GECCO 2015 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

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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)

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

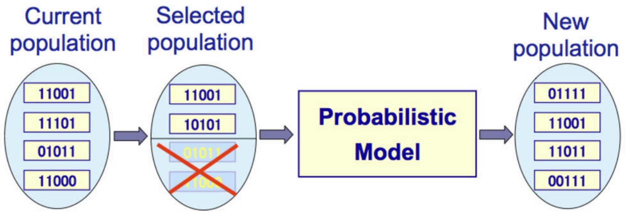
- Little known about the structure of the problem
- Clean separation optimizer from problem definition
- Easy and generally applicable

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

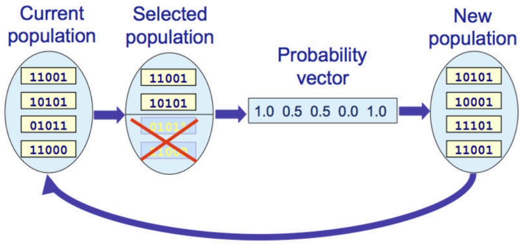
Type of Models

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

Univariate PMBGA

Model

* Model: probability vector $[p_1, \ldots, p_\ell]$ (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
000000
111111
010101
101010
000010
111000
010111
111000
000111
111111

Marginal Product (MP) FOS		
	$\hat{P}(X_0X_1X_2)$	$\hat{P}(X_3X_4X_5)$
000	0.3	0.3
001	0.0	0.0
010	0.2	0.2
011	0.0	0.0
100	0.0	0.0
101	0.1	0.1
110	0.0	0.0
111	0.4	0.4

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).

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

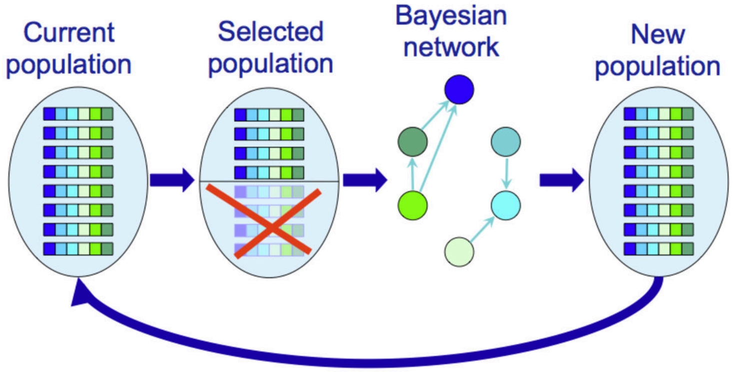
1. Start from univariate FOS:
$$\{\{0\}, \{1\}, \{2\}, \ldots, \{l-2\}, \{l-1\}\}$$
2. All possible pairs of partitions are temporarily merged:
$$\begin{gathered}\{\{0,1\}, \{2\}, \ldots, \{l-2\}, \{l-1\}\}\\ \{\{0,2\}, \{1\}, \ldots, \{l-2\}, \{l-1\}\}\\ \vdots\\ \{\{0\}, \{1,2\}, \ldots, \{l-2\}, \{l-1\}\}\\ \vdots\\ \{\{0\}, \{1\}, \{2\}, \ldots, \{l-2, l-1\}\}\end{gathered}$$
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 Netwok 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 $x_0, x_1, \ldots, x_{\ell-1}$.
- Let S be a set of all variable indices $\{0, 1, \ldots, \ell - 1\}$.
- 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:

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

where

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

- Every variable is in at least one subset in the FOS, i.e.:

$$\forall i \in \{0, 1, \ldots, l - 1\} : \left(\exists j \in \{0, 1, \ldots, |\mathcal{F}| - 1\} : i \in \mathbf{F}^j\right)$$

The Univariate Structure

- The univariate FOS is defined by:

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

- 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 varibables.

The Marginal Product Structure

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

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

- 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:

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

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

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

- Variables sometimes independent, sometimes dependent.
- ≈ 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_{F^i} and X_{F^j}: average pairwise linkage clustering (= unweighted pair group method with a arithmetic mean: UPGMA).

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

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 Algorithms (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
- Recombinative OM (ROM) and Gene-pool OM (GOM)
  - ROM is GA-like: select single solution to perform OM with
  - GOM is EDA-like: select new solution for each substructure in OM

Optimal Mixing EA (GOMEA)

- FOS linkage models specify the linked variables.
- A subset of the FOS is used as crossover mask
- Crossover is greedy: only improvements (or equal) are accepted.
- Each generation a new FOS model is build from selected solutions.
- For each solution in the population, all subsets of the FOS are tried with a donor solution randomly picked from the population
- Recombinative OM (ROM) and Gene-pool OM (GOM)
  - ROMEA: each solution uses a single donor solution.
  - GOMEA: new donor selected for each FOS subset.

