Epistasis.
Estimation-of-Distribution Algorithms.

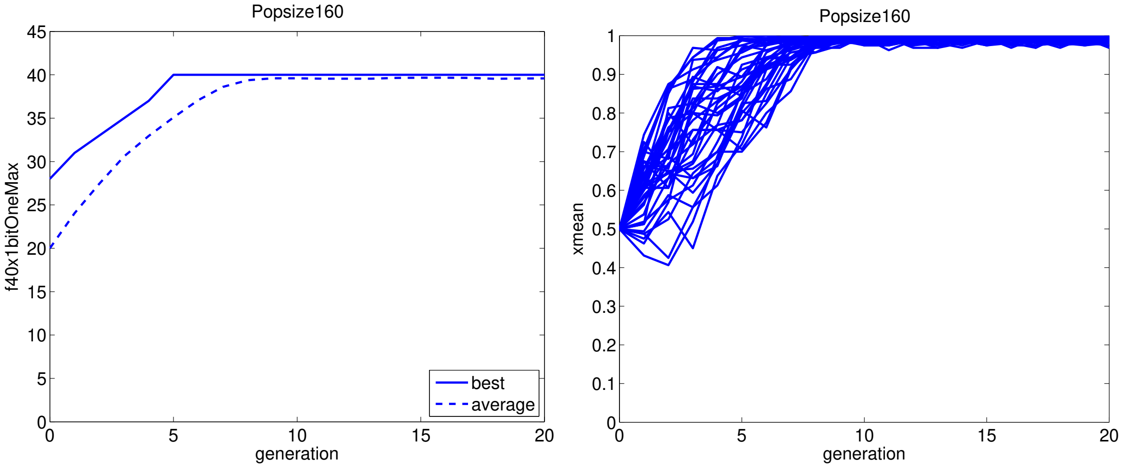
Petr Pošík

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: $x^{\text{opt}} = (1111\dots1)$.

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

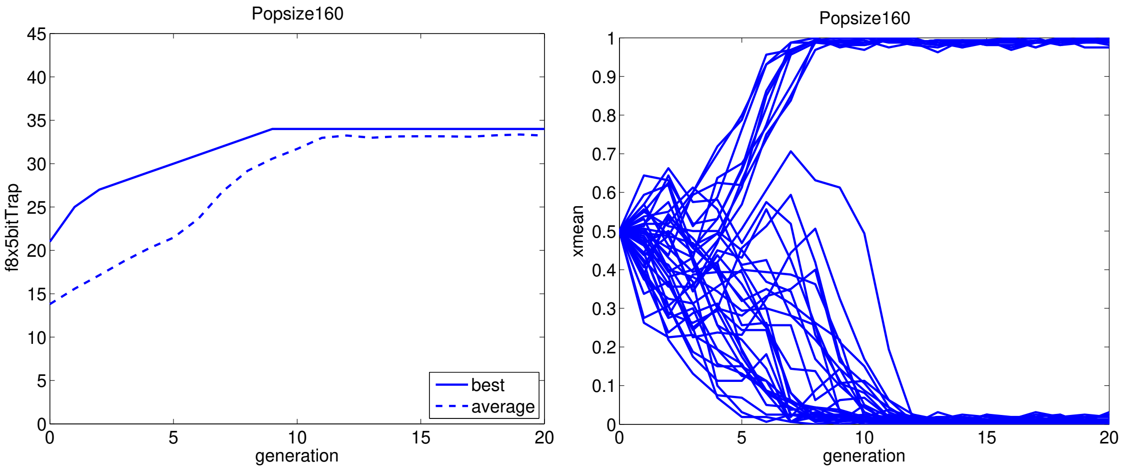


GA fails...

Problem 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: $x^{\text{opt}} = (1111\dots1)$.

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



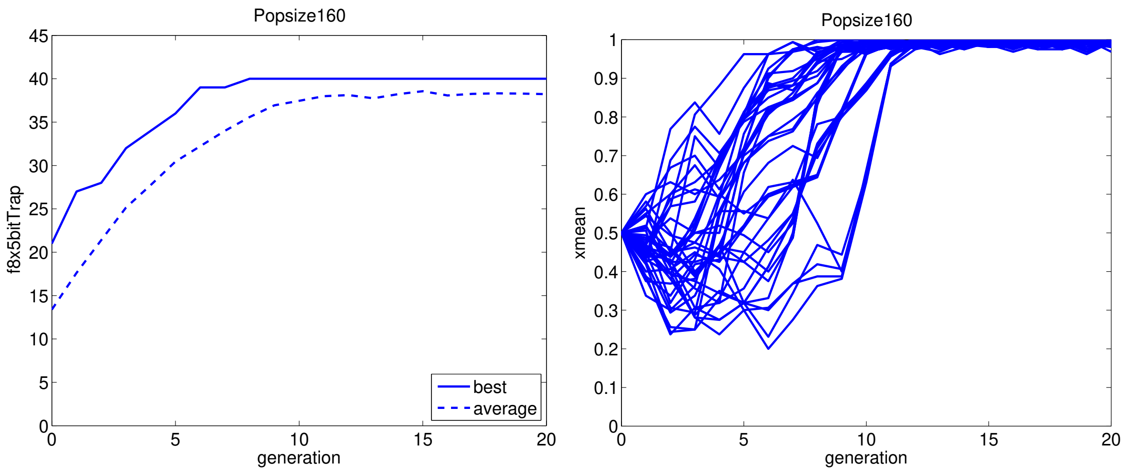
GA works again...

