

GECCO 2023 Tutorial

Model-Based Evolutionary Algorithms

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Outline

Model-Based Evolutionary Algorithms (MBEA)

- ▶ Introduction
- ▶ Part I: Discrete Representation
- ▶ Part II: Real-Valued, Permutation, and Program Representations

What ?

Evolutionary Algorithms

- ▶ Population-based, stochastic search algorithms
- ▶ **Exploitation**: selection
- ▶ **Exploration**: mutation & crossover

Model-Based Evolutionary Algorithms

- ▶ Population-based, stochastic search algorithms
- ▶ **Exploitation**: selection
- ▶ **Exploration**:
 1. Learn a model from selected solutions
 2. Generate new solutions from the model (& population)

What ?

Model-Based Evolutionary Algorithms (MBEA)

- ▶ a.k.a. Estimation of Distribution Algorithms (EDAs)
- ▶ a.k.a. Probabilistic Model-Building Genetic Algorithms
- ▶ a.k.a. Iterated Density Estimation Evolutionary Algorithms

MBEA = Evolutionary Computing + Machine Learning

Note: model not necessarily probabilistic

Why ?

Goal: Black Box Optimization

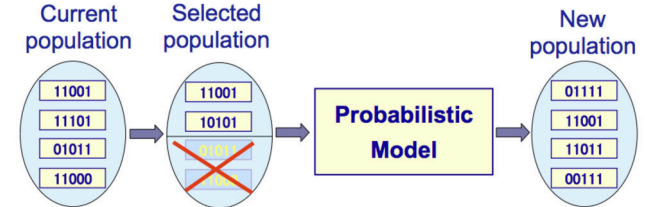
- ▶ Little known about the structure of the problem
- ▶ Clean separation optimizer from problem definition
- ▶ Easy and generally applicable

Approach

- * **Classical EAs:** need suitable representation & variation operators
- * **Model-Based EAs:** learn structure from good solutions

Discrete Representation

- ▶ Typically binary representation
- ▶ Higher order cardinality: similar approach



Probabilistic Model-Building Genetic Algorithm

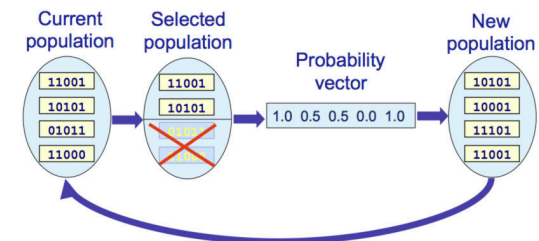
Type of Models

- ▶ **Univariate:** no statistical interaction between variables considered.
- ▶ **Bivariate:** pairwise dependencies learned.
- ▶ **Multivariate:** higher-order interactions modeled.

Univariate PMBGA

Model

- * Model: probability vector $[p_1, \dots, p_\ell]$ (ℓ : string length)
- * p_i : probability of value 1 at string position i
- * $p(X) = \prod_{i=1}^{\ell} p(x_i)$ ($p(x_i)$: univariate marginal distribution)
- ▶ **Learn** model: count proportions of 1 in selected population
- ▶ **Sample** model: generate new solutions with specified probabilities



Univariate PMBGA

Different Variants

- ▶ **PBIL** (Baluja; 1995)
 - ▶ Prob. vector incrementally updated over successive generations
- ▶ **UMDA** (Mühlenbein, Paass; 1996)
 - ▶ No incremental updates: example above
- ▶ **Compact GA** (Harik, Lobo, Goldberg; 1998)
 - ▶ Models steady-state GA with tournament selection
- ▶ **DEUM** (Shakya, McCall, Brown; 2004)
 - ▶ Uses Markov Random Field modeling

A hard problem for the univariate FOS

Data	Marginal Product (MP) FOS		
	$\hat{P}(X_0X_1X_2)$	$\hat{P}(X_3X_4X_5)$	
000000			
111111	000	0.3	0.3
010101	001	0.0	0.0
101010	010	0.2	0.2
000010	011	0.0	0.0
111000	100	0.0	0.0
010111	101	0.1	0.1
111000	110	0.0	0.0
000111	111	0.4	0.4
111111			

Univariate FOS						
	$\hat{P}(X_0)$	$\hat{P}(X_1)$	$\hat{P}(X_2)$	$\hat{P}(X_3)$	$\hat{P}(X_4)$	$\hat{P}(X_5)$
0	0.5	0.4	0.5	0.5	0.4	0.5
1	0.5	0.6	0.5	0.5	0.6	0.5

- ▶ What is the **probability** of generating 111111?
- ▶ **Univariate FOS**: $0.5 \cdot 0.6 \cdot 0.5 \cdot 0.5 \cdot 0.6 \cdot 0.5 = 0.0225$
- ▶ **MP FOS**: $0.4 \cdot 0.4 = 0.16$ (7 times larger!)

Learning problem structure on the fly

- ▶ Without a “good” **decomposition** of the problem, important **partial solutions** (building blocks) are likely to get **disrupted** in variation.
- ▶ **Disruption** leads to **inefficiency**.
- ▶ Can we **automatically** configure the model structure **favorably**?
- ▶ Selection **increases** proportion of good building blocks and thus “correlations” between variables of these building blocks.
- ▶ So, **learn** which variables are “**correlated**”.
- ▶ See the population (or selection) as a **data set**.
- ▶ Apply **statistics** / **probability theory** / **probabilistic modeling**.

Bivariate PMBGA

Model

- ▶ Need more than just probabilities of bit values
- ▶ Model pairwise interactions: conditional probabilities
- ▶ **MIMIC** (de Bonet, Isbell, Viola; 1996)
 - ▶ Dependency Chain
- ▶ **COMIT** (Baluja, Davies; 1997)
 - ▶ Dependency Tree
- ▶ **BMDA** (Pelikan, Mühlenbein; 1998)
 - ▶ Independent trees (forest)

Bivariate PMBGA

MIMIC

- ▶ Model: **chain** of pairwise dependencies.
- ▶ $p(X) = \prod_{i=1}^{\ell-1} p(x_{i+1}|x_i)p(x_1)$.
- ▶ MIMIC **greedily** searches for the optimal **permutation** of variables that minimizes Kullback-Leibler divergence.

Bivariate PMBGA

COMIT

- ▶ Optimal **dependency tree** instead of linear chain.
- ▶ Compute fully connected weighted graph between problem variables.
- ▶ Weights are the mutual information $I(X, Y)$ between the variables.
- ▶ $I(X, Y) = \sum_{y \in Y} \sum_{x \in X} p(x, y) \log \frac{p(x, y)}{p(x)p(y)}$.
- ▶ COMIT computes the **maximum spanning tree** of the weighted graph.

Bivariate PMBGA

BMDA

- ▶ BMDA also builds tree model.
- ▶ Model not necessarily fully connected: set of trees or **forrest**.
- ▶ Pairwise interactions measured by **Pearson's chi-square** statistics.

Bivariate PMBGA

DSMGA

- ▶ Dependency Structure Matrix Genetic Algorithm (Yu, Goldberg, Sastry, Lima, Pelikan; 2009)
- ▶ Dependency Structure Matrix (DSM) contains the information of pairwise interactions.
- ▶ DSMGA constructs the DSM by using mutual information metric.
- ▶ DSM clustering aims to transfer the pair-wise interaction information into higher-order interaction information.
- ▶ DSM Clustering Metric based on the minimum description length principle (MDL).

Bivariate PMBGA

DSMGA-II

- ▶ Extended version \Rightarrow DSMGA-II (Hsu, Yu; 2015).
- ▶ DSMGA-II consists of four major components:
 1. pair-wise linkage detection
 2. model building
 3. restricted mixing
 4. back mixing
- ▶ Clustering the DSM leads to the Incremental Linkage Set: starting from one gene, incrementally add the next most dependent gene one-by-one.
- ▶ Restricted mixing: focus on building-block supply.
- ▶ Back mixing: when no improvement occurs, switch to the equal-acceptance criterion to reduce unnecessary evaluations on plateaus.

Multivariate PMBGA

Marginal Product Model

- ▶ **Extended Compact GA (ECGA)** (Harik; 1999) was first EDA going beyond pairwise dependencies.
- ▶ Greedily searches for the Marginal Product Model that minimizes the minimum description length (MDL).
- ▶ $p(X) = \prod_{g=1}^G p(X_g)$
- ▶ Choose the probability distribution with the **lowest** MDL score.
- ▶ Start from **simplest** model: the **univariate** factorization.
- ▶ Join two groups that result in the **largest** improvement in the used scoring measure.
- ▶ **Stop** when no joining of two groups **improves** the score further.

Multivariate PMBGA

Minimum Description Length (MDL)

- ▶ $MDL(M, D) = D_{Model} + D_{Data}$
- ▶ **Best** factorization = the one with the **lowest MDL** score.
- ▶ MDL is a measure of **complexity**.
 1. **Compressed population** complexity: how well the population is compressed by the model (measure of **goodness** of the probability distribution **estimation**).
 2. **Model** complexity: the number of **bits** required to store all **parameters** of the model.

Multivariate PMBGA

Learning MP model

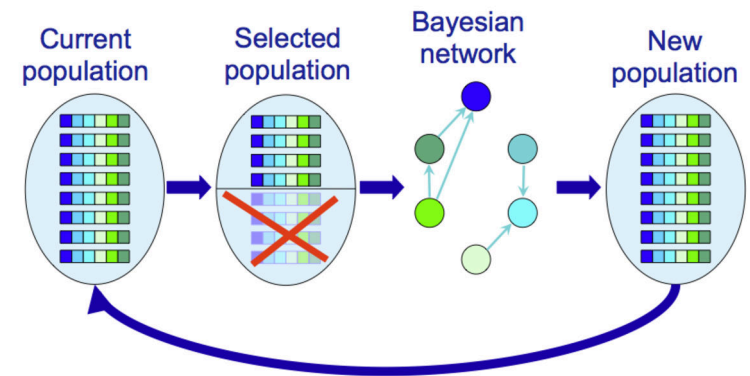
1. Start from univariate FOS:
 $\{\{0\}, \{1\}, \{2\}, \dots, \{l-2\}, \{l-1\}\}$
2. All possible **pairs** of partitions are temporarily merged:
 $\{\{0, 1\}, \{2\}, \dots, \{l-2\}, \{l-1\}\}$
 $\{\{0, 2\}, \{1\}, \dots, \{l-2\}, \{l-1\}\}$
 \vdots
 $\{\{0\}, \{1, 2\}, \dots, \{l-2\}, \{l-1\}\}$
 \vdots
 $\{\{0\}, \{1\}, \{2\}, \dots, \{l-2\}, \{l-1\}\}$
3. Compute **MDL** score of each factorization.
4. Choose the **best** scoring factorization if **better** than current.
5. **Repeat** until no better scoring factorization is found.

