



**Epistasis.  
Estimation-of-Distribution Algorithms.**

Petr Pošík



# Introduction to Epistasis



# GA works well...

Problem  $f_1$ :

- defined over 40-bit strings
- the quality of the worst solution:  $f_1(x^{\text{worst}}) = 0$ .
- the quality of the best solution:  $f_1(x^{\text{opt}}) = 40$ .
- the best solution:  $x^{\text{opt}} = (1111 \dots 1)$ .

GA: pop. size 160, uniform crossover, bit-flip mutation

## Epistasis

- GA works well...
- GA fails...
- Quiz
- GA works again...
- Epistasis
- LI techniques

## EDAs

How EDAs work?

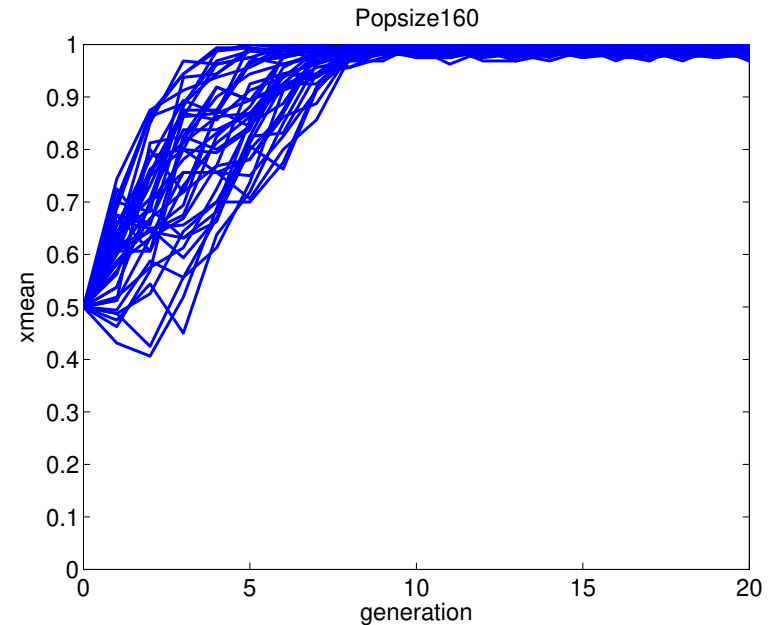
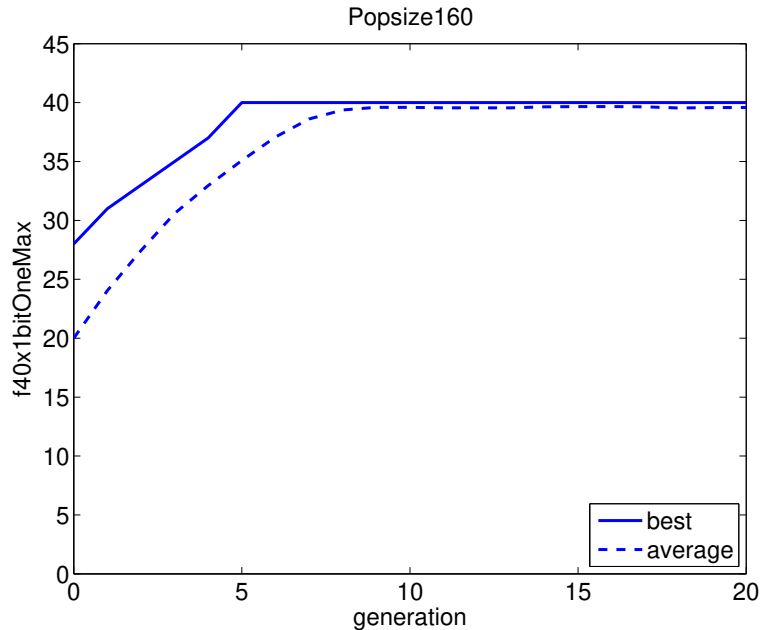
Discrete EDAs

Pairwise Interactions

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# GA fails...

Problem  $f_2$ :

- defined over 40-bit strings
- the quality of the worst solution:  $f_2(x^{\text{worst}}) = 0$ .
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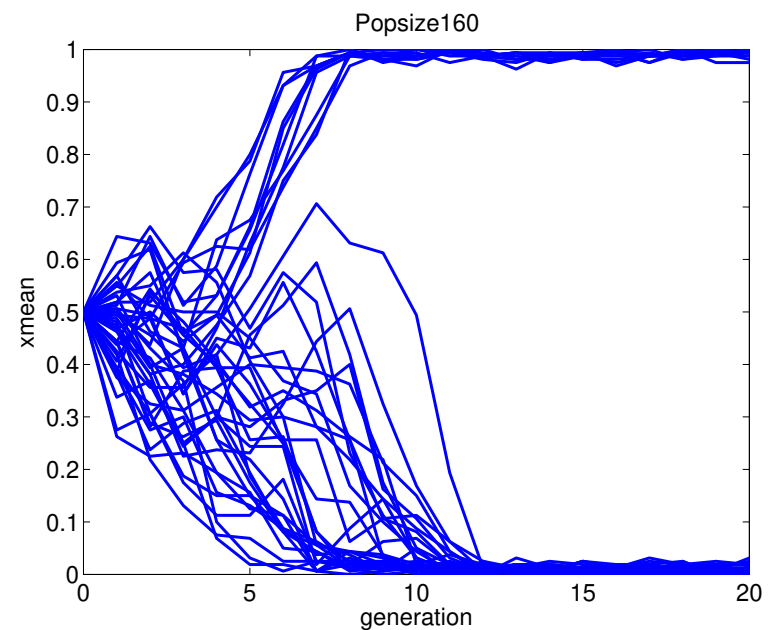
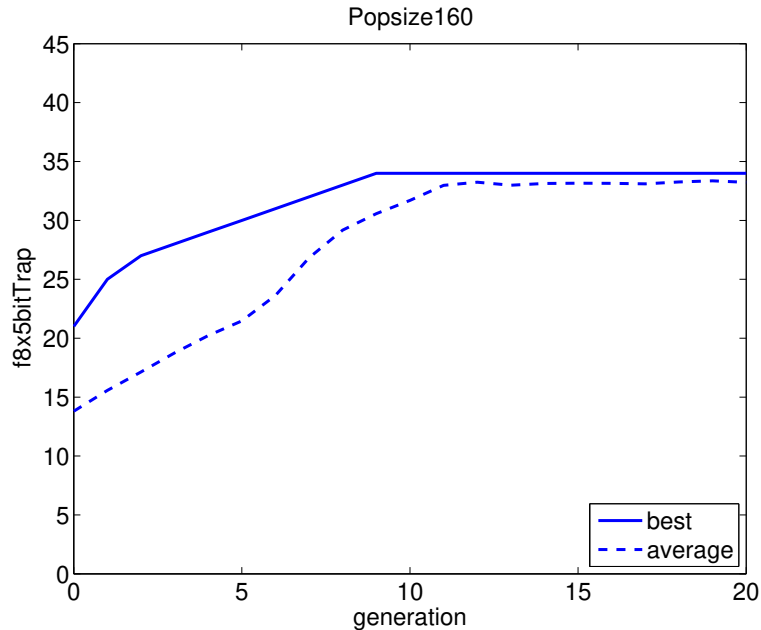
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# Quiz

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Note: Neither

- the information about the problems  $f_1$  and  $f_2$ , nor
- the information about the GA

allowed us to judge whether GA would work for the problem or not.

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# Quiz

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Note: Neither

- the information about the problems  $f_1$  and  $f_2$ , nor
- the information about the GA

allowed us to judge whether GA would work for the problem or not.

Question: Why do the results of the same GA look so different for  $f_1$  and  $f_2$ ?

- A** For  $f_1$ , we correctly tried to maximize the function, while for  $f_2$  we minimized it by mistake.
- B** Function  $f_2$  is specially designed to be extremely hard for GA that it cannot be solved efficiently, no matter what modifications we make to the GA.
- C** In function  $f_1$  all bits are independent, while  $f_2$  contains some interactions among individual bits. GA is not aware of any interactions, and treats all bits independently.
- D** I have absolutely no idea.

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# GA works again...

Still solving  $f_2$ :

- defined over 40-bit strings
- the quality of the worst solution:  $f_2(x^{\text{worst}}) = 0$ .
- the quality of the best solution:  $f_2(x^{\text{opt}}) = 40$ .
- the best solution:  $x^{\text{opt}} = (1111 \dots 1)$ .

Instead of the uniform crossover,

- let us *allow the crossover only after each 5th bit*.

