

GECCO 2019 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

Dirk Thierens & Peter A.N. Bosman. GECCO 2019 Tutorial - Model-Based Evolutionary Algorithms.

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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)

Dirk Thierens & Peter A.N. Bosman. GECCO 2019 Tutorial - Model-Based Evolutionary Algorithms.

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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

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Why ?

Goal: Black Box Optimization

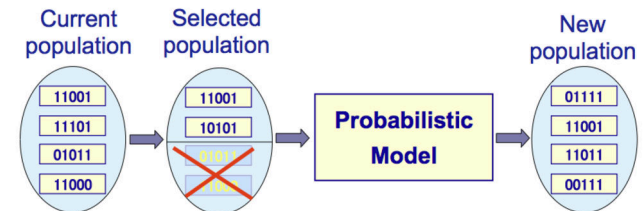
- ▶ Little known about the structure of the problem
- ▶ Clean separation optimizer from problem definition
- ▶ Easy and generally applicable

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

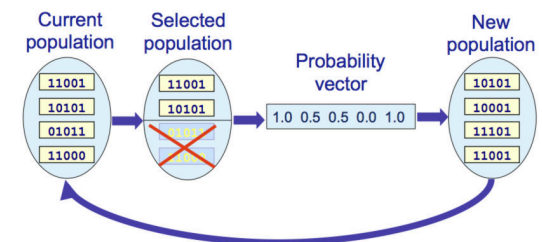
Type of Models

- ▶ **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 | 000 | 0.3 |
| 111111 | 001 | 0.0 |
| 010101 | 010 | 0.2 |
| 101010 | 011 | 0.0 |
| 000010 | 100 | 0.0 |
| 111000 | 101 | 0.1 |
| 010111 | 110 | 0.0 |
| 111000 | 111 | 0.4 |
| 000111 | | |
| 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 Kullack-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

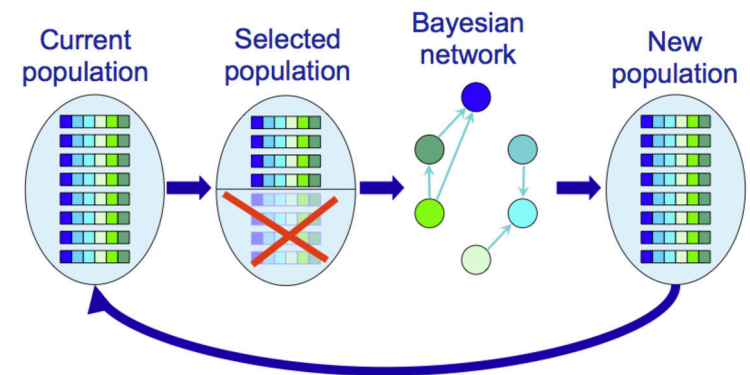
1. Start from univariate FOS:
 $\{\{0\}, \{1\}, \{2\}, \dots, \{l-2\}, \{l-1\}\}$
2. All possible **pairs** of partitions are temporarily merged:
 $\{\{0, 1\}, \{2\}, \dots, \{l-2\}, \{l-1\}\}$
 $\{\{0, 2\}, \{1\}, \dots, \{l-2\}, \{l-1\}\}$
 \vdots
 $\{\{0\}, \{1, 2\}, \dots, \{l-2\}, \{l-1\}\}$
 \vdots
 $\{\{0\}, \{1\}, \{2\}, \dots, \{l-2\}, \{l-1\}\}$
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**) (Etzeberria, 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

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

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

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 \mathcal{F} form a hierarchical clustering.

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

- ▶ 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

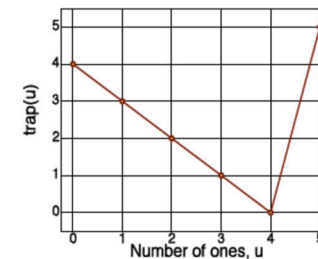
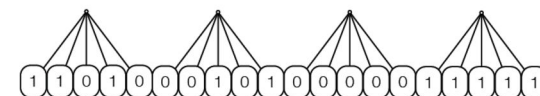
- ▶ **Onemax** (counting ones)

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

Deceptive Trap Function

Interacting, non-overlapping, deceptive groups of variables.

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

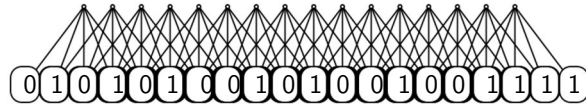


Nearest-neighbor NK-landscape

- **Overlapping**, neighboring random subfunctions

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

- 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

- **Hierarchical Trap (HTrap)**
(Pelikan and Goldberg, 2000)
- Also computed over **multiple layers**
- Nodes are combined as a **perfectly balanced k -ary tree**
- We use $k = 3$
- Problem lengths are **powers of k** (i.e., $\ell = 3, 9, 27, 81, 243, \dots$)
- Each **variable** is considered to be a **leaf**
- **Leaf** contributes 1
- **Internal node** contributes value of trap function times k^{height}
(**root**: deceptive trap, **otherwise**: trap with same value for 0s)
- **Internal node** is 0 if children **all 0**; 1 if **all 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