Multivariate PMBGA

Bayesian Network

- ▶ Probability vector, dependency tree, and marginal product model are **limited** probability models.
- ▶ Bayesian network much more **powerful** model.
 - ▶ Acyclic directed graph.
 - ▶ Nodes are problem variables.
 - ▶ Edges represent conditional dependencies.

Multivariate PMBGA



Multivariate PMBGA

Bayesian network learning

- ▶ Similar to ECGA: scoring metric + greedy search
- ▶ **Scoring metric**: MDL or Bayesian measure
- ▶ **Greedy search**:
 - ▶ Initially, no variables are connected.
 - ▶ Greedily either add, remove, or reverse an edge between two variables.
 - ▶ Until local optimum is reached.

Multivariate PMBGA

Bayesian Network PMBGAs variants

- ▶ Bayesian Optimization Algorithm (**BOA**) (Pelikan, Goldberg, Cantú-Paz; 1998)
- ▶ Estimation of Distribution Networks Algorithm (**EBNA**) (Etxeberria, Larrañaga; 1999)
- ▶ Learning Factorized Distribution Algorithm (**LFDA**) (Mühlenbein, Mahnig, Rodriguez; 1999)

- ▶ **Similarities**: All use Bayesian Network as probability model.
- ▶ **Dissimilarities**: All use different method to learn BN.

Hierarchical BOA

- ▶ hBOA (Pelikan, Goldberg; 2001)
- ▶ **Decomposition** on multiple levels.
 - ▶ Bayesian network learning by BOA
- ▶ **Compact** representation.
 - ▶ Local Structures to represent conditional probabilities.
- ▶ **Preservation** of alternative solutions.
 - ▶ Niching with Restricted Tournament Replacement

Multivariate PMBGA

Markov Network

- ▶ **Markov Network EDA**
(MN-EDA: Santana, 2005) (DEUM: Shakya & McCall, 2007).
- ▶ Probability model is **undirected graph**.
- ▶ **Factorise** the joint probability distribution in cliques of the undirected graph and sample it.
- ▶ Most recent version: **Markovian Optimisation Algorithm (MOA)** (Shakya & Santana, 2008).
- ▶ MOA does not explicitly factorise the distribution but uses the **local Markov property** and **Gibbs sampling** to generate new solutions.

Family Of Subsets (FOS) model

FOS \mathcal{F}

- ▶ PMBGAs learn a **probabilistic model** of good solutions to match the **structure** of the optimization problem
- ▶ Key idea is to identify **groups** of **problem variables** that together make an important contribution to the quality of solutions.
- ▶ Dependency structure generally called a **Family Of Subsets (FOS)**.
- ▶ Let there be ℓ **problem variables** $x_0, x_1, \dots, x_{\ell-1}$.
- ▶ Let S be a set of all variable **indices** $\{0, 1, \dots, \ell - 1\}$.
- ▶ A FOS \mathcal{F} is a **set of subsets** of the set S .
- ▶ FOS \mathcal{F} is a **subset** of the **powerset** of S ($\mathcal{F} \subseteq \mathcal{P}(S)$).

Family Of Subsets (FOS) model

- ▶ FOS can be written more **specifically** as:

$$\mathcal{F} = \{\mathbf{F}^0, \mathbf{F}^1, \dots, \mathbf{F}^{|\mathcal{F}|-1}\}$$

where

$$\mathbf{F}^i \subseteq \{0, 1, \dots, l - 1\}, \quad i \in \{0, 1, \dots, |\mathcal{F}| - 1\}$$

- ▶ Every variable is in **at least one** subset in the FOS, i.e.:
 $\forall i \in \{0, 1, \dots, l - 1\} : (\exists j \in \{0, 1, \dots, |\mathcal{F}| - 1\} : i \in \mathbf{F}^j)$

The Univariate Structure

- ▶ The **univariate** FOS is defined by:

$$\mathbf{F}^i = \{i\}, \quad i \in \{0, 1, \dots, l-1\}$$

- ▶ For $l = 10$ the **univariate** FOS is:

$$\mathcal{F} = \{\{0\}, \{1\}, \{2\}, \{3\}, \{4\}, \{5\}, \{6\}, \{7\}, \{8\}, \{9\}\}$$

- ▶ Every variable is modeled to be **independent** of other variables.

The Marginal Product Structure

- ▶ The **marginal product** (MP) FOS is a FOS such that:

$$\mathbf{F}^i \cap \mathbf{F}^j = \emptyset, \quad i, j \in \{0, 1, \dots, l-1\}.$$

- ▶ **Univariate** FOS is a **MP** FOS.

- ▶ For $l = 10$ a possible MP FOS is:

$$\mathcal{F} = \{\{0, 1, 2\}, \{3\}, \{4, 5\}, \{6, 7, 8, 9\}\}$$

- ▶ Every group of variables is modeled to be **independent** of other variables.

The Linkage Tree Structure

- ▶ The **linkage tree** (LT) FOS is a **hierarchical** structure.

- ▶ Group of **all variables** is in there.

- ▶ For **any** subset \mathbf{F}^i with **more than one variable**, there are subsets \mathbf{F}^j and \mathbf{F}^k such that:

$$\mathbf{F}^j \cap \mathbf{F}^k = \emptyset, \quad |\mathbf{F}^j| < |\mathbf{F}^i|, \quad |\mathbf{F}^k| < |\mathbf{F}^i| \quad \text{and} \quad \mathbf{F}^j \cup \mathbf{F}^k = \mathbf{F}^i$$

- ▶ For $l = 10$ a possible **LT** FOS is

$$\begin{aligned} \mathcal{F} = \{ & \{7, 5, 8, 6, 9, 0, 3, 2, 4, 1\}, \\ & \{7, 5, 8, 6, 9\}, \{0, 3, 2, 4, 1\}, \{7\}, \{5, 8, 6, 9\}, \\ & \{0, 3, 2, 4\}, \{1\}, \{5, 8, 6\}, \{9\}, \{0, 3\}, \{2, 4\}, \\ & \{5, 8\}, \{6\}, \{0\}, \{3\}, \{2\}, \{4\}, \{5\}, \{8\} \} \end{aligned}$$

- ▶ Variables sometimes **independent**, sometimes **dependent**.
- ▶ \approx **Path** through dependency space, from **univariate** to **joint**.

Linkage Tree

- ▶ **Linkage Tree** structure: subsets of FOS F form a hierarchical clustering.

- ▶ $F = \{\{0,1,2,3,4,5,6,7,8,9\}, \{0,1,2,3,4,5\}, \{6,7,8,9\}, \{0,1,2\}, \{3,4,5\}, \{7,8,9\}, \{0,1\}, \{4,5\}, \{8,9\}, \{0\}, \{1\}, \{2\}, \{3\}, \{4\}, \{5\}, \{6\}, \{7\}, \{8\}, \{9\}\}$

- ▶ Each subset (of length > 1) is split in two **mutually exclusive** subsets.

- ▶ Problem variables in subset are considered to be **dependent** on each other but become **independent** in a child subset.

- ▶ For a problem of length ℓ the linkage tree has ℓ **leaf** nodes (the clusters having a single problem variable) and $\ell - 1$ **internal** nodes.

Linkage Tree Learning

- ▶ Start from **univariate** structure.
- ▶ Build linkage tree using **bottom-up** hierarchical clustering algorithm.
- ▶ **Similarity** measure:
 1. Between individual variables X and Y : **mutual information** $I(X, Y)$.
 2. Between cluster groups X_{Fi} and X_{Fj} : **average pairwise linkage** clustering (= unweighted pair group method with a arithmetic mean: UPGMA).

$$I^{UPGMA}(X_{Fi}, X_{Fj}) = \frac{1}{|X_{Fi}||X_{Fj}|} \sum_{X \in X_{Fi}} \sum_{Y \in X_{Fj}} I(X, Y).$$

Linkage Tree Learning

- ▶ This agglomerative hierarchical clustering algorithm is computationally **efficient**.
- ▶ Only the mutual information between pairs of variables needs to be computed once, which is a $O(\ell^2)$ operation.
- ▶ The bottom-up hierarchical clustering can also be done in $O(\ell^2)$ computation by using the **reciprocal nearest neighbor chain** algorithm.

Optimal Mixing Evolutionary Algorithm (OMEA)

- ▶ **OMEA** is a Model-Building EA that uses a **FOS** as its linkage model (Thierens & Bosman, 2011).
- ▶ Characteristic of **Optimal Mixing Evolutionary Algorithm** (OMEA) is the use of **intermediate** function evaluations (inside variation)
- ▶ Can be regarded as **greedy improvement** of existing solutions
- ▶ Coined “**Optimal**” **Mixing** because **better** instances for substructures are **immediately accepted** and not dependent on “**noise**” coming from other parts of the solution

Gene-pool Optimal Mixing EA (GOMEA)

- ▶ **FOS** linkage models specify the linked variables.
- ▶ A subset of the FOS is used as **mixing mask**
- ▶ Mixing is **greedy**: accept only **improvements** (or **equal**).
- ▶ A new FOS model is built from the population every generation.
- ▶ FOS model may also be pre-specified, of course.
- ▶ **Gene-pool Optimal Mixing Evolutionary Algorithm** (GOMEA)
 - ▶ For each solution in the population
 - ▶ **all subsets** of the FOS are tried with a **donor** solution randomly picked from the population

Gene-pool Optimal Mixing EA

GOMEA()

```

Pop ← InitPopulation()
while NotTerminated(Pop)
  FOS ← BuildFOS(Pop)
  forall Sol ∈ Pop
    forall SubSet ∈ FOS
      Donor ← Random(Pop)
      Sol ← OptimalMixing(Sol, Donor, SubSet, Pop)
return Sol

```

OptimalMixing(Sol, Donor, SubSet, Pop)

```

NewSol ← ReplaceSubSetValues(Sol, SubSet, Donor)
if ImprovementOrEqual(NewSol, Sol)
  then Sol ← NewSol
return Sol

```

Linkage Tree Genetic Algorithm

- ▶ The LTGA is an instance of **GOMEA** that uses a Linkage Tree as FOS model (Thierens & Bosman, 2010, 2011).
- ▶ AKA **LT-GOMEA**.
- ▶ Each generation a new **hierarchical cluster tree** is built.
- ▶ For each solution in population, traverse **tree** (random order).
- ▶ Nodes (= clusters) in the linkage tree form **FOS**.