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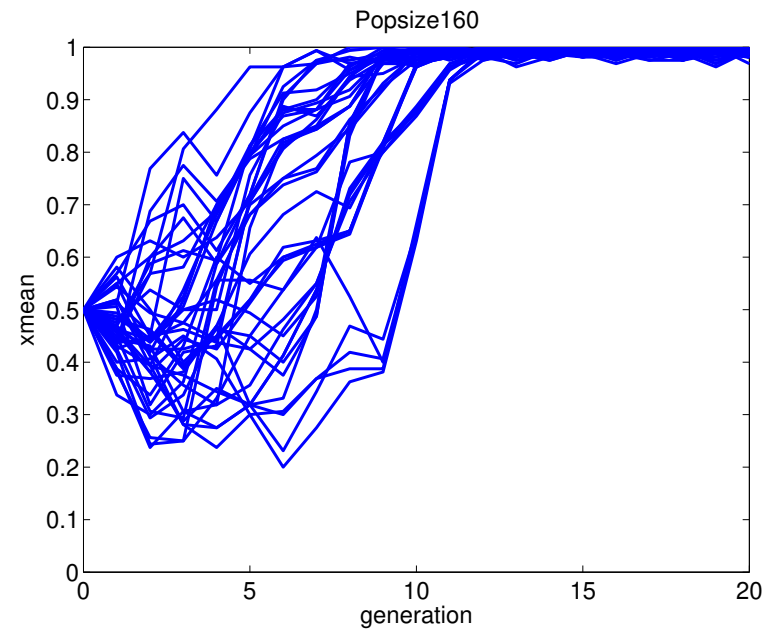
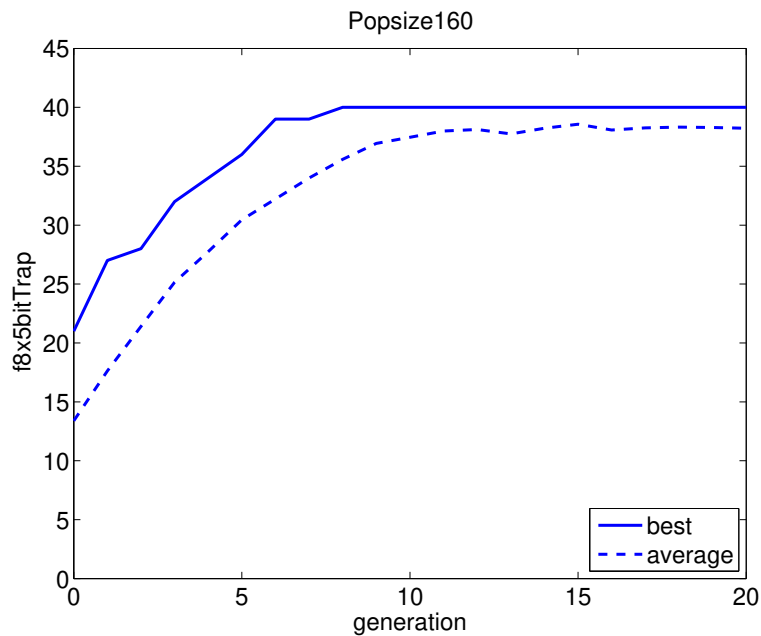
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Problem  $f_2$  contains some interactions among variables and *GA knows about them*.



# Epistasis

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## Epistasis:

- Effects of one gene are dependent on (influenced, conditioned by) other genes.
- Other names: dependencies, interdependencies, interactions.

## Linkage:

- Tendency of certain loci or alleles to be inherited together.

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# Epistasis

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## Epistasis:

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- Other names: dependencies, interdependencies, interactions.

## Linkage:

- Tendency of certain loci or alleles to be inherited together.

When optimizing the following functions, which of the variables are linked together?

$$f = x_1 + x_2 + x_3 \quad (1)$$

$$f = 0.1x_1 + 0.7x_2 + 3x_3 \quad (2)$$

$$f = x_1x_2x_3 \quad (3)$$

$$f = x_1 + x_2^2 + \sqrt{x_3} \quad (4)$$

$$f = \sin(x_1) + \cos(x_2) + e^{x_3} \quad (5)$$

$$f = \sin(x_1 + x_2) + e^{x_3} \quad (6)$$

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$$f = \sin(x_1 + x_2) + e^{x_3} \quad (6)$$

Notes:

- Almost all real-world problems contain interactions among design variables.
- The “amount” and “type” of interactions depend on the representation and the objective function.
- Sometimes, by a clever choice of the representation and the objective function, we can get rid of the interactions.

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# Linkage Identification Techniques

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Problems:

- How to detect dependencies among variables?
- How to use them?

Techniques used for linkage identification:

1. Indirect detection along genetic search (messy GAs)
2. Direct detection of fitness changes by perturbation
3. Model-based approach: classification
4. Model-based approach: distribution estimation (EDAs)

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# Introduction to EDAs



# Genetic Algorithms

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## Algorithm 1: Genetic Algorithm

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```
1 begin
2   Initialize the population.
3   while termination criteria are not met do
4     Select parents from the population.
5     Cross over the parents, create offspring.
6     Mutate offspring.
7     Incorporate offspring into the population.
```

---

“Select → cross over → mutate” approach

### Conventional GA operators

- are not adaptive, and
- cannot (or usually do not) discover and use *the interactions among solution components*.

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- Genetic Algorithms
- GA vs EDA
- EDAs

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# Genetic Algorithms

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### Conventional GA operators

- are not adaptive, and
- cannot (or usually do not) discover and use *the interactions among solution components*.

The goal of recombination operators:

- Intensify the search in areas which contained “good” individuals in previous iterations.
- Must be able to take the interactions into account.
- Why not directly describe the distribution of “good” individuals???

# GA vs EDA

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## Algorithm 1: Genetic Algorithm

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---

“Select → cross over → mutate” approach

Why not use directly...

---

## Algorithm 2: Estimation-of-Distribution Alg.

---

```
1 begin
2   Initialize the population.
3   while termination criteria are not met do
4     Select parents from the population.
5     Learn a model of their distribution.
6     Sample new individuals.
7     Incorporate offspring into the
      population.
```

---

“Select → update model → sample” approach

# GA vs EDA

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## Algorithm 1: Genetic Algorithm

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1 begin
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Why not use directly...

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## Algorithm 2: Estimation-of-Distribution Alg.

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1 begin
2   Initialize the population.
3   while termination criteria are not met do
4     Select parents from the population.
5     Learn a model of their distribution.
6     Sample new individuals.
7     Incorporate offspring into the
      population.
```

---

“Select → update model → sample” approach

Or even...

---

## Algorithm 3: Estimation-of-Distribution Alg. (Type 2)

---

```
1 begin
2   Initialize the model.
3   while termination criteria are not met do
4     Sample new individuals.
5     Select better ones.
6     Update the model based on selected
      ones.
```

---

“Sample → select → update model” approach





# EDAs

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## Explicit probabilistic model:

- Sound and principled way of working with dependencies.
- Adaptation ability (different behavior in different stages of evolution).

## Names:

**EDA** Estimation-of-Distribution Algorithm

**PMBGA** Probabilistic Model-Building Genetic Algorithm

**IDEA** Iterated Density Estimation Algorithm

## Continuous EDAs (a very simplified view):

- Histograms and (Mixtures of) Gaussian distributions are used most often as the probabilistic model.
- Algorithms with Gaussians usually become very similar to CMA-ES.

In the following, we shall talk only about discrete (binary) EDAs.

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## How EDAs work?



# Example

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## 5-bit OneMax (CountOnes) problem:

- $f_{D \times 1 \text{bitOneMax}}(\mathbf{x}) = \sum_{d=1}^D x_d$
- Optimum: 11111, fitness: 5

## Algorithm: **Univariate Marginal Distribution Algorithm (UMDA)**

- Population size: 6
- Tournament selection:  $t = 2$
- **Model:** vector of probabilities  $p = (p_1, \dots, p_D)$ 
  - each  $p_d$  is the probability of observing 1 at  $d$ th element
- **Model learning:**
  - estimate  $p$  from selected individuals
- **Model sampling:**
  - generate 1 on  $d$ th position with probability  $p_d$  (independently of other positions)

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- Example
- UMDA Pipeline
- UMDA: OneMax
- Trap function
- UMDA: Traps
- Beating traps
- Good news!

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# Selection, Modeling, Sampling

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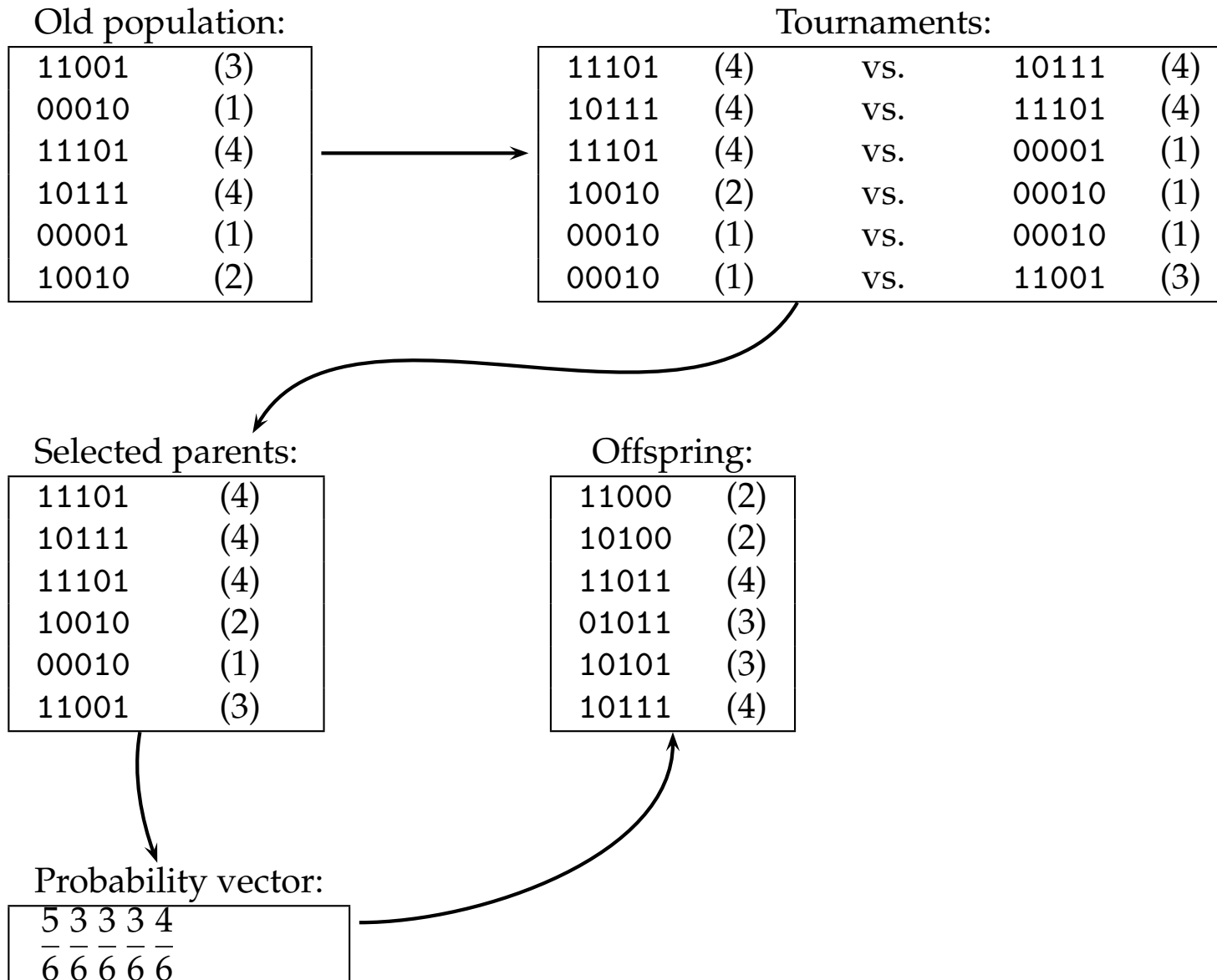
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# UMDA Behaviour for OneMax problem