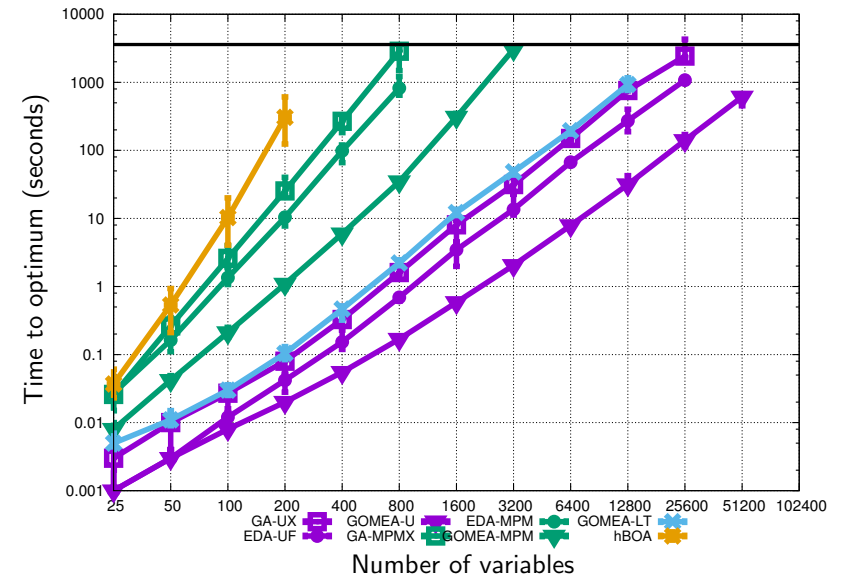
$$f_{\text{Weighted MAX-CUT}}(\mathbf{x}) = \sum_{(v_i, v_j) \in E} \begin{cases} w_{ij} & \text{if } x_i \neq x_j \\ 0 & \text{otherwise} \end{cases}$$

- 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

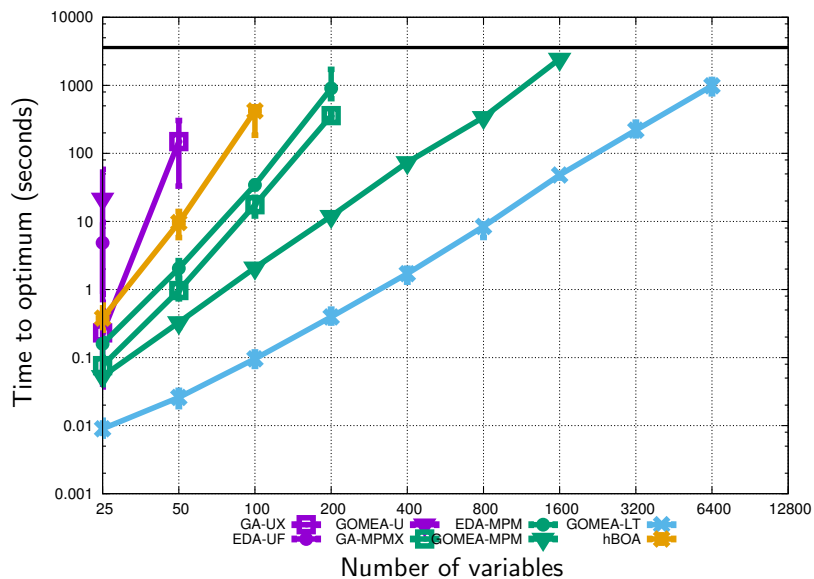
Experimental setup

- ▶ 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!