Benchmark problems

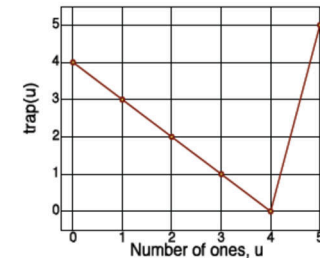
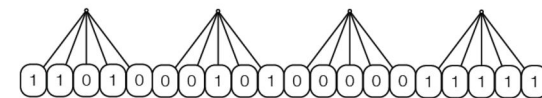
- ▶ **Onemax** (counting ones)

$$f_{\text{Onemax}}(\mathbf{x}) = \sum_{i=0}^{\ell-1} x_i$$

Deceptive Trap Function

Interacting, non-overlapping, deceptive groups of variables.

$$f_{\text{DT}}(x) = \sum_{i=0}^{l-k} f_{\text{DT}}^{\text{sub}}(x_{(i, \dots, i+k-1)})$$

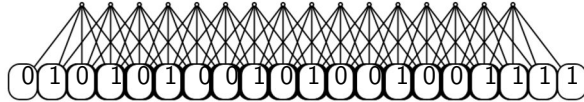


Nearest-neighbor NK-landscape

- ▶ **Overlapping**, neighboring random subfunctions

$$f_{\text{NK-S1}}(\mathbf{x}) = \sum_{i=0}^{l-k} f_{\text{NK}}^{\text{sub}}(x_{(i, \dots, i+k-1)}) \quad \text{with } f_{\text{NK}}^{\text{sub}}(x_{(i, \dots, i+k-1)}) \in [0..1]$$

- ▶ eg. 16 subfcts, length $k = 5$, overlap $o = 4 \Rightarrow$ stringlength $\ell = 20$



- ▶ **Global optimum** computed by dynamic programming
- ▶ Benchmark function: **structural information is not known!**
- ▶ \Rightarrow **Randomly shuffled** variable indices.

Benchmark problems

- ▶ **Hierarchical If-and-only-iFF (HIFF)**
(Watson, Hornby and Pollack, 1998)
- ▶ Computed over multiple **layers**
- ▶ Nodes are combined as a **perfectly balanced binary tree**
- ▶ Problem lengths are **powers of two** (i.e., $\ell = 2, 4, 8, 16, 32, \dots$)
- ▶ Each **variable** is considered to be a **leaf**
- ▶ **Leaf** contributes 1
- ▶ **Internal node** contributes 2^{height} if children **both 0** or **both 1**
- ▶ **Internal node** is 0 if children **both 0**; 1 if **both 1**; **NIL** else

Benchmark problems

- ▶ **Weighted MAX-CUT**
(Karp, 1972)
- ▶ Given a **weighted graph** (V, E) , divide nodes into two sets so that **total weight** of edges between sets is **maximized**
- ▶ Identify **binary variable** x_i with each **node** v_i

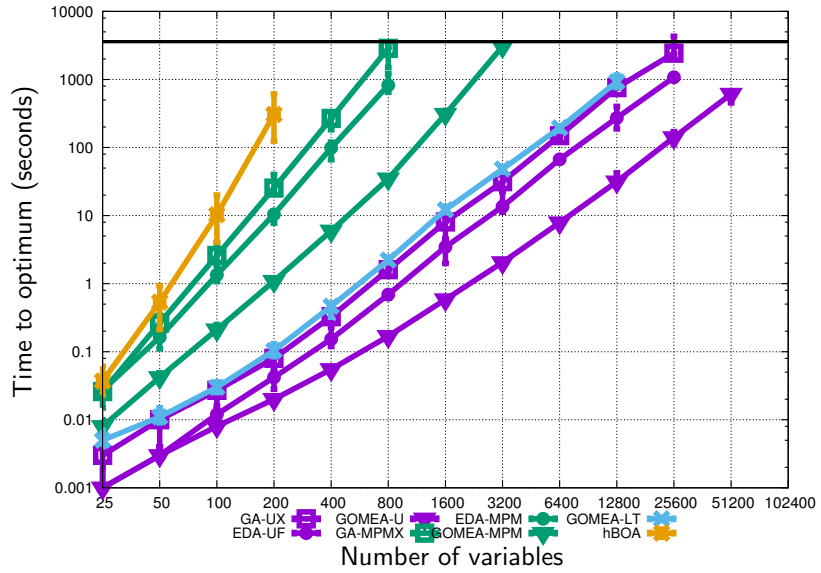
$$f_{\text{Weighted MAX-CUT}}(\mathbf{x}) = \sum_{(v_i, v_j) \in E} \begin{cases} w_{ij} & \text{if } x_i \neq x_j \\ 0 & \text{otherwise} \end{cases}$$

- ▶ For now, considered as a **black-box problem**
(no **partial evaluations** allowed)
- ▶ 5 instance **types**:
 - ▶ Fully connected graphs (β -distributed, $\alpha = 100, \beta = 1$)
 - ▶ 2D Square-grid graphs (β -distributed, $\alpha = 100, \beta = 1$)
 - ▶ 3D Square-torus graphs (β -distributed, $\alpha = 100, \beta = 1$)
 - ▶ Uniformly distributed in a box, fully connected
 - ▶ Uniformly distributed in a box, $\lfloor \sqrt{\ell} \rfloor$ nearest neighbors

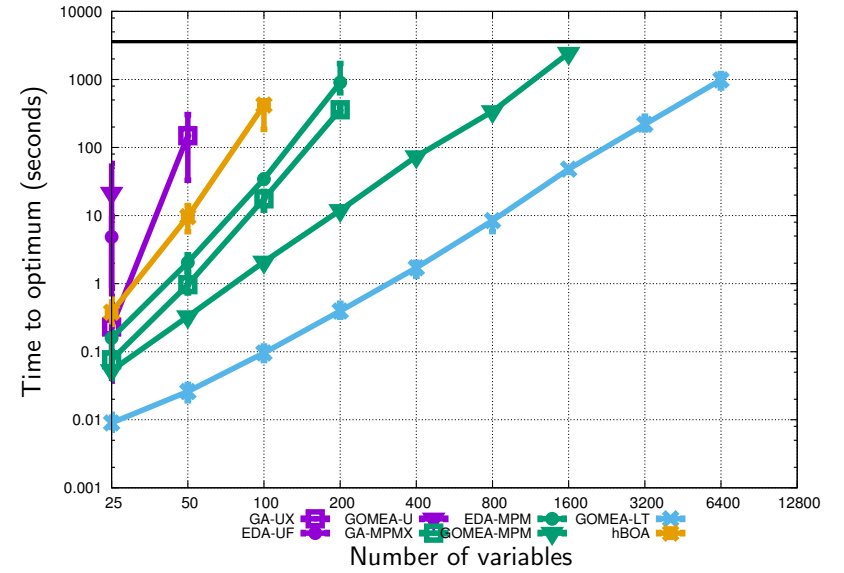
Experimental setup

- ▶ 100 **independent runs**
- ▶ Fully **black-box** evaluated
- ▶ Observe **time** required to reach **optimum**
- ▶ On a **relatively slow** CPU: 2.8 GHz AMD core
- ▶ Harik-Lobo **Population-sizing-free** scheme
 - ▶ Setting population size **optimally** is **hard/impossible**
 - ▶ Use **interleaving** of different runs with **different population sizes**
 - ▶ Generations in **larger** population sizes tick **slower**
 - ▶ **Smaller** populations converge **first**
 - ▶ **Overhead**: typically somewhere between **1-4 times slower**
 - ▶ Can actually also be **faster!**
 - ▶ **Gains** outweigh the overhead!