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: $x^{\text{opt}} = (1111\ldots1)$.

Instead of the uniform crossover,

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



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

Epistasis

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.

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

$$f = x_1 + x_2 + x_3 \tag{1}$$
$$f = 0.1x_1 + 0.7x_2 + 3x_3 \tag{2}$$
$$f = x_1x_2x_3 \tag{3}$$
$$f = x_1 + x_2^2 + \sqrt{x_3} \tag{4}$$
$$f = \sin(x_1) + \cos(x_2) + e^{x_3} \tag{5}$$
$$f = \sin(x_1 + x_2) + e^{x_3} \tag{6}$$

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.

Linkage Identification Techniques

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)

Introduction to EDAs

Genetic Algorithms

Algorithm 1: Genetic Algorithm

```
begin
    Initialize the population.
    while termination criteria are not met do
        Select parents from the population.
        Cross over the parents, create offspring.
        Mutate offspring.
        Incorporate offspring into the population.
```

"Select → cross over → mutate" approach

Conventional GA operators

- are not adaptive, and
- cannot (or ususally 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

Algorithm 1: Genetic Algorithm

```
begin
    Initialize the population.
    while termination criteria are not met do
        Select parents from the population.
        Cross over the parents, create offspring.
        Mutate offspring.
        Incorporate offspring into the population.
```

"Select → cross over → mutate" approach

Why not use directly…

Algorithm 2: Estimation-of-Distribution Alg.

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

"Select → update model → sample" approach

Or even…

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

```
begin
    Initialize the model.
    while termination criteria are not met do
        Sample new individuals.
        Select better ones.
        Update the model based on selected ones.
```

"Sample → select → update model" approach

EDAs

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.

Example

5-bit OneMax (CountOnes) problem:

- $f_{\text{Dx1bitOneMax}}(\mathbf{x}) = \sum_{d=1}^{D} x_d$
- Optimum: `11111`, fitness: 5

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

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

Selection, Modeling, Sampling

Old population:

11001	(3)
00010	(1)
11101	(4)
10111	(4)
00001	(1)
10010	(2)

Tournaments:

11101	(4)	vs.	10111	(4)
10111	(4)	vs.	11101	(4)
11101	(4)	vs.	00001	(1)
10010	(2)	vs.	00010	(1)
00010	(1)	vs.	00010	(1)
00010	(1)	vs.	11001	(3)

Selected parents:

11101	(4)
10111	(4)
11101	(4)
10010	(2)
00010	(1)
11001	(3)

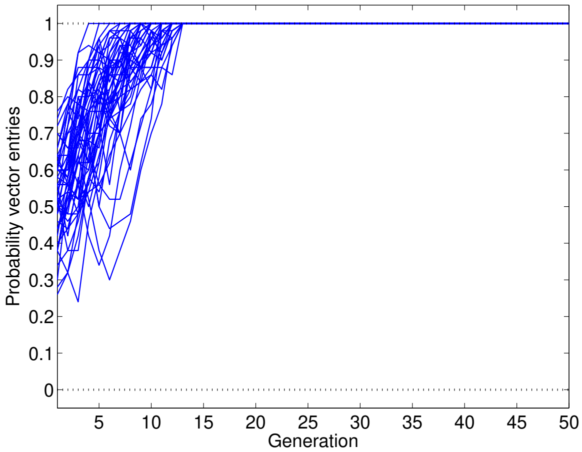
Offspring:

11000	(2)
10100	(2)
11011	(4)
01011	(3)
10101	(3)
10111	(4)

Probability vector:

$\frac{5}{6}\ \frac{3}{6}\ \frac{3}{6}\ \frac{3}{6}\ \frac{4}{6}$

UMDA Behaviour for OneMax problem



- 1s are better then 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 xover	approx. $\mathcal{O}(D \ln D)$
GA with 1-point xover	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. :-(

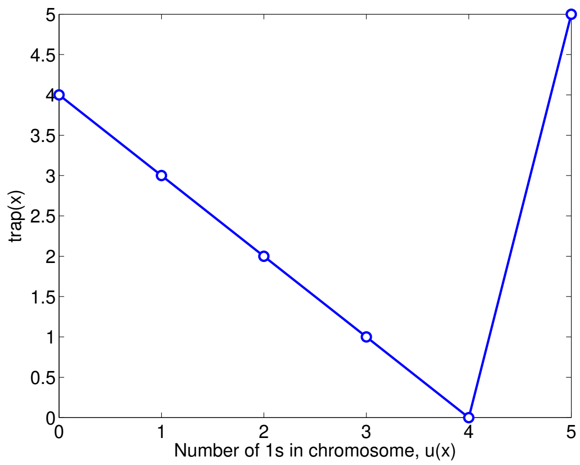
Problem: **Concatanated 5-bit traps**

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

The *trap* function is defined as

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

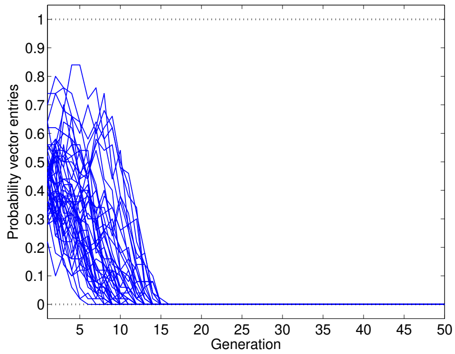
where $u(\mathbf{x})$ is the so called *unity* function and returns the number of 1s in $\mathbf{x}$ (it is actually the One Max function).