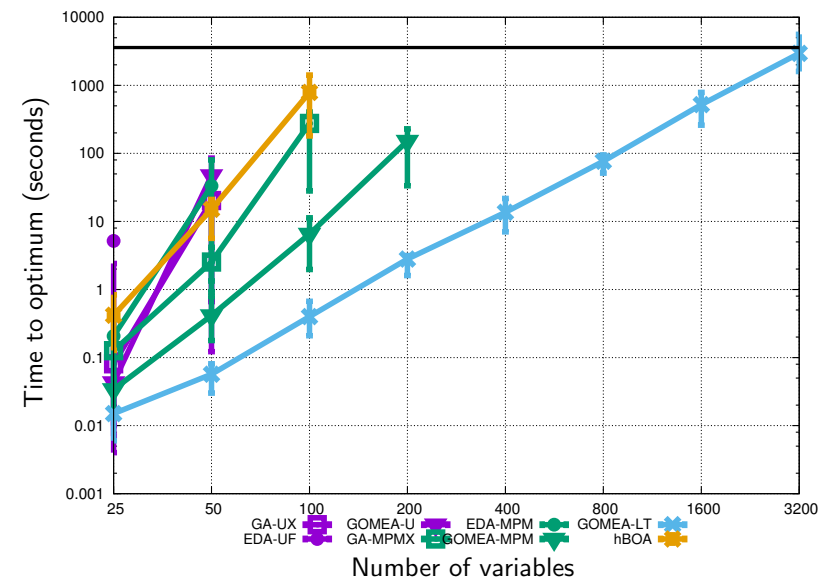
Experiments - Onemax



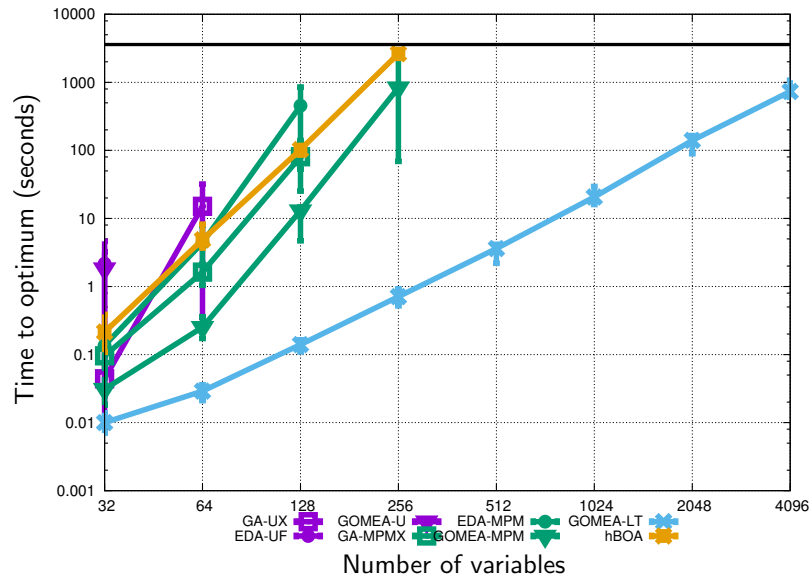
Experiments - Deceptive trap



Experiments - Overlapping NK



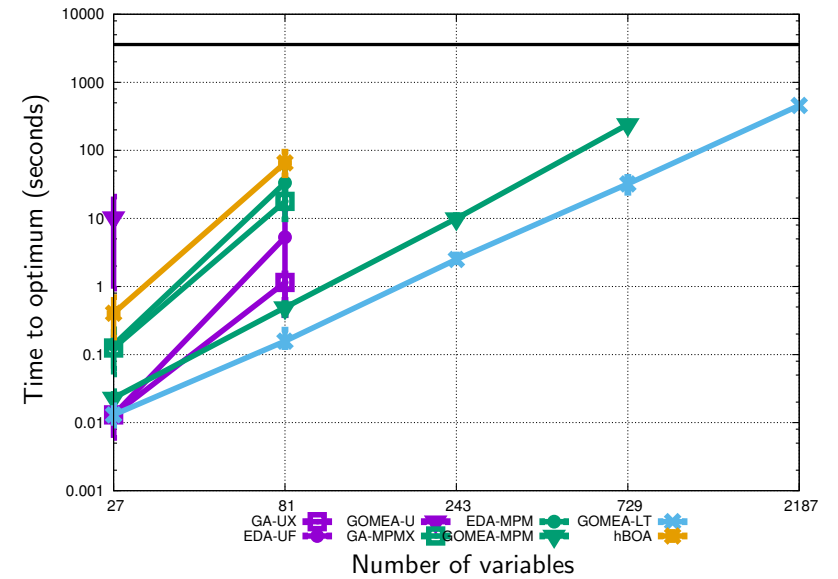
Experiments - HIFF



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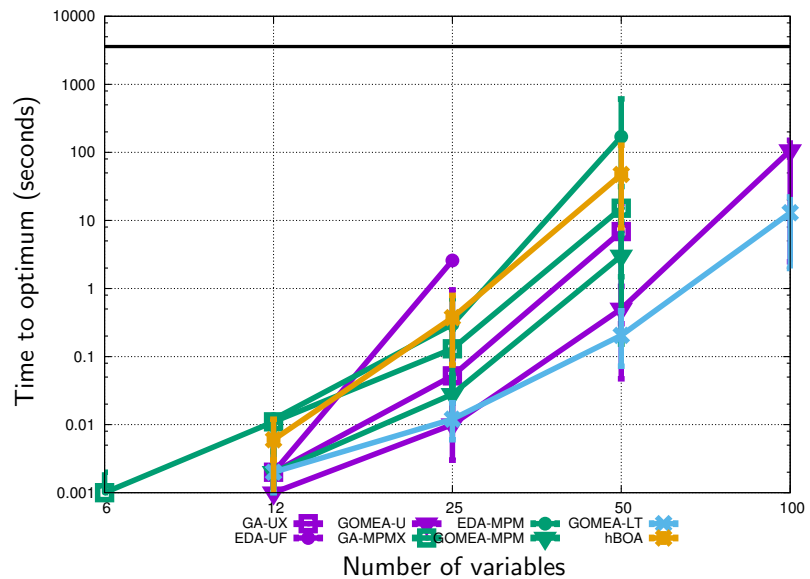
Experiments - HTrap



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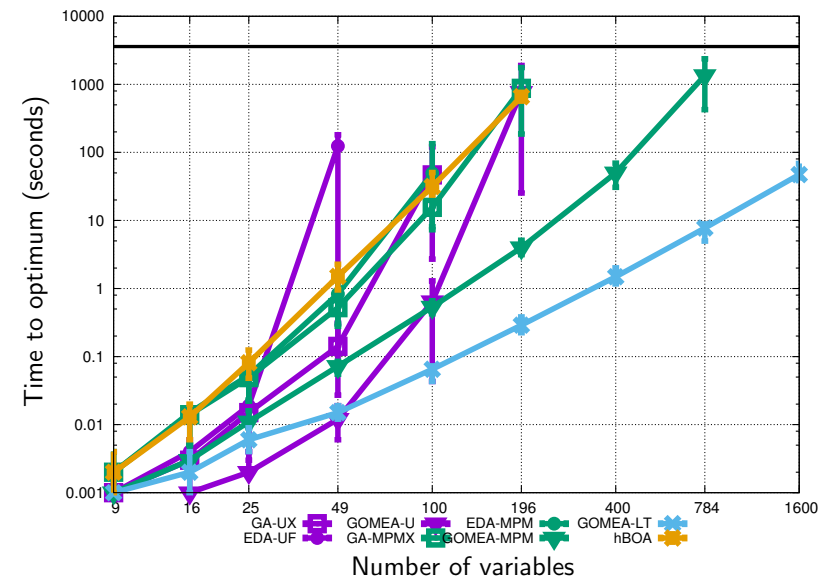
Experiments - MAX-CUT fully connected