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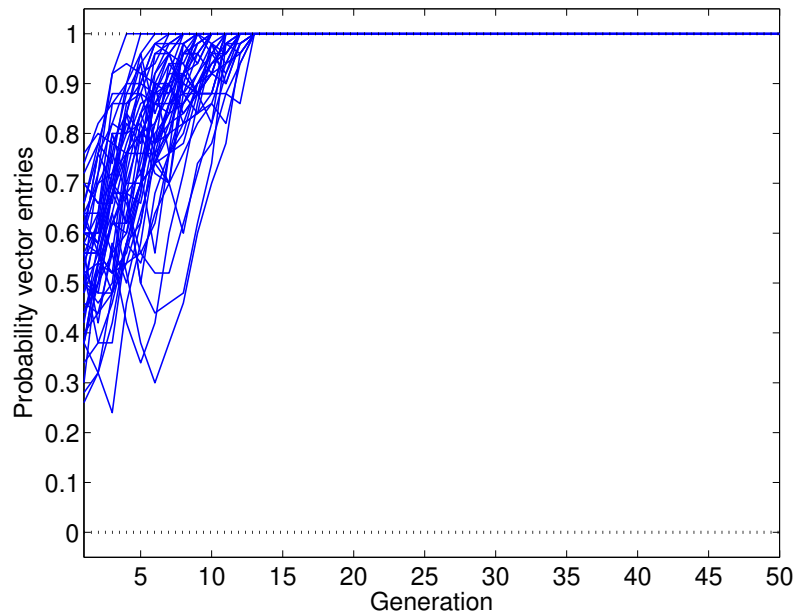
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- 1s are better than 0s on average, selection increases the proportion of 1s
- Recombination preserves and combines 1s, the ratio of 1s increases over time
- If we have many 1s in population, we cannot miss the optimum

The number of evaluations needed for reliable convergence:

Algorithm	Nr. of evaluations
UMDA	$\mathcal{O}(D \ln D)$
Hill-Climber	$\mathcal{O}(D \ln D)$
GA with uniform crossover	approx. $\mathcal{O}(D \ln D)$
GA with 1-point crossover	a bit slower

**UMDA behaves similarly to GA with uniform crossover!**



# What about a different fitness?

For OneMax function:

- UMDA works well, all the bits probably eventually converge to the right value.

Will UMDA be similarly successful for other fitness functions?

- Well, .....no. :-)

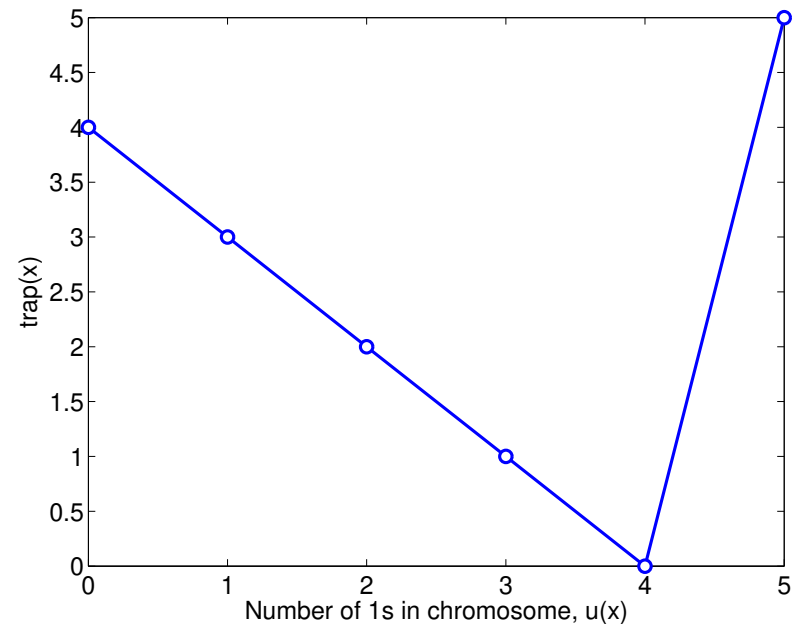
**Problem: Concatanated 5-bit traps**

$$f = f_{\text{trap}}(x_1, x_2, x_3, x_4, x_5) + \\ + f_{\text{trap}}(x_6, x_7, x_8, x_9, x_{10}) + \\ + \dots$$

The *trap* function is defined as

$$f_{\text{trap}}(\mathbf{x}) = \begin{cases} 5 & \text{if } u(\mathbf{x}) = 5 \\ 4 - u(\mathbf{x}) & \text{otherwise} \end{cases}$$

where  $u(\mathbf{x})$  is the so called *unity* function and returns the number of 1s in  $\mathbf{x}$  (it is actually the One Max function).



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# UMDA behaviour on concatenated traps

## Traps:

- Optimum in 111111...1
- But  $f_{\text{trap}}(0****) = 2$  while  $f_{\text{trap}}(1****) = 1.375$
- 1-dimensional probabilities lead the GA to the wrong way!
- Exponentially increasing population size is needed, otherwise GA will not find optimum reliably.

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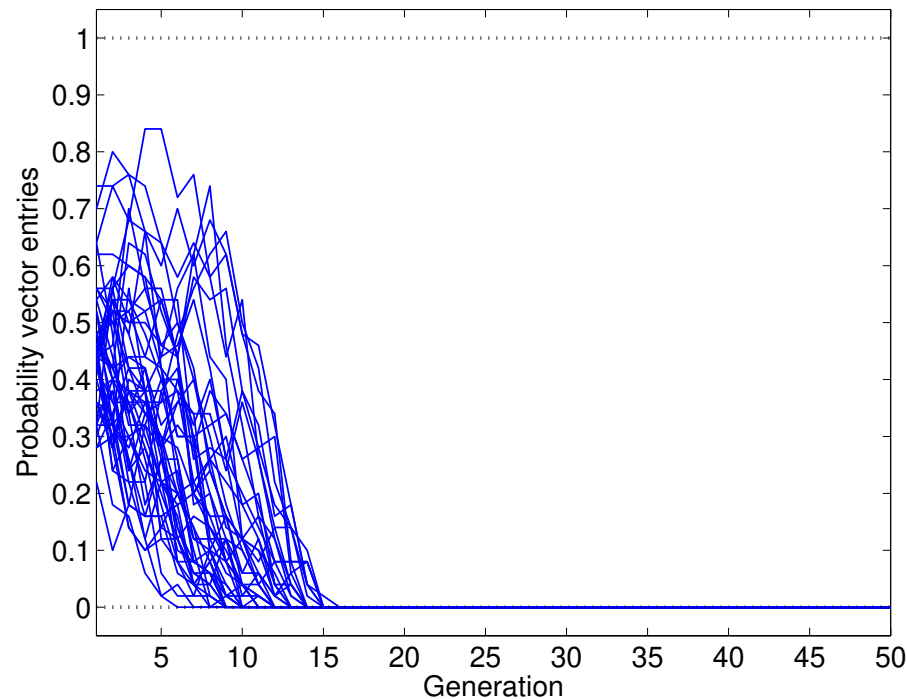
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# What can be done about traps?

---

The  $f_{\text{trap}}$  function is *deceptive*:

- Statistics over 1\*\*\*\* and 0\*\*\*\* do not lead us to the right solution
- The same holds for statistics over 11\*\*\* and 00\*\*\*, 111\*\* and 000\*\*, 1111\* and 0000\*

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- Harder than the *needle-in-the-haystack* problem:
  - regular haystack simply does not provide any information, where to search for the needle
  - $f_{\text{trap}}$ -haystack actively lies to you—it points you to the wrong part of the haystack

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- But:  $f_{\text{trap}}(00000) < f_{\text{trap}}(11111)$ , 11111 will be better than 00000 on average
- 5bit statistics should work for 5bit traps in the same way as 1bit statistics work for OneMax problem!