Gene-pool Optimal Mixing EA

```
GOMEA()
    Pop ← InitPopulation()
    while NotTerminated(Pop)
       FOS ← BuildFOS(Pop)
       forall Sol ∈ Pop
          forall SubSet ∈ FOS
             Donor ← Random(Pop)
             Sol ← GreedyRecomb(Sol,Donor,Subset,Pop)
    return Sol

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

Recombinative Optimal Mixing EA

```
ROMEA()
    Pop ← InitPopulation()
    while NotTerminated(Pop)
       FOS ← BuildFOS(Pop)
       forall Sol ∈ Pop
          Donor ← Random(Pop)
          forall SubSet ∈ FOS
             Sol ← GreedyRecomb(Sol,Donor,Subset,Pop)
    return Sol

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

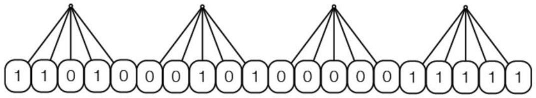
Linkage Tree Genetic Algorithm

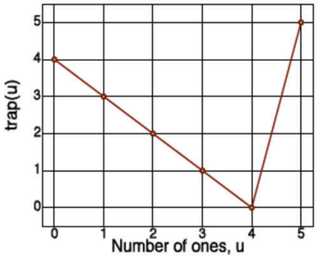
- The LTGA is an instance of GOMEA that uses a Linkage Tree as FOS model (Thierens & Bosman, 2010, 2011).
- Each generation a new hierarchical cluster tree is build.
- For each solution in population, traverse tree starting at the top.
- Nodes (= clusters) in the linkage tree used as crossover masks.
- Select random donor solution, and its values at the crossover mask replace the variable values from the current solution.
- Evaluate new solution and accept if better/equal, otherwise reject.

Deceptive Trap Function

Interacting, non-overlapping, deceptive groups of variables.

$$f_{\mathrm{DT}}(x) = \sum_{i=0}^{l-k} f_{\mathrm{DT}}^{\mathrm{sub}}\left(x_{(i,\ldots,i+k-1)}\right)$$



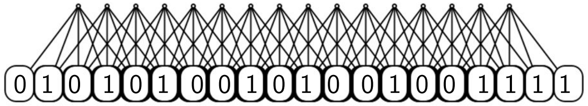


Nearest-neighbor NK-landscape

- Overlapping, neighboring random subfunctions

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

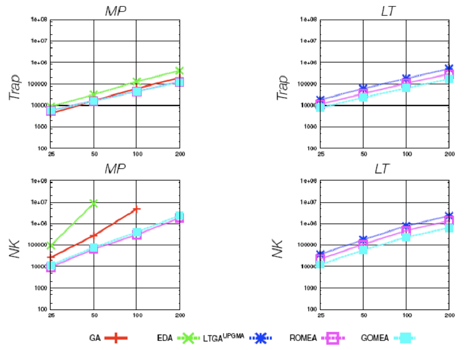
- eg. 16 subsfcts, length $k = 5$, overlap $o = 4 \Rightarrow$ stringlength $\ell = 20$