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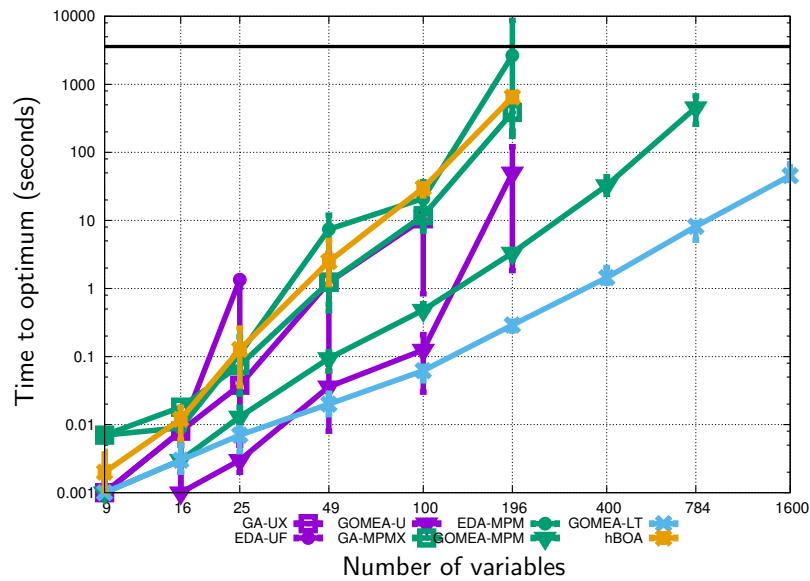
Experiments - MAX-CUT 2D square grid



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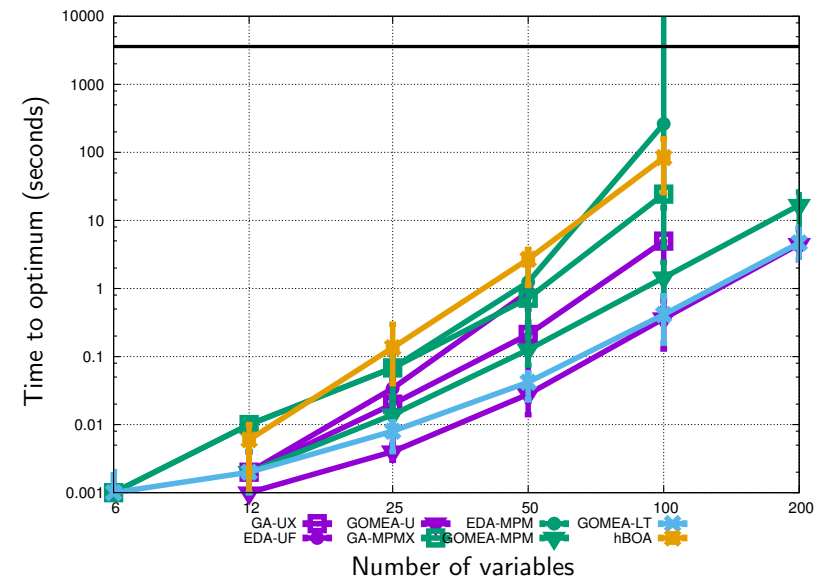
Experiments - MAX-CUT 2D square torus



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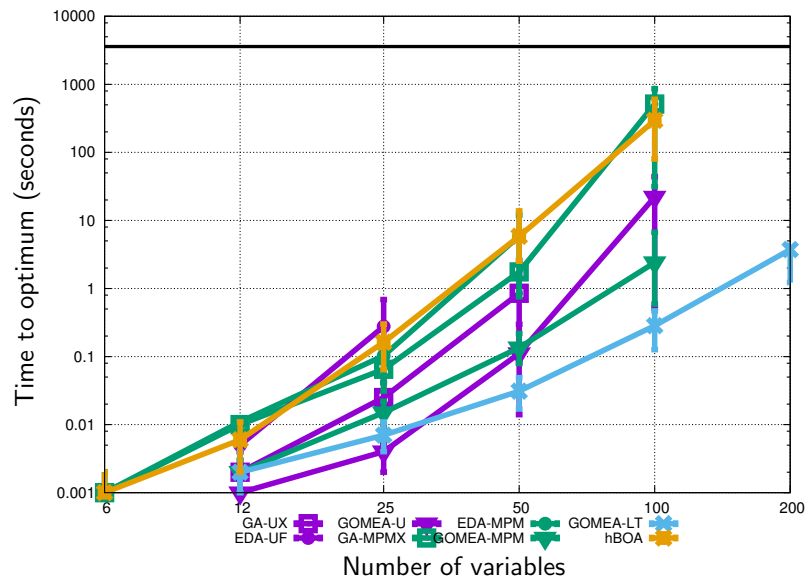
Experiments - MAX-CUT box, fully connected



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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 Trap** 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.