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Model learning:

- build model for each 5-tuple of bits
- compute  $p(00000), p(00001), \dots, p(11111)$ ,

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Model learning:

- build model for each 5-tuple of bits
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Model sampling:

- Each 5-tuple of bits is generated independently
- Generate 00000 with probability  $p(00000)$ , 00001 with probability  $p(00001), \dots$

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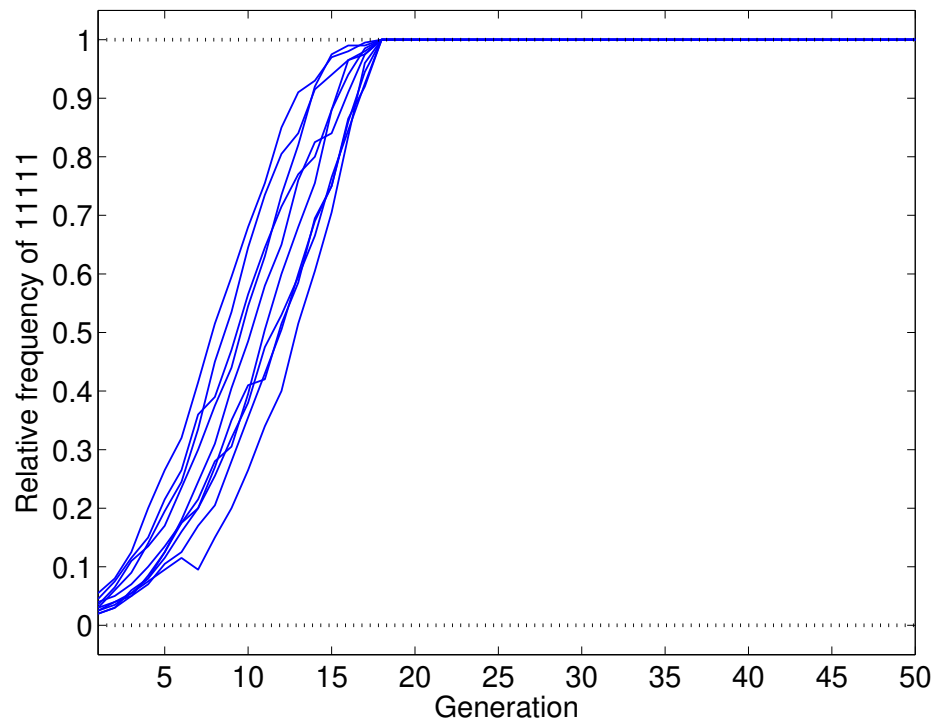
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# Good news!

## The right statistics work great!



Algorithm

Nr. of evaluations

UMDA with 5bit BB

$\mathcal{O}(D \ln D)$  (WOW!)

Hill-Climber

$\mathcal{O}(D^k \ln D)$ ,  $k = 5$

GA with uniform xover

approx.  $\mathcal{O}(2^D)$

GA with 1-point xover

similar to unif. xover

## What shall we do next?

If we were able to

- find the right statistics with a small overhead, and
- use them in the UMDA framework,

we would be able to solve order- $k$  separable problems using  $\mathcal{O}(D^2)$  evaluations.

- ...and there are many problems of this type.

The problem solution is closely related to the so-called *linkage learning*, i.e. discovering and using statistical dependencies among variables.



## Discrete EDAs



# EDAs without interactions

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- EDAs without interactions

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1. **Population-based incremental learning (PBIL)**  
Baluja, 1994
2. **Univariate marginal distribution algorithm (UMDA)**  
Mühlenbein and Paaß, 1996
3. **Compact genetic algorithm (cGA)**  
Harik, Lobo, Goldberg, 1998

## Similarities:

- all of them use a vector of probabilities

## Differences:

- PBIL and cGA do not use population (only the vector  $p$ ); UMDA does
- PBIL and cGA use different rules for the adaptation of  $p$

## Advantages:

- Simplicity
- Speed
- Simple simulation of large populations

## Limitations:

- Reliable only for order-1 decomposable problems (i.e., problems without interactions).



# EDAs with Pairwise Interactions

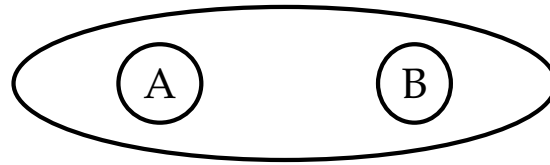




# From single bits to pairwise models

How to describe two positions together?

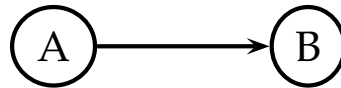
- Using the joint probability distribution:



Number of free parameters: 3

$p(A, B)$		B	
		0	1
A	0	$p(0, 0)$	$p(0, 1)$
	1	$p(1, 0)$	$p(1, 1)$

- Using conditional probabilities:



Number of free parameters: 3

$$p(A, B) = p(B|A) \cdot p(A):$$

$$p(B = 1|A = 0)$$

$$p(B = 1|A = 1)$$

$$p(A = 1)$$

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- Graph. models

- Quiz

- Dependency tree

- DT learning

- DT model

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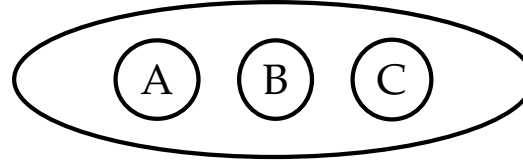


# Quiz

---

Question: What is the number of free parameters for the following models?  
(A, B, C are binary random variables.)

Joint probability distribution:



Epistasis

EDAs

How EDAs work?

Discrete EDAs

Pairwise Interactions

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**A** 5

**B** 6

**C** 7

**D** 8

Multivar. Interactions

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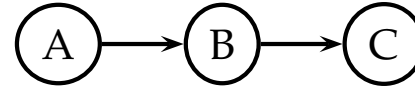


# Quiz

---

Question: What is the number of free parameters for the following models?  
(A, B, C are binary random variables.)

Distribution using the following conditioning structure:



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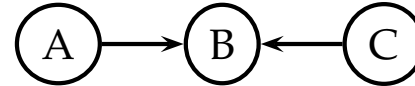


# Quiz

---

Question: What is the number of free parameters for the following models?  
(A, B, C are binary random variables.)

Distribution using the following conditioning structure:



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# How to learn pairwise dependencies: dependency tree

---

- Nodes: binary variables (loci of chromosome)
- Edges: the strength of dependencies among variables
- Features:
  - Each node depends on at most 1 other node
  - Graph does not contain cycles
  - Graph is connected

Learning the structure of dependency tree:

1. Score the edges using mutual information:

$$I(X, Y) = \sum_{x,y} p(x, y) \cdot \log \frac{p(x, y)}{p(x)p(y)}$$

2. Use any algorithm to determine the maximum spanning tree of the graph, e.g. Prim (1957)
  - (a) Start building the tree from any node
  - (b) Add such a node that is connected to the tree by the edge with maximum score

Epistasis

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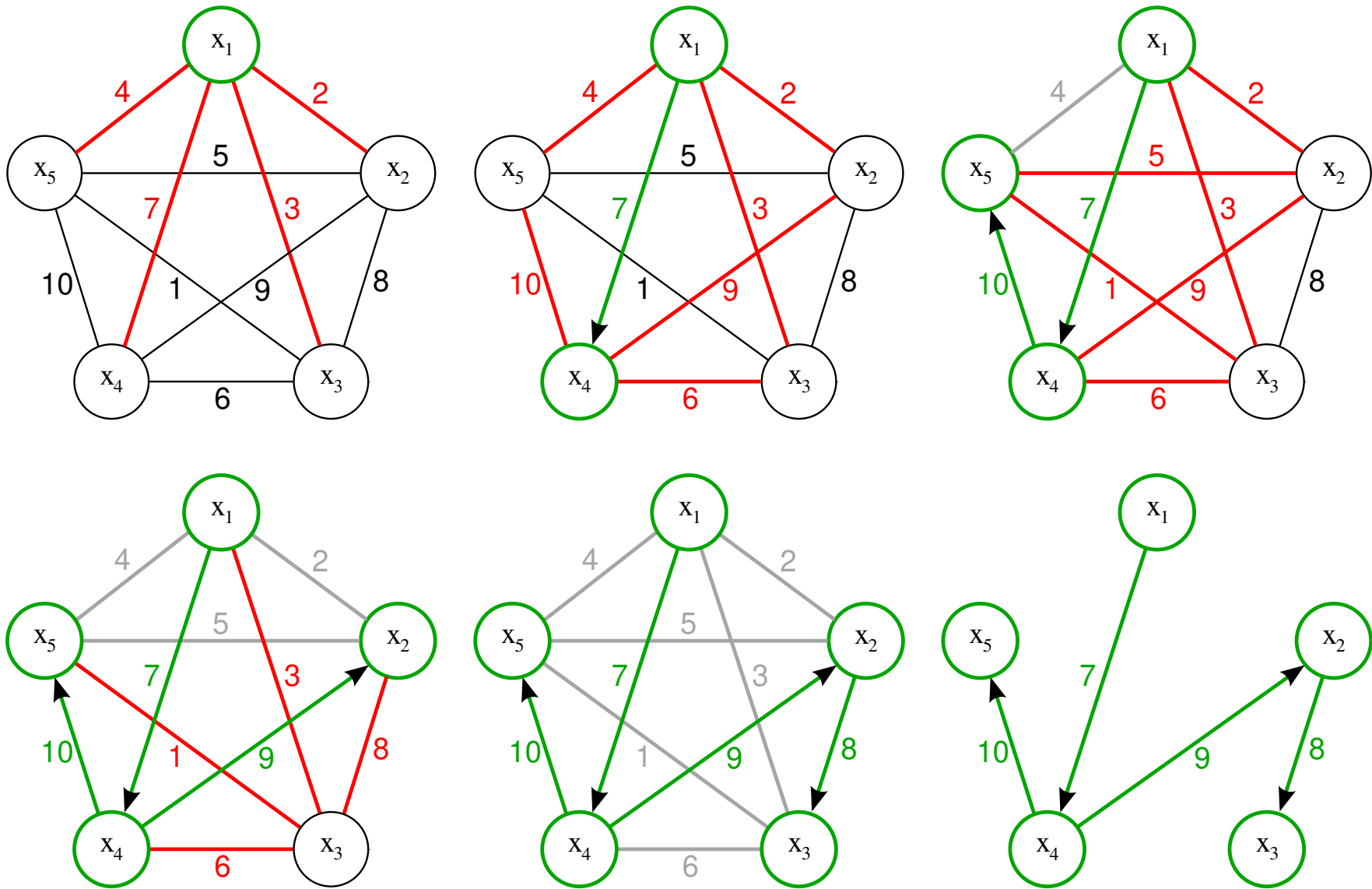
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# Example of dependency tree learning (Max. spanning tree, Prim)