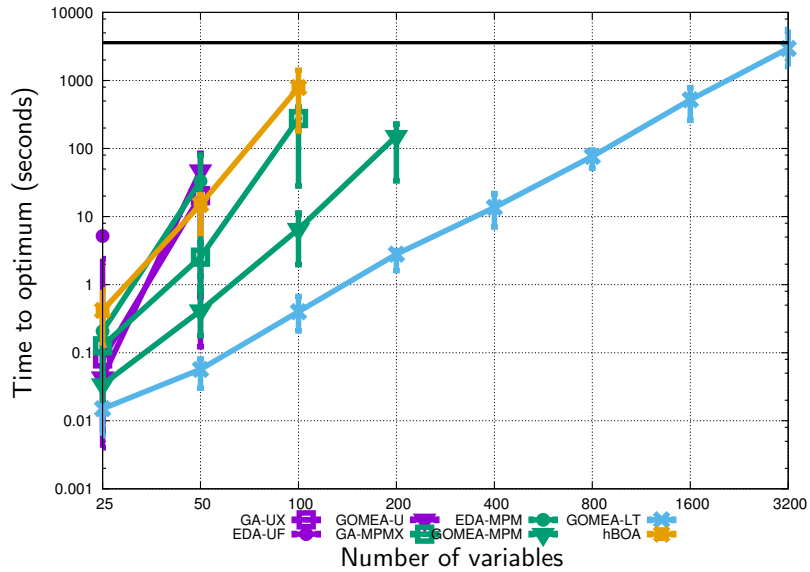
Experiments - Onemax



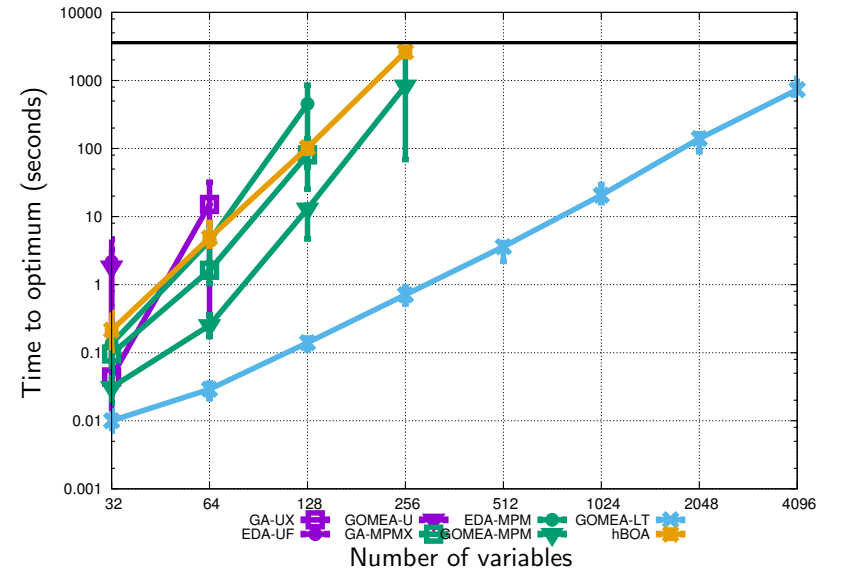
Experiments - Deceptive trap



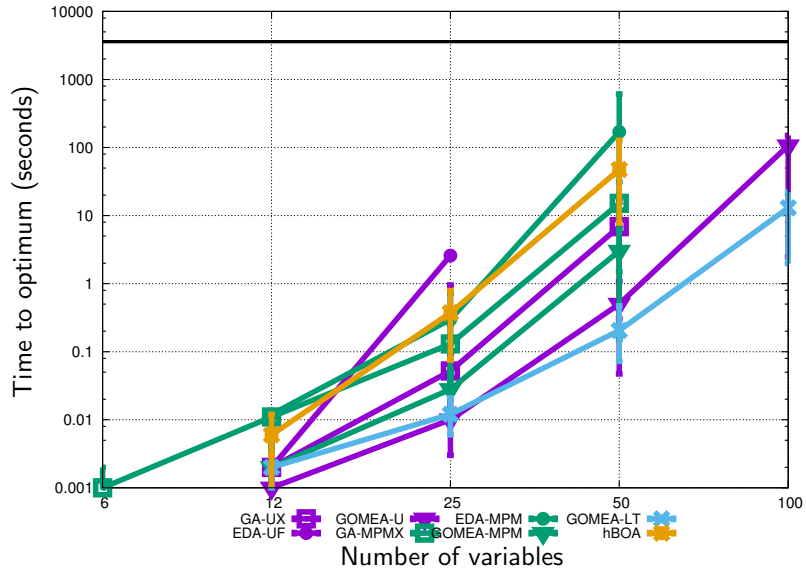
Experiments - Overlapping NK



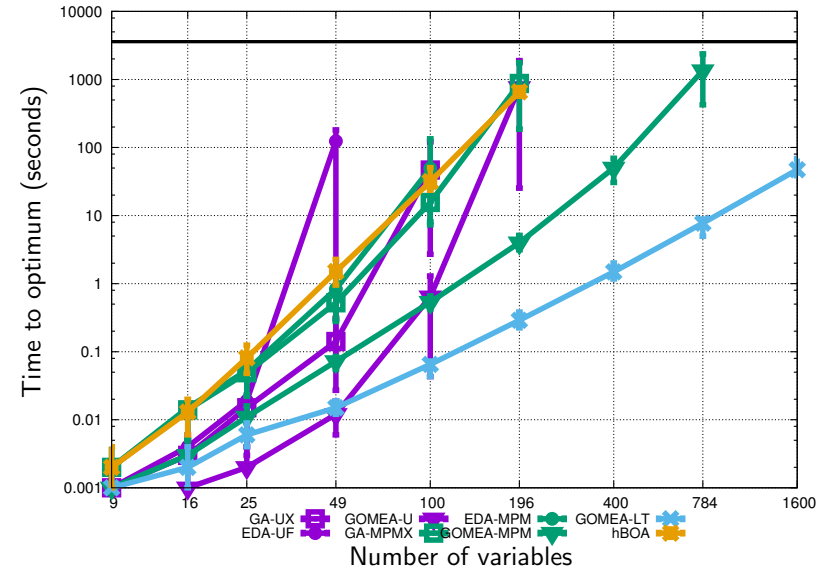
Experiments - HIFF



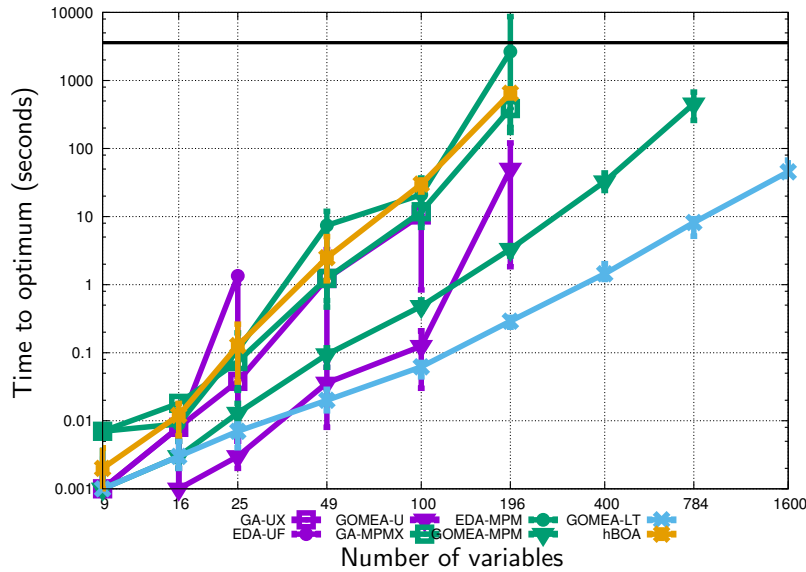
Experiments - MAX-CUT fully connected



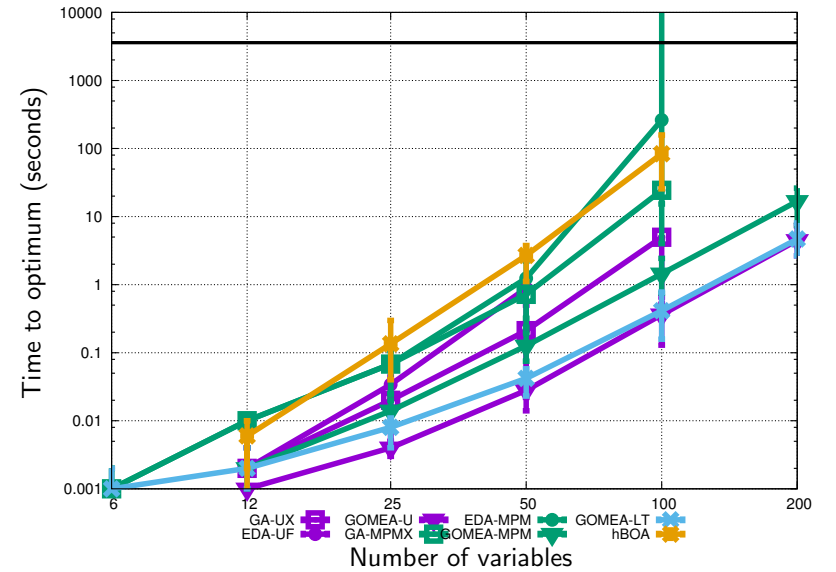
Experiments - MAX-CUT 2D square grid



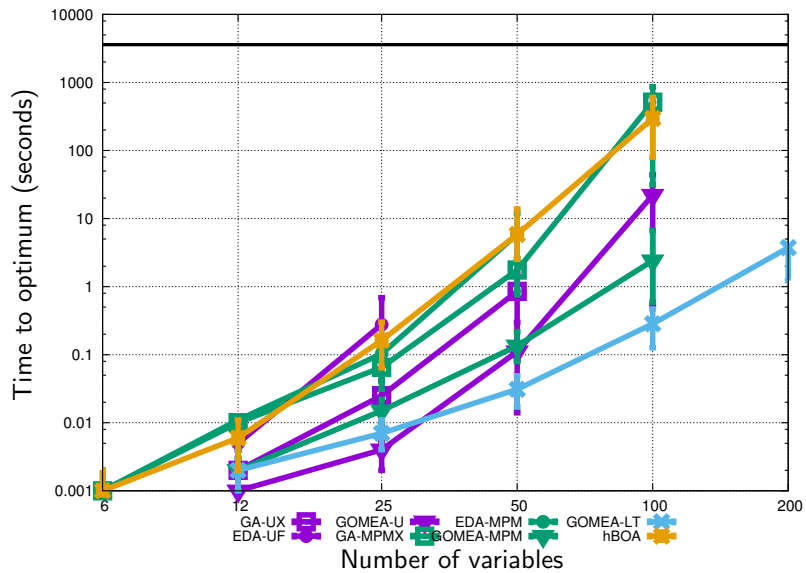
Experiments - MAX-CUT 2D square torus



Experiments - MAX-CUT box, fully connected



Experiments - MAX-CUT box, $\lfloor \sqrt{\ell} \rfloor$ nearest neighbors



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Discussion

- ▶ Use of **univariate structure** leads to **exponential** scale-up on **non-trivial** problems
- ▶ **GOMEA mixing** is then the **worst**
- ▶ Use of **learned** structure leads to **polynomial** scale-up
- ▶ **GOMEA mixing** is then the **best**
- ▶ Most **efficient**: **LT-GOMEA** (a.k.a. LTGA)

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Experiments: conclusion

- ▶ LTGA (= GOMEA with LT FOS) very efficient on **Deceptive Trap** function, **Nearest-Neighbor NK** landscape, and **Hierarchical IFF** function.
- ▶ Other FOS models possible: **Linkage Neighborhood OM** (Bosman & Thierens, 2012).
- ▶ **Linkage Tree** seems to be good compromise between FOS model complexity and search efficiency.

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Predetermined vs. Learned FOS

- ▶ Problem structure unknown: **learn** a FOS model.
- ▶ Problem structure Information available: **predetermined** FOS model.
- ▶ What is a **good** predetermined FOS model ?
- ▶ **Direct mapping** of dependency structure of problem definition to a predetermined FOS model ?
- ▶ **Predetermined linkage models** mirroring the static structure of the problem **not sufficient** (Thierens & Bosman, 2012).
- ▶ **Dynamically learned tree model superior** to mirror structured models and to static tree model.
- ▶ **Question**: is there an optimal, predetermined linkage model that outperforms the learned (tree) model ?

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Parameter-less Population Pyramid

- ▶ P3 (Goldman, Punch; 2014)
 - ▶ Similar to Harik-Lobo scheme: eliminates population-size parameter
- ▶ Each level of a pyramid-like structure is a population of solutions.
- ▶ Solutions are always hill-climbed.
- ▶ All solutions encountered are stored in the pyramid structure.
- ▶ At each level a Linkage Tree GA is run.
- ▶ Solutions climb the pyramid ladder with increasing fitness.
- ▶ Whenever a solution enters a level the linkage tree is released.

Conclusions

- ▶ “Blind” Evolutionary Algorithms are **limited** in their capability to **detect** and **mix/exploit/re-use** partial solutions (building blocks).
- ▶ One requires **luck** or **analyzing** and **designing** ways of **structure exploitation** directly into problem **representation** and **search** operators.
- ▶ Having a configurable **model** can help overcome this.
- ▶ Algorithm then must **learn** to configure the model and thereby **exploit structure** online during optimization (e.g. **EDAs**, **OMEAs**).