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 ?

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 relearned.

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 |
|---|
| <ol style="list-style-type: none"> 1 Initialize \mathcal{P} with n random solutions 2 Repeat until termination criterion met <ol style="list-style-type: none"> 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

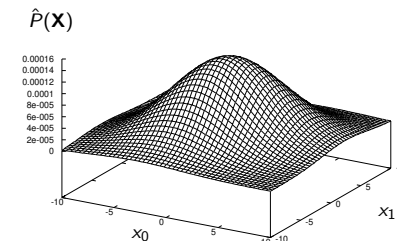
- **General concepts**
- Can be applied to **different types** of optimization problems/domains
- In second part of tutorial: focus on **other domains** than binary/integer

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

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

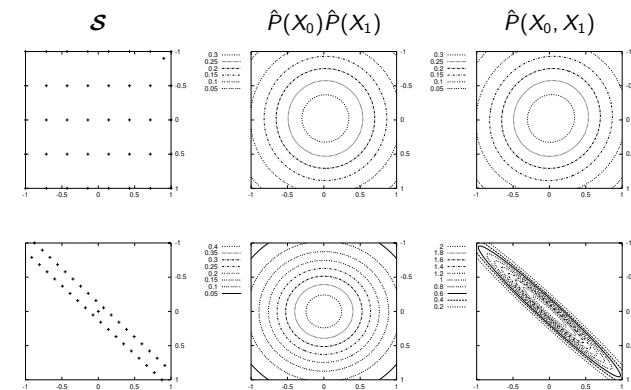
- Can **only** model **linear** dependencies

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. $\hat{P}(X_0)\hat{P}(X_1)$)

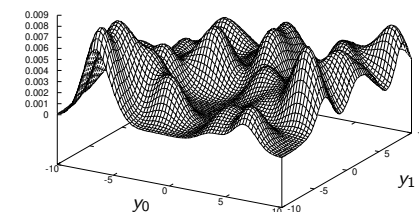


EDAs based on the Normal Distribution

- EDAs with factorized Normal Distributions (MIMIC, COMIT, Bayesian, Copula selection, Multivariate (Markov networks))
 - Bosman and Thierens (2000, 2001)
 - Larrañaga, Etxeberria, 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

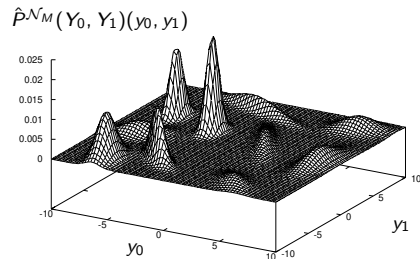
EDAs based on the Normal-kernels distribution

$$\hat{P}^{\mathcal{N}_K}(Y_0, Y_1)(y_0, y_1)$$



- 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

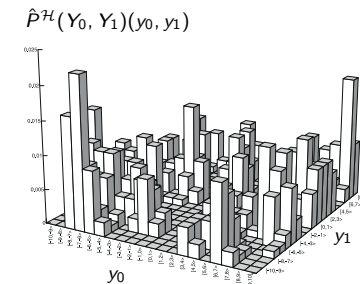


- ▶ Gallagher, Fream, and Downs (1999)
- ▶ Bosman and Thierens (2001)
- ▶ Cho and Zhang (2002)
- ▶ Ahn, Ramakrishna, and Goldberg (2004)
- ▶ Li, Goldberg, Sastry, and Yu (2007)
- ▶ Maree, Alderliesten, Thierens, and Bosman (2017)
- ▶ Trade-off between normal and normal kernels.
- ▶ Maximum-Likelihood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

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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.

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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

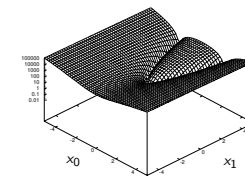
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Direct use of normal distribution

- ▶ **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

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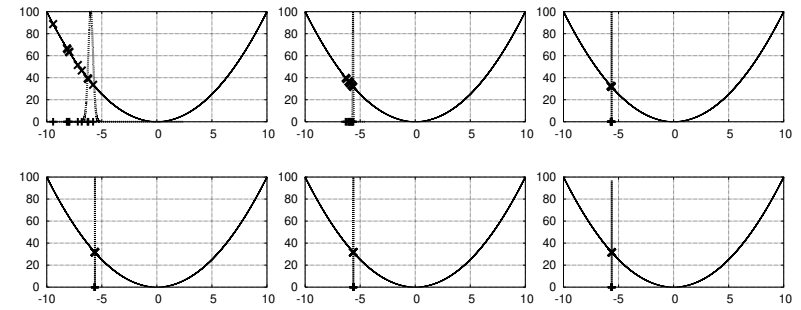
No attention for the gradient

- 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

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

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

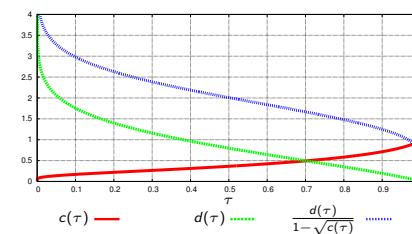
- Variance **decreases** (exponentially fast)

$$\lim_{t \rightarrow \infty} \{\hat{\sigma}(t)\} = \lim_{t \rightarrow \infty} \{\hat{\sigma}(0)c(\tau)^t\} = 0$$