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

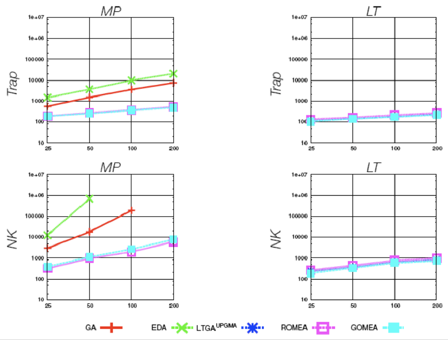
Experiments

Function Evaluations / Problem size



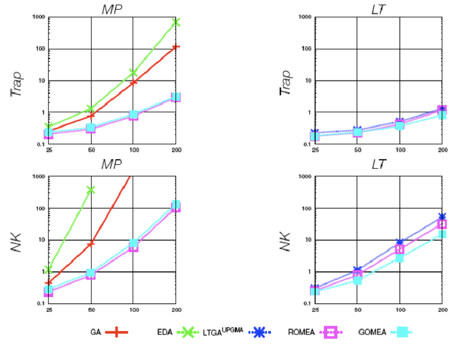
Experiments

Minimal Population Size / Problem Size



Experiments

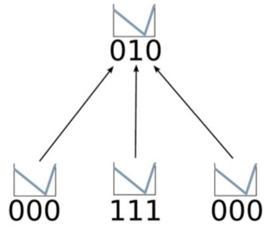
Runtime (seconds) / Problem Size



Hierarchical Trap function

HTrap

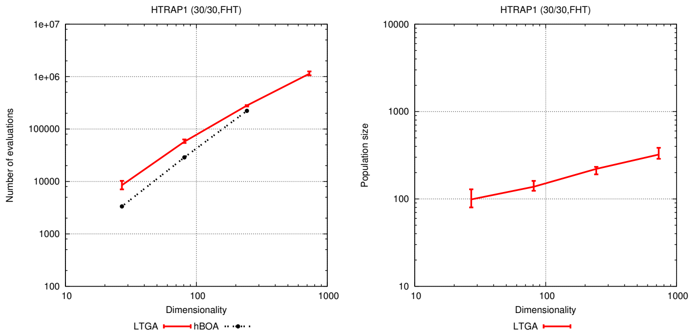
- Combine deceptive trap functions at each level in tree.
- Balanced $k-$ary tree
- Internal nodes are 0 (resp. 1) if all their children are 0 (resp. 1).
- Global optimum is all ones, yet at each level search is biased towards zeroes.



Hierarchical Trap function

HTrap: LTGA and hBOA

- HTrap problems:
  block length $k = 3$; problem lengths $27, 81, 243$ & 729.
- Number of evaluations & minimal population size.



Experiments: conclusion

- LTGA (= GOMEA with LT FOS) very efficient on Deceptive Trap function, Nearest-Neighbor NK landscape, and Hierarchical Trap function.
- Tree not always suitable linkage model: for instance spin-glasses LTGA vs. hBOA (Pelikan, Hauschild & Thierens, 2011).
- 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: no parameter values to choose (Goldman, Punch; 2014)
- 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).

Black-Box Optimization (BBO)

- Maximize $\mathfrak{F}(\mathbf{x})$, $\mathbf{x} \in \mathbb{P}$
- No prior knowledge of $\mathfrak{F}$
- Guess a new $\mathbf{x}$ and evaluate it
- Can only use previously evaluated solutions
- Minimize number of evaluations and/or actual time
- Needed when not much known about a problem (e.g. simulations)

Black-Box Optimization (BBO)

- Assumption: problems are somehow structured
- Use induction to find structure
- Exploit structure for increased efficiency
- Preferable to enumeration or iterated random sampling

Model-based optimization

- What to induce?
- Use a model that defines reasonable structures
- Induce instance of the model
- Model capacity determines bias strength

Stochastic optimization

- Random initial populations
- Randomized (but potentially structured) variation operators
- Why optimize stochastically?
- More robust against
  - Noise
  - Unreliable gradients (e.g. numerically unstable)
  - Discontinuities
  - Local optima
  - . . .

Stochastic model-based optimization

- Model: a parameterized (function) class
- Given observed solutions $\left\{\left(\mathbf{x}^i, \mathfrak{F}(\mathbf{x}^i)\right)\right\}$
  - Induction: configure the model (construct an instance)
  - Variation: generate new solution(s) from model (stochastically)
  - Repeat

Stochastic 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 $\mathcal{O}$
```

Stochastic model-based optimization

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

- Optimal Mixing Evolutionary Algorithm (OMEA)

The Estimation-of-Distribution Algorithm (EDA)

- 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

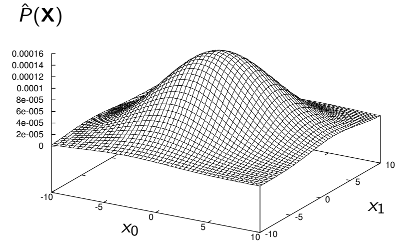
```
OMEA
1 Initialize $\mathcal{P}$ with $n$ random solutions
2 Repeat until termination criterion met
    2.1 Select subset $\mathcal{S}$ from $\mathcal{P}$
    2.2 Learn linkage model from $\mathcal{S}$
    2.3 Apply linkage-model guided optimal mixing
        to every individual in $\mathcal{P}$ to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