UMDA behaviour on concatanated 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.



What can be done about traps?

The f_{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*`.
- Harder than the *needle-in-the-haystack* problem:
  - Regular haystack simply does not provide any information, where to search for the needle.
  - f_{trap}-haystack actively lies to you—it points you to the wrong part of the haystack.
- 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!

Model learning:

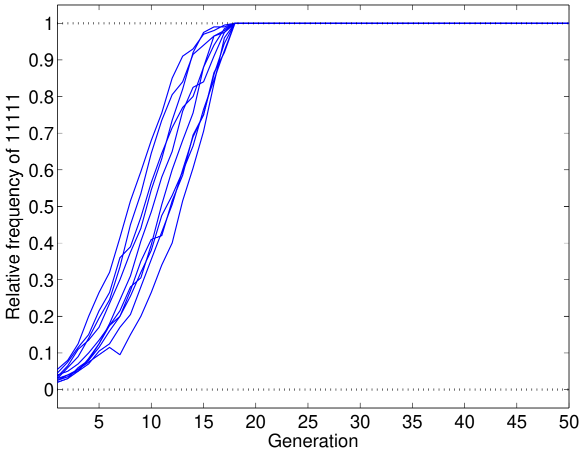
- build model for each 5-tuple of bits
- compute $p(00000)$, $p(00001)$, ..., $p(11111)$,

Model sampling:

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

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.

EDAs without interactions

1. **Population-based incremental learning (PBIL)** [Bal94]
2. **Univariate marginal distribution algorithm (UMDA)** [MP96]
3. **Compact genetic algorithm (cGA)** [HLG97]

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).

[Bal94] Shumeet Baluja. Population based incremental learning: A method for integrating genetic search based function optimization and competitive learning. Technical Report CMU-CS-94-163, Carnegie Mellon University, Pittsburgh, PA, 1994.

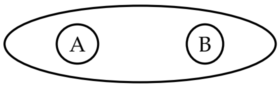
[HLG97] Georges Harik, Fernando Lobo, and David E. Goldberg. The compact genetic algorithm. Technical Report IlliGAL Report No. 97006, University of Illinois, Urbana-Champaign, 1997.

[MP96] Hans Mühlenbein and G. Paass. From recombination of genes to the estimation of distributions i. binary parameters. In *Parallel Problem Solving from Nature*, pages 178–187, 1996.

From single bits to pairwise models

How to describe two positions together?

- Using the joint probability distribution:

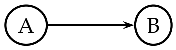


Number of free parameters: 3

$p(A, B)$

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

- Using conditional probabilities:



Number of free parameters: 3

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

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

How to learn pairwise dependencies: dependency tree

- Nodes: binary variables (loci of chromozome)
- 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

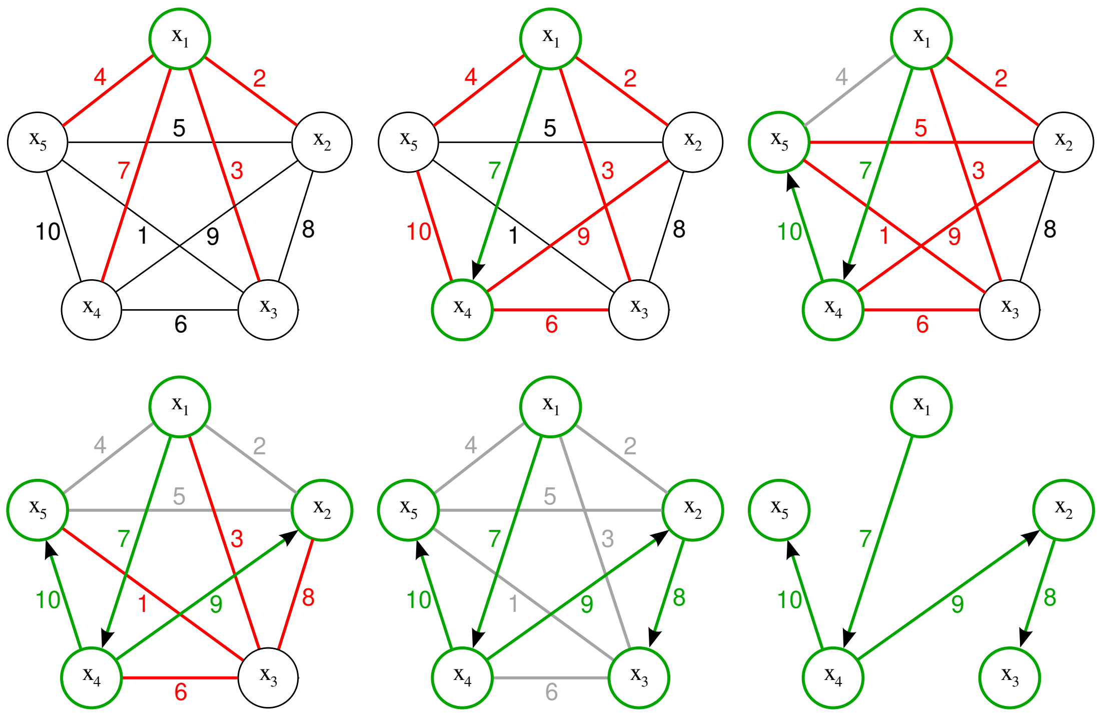
Learning the structure of dependency tree:

1. Score the edges using mutual information:

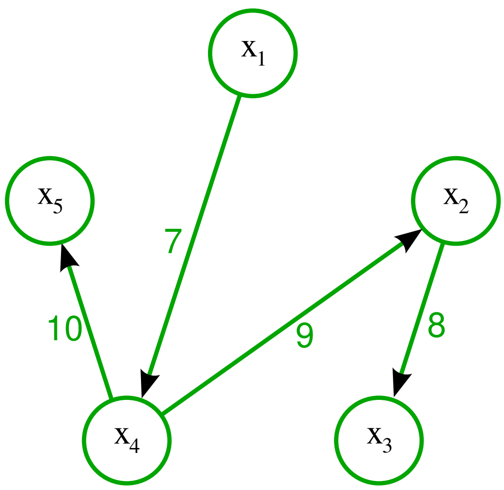
$$I(X, Y) = \sum_{x,y} p(x, y) \cdot \log \frac{p(x, y)}{p(x)p(y)}$$

2. Use any algorithm to determine the maximum spanning tree of the graph, e.g. Prim's algorithm.
   (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

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



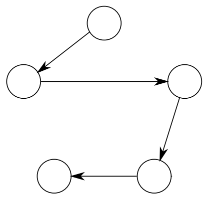
Dependency tree: probabilities



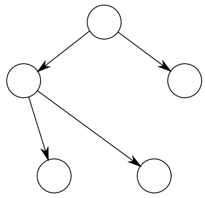
Probability	Number of free params
$p(X_1 = 1)$	1
$p(X_4 = 1\|X_1)$	2
$p(X_5 = 1\|X_4)$	2
$p(X_2 = 1\|X_4)$	2
$p(X_3 = 1\|X_2)$	2
Whole model	9

EDAs with pairwise interactions

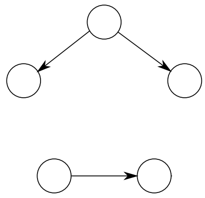
1. **MIMIC** (sequences)
   - Mutual Information Maximization for Input Clustering
   - [dBIV97]



2. **COMIT** (trees)
   - Combining Optimizers with Mutual Information Trees
   - [BD97]



3. **BMDA** (forrest)
   - Bivariate Marginal Distribution Algorithm
   - [PM99]



[BD97] Shumeet Baluja and Scott Davies. Using optimal dependency-trees for combinatorial optimization: Learning the structure of the search space. In D.H. Fisher, editor, *14th International Conference on Machine Learning*, pages 30–38. Morgan Kaufmann, 1997.

[dBIV97] Jeremy S. de Bonet, Charles L. Isbell, and Paul Viola. MIMIC: Finding optima by estimating probability densities. *Advances in Neural Information Processing Systems*, 9:424–431, 1997.

[PM99] Martin Pelikan and Hans Mühlenbein. The bivariate marginal distribution algorithm. In *Advances in Soft Computing – Engineering Design and Manufacturing*, pages 521–535, 1999.

Summary

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

ECGA

Extended Compact GA [Har99]

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]

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 (MDL) best.
   (c) Finish if no join improves the score.

[Har99] Georges Harik. Linkage learning via probabilistic modeling in the ECGA. Technical Report IlliGAL Report No. 99010, University of Illinois, Urbana-Champaign, 1999.

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):

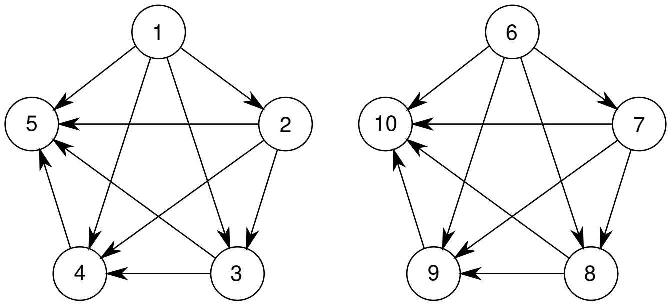
$$DL_{Data} = N \sum_{g \in G} h(X_g) = -N \sum_{g \in G} \sum_{x_g} p(X_g = x_g) \log p(X_g = x_g)$$

BOA: Bayesian Optimization Algorithm

Bayesian Optimization Algorithm [PGCP99]

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 Algorithm (EBNA) [EL99]
  - Learning Factorized Density Algorithm (LFDA) [MM99]

[EL99] R. Etxeberria and Pedro Larrañaga. Global optimization using bayesian networks. In A.A.O. Rodriguez, M.R.S. Ortiz, and R.S. Hermida, editors, *CIMAF 99, Second Symposium on Artificial Intelligence*, Adaptive Systems, pages 332–339, La Habana, 1999.