- 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)

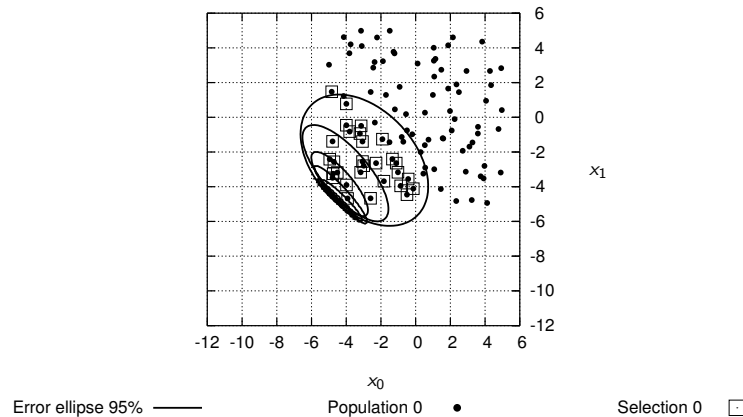


(Bosman and Grahl (2005))

Illustration on the 2-D plane function

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

Progression in first 6 generations



What is missing?

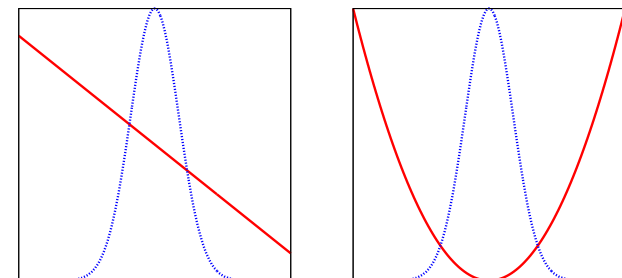
- ▶ Structure of landscape can be very complicated
- ▶ “Simple” normal distr. hardly matches global structure
- ▶ More involved distributions possible, but
 - ▶ harder, or even impossible, to estimate with ML
 - ▶ requires lots of data
- ▶ Local structure can be approximated but...
 - ▶ there is no generalization 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

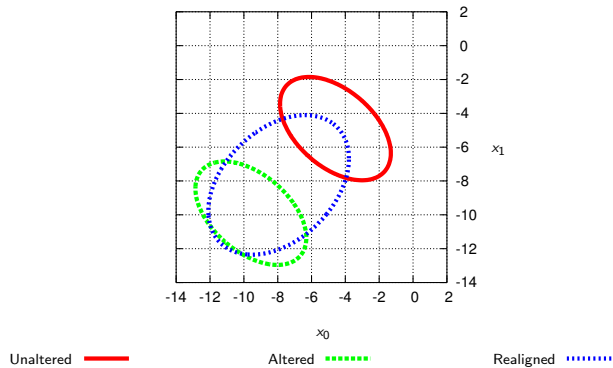


- a) far from the mean, enlarge $\hat{\Sigma}$
- b) close to the mean, do nothing

- ▶ 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



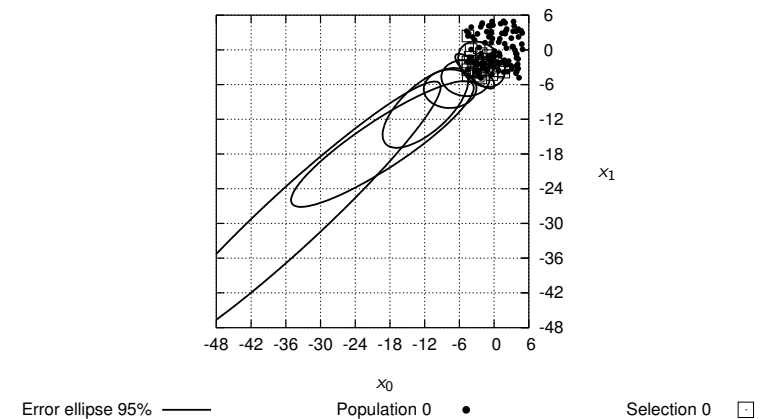
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Illustration on a 2-D slope

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

Progression in first 6 generations



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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.

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AMaLGaM, CMA-ES, NES, and RP

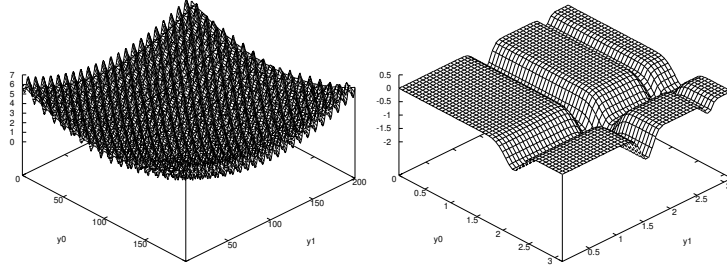
- ▶ Differences are only in how the **distribution** is obtained.
Where **AMaLGaM** uses maximum-likelihood estimates from the current generation, **CMA-ES** and **NES** base estimates on **differences** between **subsequent** generations as well as many elaborate **enhancements** (see tutorial on CMA-ES) 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

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Parameter-free Gaussian EDAs