# Dependency tree: probabilities

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EDAs

How EDAs work?

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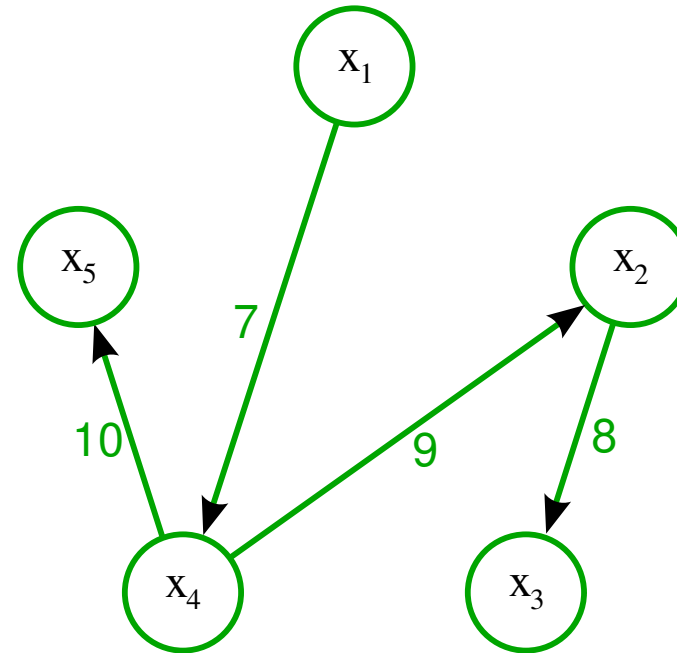
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Probability	Number of free params
$p(X_1 = 1)$	1
$p(X_4 = 1 X_1)$	2
$p(X_5 = 1 X_4)$	2
$p(X_2 = 1 X_4)$	2
$p(X_3 = 1 X_2)$	2
Whole model	9



# EDAs with pairwise interactions

Epistasis

EDAs

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Discrete EDAs

Pairwise Interactions

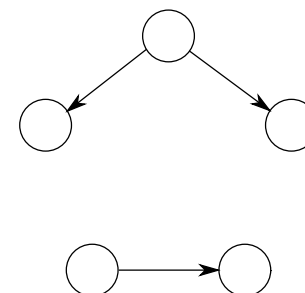
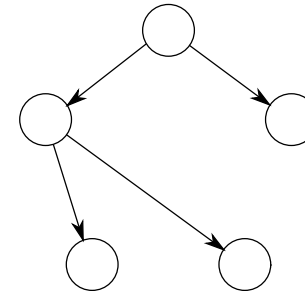
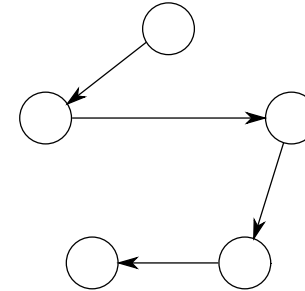
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1. **MIMIC** (sequences)
  - Mutual Information Maximization for Input Clustering
  - de Bonet et al., 1996
2. **COMIT** (trees)
  - Combining Optimizers with Mutual Information Trees
  - Baluja and Davies, 1997
3. **BMDA** (forrest)
  - Bivariate Marginal Distribution Algorithm
  - Pelikan and Mühlenbein, 1998







# Summary

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- Advantages:
  - Still simple
  - Still fast
  - Can learn *something* about the structure
- Limitations:
  - Reliable only for order-1 or order-2 decomposable problems

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## EDAs with Multivariate Interactions



# ECGA

Extended Compact GA, Harik, 1999

Marginal Product Model (MPM)

- Variables are treated in groups
- Variables in different groups are considered statistically independent
- Each group is modeled by its joint probability distribution
- The algorithm adaptively searches for the groups during evolution

Problem	Ideal group configuration
OneMax	[1] [2] [3] [4] [5] [6] [7] [8] [9] [10]
5bitTraps	[1 2 3 4 5] [6 7 8 9 10]

Epistasis

EDAs

How EDAs work?

Discrete EDAs

Pairwise Interactions

Multivar. Interactions

- ECGA
- MDL Metric
- BOA
- BOA: Learning

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# ECGA

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- Each group is modeled by its joint probability distribution
- The algorithm adaptively searches for the groups during evolution

Problem	Ideal group configuration									
OneMax	[1]	[2]	[3]	[4]	[5]	[6]	[7]	[8]	[9]	[10]
5bitTraps	[1	2	3	4	5]	[6	7	8	9	10]

Learning the structure

1. Evaluation metric: Minimum Description Length (MDL)
2. Search procedure: greedy
  - (a) Start with each variable belonging to its own group
  - (b) Perform such a join of two groups which improves the score best
  - (c) Finish if no join improves the score

Epistasis

EDAs

How EDAs work?

Discrete EDAs

Pairwise Interactions

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- ECGA
- MDL Metric
- BOA
- BOA: Learning

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# ECGA: Evaluation metric

## Minimum description length:

Minimize the number of bits required to store the model and the data encoded using the model

$$DL(Model, Data) = DL_{Model} + DL_{Data}$$

## Model description length:

Each group  $g$  has  $|g|$  dimensions, i.e.  $2^{|g|} - 1$  frequencies, each of them can take on values up to  $N$

$$DL_{Model} = \log N \sum_{g \in G} (2^{|g|} - 1)$$

## Data description length using the model:

Defined using the entropy of marginal distributions ( $X_g$  is  $|g|$ -dimensional random vector,  $x_g$  is its realization):

$$DL_{Data} = N \sum_{g \in G} h(X_g) = -N \sum_{g \in G} \sum_{x_g} p(X_g = x_g) \log p(X_g = x_g)$$

Epistasis

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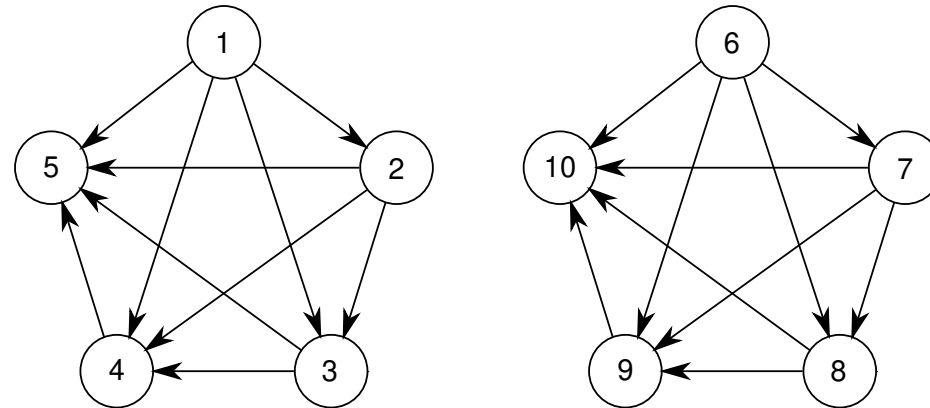


# BOA

**Bayesian Optimization Algorithm:** Pelikán, Goldberg, Cantù-Paz, 1999

Bayesian network (BN)

- Conditional dependencies (instead groups)
- Sequence, tree, forrest — special cases of BN
- For trap function:



- The same model used independently in
  - Estimation of Bayesian Network Alg. (EBNA), Etxeberria et al., 1999
  - Learning Factorized Density Alg. (LFDA), Mühlenbein et al., 1999

Epistasis

EDAs

How EDAs work?

Discrete EDAs

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- **BOA**
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# BOA: Learning the structure

---

1. Evaluation metric:
  - Bayesian-Dirichlet metric, or
  - Bayesian information criterion (BIC)
2. Search procedure: greedy
  - (a) Start with graph with no edges (univariate marginal product model)
  - (b) Perform one of the following operations, choose the one which improves the score best
    - Add an edge
    - Delete an edge
    - Reverse an edge
  - (c) Finish if no operation improves the score

**BOA solves order- $k$  decomposable problems in less than  $\mathcal{O}(D^2)$  evaluations!**

$$n_{evals} = \mathcal{O}(D^{1.55}) \text{ to } \mathcal{O}(D^2)$$

Epistasis

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EDAs

---

How EDAs work?