[MM99] Heinz Mühlenbein and Thilo Mahnig. FDA -a scalable evolutionary algorithm for the optimization of additively decomposed functions. *Evolutionary Computation*, 7(4):353–376, December 1999.

[PGCP99] Martin Pelikan, David E. Goldberg, and Erick Cantu-Paz. BOA: The bayesian optimization algorithm. In *Proceedings of the Genetic and Evolutionary Computation Conference GECCO-99*, pages 525–532. Morgan Kaufmann, 1999.

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 then $\mathcal{O}(D^2)$ evaluations!

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

Test functions

One Max:

$$f_{D\text{x1bitOneMax}}(\boldsymbol{x}) = \sum_{d=1}^{D} x_d$$

Trap:

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

Equal Pairs:

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

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

Sliding XOR:

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

$$f_{\text{AllEqual}}(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{x} = (000\ldots0) \\ 1 & \text{if } \boldsymbol{x} = (111\ldots1) \\ 0 & \text{otherwise} \end{cases}$$

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

Concatenated short basis functions:

$$f_{N\text{x}K\text{bitBasisFunction}} = \sum_{n=1}^{N} f_{\text{KbitBasisFunction}}(x_{K(n-1)+1}, \ldots, x_{Kn})$$

Test function (cont.)

1. $f_{\text{40x1bitOneMax}}$
   - order-1 decomposable function, no interactions
2. $f_{\text{1x40bitEqualPairs}}$
   - non-decomposable function
   - weak interactions: optimal setting of each bit depends on the value of the preceding bit
3. $f_{\text{8x5bitEqualPairs}}$
   - order-5 decomposable function
4. $f_{\text{1x40bitSlidingXOR}}$
   - non-decomposable function
   - stronger interactions: optimal setting of each bit depends on the value of the 2 preceding bits
5. $f_{\text{8x5bitSlidingXOR}}$
   - order-5 decomposable function
6. $f_{\text{8x5bitTrap}}$
   - order-5 decomposable function
   - interactions in each 5-bit block are very strong, the basis function is deceptive

Scalability analysis

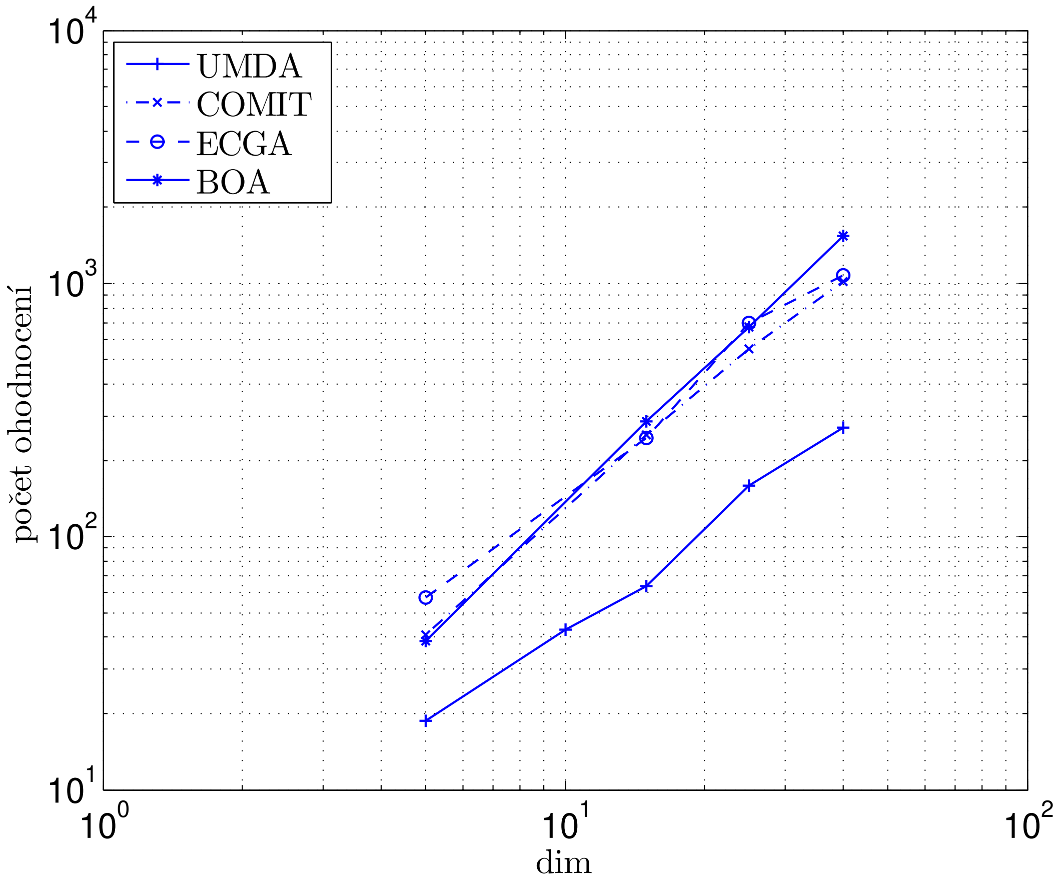
Facts:

- 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 resources.