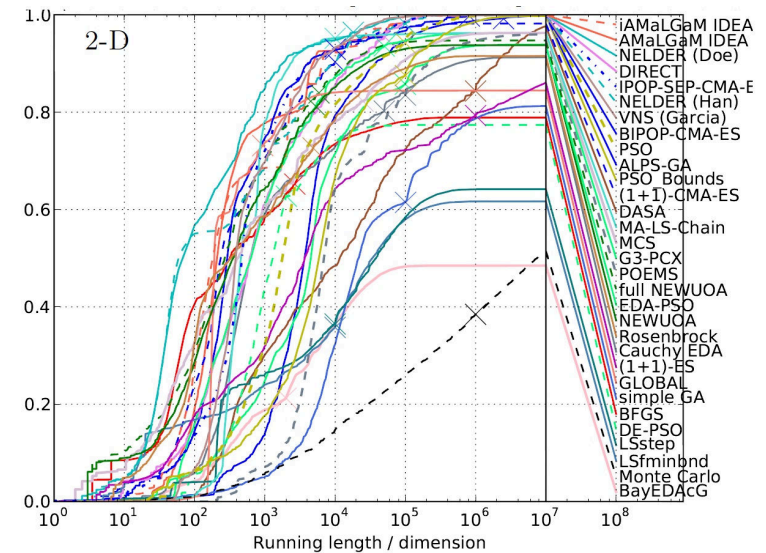
- Parameters get in the way of **ease-of-use**
- Remove** all parameters: derive and implement **guidelines**
- Restart** mechanism to increase success probability
- Typical restart scheme: increase size **exponentially**
- Works well on **Griewank** (left),
not so much on **Michalewicz** (right)
- Many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



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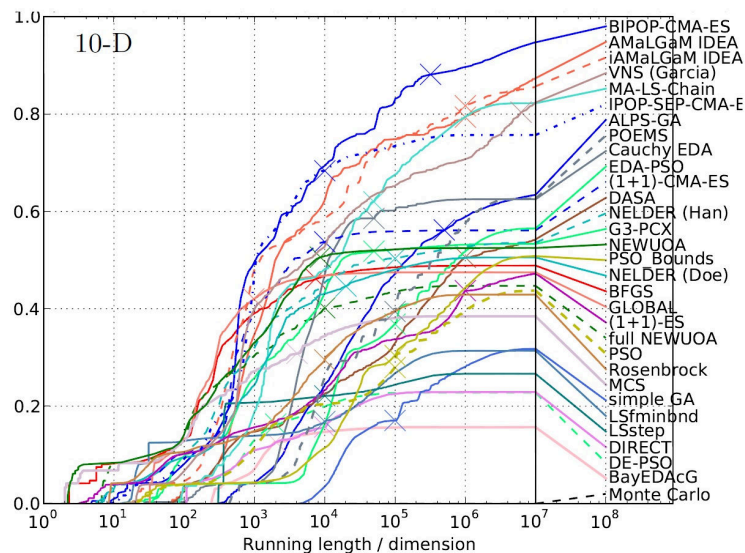
Noiseless BBOB comparison with other algorithms



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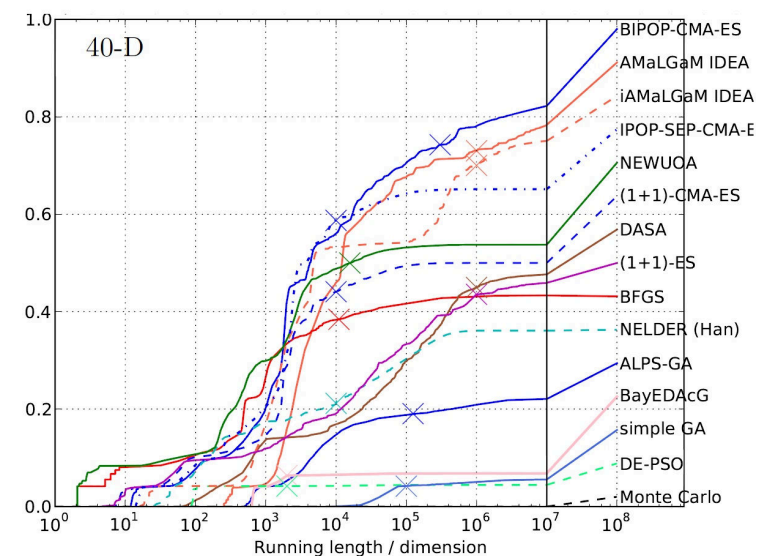
Noiseless BBOB comparison with other algorithms



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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))

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

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 | \Rightarrow | 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**: $P(\mathbf{X}) = \frac{2!1!1!2!}{5!}P(X_0, X_4)P(X_1)P(X_3, X_2)$.
- ▶ 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)