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

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

- 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

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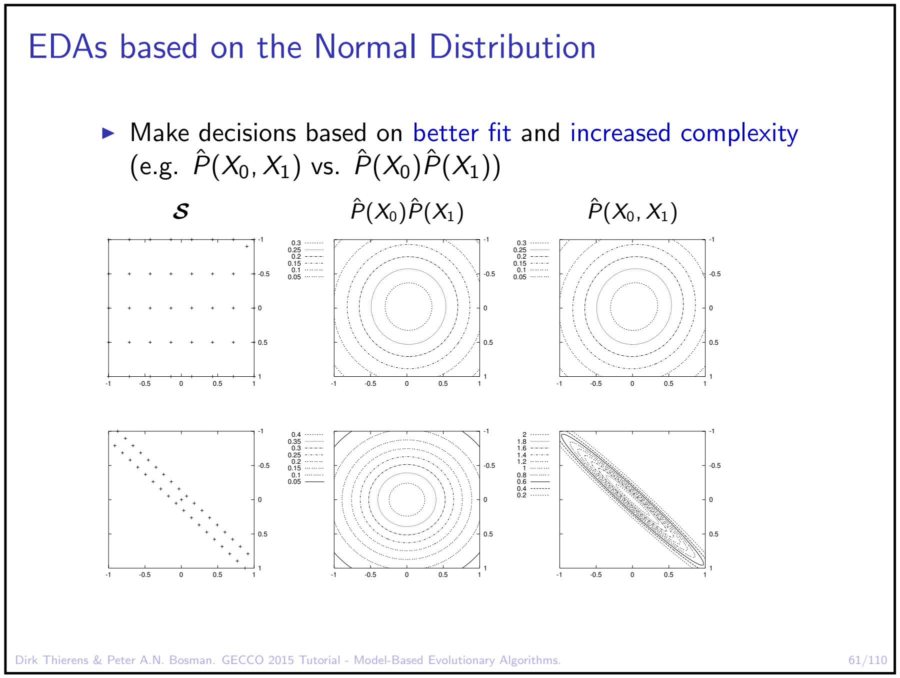
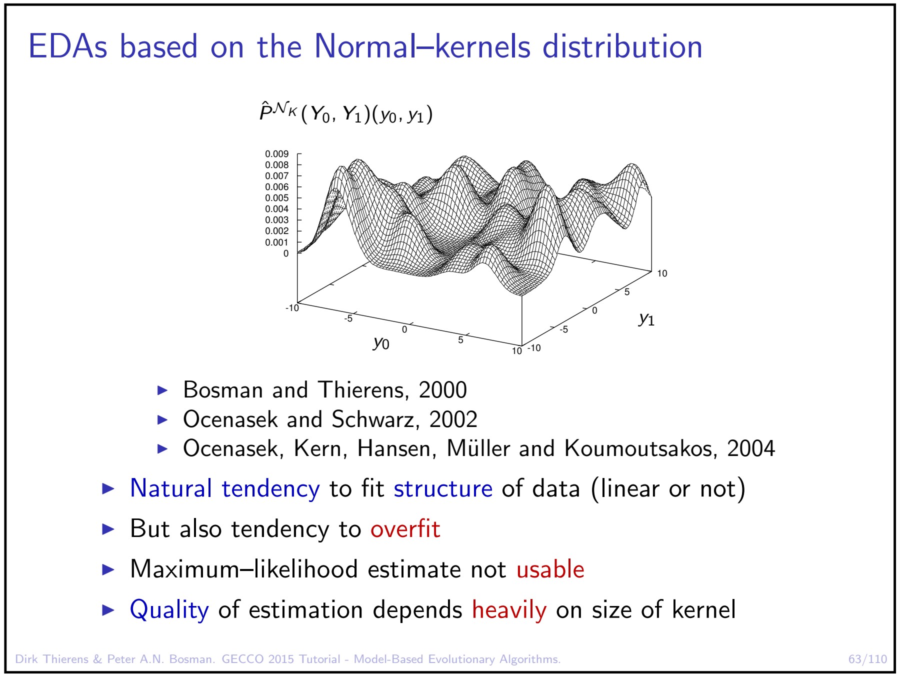


EDAs based on the Normal Distribution

- 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

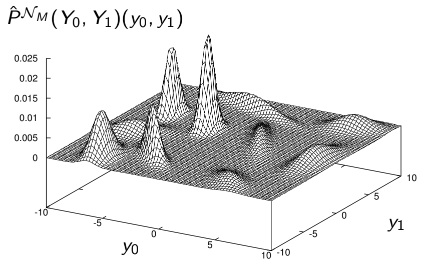
- EDAs with factorized Normal Distributions (MIMIC, COMIT, Bayesian, Copula selection, Multivariate (Markov networks))
  - Bosman and Thierens, 2000, 2001
  - Larrañaga, Etxeberria, Lozano and Peña, 2000
  - Salinas-Gutièrrez, Hernàndez-Aguirre and Villa-Diharce (2011)
  - Karshenas, Santana, Bielza 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