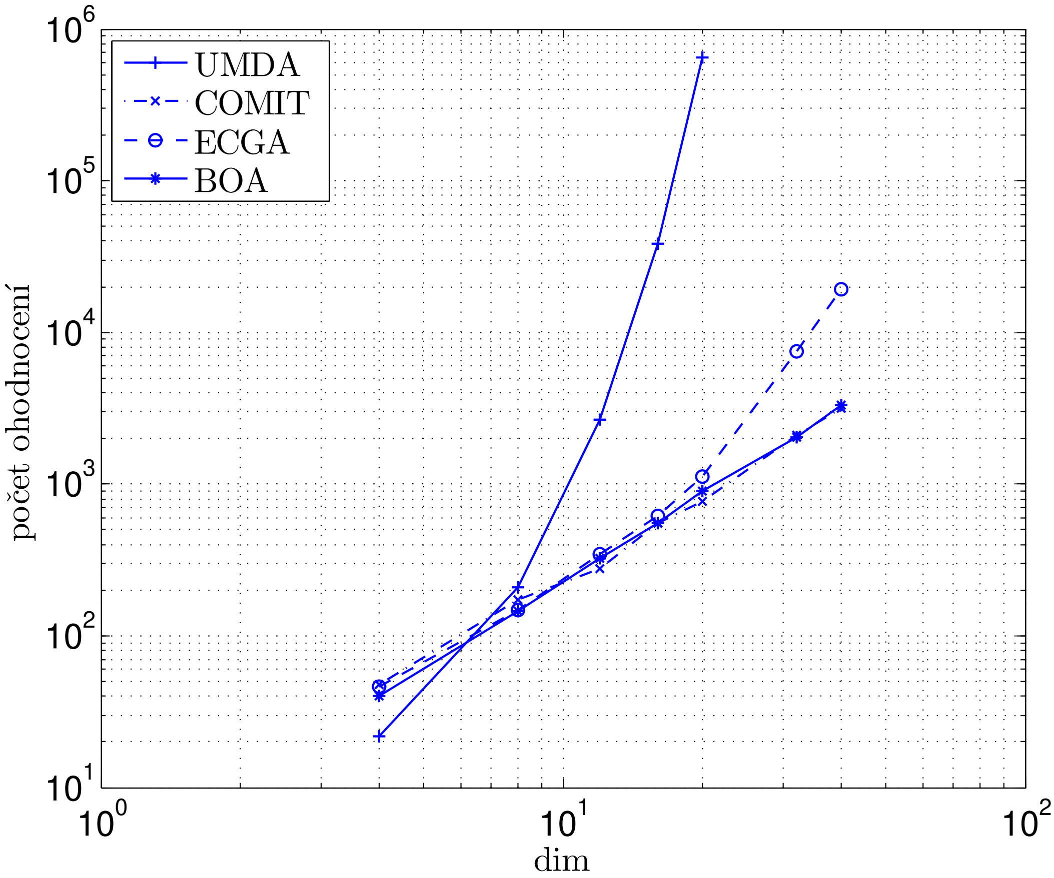
Scalability analysis:

- 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.