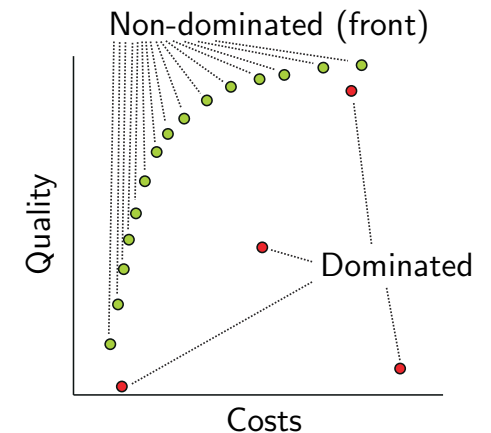
| Representation | | | Models | | Positional | | Context (Label) | | Context (Ancestral) | |
|-----------------|------------------|----------------------------|----------------|--|------------|--------|-----------------|------|---------------------|------|
| Genotype | Model | | | | Det. | Dep. | Det. | 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 |
| | N-gram | Stochastic Chomsky Grammar | AP | | 1 | | -1 | -1 | -1 | -1 |
| | | | OFGP | | -1 | -1 | 1 | | -1 | 1 |
| | | | sSG-GP | | -1 | -1 | 1 | | -1 | -1 |
| | | | vSG-GP | | -1 | 1 | | | -1 | 1 |
| Graph | Derivation Tree | Stochastic Chomsky Grammar | PEEL | | -1 | 1 | | | (-1,1) | 1 |
| | | | GMPE | | -1 | (-1,1) | 1 | | (-1,1) | 1 |
| | | | PAGE | | -1 | (-1,1) | 1 | | (-1,1) | 1 |
| | | | CRGT | | -1 | (-1,1) | 1 | | (-1,1) | 1 |
| | GNP-EDA | | CSGR | | -1 | (0,1) | 1 | | -1 | 1 |
| | | | | | | | | | | |
| | | | | | | | | | | |
| | | | | | | | | | | |
| GA like | Prefix Exp. Tree | | hACP | | -1 | | -1 | -1 | -1 | |
| | | | gACP | | 1 | | -1 | -1 | -1 | 1 |
| | | | GACP | | -1 | (0,1) | 1 | | (-1,1) | 1 |
| | | | DAP | | -1 | | 1 | | 1 | |
| | Prefix Per. Tree | | GAP | | -1 | -1 | 1 | | 1 | |
| | | | EGAP | | -1 | -1 | 1 | | 1 | |
| | | | GBAP | | -1 | -1 | 1 | | 1 | |
| | | | | | | | | | | |
| Linear Genotype | | | BAP | | 1 | | -1 | -1 | -1 | 1 |
| | | | BOAP | | 1 | | -1 | -1 | -1 | 1 |
| | | | CGP-EDA | | 1 | | -1 | -1 | -1 | 1 |
| | | | N-gramGP | | -1 | -1 | | | -1 | 1 |
| | | | AntTAG | | -1 | -1 | 1 | | -1 | -1 |
| | | | | | | | | | | |
| | | | | | | | | | | |
| | | | | | | | | | | |
| Hybrid | | | CFGR | | | | | | | |
| | | | MOSSES 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

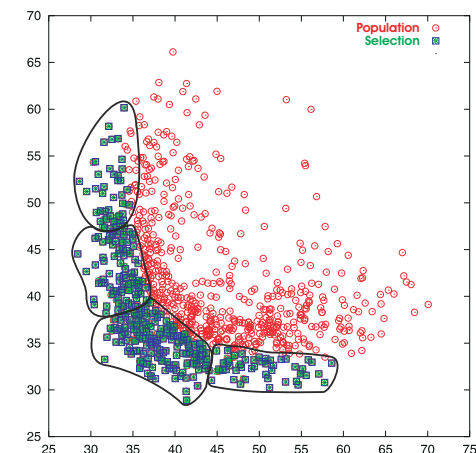
- ▶ Multiple objectives should be optimized simultaneously
- ▶ Conflicting objectives, no expression of weights
- ▶ Can't combine the objectives in a single scalar objective
- ▶ Want to present a set of promising alternatives to a decision maker
- ▶ Example: Maximize the quality and minimize the production 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

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

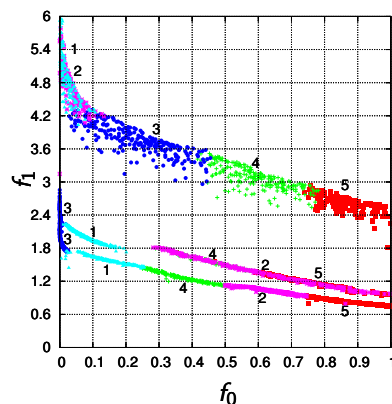
- **Cluster** solutions in **objective** space (e.g. k-means)
- Estimate a **simpler** distribution $P_{(\zeta_i, \theta_i)}(\mathcal{Z})$ in each cluster
- Set all **mixing coefficients** to $\beta_i = \frac{1}{k}$
- **Parallel**, specialized exploration **along** front

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)

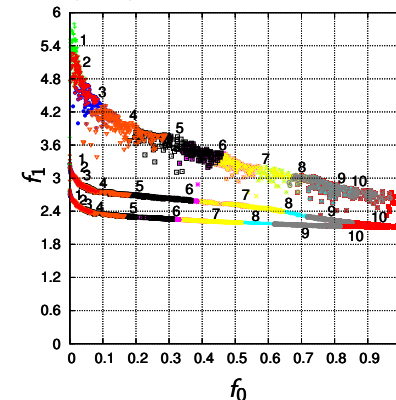
Multi-objective Model-Based Evolutionary Algorithms

- **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



Multi-objective Model-Based Evolutionary Algorithms

- **Explicit** cluster registration
- Minimize **sum of cluster distance** over all permutations of clusters in subsequent generations
 - Bosman (2010)



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)

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

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

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