Model-based optimization

- ▶ Assumption: problems are somehow **structured**
- ▶ Use **induction** to find structure
- ▶ **Exploit** structure for increased **efficiency**
- ▶ **Preferable** to **enumeration** or **iterated random sampling**
- ▶ What to **induce**?
- ▶ Use a **model** that defines **reasonable structures**
- ▶ Induce **instance** of the model
- ▶ Model **capacity** determines **bias strength**

Model-based optimization

- ▶ Model = **probability distribution**
- ▶ Induction = **learning/estimation**
- ▶ Variation = **sampling**

- ▶ Estimation-of-Distribution Algorithm (EDA)

The Estimation-of-Distribution Algorithm (EDA)

- ▶ Use a set of n solutions for **distribution estimation**
- ▶ Focus on better solutions by **selection**
- ▶ Estimate from **selection**
 - ▶ EDA: Mühlenbein and Paaß(1996)

EDA

- 1 Initialize \mathcal{P} with n random solutions
- 2 Repeat until termination criterion met
 - 2.1 Select subset \mathcal{S} from \mathcal{P}
 - 2.2 Estimate distribution from \mathcal{S}
 - 2.3 Draw new set of solutions \mathcal{O} from distribution
 - 2.4 Update \mathcal{P} with \mathcal{O}

Model-based optimization

- ▶ Model = **description of linkages/dependencies**
- ▶ Induction = **learning/statistical testing**
- ▶ Variation = **mixing**

- ▶ Optimal Mixing Evolutionary Algorithm (OMEA)

The Optimal Mixing Evolutionary Algorithm (OMEA)

- ▶ Use a set of n solutions for **linkage detection**
- ▶ Focus on better solutions by **selection within variation**
- ▶ Estimate from **selection**
 - ▶ OMEA: Thierens and Bosman (2011)

OMEA

- 1 Initialize \mathcal{P} with n random solutions
- 2 Repeat until termination criterion met
 - 2.1 Select subset \mathcal{S} from \mathcal{P}
 - 2.2 Learn linkage model from \mathcal{S}
 - 2.3 Apply linkage-model guided optimal mixing to every individual in \mathcal{P} to generate \mathcal{O}
 - 2.4 Replace \mathcal{P} by \mathcal{O}

Model-based optimization

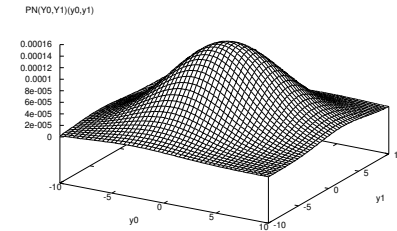
- ▶ **General concepts**
- ▶ Can be applied to **different types** of optimization problems/domains
- ▶ In second part of tutorial: focus on **other domains** than binary/integer

Real-valued Model-Based Evolutionary Algorithms

- ▶ Essentially **similar questions** to case of **binary/integer** variables
- ▶ We **don't have** the optimal model...
- ▶ **Approximate** the **optimal** model
- ▶ **Match** inductive search bias and problem structure
- ▶ How to **learn** and **perform variation** efficiently and effectively
- ▶ Trade-offs:
 - ▶ **Quality** versus complexity of **approximation**
 - ▶ **Efficiency in # evaluations** versus **time**
- ▶ **Essential model questions**:
 - ▶ Can key problem structure be represented?
 - ▶ Can key problem structure be represented efficiently?
 - ▶ Can the model be learned from data?
 - ▶ Can the model be learned (and used for variation) efficiently?

Normal distribution

- ▶ Require **practically useful** models.
- ▶ For instance **normal distribution**:



- ▶ Only $\mathcal{O}(I^2)$ **parameters** (mean, covariance matrix)
- ▶ **maximum-likelihood** (ML) estimates well known

$$\hat{\mu} = \frac{1}{|\mathcal{S}|} \sum_{j=0}^{|\mathcal{S}|-1} (\mathcal{S}_j), \quad \hat{\Sigma} = \frac{1}{|\mathcal{S}|} \sum_{j=0}^{|\mathcal{S}|-1} ((\mathcal{S}_j) - \hat{\mu})(\mathcal{S}_j - \hat{\mu})^T$$

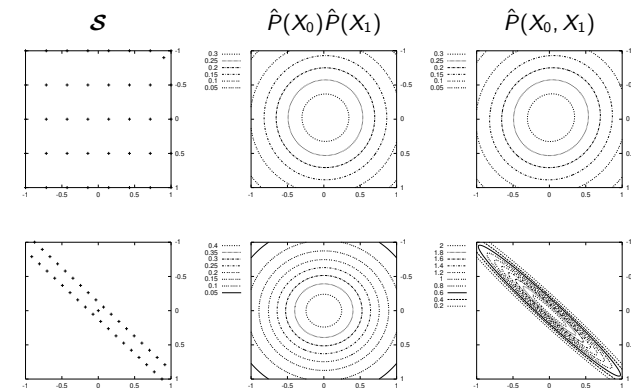
- ▶ Can **only** model **linear** dependencies

EDAs based on the Normal Distribution

- ▶ First uses were adaptations of **PBIL**
 - ▶ Rudlof and Köppen (1996)
 - ▶ Sebag and Ducoulombier (1998)
- ▶ Although initial results were **interesting**, quickly found that some problems were solved **more efficiently** if **dependencies** were modeled

EDAs based on the Normal Distribution

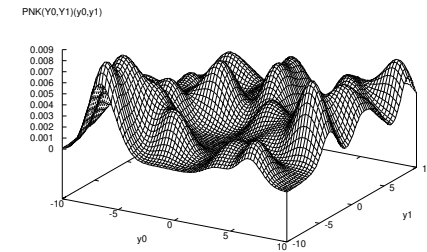
- ▶ Make decisions based on **better fit** and **increased complexity** (e.g. $\hat{P}(X_0, X_1)$ vs. $\hat{P}(X_0)\hat{P}(X_1)$)



EDAs based on the Normal Distribution

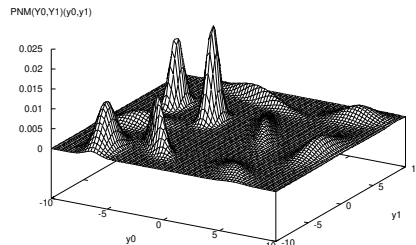
- ▶ EDAs with factorized **Normal** Distributions (MIMIC, COMIT, Bayesian, Copula selection, Multivariate (Markov networks))
 - ▶ Bosman and Thierens (2000, 2001)
 - ▶ Larrañaga, Etxebarria, Lozano, and Peña (2000)
 - ▶ Salinas-Gutiérrez, Hernández-Aguirre, and Villa-Diharce (2011)
 - ▶ Karshenas, Santana, Bielza, and Larrañaga (2012)
- ▶ On selected problems, **improvements** were found when using **higher-order dependencies**
- ▶ On some problems, results **didn't** get much better however
- ▶ Initially mainly attributed to **mismatch** between **model** and **search space**
- ▶ Clearly **true** to some extent

EDAs based on the Normal-kernels distribution



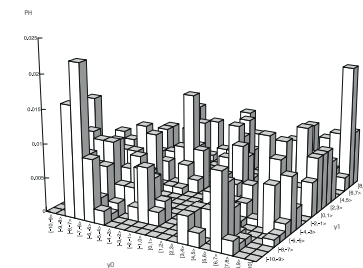
- ▶ Bosman and Thierens (2000)
- ▶ Ocenasek and Schwarz (2002)
- ▶ Ocenasek, Kern, Hansen, Müller, and Koumoutsakos (2004)
- ▶ **Natural tendency** to fit **structure** of data (linear or not)
- ▶ But also tendency to **overfit**
- ▶ Maximum-likelihood estimate not **usable**
- ▶ **Quality** of estimation depends **heavily** on size of kernel

EDAs based on the Normal-mixture distribution



- ▶ Gallagher, Fream, and Downs (1999)
- ▶ Bosman and Thierens (2001)
- ▶ Cho and Zhang (2002)
- ▶ Ahn, Ramakrishna, and Goldberg (2004)
- ▶ Li, Goldberg, Sastry, and Yu (2007)
- ▶ Maree, Alderliesten, Thierens, and Bosman (2017)
- ▶ **Trade-off** between normal and normal kernels.
- ▶ Maximum-Likelihood Estimate is **lot of effort** (**EM algorithm**).
- ▶ Alternative: cluster, then est. normal (with max. likelihood).

EDAs based on the Histogram Distribution



- ▶ Bosman and Thierens (2000)
- ▶ Tsutsui, Pelikan, and Goldberg (2001)
- ▶ **Easy** to implement and **map** to integers.
- ▶ Require **many** bins to get a **good** estimate.
- ▶ **Curse of dimensionality**.
- ▶ Greedy incr. factorization selection **hardly** possible.

EDAs based on latent variable models

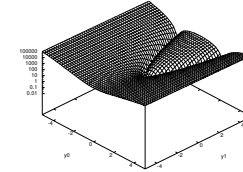
- ▶ Build models by **projecting** data onto model of **lower** dimensionality
- ▶ Helmholtz machines, mixture of factor analyzers, etc
 - ▶ Shin and Zhang (2001)
 - ▶ Cho and Zhang (2001)
 - ▶ Shin, Cho, and Zhang (2001)
 - ▶ Cho and Zhang (2002)
 - ▶ Cho and Zhang (2004)
- ▶ **Better** results than **standard** normal EDA on some problems, but still **unable** to come close to the **optimum** of 10-dimensional **Rosenbrock** function

Direct use of normal distribution

▶ Bad results

- ▶ Rosenbrock:

$$\mathfrak{F}(\mathbf{x}) = \sum_{i=0}^{n-2} 100(x_{i+1} - x_i^2)^2 + (1 - x_i)^2$$



▶ because...