---

Discrete EDAs

---

Pairwise Interactions

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Multivar. Interactions

---

- ECGA
- MDL Metric
- BOA
- **BOA: Learning**

Scalability Analysis

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Summary

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# Scalability Analysis



# Test functions

**One Max:**

$$f_{D \times 1 \text{bitOneMax}}(\mathbf{x}) = \sum_{d=1}^D x_d$$

**Trap:**

$$f_{D \text{bitTrap}}(\mathbf{x}) = \begin{cases} D & \text{if } u(\mathbf{x}) = D \\ D - 1 - u(\mathbf{x}) & \text{otherwise} \end{cases}$$

**Equal Pairs:**

$$f_{D \text{bitEqualPairs}}(\mathbf{x}) = 1 + \sum_{d=2}^D f_{\text{EqualPair}}(x_{d-1}, x_d)$$

$$f_{\text{EqualPair}}(x_1, x_2) = \begin{cases} 1 & \text{if } x_1 = x_2 \\ 0 & \text{if } x_1 \neq x_2 \end{cases}$$

**Sliding XOR:**

$$f_{D \text{bitSlidingXOR}}(\mathbf{x}) = 1 + f_{\text{AllEqual}}(\mathbf{x}) + \sum_{d=3}^D f_{\text{XOR}}(x_{d-2}, x_{d-1}, x_d)$$

$$f_{\text{AllEqual}}(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{x} = (000 \dots 0) \\ 1 & \text{if } \mathbf{x} = (111 \dots 1) \\ 0 & \text{otherwise} \end{cases}$$

$$f_{\text{XOR}}(x_1, x_2, x_3) = \begin{cases} 1 & \text{if } x_1 \oplus x_2 = x_3 \\ 0 & \text{otherwise} \end{cases}$$

**Concatenated short basis functions:**

$$f_{N \times K \text{bitBasisFunction}} = \sum_{k=1}^K f_{\text{BasisFunction}}(x_{K(k-1)+1}, \dots, x_{Kk})$$

## Test function (cont.)

---

1.  $f_{40 \times 1 \text{bitOneMax}}$ 
  - order-1 decomposable function, no interactions
2.  $f_{1 \times 40 \text{bitEqualPairs}}$ 
  - non-decomposable function
  - weak interactions: optimal setting of each bit depends on the value of the preceding bit
3.  $f_{8 \times 5 \text{bitEqualPairs}}$ 
  - order-5 decomposable function
4.  $f_{1 \times 40 \text{bitSlidingXOR}}$ 
  - non-decomposable function
  - stronger interactions: optimal setting of each bit depends on the value of the 2 preceding bits
5.  $f_{8 \times 5 \text{bitSlidingXOR}}$ 
  - order-5 decomposable function
6.  $f_{8 \times 5 \text{bitTrap}}$ 
  - order-5 decomposable function
  - interactions in each 5-bit block are very strong, the basis function is deceptive



# Scalability analysis

---

Facts:

- using small population size, population-based optimizers can solve only easy problems
- increasing the population size, the optimizers can solve increasingly harder problems
- ... but using a too big population is wasting of resources.

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# Scalability analysis

---

Facts:

- using small population size, population-based optimizers can solve only easy problems
- increasing the population size, the optimizers can solve increasingly harder problems
- ... but using a too big population is wasting of resources.

Scalability analysis:

- determines the optimal (smallest) population size, with which the algorithm solves the given problem reliably
  - reliably: algorithm finds the optimum in 24 out of 25 runs)
  - for each problem complexity, the optimal population size is determined e.g. using the bisection method
- studies the influence of the problem complexity (dimensionality) on the optimal population size and on the number of needed evaluations

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# Scalability on the One Max function

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How EDAs work?

Discrete EDAs

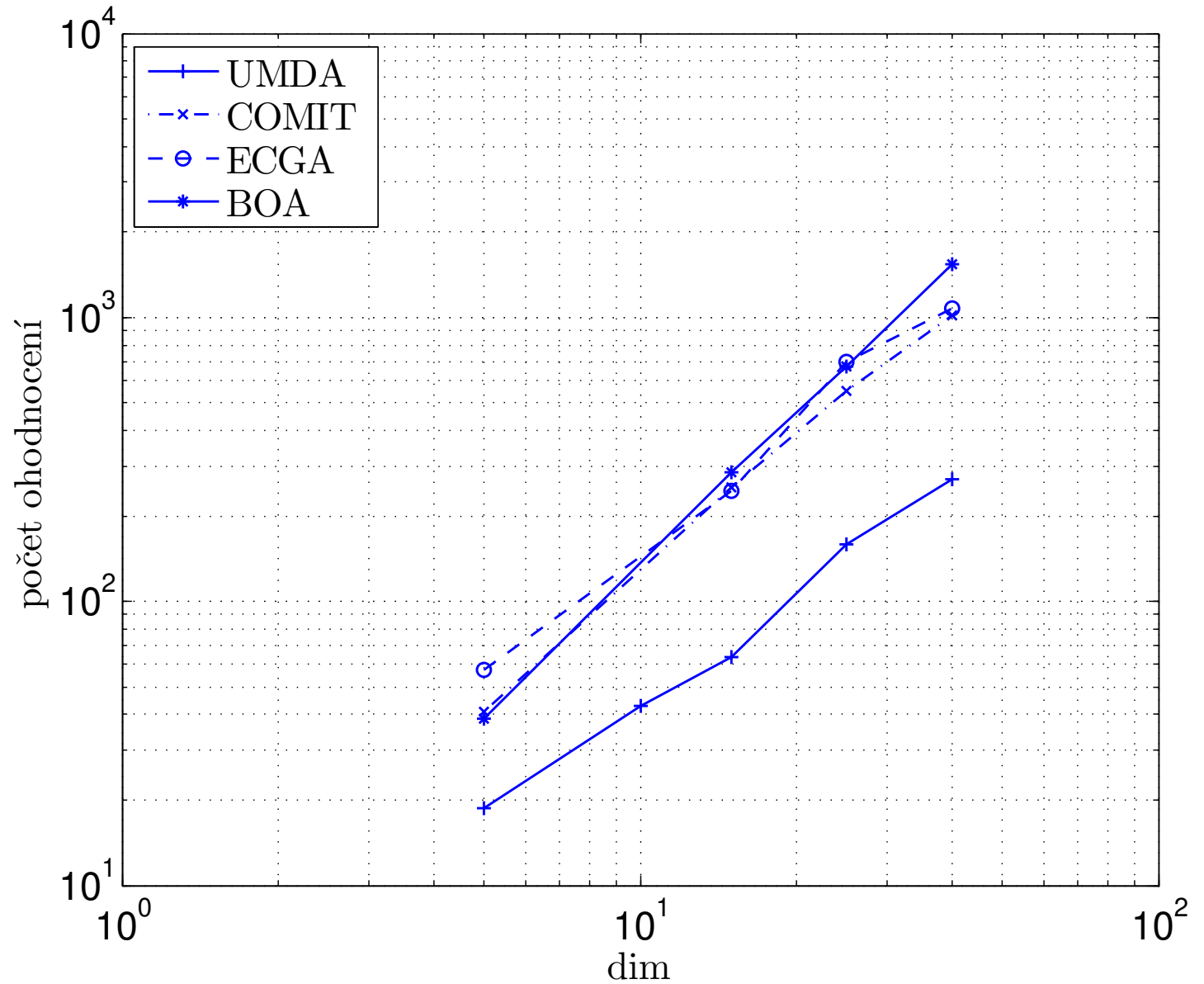
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# Scalability on the non-decomposable Equal Pairs function