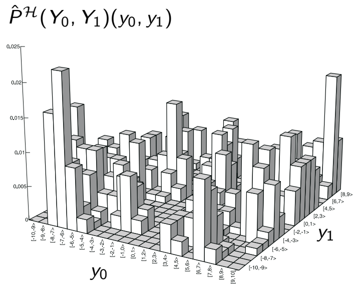
EDAs based on the Normal–mixture distribution



- Gallagher, Fream and Downs, 1999
- Bosman and Thierens, 2001
- Ahn, Ramakrishna and Goldberg, 2004

- Trade–off between normal and normal kernels.
- Requires a lot of effort to estimate with maximum likelihood (EM algorithm).
- Clustering, followed by normal–distribution estimate can be used alternatively.

EDAs based on the Histogram Distribution

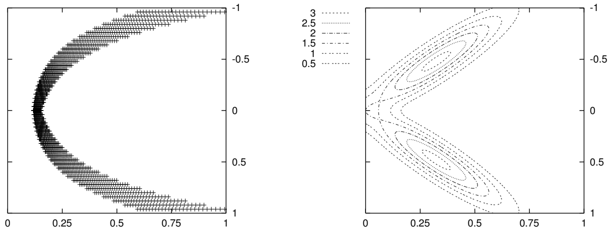


- Bosman and Thierens, 2000
- Tsutsui, Pelikan and Goldberg, 2001

- 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 the Normal–mixture Distribution Revisited

- Cluster first, then estimate (factorized) normal distribution in each cluster
  - Bosman and Thierens, 2001
  - Cho and Zhang, 2002



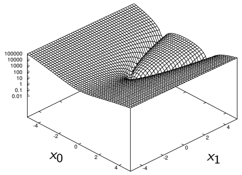
- “Reverse” also possible (more focus on seperability)
- Factorize, then estimate mixture distr. per set of variables
- Still need to way to factorize however (select pdf to base on)
  - Li, Goldberg, Sastry and Yu (2007)

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



- because...
  - Rosenbrock has narrow valley leading to minimum
  - Quickly samples no longer centered around minimum

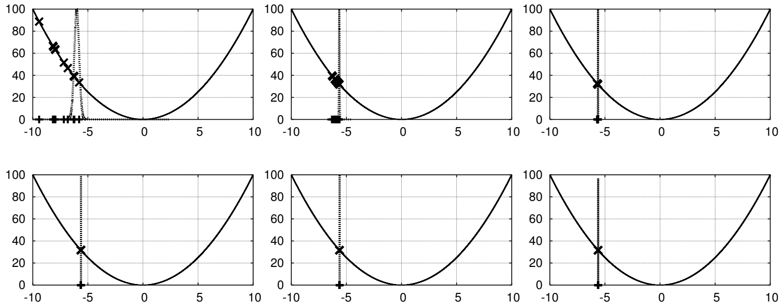
No attention for the gradient

- 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

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

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

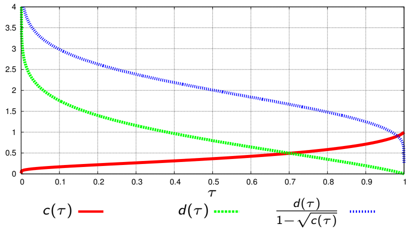
- Variance decreases (exponentially fast)

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

- This limits mean shift to a fixed factor times initial spread!

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

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

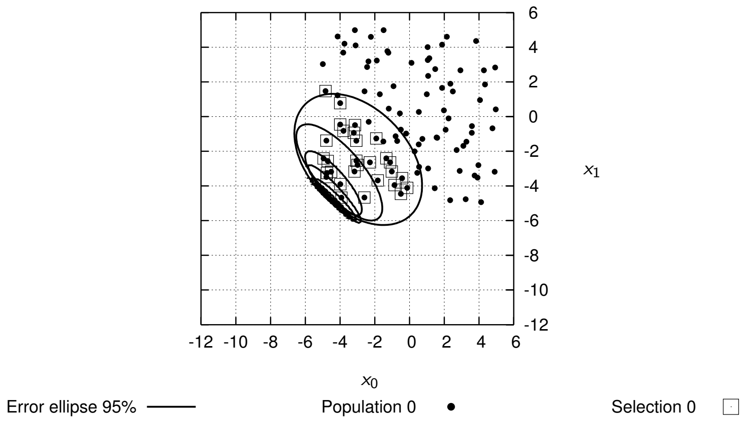


(Bosman and Grahl, 2005)

Illustration on the 2-D plane function

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

Progression in first 6 generations



What is missing?