- ▶ Rosenbrock has **narrow valley** leading to minimum
- ▶ Quickly samples **no longer centered** around minimum

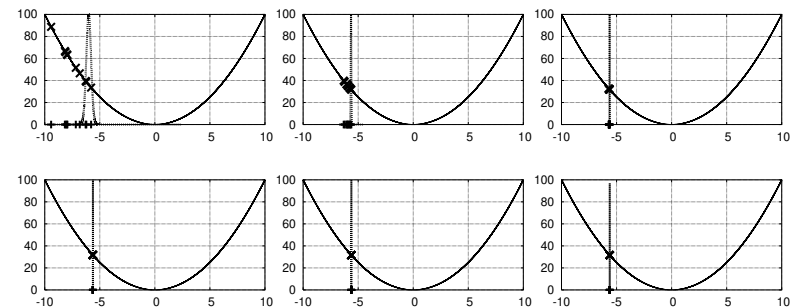
No attention for the gradient

- ▶ Distribution estimation makes **no assumption** on source
- ▶ Source is just **selected points** in parameter space
- ▶ Gradient info is **ignored** in maximum-likelihood estimate
- ▶ For normal distribution:
Variance goes to zero **too fast**

Illustration on the 1-D sphere function

$$\mathfrak{F}(x) = x_0^2$$

Progression in first 6 generations (top-left to bottom-right)



Analysis of the premature-convergence problem

- ▶ Theoretical **analysis** reveals indeed **limits**
 - ▶ Gonzalez, Lozano, and Larrañaga (2000)
 - ▶ Grahl, Minner, and Rothlauf (2005)
 - ▶ Bosman and Grahl (2005)
 - ▶ Yuan and Gallagher (2006)
- ▶ There is for instance a **bound** on how far the mean can **shift**

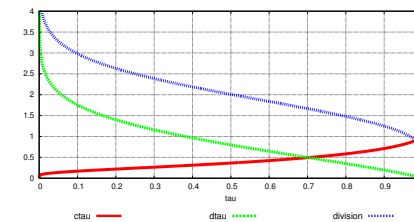
Analysis of the premature-convergence problem

- ▶ Variance **decreases** (exponentially fast)

$$\lim_{t \rightarrow \infty} \{\hat{\sigma}(t)\} = \lim_{t \rightarrow \infty} \{\hat{\sigma}(0)c(\tau)^t\} = 0$$
- ▶ This **limits** mean shift to a **fixed factor** times **initial spread!**

$$\lim_{t \rightarrow \infty} \{\hat{\mu}(t)\} = \hat{\mu}(0) + \frac{d(\tau)}{1 - \sqrt{c(\tau)}} \hat{\sigma}(0)$$

- ▶ $c(\tau)$ and $d(\tau)$ functions of
 - ▶ $\phi()$ (standard normal distribution) and
 - ▶ $\Phi()$ (inverse cumulative normal distribution)

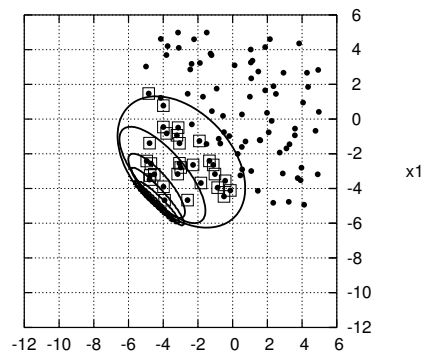


(Bosman and Grahl (2005))

Illustration on the 2-D plane function

$$\mathfrak{F}(\mathbf{x}) = x_0 + x_1$$

Progression in first 6 generations



Error ellipse 95% — Population 0 • Selection 0 □

What is missing?

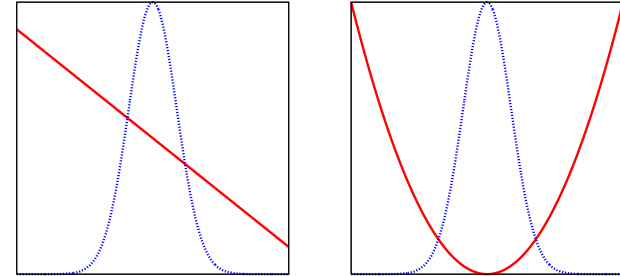
- ▶ **Structure** of landscape can be very **complicated**
- ▶ “Simple” normal distr. **hardly** matches global structure
- ▶ More **involved** distributions possible, but
 - ▶ **harder**, or even **impossible**, to estimate with **ML**
 - ▶ requires **lots** of **data**
- ▶ **Local** structure can be **approximated** but...
 - ▶ there is **no** generalization outside of the **data range**
 - ▶ Once **optimum** “lost” outside data range, EDA converges **elsewhere**, possibly **not** even a **local** optimum!
- ▶ EDA based on **maximum-likelihood estimate** **not efficient**

Ways to improve

- ▶ Gradient hybridization
 - ▶ Explicit use of gradient information
 - ▶ Apply gradient-based search to certain solutions (e.g. conjugate gradients)
 - ▶ Requires gradient computation
 - ▶ not always possible
 - ▶ not always reliable
- ▶ Adapt(ive) (ML) estimation
 - ▶ Derivative Free
 - ▶ Maintain EDA properties for valley case
 - ▶ Adapt in other cases (to explore beyond selected solutions)
 - ▶ How to distinguish?
 - ▶ Three ingredients:
 - ▶ Adaptive Variance Scaling (AVS)
 - ▶ Standard-Deviation Ratio (SDR)
 - ▶ Anticipated Mean Shift (AMS)

Adapted Maximum-Likelihood Gaussian Model

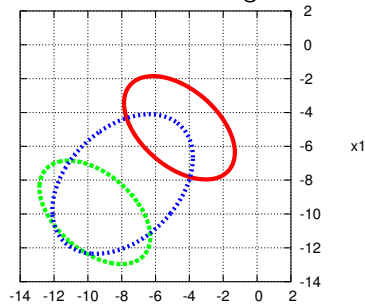
- ▶ Adaptive Variance Scaling (AVS) & Standard-Deviation Ratio (SDR)
- ▶ If improvements are found



- a) far from the mean, enlarge $\hat{\Sigma}$
- b) close to the mean, do nothing
- ▶ Close to the mean: within one standard deviation

Adapted Maximum-Likelihood Gaussian Model

- ▶ Anticipated Mean Shift (AMS)
- ▶ Anticipate where the mean is shifting
- ▶ Alter part of generated solutions by shifting
- ▶ On a slope, predictions are better (further down slope)
- ▶ Require balanced selection to re-align covariance matrix

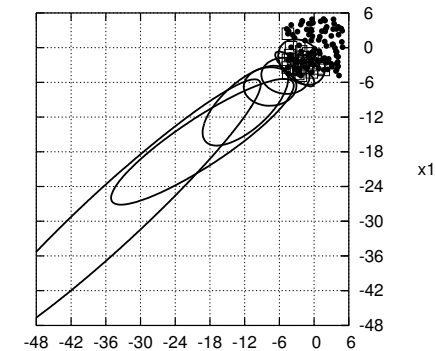


unaltered ——— altered x_0 realigned

Illustration on a 2-D slope

$$\tilde{f}(\mathbf{x}) = x_0 + x_1$$

Progression in first 6 generations



Error ellipse 95% ——— Population 0 • Selection 0 □

AMaLGaM, CMA-ES, NES, and RP

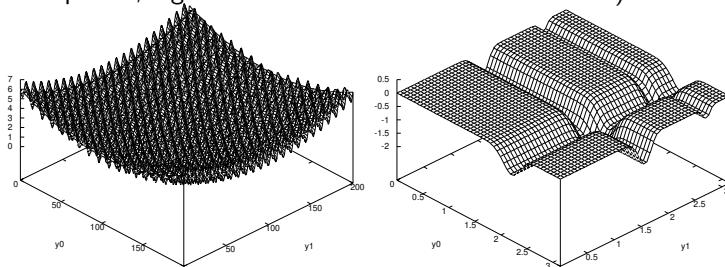
- ▶ AMaLGaM IDEA (or AMaLGaM for short)
Adapted Maximum-Likelihood Gaussian Model Iterated Density-Estimation Evolutionary Algorithm
- ▶ Natural question:
what is the relation to CMA-ES (Hansen (2001)) and NES (Wierstra, Schaul, Peters, and Schmidhuber (2008))
- ▶ Answer: the probability distribution
- ▶ All can be seen to be EDAs: every generation they estimate/update a probability distribution (which also happens to be the normal distribution in all three cases) and perform variation by generating new samples from this distribution.

AMaLGaM, CMA-ES, NES, and RP

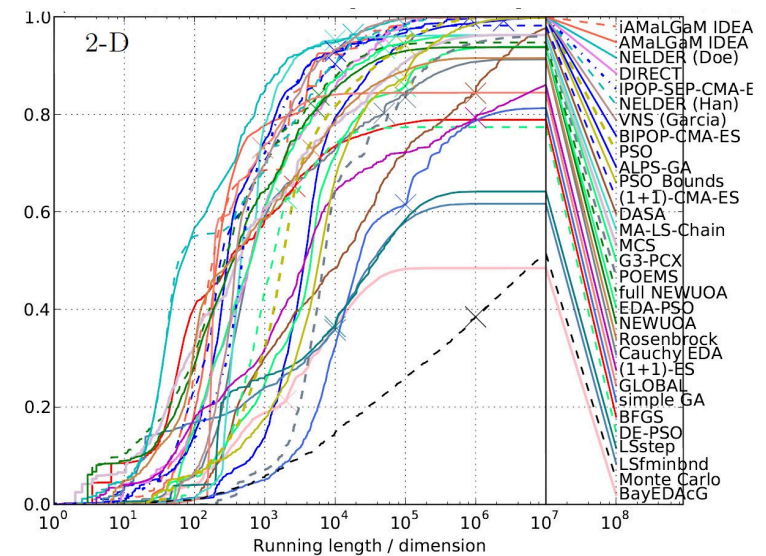
- ▶ Differences are only in how the distribution is obtained.
Where AMaLGaM uses maximum-likelihood estimates from the current generation, CMA-ES and NES base estimates on differences between subsequent generations as well as many elaborate enhancements (see tutorial on CMA-ES) and RP uses ensembles of random projections to lower dimensions to estimate covariance matrices more efficiently.
- ▶ On typical unimodal benchmark problems (sphere, (rotated) ellipsoid, cigar, etc) these algorithms exhibit polynomial scalability in both minimally required population size and required number of function evaluations
- ▶ CMA-ES, NES scale better than AMaLGaM on such problems