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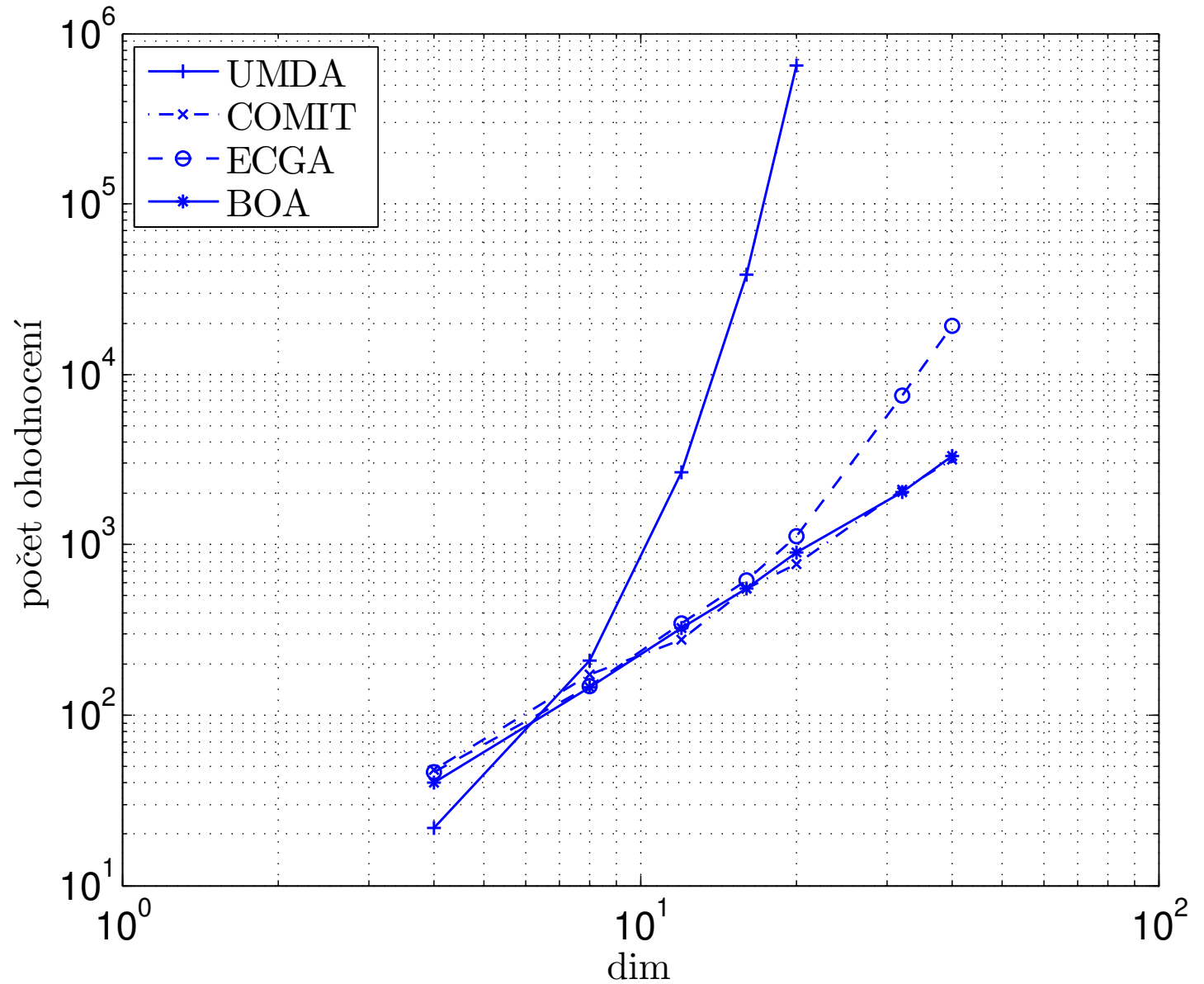
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# Scalability on the decomposable Equal Pairs function

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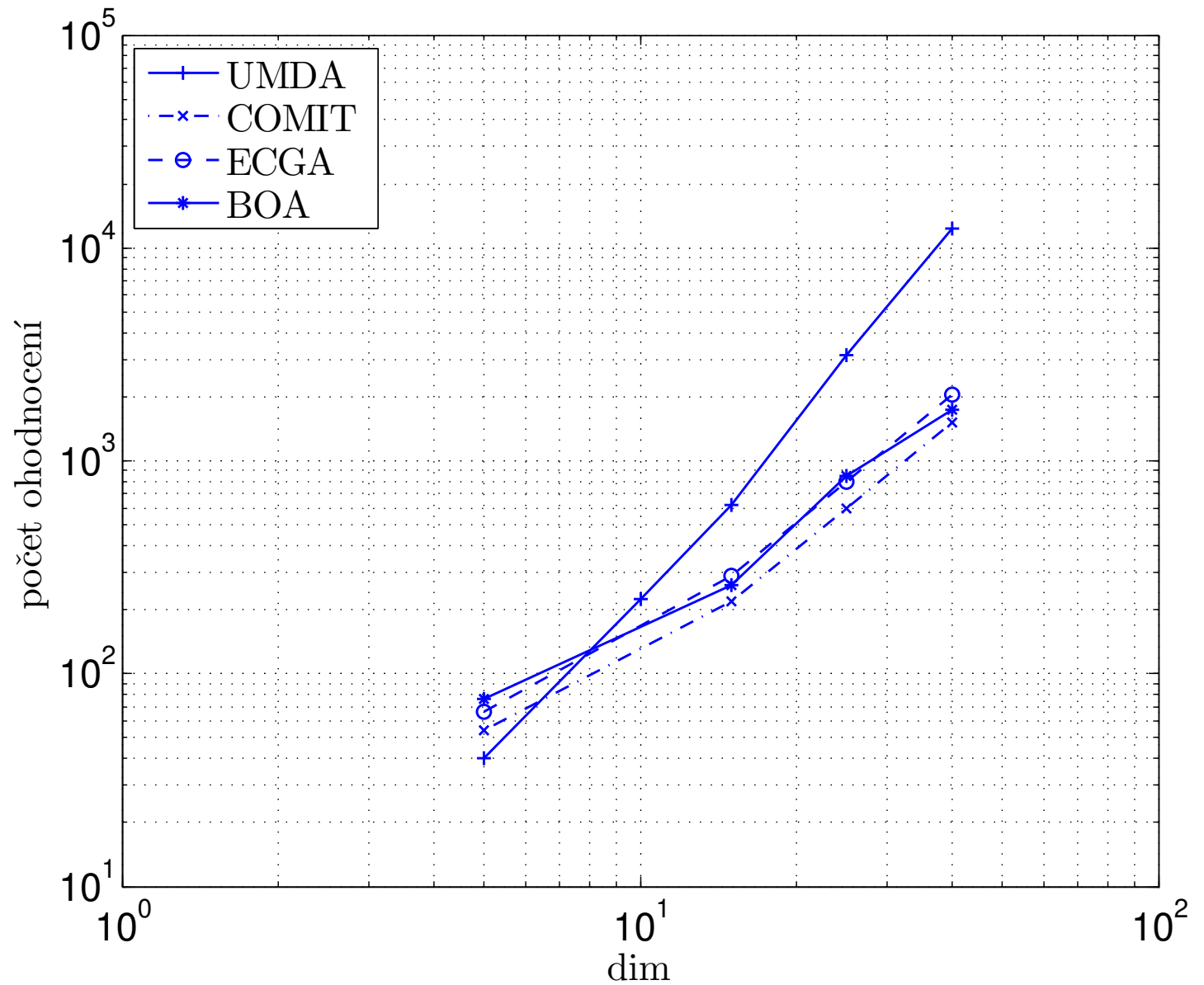
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# Scalability on the non-decomposable Sliding XOR function

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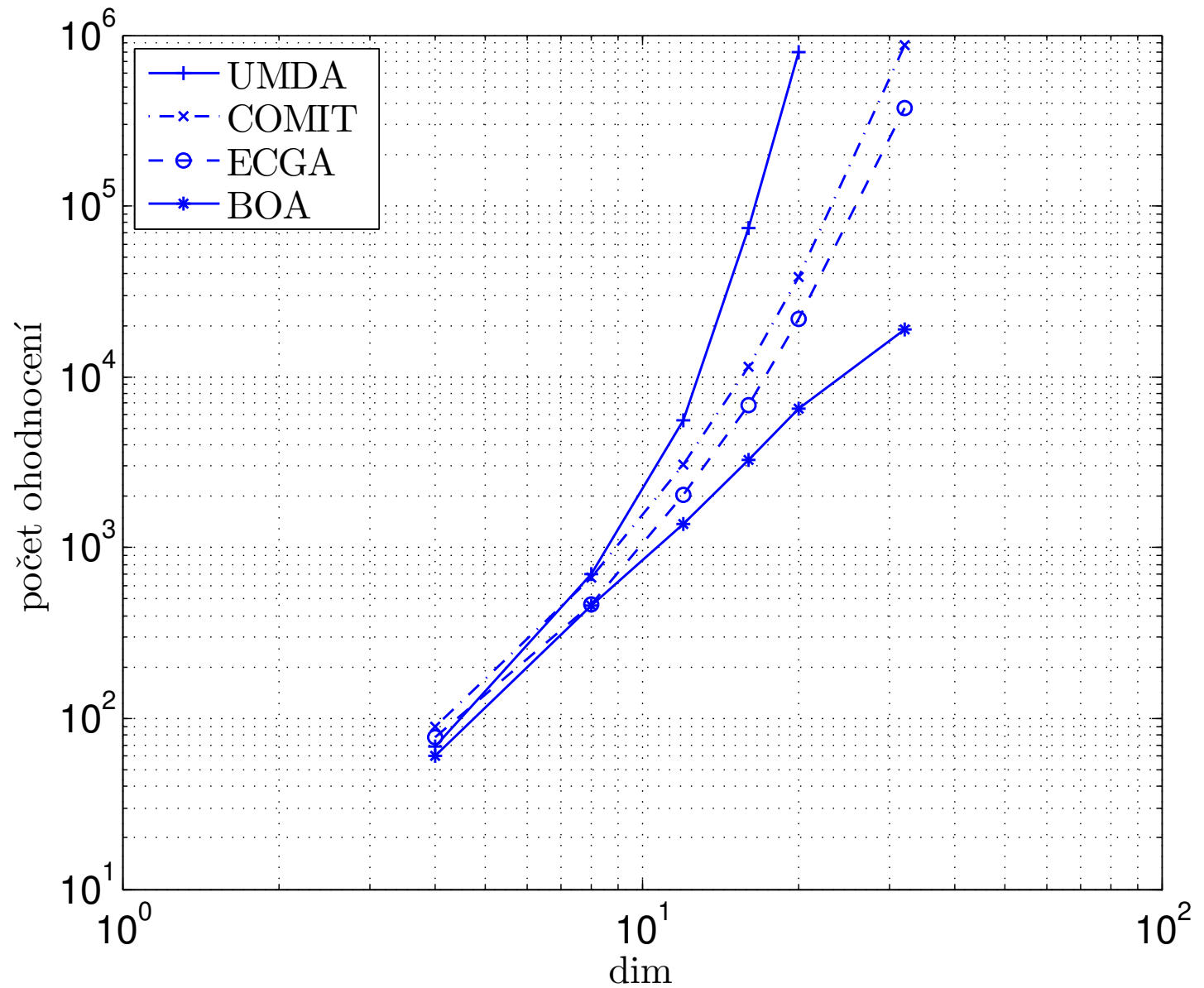
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# Scalability on the decomposable Sliding XOR function