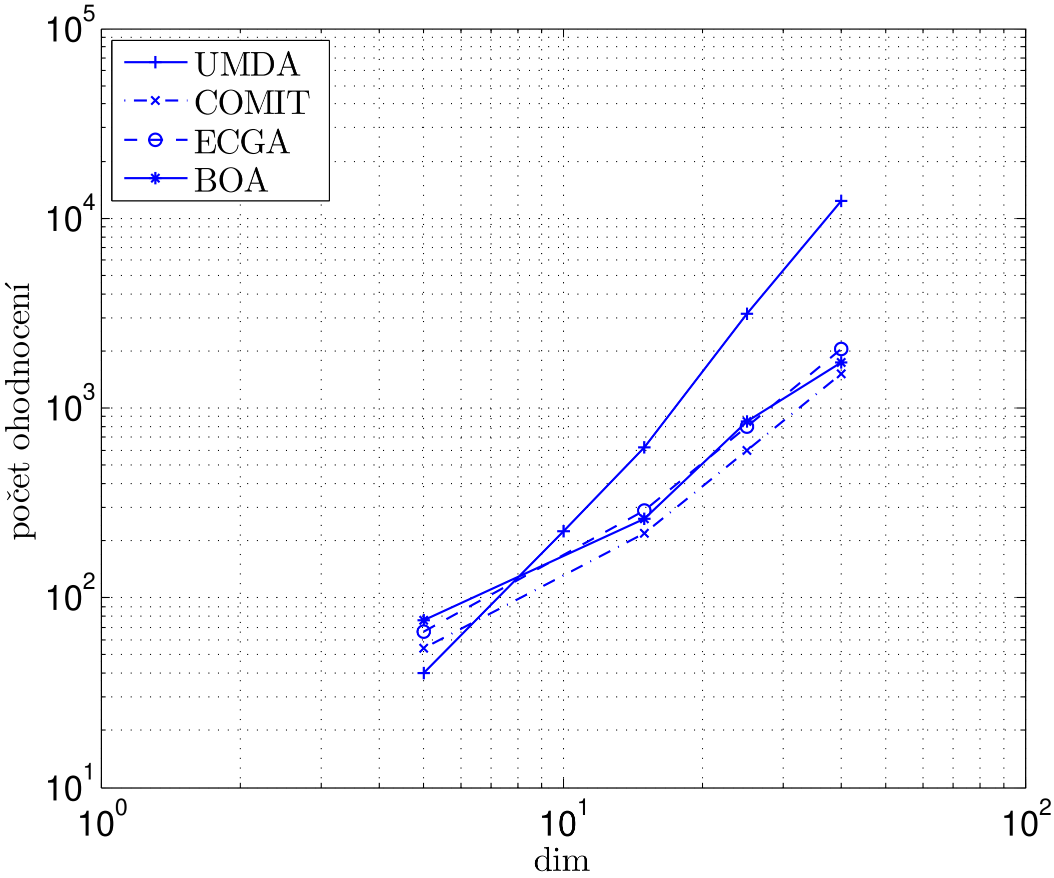
Scalability on the One Max function



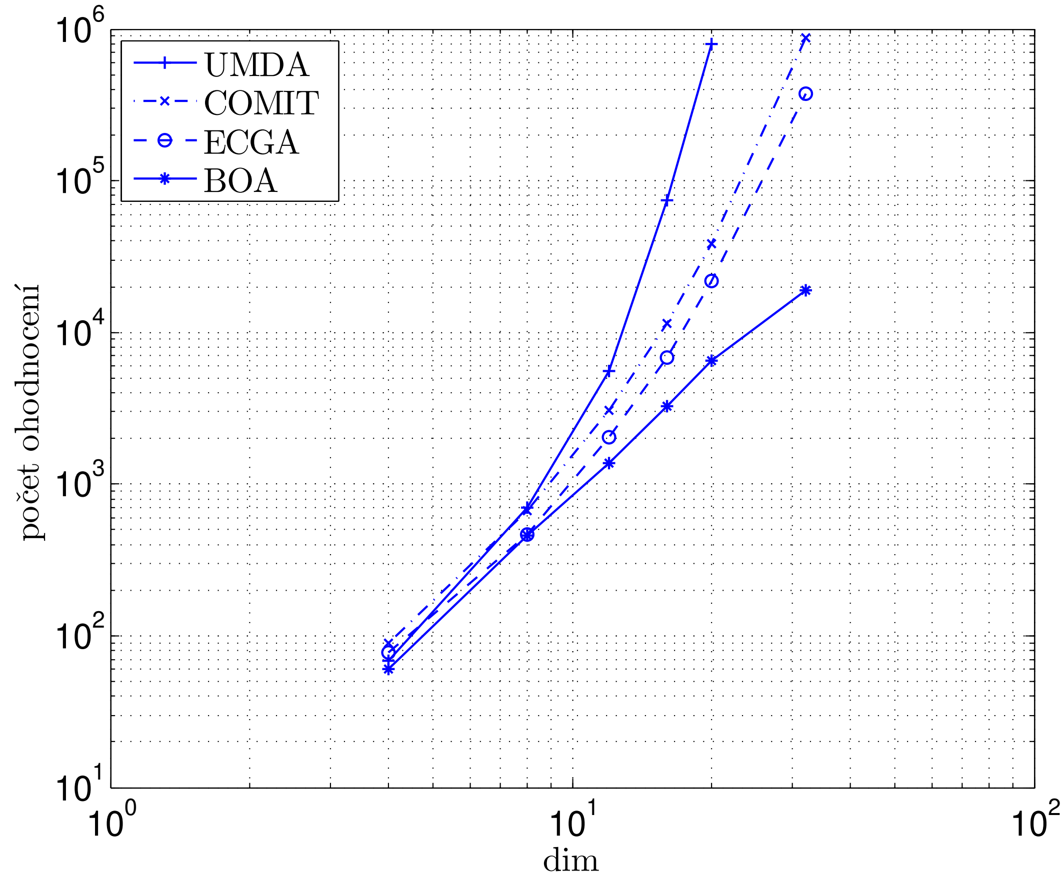
Scalability on the non-decomposable Equal Pairs function