Parameter-free Gaussian EDAs

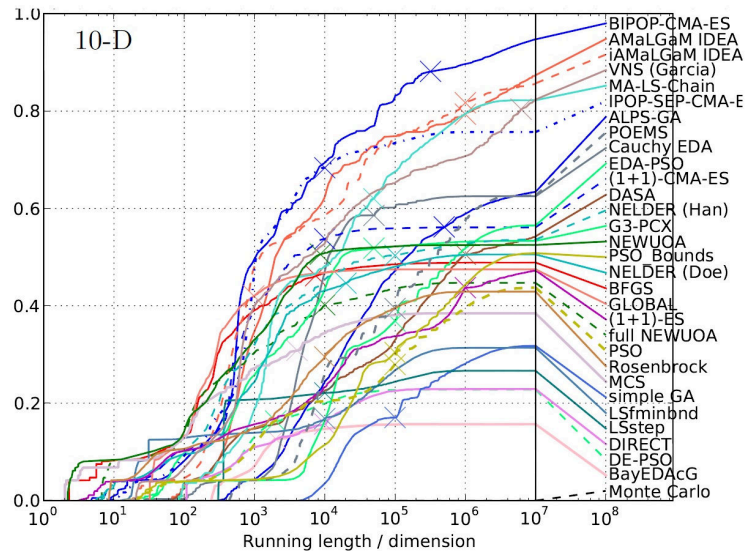
- ▶ Parameters get in the way of ease-of-use
- ▶ Remove all parameters: derive and implement guidelines
- ▶ Restart mechanism to increase success probability
- ▶ Typical restart scheme: increase size exponentially
- ▶ Works well on Griewank (left), not so much on Michalewicz (right)
- ▶ Many different schemes exist therefore (also algorithm specific, e.g. BIPOP-CMA-ES and IPOP-CMA-ES)



Noiseless BBOB comparison with other algorithms



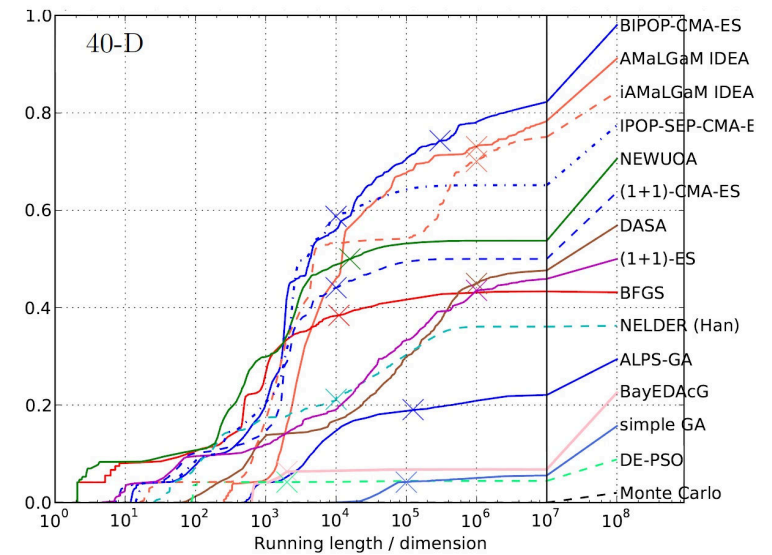
Noiseless BBOB comparison with other algorithms



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Noiseless BBOB comparison with other algorithms



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Dimensionality reduction and problem-specific models

- ▶ Real-world problems may be high(er) dim. (at least, $\ell \gg 40$)
- ▶ Handling a full covariance matrix becomes expensive
- ▶ Restrict size of covariance matrix somehow
 - ▶ Random projections, tested up to $\ell = 10^3$ (Kabán, Bootkrajang, and Durrant (2013))
 - ▶ Projection-based restricted CMA-ES, tested up to $\ell = 10^3$ (Akimoto and Hansen (2016))
 - ▶ GOMEA-based, tested up to $\ell = 5 \cdot 10^6$ (with partial eval.'s) (Bouter, Alderliesten, Witteveen, and Bosman (2017))

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Permutation Model-Based Evolutionary Algorithms

- ▶ Binary/Integer representations are discrete, but also **Cartesian**
- ▶ Other discrete search spaces exist that are **non-Cartesian**
- ▶ Most notably: **permutation**-based problems
- ▶ Important real-world relevance, e.g. **routing** and **scheduling**
- ▶ Brings **different challenges** than Cartesian spaces however
 - ▶ **Relative** ordering problems
 - ▶ **Absolute** ordering problems
 - ▶ **Neighbor** ordering problems
 - ▶ **Combinations** of these
- ▶ Different **types** of models are more suited for specific **types** of ordering problem

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Permutation Model-Based Evolutionary Algorithms

- ▶ Building **permutation** models directly **not straightforward**
- ▶ Potential aid in the form of **random keys** (Bean (1997))
- ▶ Random keys **encode** permutations in **real-valued** space (via sorting)

0	1	2	3	⇒	3	1	0	2
0.61	0.51	0.62	0.31		0.31	0.51	0.61	0.62

- ▶ **Real-valued** approaches can thus be used **directly**
 - ▶ Bosman and Thierens (2001) (normal EDA)
 - ▶ Larrañaga et al (2001) (normal EDA)
- ▶ **Inefficient scale-up** behavior on deceptive additively decomposable relative ordering problems
- ▶ Highly **redundant** encoding that is hard to model with a **normal distribution**

Permutation Model-Based Evolutionary Algorithms

- ▶ Use **crossover** on the basis of a **factorization** of the normal distribution instead
 - ▶ Bosman and Thierens (2001)
- ▶ Now obtain **polynomial scale-up** behavior, but redundant encoding
- ▶ How about a **direct** modelling of probabilities of permutations?
- ▶ Consider a **marginal product factorization** (i.e. mutually exclusive subsets of variables as in ECGA)
- ▶ Once an instance is **sampled** for a subset of variables, other variables **can't** use these values anymore
- ▶ One way to deal with this is **explicit repair** of probability tables during sampling
 - ▶ Bengoetxea et al (2000)
 - ▶ Pelikan et al (2007)
- ▶ Requires **very large** sample sizes
- ▶ Sampling **repair** can introduce **unwanted biases**

Permutation Model-Based Evolutionary Algorithms

- ▶ For relative-ordering variables, a **probabilistically correct** factorization approach is **possible**
 - ▶ Bosman (2003)
- ▶ **Continuous, Binary**: $P(\mathbf{X}) = P(X_0, X_4)P(X_1)P(X_3, X_2)$.
- ▶ **Permutation**: $P(\mathbf{X}) = \frac{2!1!2!}{5!}P(X_0, X_4)P(X_1)P(X_3, X_2)$.
- ▶ Random variable X_i : **position** of integer i in the permutation
→ tackle **relative-ordering permutation problems**.
- ▶ **Normalization** required, because there are $5!$ permutations.
- ▶ “Oddities” specific to **permutations** exist (spurious dependencies between “low” variables in one building block and “high” variables in another)
- ▶ Require **specialized adaptations** of standard linkage learning / factorization techniques

Permutation Model-Based Evolutionary Algorithms

- ▶ Generate **instance** for each subset of variables **independently**
- ▶ Then **map** to the **real-valued** domain using **random keys** and then translate the entire string into a valid **permutation**
- ▶ **Preserves** relative ordering of variables in subsets
- ▶ Can sample **directly** instead of using crossover (**crossover** still more robust however)
- ▶ Scales **polynomially** and much better than normal-pdf induced crossover

Permutation Model-Based Evolutionary Algorithms

- ▶ **Edge-histogram** based sampling
 - ▶ Tsutsui, Pelikan, and Goldberg (2003)
- ▶ Maps well to problems with **neighboring variable** relations
- ▶ Model is a **matrix** with probabilities of edges
- ▶ Matrix needs to be **adjusted while sampling**
- ▶ For problems with neighboring relations works **better** than **random keys**

Permutation Model-Based Evolutionary Algorithms

- ▶ **Gaussian** “equivalent” in permutation space: **Mallows** model (GM-EDA)
 - ▶ Ceberio, Mendiburu, and Lozano (2011)
- ▶ Requires a **distance measure** between permutations and a **central permutation**
- ▶ Also requires a **spread parameter** (not estimated from data)
- ▶ Most commonly used **distance**: Kendall- τ , allows **factorization**
- ▶ Finding central permutation is **NP-hard** however
- ▶ Fast **heuristics** are **possible** (linear in l and n)
- ▶ Final **parameter estimation** and **sampling** are not trivial and require **dedicated** algorithms
- ▶ First results are **promising** (permutation flow shop), outperforming Tsutsui
 - ▶ Ceberio, Irurozki, Mendiburu, and Lozano (2014)

Permutation Model-Based Evolutionary Algorithms

- ▶ **GOMEA** variant for permutations based on random keys
 - ▶ Bosman, Luong, and Thierens (2016)
- ▶ Requires a **distance measure** between permutations. Used product of:
 - ▶ Relative ordering information
 - ▶ Adjacency information
- ▶ Possibly add **random rescaling** and **re-encoding**
- ▶ First results are **promising** (permutation flow shop), mostly outperforming GM-EDA

Model-Based Genetic Programming

- ▶ Estimation-of-Distribution Programming (**EDP**)
- ▶ Typically **grammar** based, but not always
- ▶ Grammar Guided Genetic Programming (**GGGP**)
- ▶ Grammars very **useful** to limit search space
- ▶ But how do we use it **learn** structural features?

Model-Based Genetic Programming

- ▶ Early works did not use **grammar**, e.g **PIPE** (Probabilistic Incremental Program Evolution)
 - ▶ Salustowicz and Schmidhuber (1997)
- ▶ Store **probabilities** of options (operators/terminals) for any **node** in the solution tree, bound maximum size
- ▶ All nodes thus **independent**

Model-Based Genetic Programming

- ▶ If looking at solutions **node-based**, and using a **fixed template**, essentially have **Cartesian fixed-length** representation
- ▶ Can use existing **integer-based** model-based EAs on this
- ▶ **eCGP** (ECGA for GP) does exactly this
 - ▶ Sastry and Goldberg (2003)
- ▶ **Better** results for selected problems, but use of a template has its **limitations**

Model-Based Genetic Programming

- ▶ Extensions to **Bayesian factorizations** are also possible
- ▶ **POLE** does exactly this
 - ▶ Hasegawa and Iba (2008)
- ▶ **MOSES** does not use fixed template, but has **incremental** tree complexity (and model complexity) using **special** operators
 - ▶ Looks, Goertzel, and Pennachin (2004)
 - ▶ Looks (2006)

Model-Based Genetic Programming

- ▶ Alternative approach: **grammar-based**
- ▶ Start with **basic production rules**
- ▶ **Learning**: assign probabilities to rules and increase **complexity** and **specificity** of rules using **heuristics**
- ▶ **Sampling**: select probabilistically from **appropriate** production rules
- ▶ Results are **promising** in that less function **evaluations** are often needed than standard GP, but time-complexity is (much) **larger**
 - ▶ Shan, McKay, Baxter, Abbass, and Essam (2003)
 - ▶ Bosman and de Jong (2004)
 - ▶ Shan, McKay, Baxter, Abbass, Essam, and Hoai (2004)
 - ▶ Hasegawa and Iba (2007)