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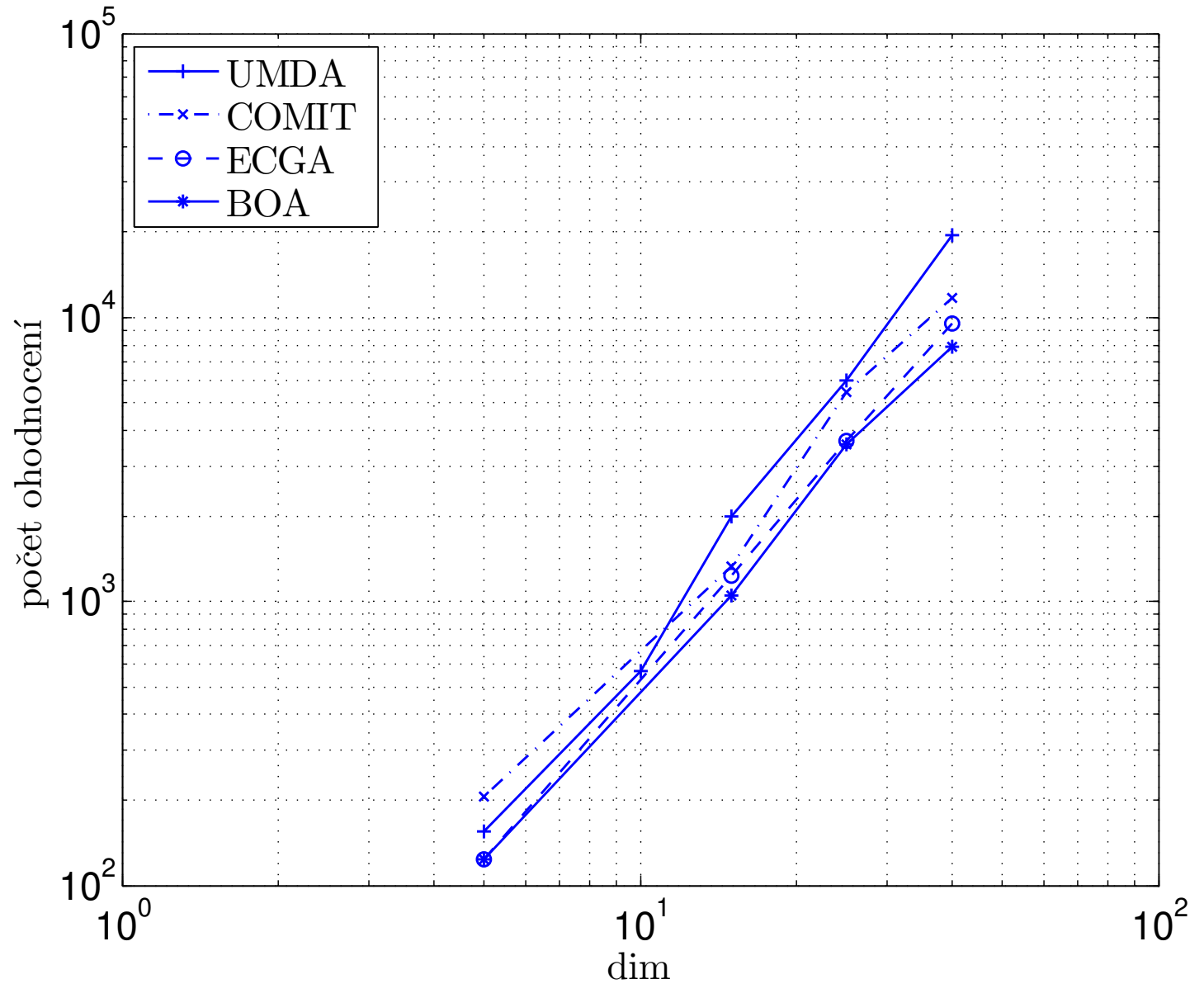
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# Scalability on the decomposable Trap function

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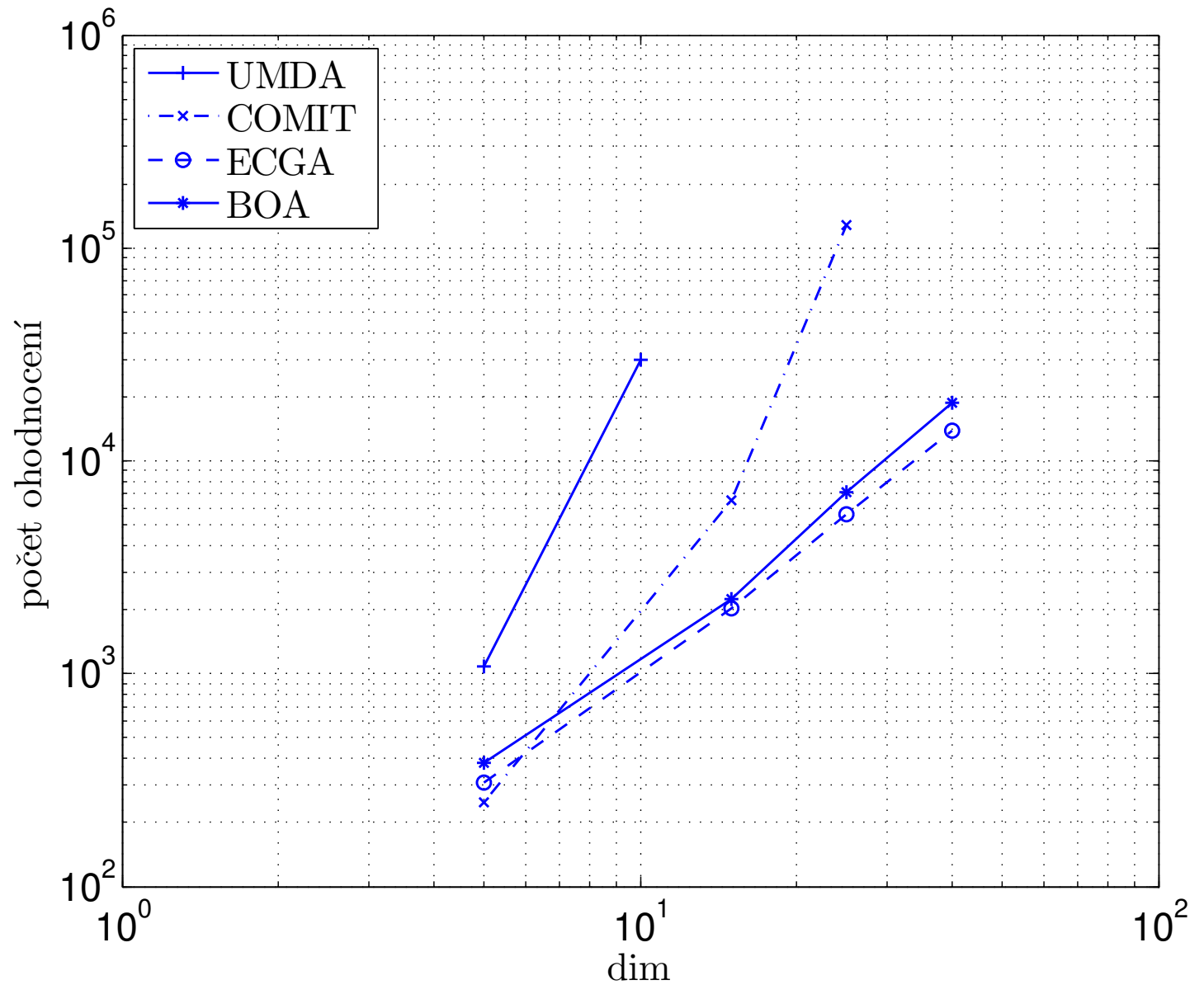
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# Model structure during evolution

---

During the evolution, the model structure is increasingly precise and at the end of the evolution, the model structure describes the problem structure exactly.

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---

## NO! That's not true!

### Why?

- In the beginning, the distribution patterns are not very discernible, models similar to uniform distributions are used.
- In the end, the population converges and contains many copies of the same individual (or a few individuals). No interactions among variables can be learned. Model structure is wrong (all bits independent), but the model describes the position of optimum very precisely.
- The model with the best matching structure is found somewhere in the middle of the evolution.
- Even though the right structure is never found during the evolution, the problem can be solved successfully.



# Summary



# Learning outcomes

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After this lecture, a student shall be able to

- explain what an epistasis is and show an example of functions with and without epistatic relations;
- demonstrate how epistatic relationships can destroy the efficiency of the search performed by an optimization algorithm, and explain it using schemata;
- describe an Estimation-of-Distribution algorithm and explain its differences from an ordinary EA;
- describe in detail and implement a simple UMDA algorithm for binary representations;
- understand, fit to data, and use simple Bayesian networks;
- explain the commonalities and differences among EDAs not able to work with any interactions (PBIL, cGA, UMDA);
- explain the commonalities and differences among EDAs able to work with only pairwise interactions (MIMIC, COMIT, BMDA);
- explain the commonalities and differences among EDAs able to work with multivariate interactions (ECGA, BOA);
- explain the model learning procedures used in ECGA and BOA;
- understand what effect the use of a more complex model has on the efficiency of the algorithm when used on problems with increasingly hard interactions.

Epistasis

EDAs

How EDAs work?

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- Learning outcomes