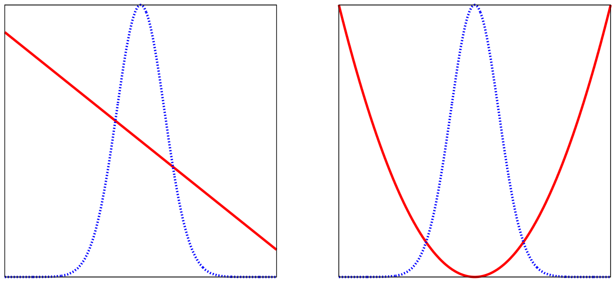
- Structure of landscape can be very complicated
- “Simple” normal distr. hardly matches global structure
- More involved distributions possible, but
  - harder, or even impossible, to estimate with ML
  - requires lots of data
- Local structure can be approximated but. . .
  - there is no generalization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

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

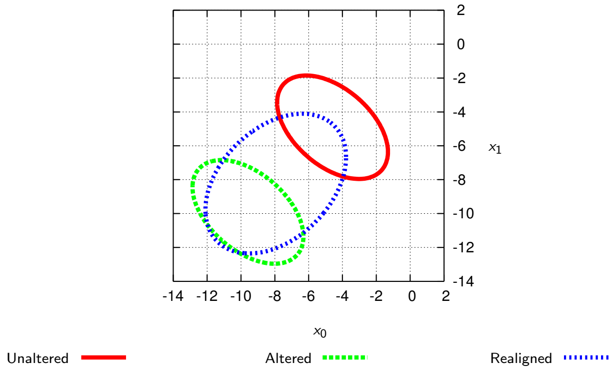
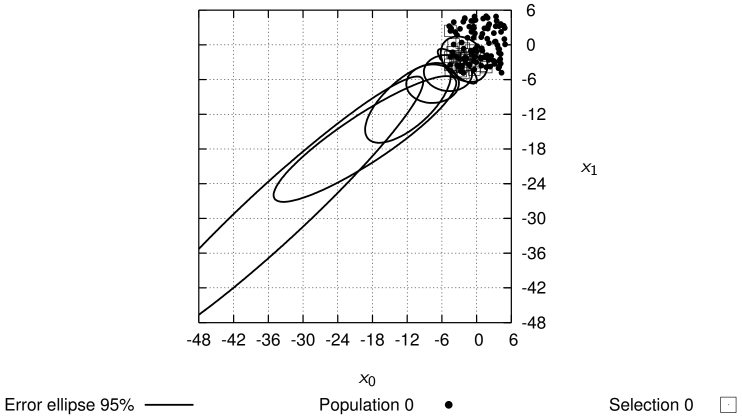


Illustration on a 2-D slope

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

Progression in first 6 generations



AMaLGaM, CMA-ES, NES, and RP

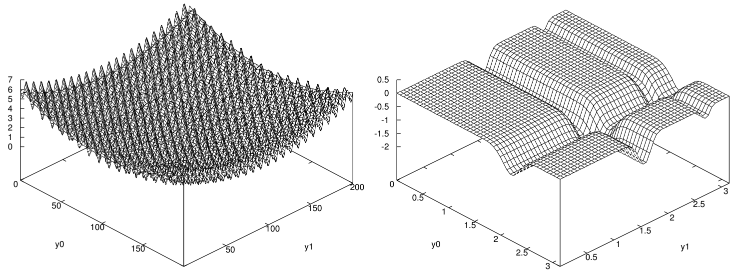
- AMaLGaM IDEA (or AMaLGaM for short)
  Adapted Maximum–Likelihood Gaussian Model Iterated Density-Estimation Evolutionary Algorithm
- Natural question:
  what is the relation to CMA-ES (Hansen, 2001), NES (Wierstra, Schaul, Peters and Schmidhuber, 2008) and the approach using Random Projections (Kabán, Bootkrajang and Durrant, 2013)?
- 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