Model-Based Genetic Programming

- ▶ **Intermediate** approach: n -grams
- ▶ Focus **probabilities** on most important **relationships** (local, e.g. with **parents** and **grandparents**)
- ▶ Enumerate all possible relationships **beforehand**
- ▶ Learning: **estimate probabilities** for the n -grams
- ▶ Sampling: **recursively employ** the n -grams
- ▶ Advantage: learning is **much faster** than with **grammar transformations**
 - ▶ Hemberg, Veeramachaneni, McDermott, Berzan, and O'Reilly (2012)

Model-Based Genetic Programming

- ▶ Impossible to cover everything in this tutorial, see literature
 - ▶ Kim, Shan, Nguyen, and McKay (2014)

Representation			Models	Positional		Context (Label)		Context (Ancestral)	
Genotype	Model	Det.		Dep.	Det.	Dep.	Det.	Dep.	
Tree GP like	Expression Tree	PPT	PIPE	1		-1	-1	-1	-1
			EDP	1		-1	-1	-1	1
			ECGP	1		-1	-1	-1	1
			POLE	1		-1	-1	-1	1
			AP	1		-1	-1	-1	-1
	Derivation Tree	Stochastic Chomsky Grammar	N-gram			1		-1	-1
			sSG-GP	-1	-1	1		-1	-1
			vSG-GP	-1	1	1		-1	1
			PEEL	-1	1	1		(-1,1)	1
			GMFE	-1	(-1,1)	1		(-1,1)	1
Graph		GNP-EDA							
GA like	Prefix Exp. Tree		bACP	-1		-1	-1	-1	
			gACP	1		-1	-1	-1	1
			DAP	-1	(0,1)	1		(-1,1)	1
	Prefix Der. Tree			GAP	-1	-1	1		1
				EGAP	-1	-1	1		1
	Linear Genotype			GBAP	-1	-1	1		1
				BAP	1		-1	-1	-1
Hybrid			BOAP	1		-1	-1	-1	1
			CGP-EDA	1		-1	-1	-1	-1
			N-gram GP	-1	-1	1		-1	1
			AntTAG	-1	-1	1		-1	-1
			CFGR						
			MOSES						
			PAM-DGP						

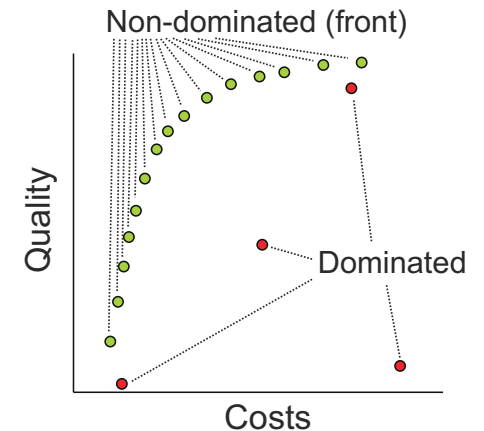
Model-Based Genetic Programming

- ▶ Hybrid approach:
 - ▶ Use **GOMEA** on template
 - ▶ Learn new candidate **functions** using entropy of wrong cases
 - ▶ **Best-ever performance** by non-specific EA on even-parity problem
 - ▶ Virgolin, Alderliesten, Witteveen, and Bosman (2017)

Multi-objective Model-Based Evolutionary Algorithms

- ▶ Multiple **objectives** should be optimized **simultaneously**
- ▶ **Conflicting** objectives, no expression of **weights**
- ▶ **Can't** combine the objectives in a single **scalar** objective

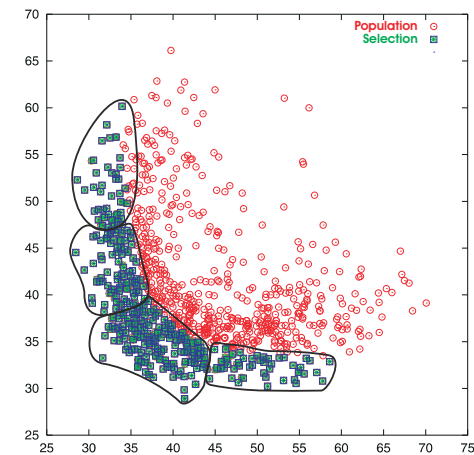
- ▶ Want to present a set of **promising** alternatives to a **decision maker**
- ▶ **Example:** Maximize the **quality** and minimize the **production costs** of a product
- ▶ **NOTE:** This is **NOT** an MO tutorial



Multi-objective Model-Based Evolutionary Algorithms

- ▶ Algorithm attempts to obtain **improvements** all **along** the current Pareto front
- ▶ Different **regions** along Pareto front may be very **different**
- ▶ E.g. what are far ends of the **optimal** Pareto front? **Optimal** solutions for individual objectives f_i
- ▶ **Restrict** variation to **clusters** (restricted mating)
- ▶ For instance: obtain clusters **along** Pareto front: cluster **selected solutions**
 - ▶ Bosman and Thierens (2002)
 - ▶ Pelikan, Sastry, and Goldberg (2009)

Multi-objective Model-Based Evolutionary Algorithms



Multi-objective Model-Based Evolutionary Algorithms

- ▶ In **EDAs**, this clustering corresponds to use of **mixture** probability distributions

$$P_{(\varsigma, \theta)}(\mathcal{Z}) = \sum_{i=0}^{k-1} \beta_i P_{(\varsigma_i, \theta_i)}(\mathcal{Z})$$

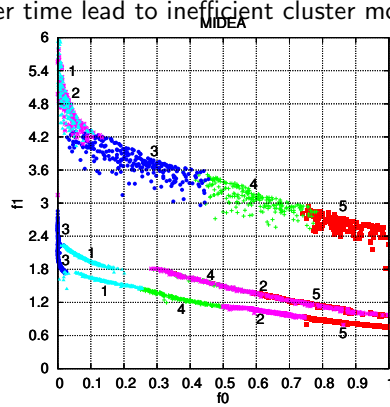
- ▶ **Cluster** solutions in **objective** space (e.g. k-means)
- ▶ Estimate a **simpler** distribution $P_{(\varsigma_i, \theta_i)}(\mathcal{Z})$ in each cluster
- ▶ Set all **mixing coefficients** to $\beta_i = \frac{1}{k}$
- ▶ **Parallel**, specialized exploration **along** front

Multi-objective Model-Based Evolutionary Algorithms

- ▶ Each distribution explores **own region**
- ▶ Learning may however by incremental (CMA-ES, iAMaLGaM, iBOA, etc)
- ▶ Assign each distribution **own adaptive** incremental mechanisms
- ▶ **Cannot** combine directly with clustering each generation
- ▶ Need **correspondence** over generations
- ▶ Number of clusters fixed beforehand (k)

Multi-objective Model-Based Evolutionary Algorithms

- ▶ **Implicit** cluster registration
- ▶ Keep clusters **spatially separated** during run.
- ▶ Assign new solution to its nearest, non-full cluster
- ▶ Can over time lead to inefficient cluster movement

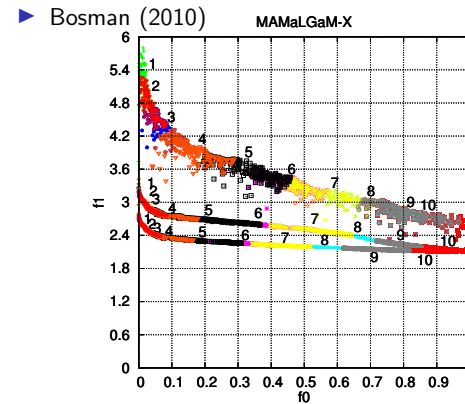


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Multi-objective Model-Based Evolutionary Algorithms

- ▶ **Explicit** cluster registration
- ▶ Minimize **sum of cluster distance** over all permutations of clusters in subsequent generations



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Multi-objective Model-Based Evolutionary Algorithms

- ▶ Other model-based MOEAs or MOEA concepts:
 - ▶ **MOEA/D**: simultaneously evolve different directions (Tchebycheff)
 - ▶ Can be combined with model-based EAs
 - ▶ e.g. CMA-ES, see: Wang, Liaw, and Ting (2016)
 - ▶ Copula-based EDAs
 - ▶ Martí, de Mello Jr., Sanchez-Pi, and Vellasco (2016)

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Conclusions

- ▶ “Blind” metaheuristics are **limited** in their capability to **detect** and **mix/exploit/re-use** structural features of an optimization problem (e.g. partial solutions, building blocks, promising search directions, etc).
- ▶ One requires **luck** or **analyzing** and **designing** ways of **structure exploitation** directly into problem **representation** and **search** operators.
- ▶ Having a configurable **model** can help “overcome” this / help to do this automatically.
- ▶ Algorithm then must **learn** to configure the model and thereby **exploit structure** online during optimization.
- ▶ Having an **explicitly tunable model** can really help

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Conclusions

- ▶ We **don't have** the optimal model...
- ▶ **Approximate** the **optimal** model
- ▶ **Match** inductive search bias and problem structure
- ▶ How to **learn** and **perform variation** efficiently and effectively
- ▶ Trade-offs:
 - ▶ **Quality** versus complexity of **approximation**
 - ▶ **Efficiency** in **# evaluations** versus **time**
- ▶ **Essential model questions**:
 - ▶ Can key problem structure be represented?
 - ▶ Can key problem structure be represented efficiently?
 - ▶ Can the model be learned from data?
 - ▶ Can the model be learned (and used for variation) efficiently?

Conclusions

- ▶ **Efficient model-based evolutionary algorithms** (EDAs/IDEAs/PMBGAs/OMEAs) exist
- ▶ Binary/Integer/Permutation/Real-valued/GP & multi-objective
- ▶ Research is **ongoing**
- ▶ Especially useful when optimizing from a **black-box** perspective (e.g. complex simulations)
- ▶ Also useful from a **white-box** perspective
 - ▶ Can **learn more** about the problem through **learnt models**
 - ▶ Models **configurable** by hand (remove "expensive" learning overhead)

Conclusions

- ▶ **Books**
 - ▶ Larrañaga and Lozano (eds) (2001). **Estimation of Distribution Algorithms: A New Tool for Evolutionary Computation**. Kluwer.
 - ▶ Lozano, Larrañaga, Inza, Bengoetxea (2006). **Towards a New Evolutionary Computation: Advances on Estimation of Distribution Algorithms**, Springer.
 - ▶ Pelikan, Sastry, Cantú-Paz (eds) (2006). **Scalable Optimization via Probabilistic Modeling: From Algorithms to Applications**, Springer.

Acknowledgements

- ▶ Selected images were re-used from the 2012 GECCO tutorial "Probabilistic Model-building Genetic Algorithms" by Martin Pelikan.