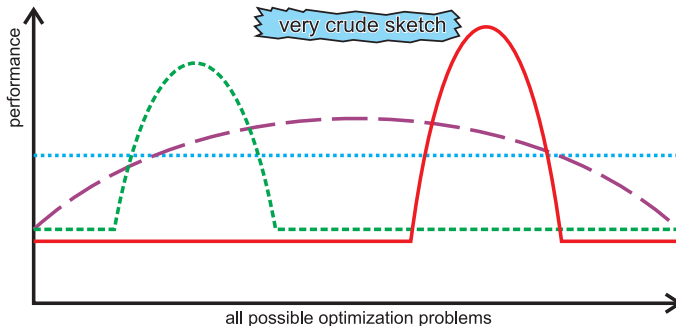
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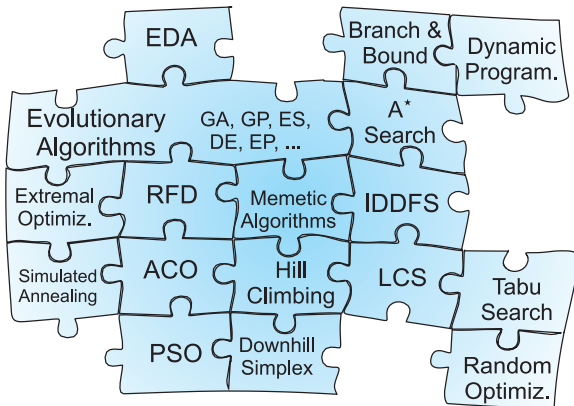


- Different algorithms are good for different problems



- random walk or exhaustive enumeration or ...
- - - general optimization algorithm - an EA, for instance
- - - specialized optimization algorithm 1; a hill climber, for instance
- specialized optimization algorithm 2; a depth-first search, for instance

- Different algorithms are good for different problems and not all possible problems actually occur in practice [1, 15, 39]



- 1 Complexity
- 2 Unsatisfying Convergence
- 3 Ruggedness & Causality
- 4 Deceptiveness
- 5 Neutrality
- 6 Epistasis
- 7 Scalability
- 8 No Free Lunch Theorem

- Optimization is difficult: This was the first batch of problems
- Many problems can only be solved exactly with algorithms of high complexity
- Metaheuristic optimizers may converge prematurely or non-uniformly
- Ruggedness is not good
- Deceptiveness is not good
- Neutrality can be good or bad
- Epistasis is always bad – and often a representation issue!
- No Free Lunch Theorem

谢谢

Thank you

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