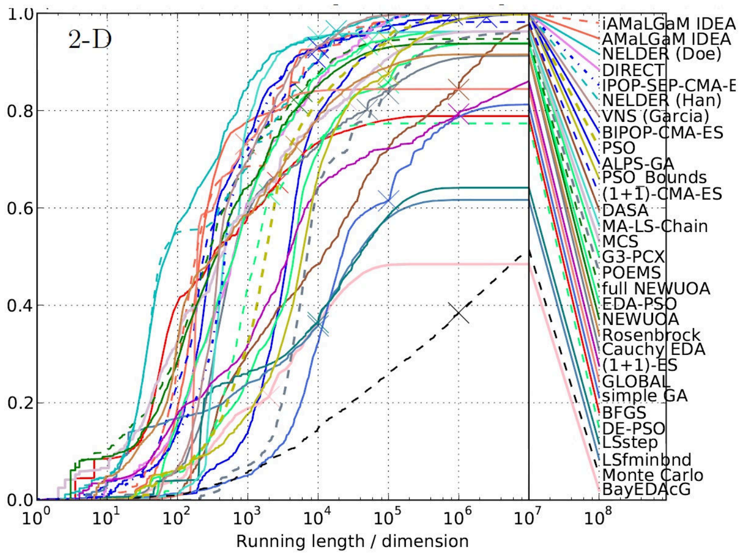
- Differences are only in how the distribution is obtained. Where AMaLGaM uses maximum-likelihood estimates from the current generation, CMA-ES and NES base estimates on differences between subsequent generations as well as many elaborate enhancements (see tutorial on CMA-ES) and RP uses ensembles of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

Parameter-free Gaussian EDAs

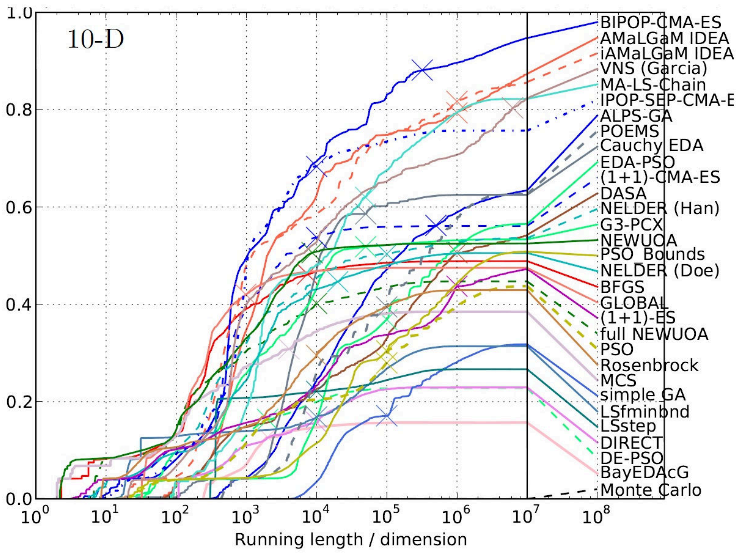
- Parameters get in the way of ease–of–use
- Remove all parameters: derive and implement guidelines
- Restart mechanism to increase success probability
- Typical restart scheme: increase size exponentially
- Works well on Griewank (left), not so much on Michalewicz (right)
- Many different schemes exist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



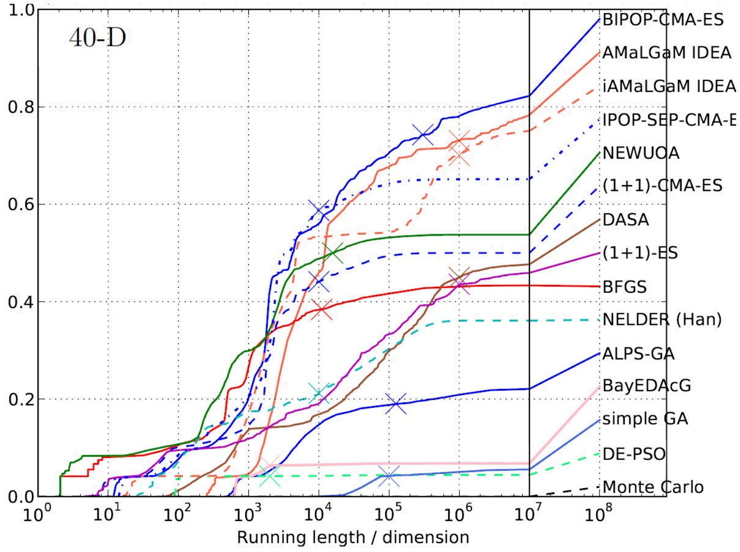
Noiseless BBOB comparison with other algorithms



Noiseless BBOB comparison with other algorithms



Noiseless BBOB comparison with other algorithms



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
0.61	0.51	0.62	0.31

⇒

3	1	0	2
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
- 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 $\rightarrow$ 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
  - 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

Tree (GP) Model-Based Evolutionary Algorithms

- Not tree-models for dependencies, but tree-models for tree-based solutions
- 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?