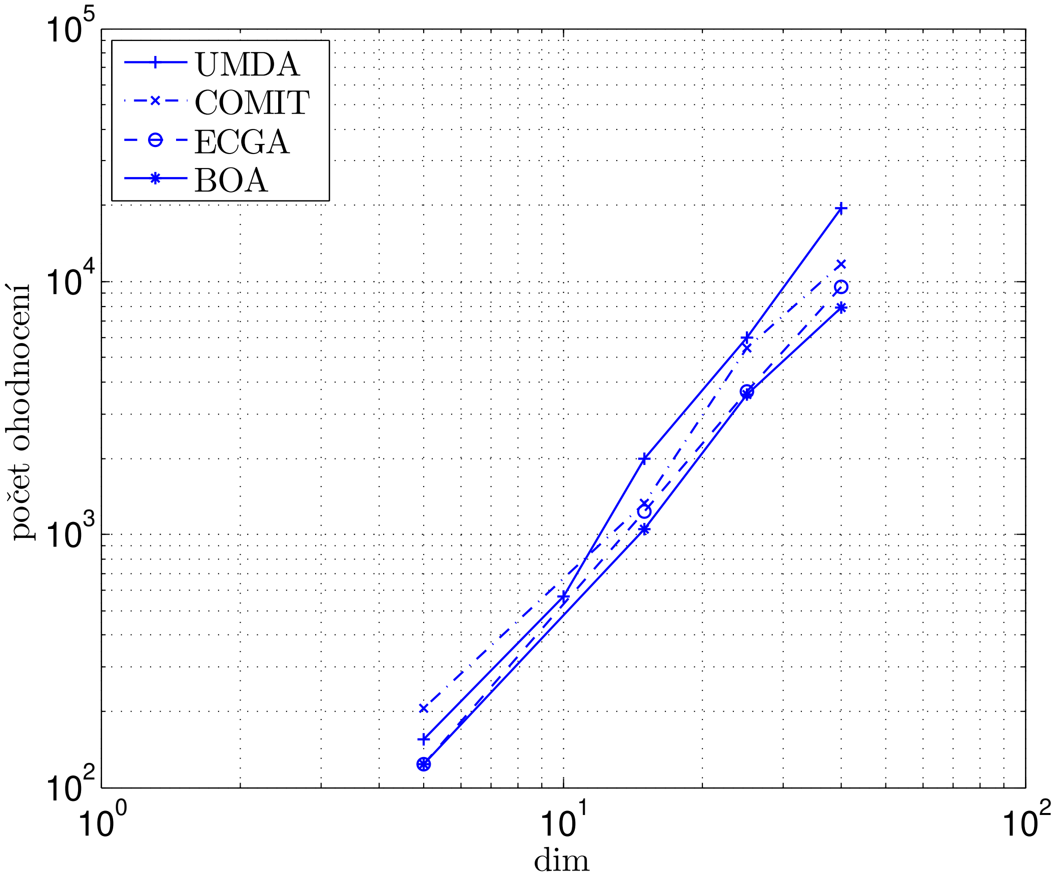
Scalability on the decomposable Equal Pairs function



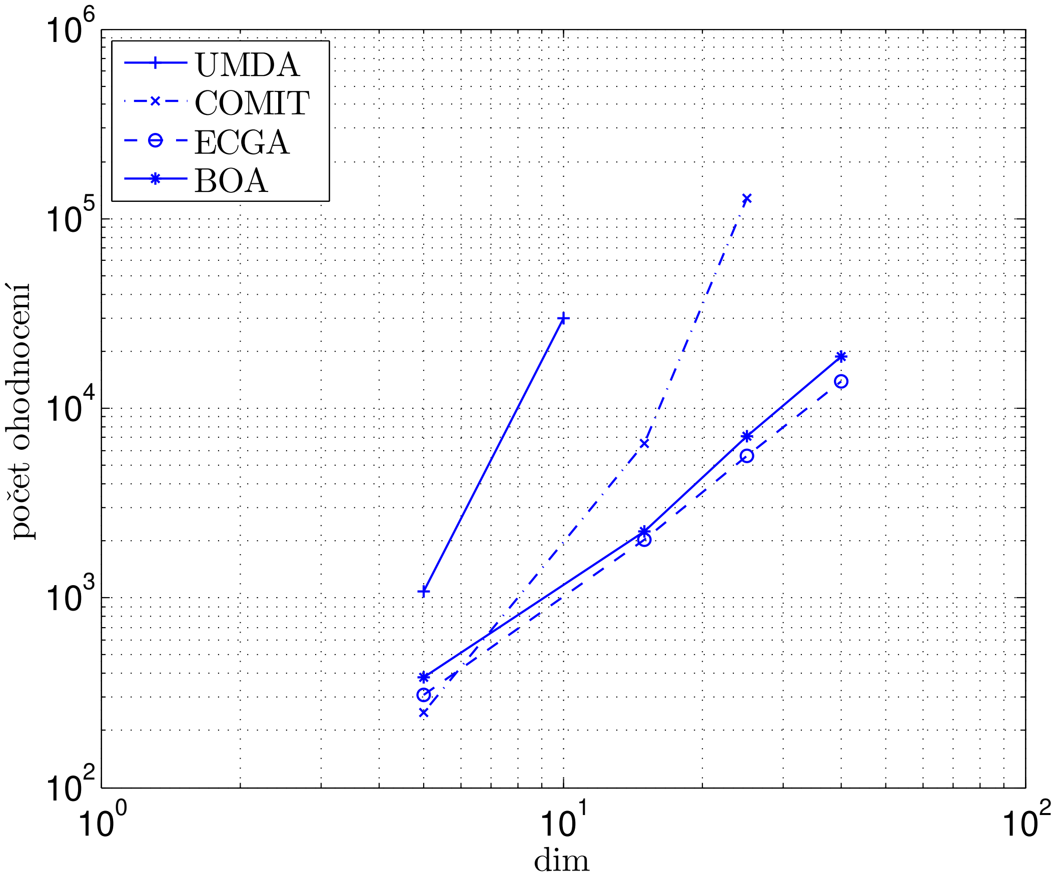
Scalability on the non-decomposable Sliding XOR function



Scalability on the decomposable Sliding XOR function



Scalability on the decomposable Trap function



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.

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.

Learning outcomes

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.