Tree (GP) Model-Based Evolutionary Algorithms

- 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

Tree (GP) Model-Based Evolutionary Algorithms

- 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 it limitations

Tree (GP) Model-Based Evolutionary Algorithms

- Extensions to Bayesian factorizations are also possible
- Incremental tree complexity (and model complexity) using special operators
  - Looks, Goertzel and Pennachin (2004)
  - Looks (2006)

Tree (GP) Model-Based Evolutionary Algorithms

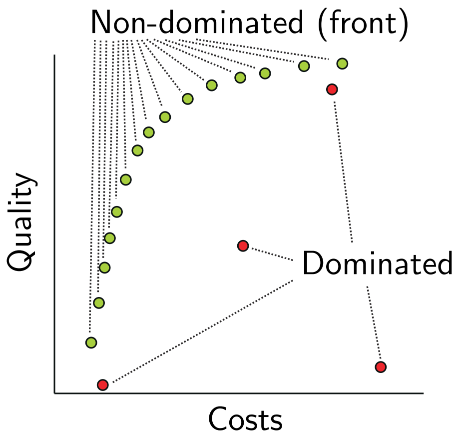
- Alternative approach: grammar-based
- Start with basic production rules
- Learning: assign probabilities to rules and increase complexity and specificity of rules using heuristics
- Sampling: select probabilistically from appropriate production rules
- Results are promising in that less function evaluations 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

Tree (GP) Model-Based Evolutionary Algorithms

- 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)

Multi-objective Model-Based Evolutionary Algorithms

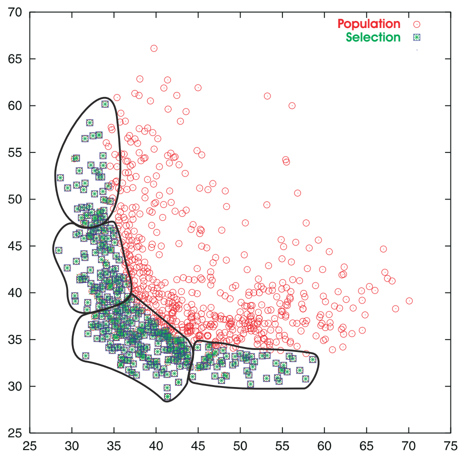
- Multiple objectives should be optimized simultaneously
- Conflicting objectives, no expression of weights
- Can't combine the objectives in a single scalar objective
- Want to present a set of promising alternatives to a decision maker
- Example: Maximize the quality and minimize the production costs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

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

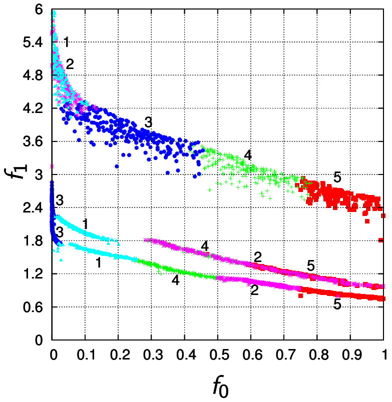
- Cluster solutions in objective space (e.g. k-means)
- Estimate a simpler distribution $P_{(\varsigma_i,\theta_i)}(\mathcal{Z})$ in each cluster
- Set all mixing coefficients to $\beta_i = \frac{1}{k}$
- Parallel, specialized exploration along front

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)

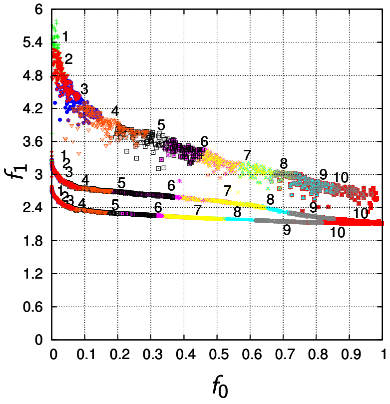
Multi-objective Model-Based Evolutionary Algorithms

- 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



Multi-objective Model-Based Evolutionary Algorithms

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



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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