Estimation-of-Distribution Algorithms for Numerical Optimization

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Introduction to EDAs

Genetic Algorithms GA vs EDA EDAs in Binary Spaces Agenda

Personal History in EDAs

State of the Art

COCO Benchmarking

Introduction to EDAs

Algorithm 1: Genetic Algorithm

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

Select \rightarrow cross over \rightarrow mutate approach

Conventional GA operators

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

Algorithm 1: Genetic Algorithm

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Interactions:

- ✓ we would like to create a new offspring by mutation
- ✓ we would like the offspring to have better, or at least the same, quality as the parent
- ✓ if we must modify x_i together with x_j to reach the desired goal (if it is not possible to improve the solution by modifying either x_i or x_j only), then x_i interacts with x_j.

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The goal of recombination operators:

✓ Intensify the search in areas which contained "good" individuals in previous iterations.

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The goal of recombination operators:

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

GA vs EDA

Algorithm 1: Genetic Algorithm
1 begin
2 Initialize the population.

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7

Incorporate offspring into the population.

Select \rightarrow cross over \rightarrow mutate approach

Algorithm 2: Estimation-of-Distribution Alg.

1 begin

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- 2 **Initialize** the population.
- 3 **while** *termination criteria are not met* **do**
 - **Select** parents from the population.
 - **Learn** a model of their distribution.
 - **Sample** new individuals.

Incorporate offspring into the population.

 $Select \rightarrow model \rightarrow sample \ approach$

GA vs EDA

Algorithm 1: Genetic Algorithm

1	begin
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Select \rightarrow cross over \rightarrow mutate approach

Explicit probabilistic model:

- ✓ principled way of working with dependencies
- ✔ adaptation ability (different behavior in different stages of evolution)

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Names:

- EDA Estimation-of-Distribution Algorithm
- **PMBGA** Probabilistic Model-Building Genetic Algorithm
- **IDEA** Iterated Density Estimation Algorithm

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EDAs in Binary Spaces

Introduction to EDAs Genetic Algorithms GA vs EDA

EDAs in Binary Spaces

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COCO Benchmarking

Usually classified on the basis of interactions complexity they can handle:

- ✓ Without interactions
 - ★ 1-dimensional marginal probabilities p(X = x)
 - ✗ PBIL, UMDA, cGA
- ✓ Pairwise interactions
 - **×** conditional probabilities p(X = x | Y = y)
 - ★ sequences (MIMIC), trees (COMIT), forrest (BMDA)
- ✓ Multivariate interactions
 - ★ conditional probabilities p(X = x | Y = y, Z = z,...)
 - ★ Bayesian networks (BOA, EBNA, LFDA)

EDAs in Binary Spaces (cont.)

Scalability of some algorithms:



Left:

✔ All bits independent

Middle:

✔ All bits weekly dependent

Right:

✓ Each 5 bits strongly dependent, but independent of all others

Agenda

- Introduction to EDAs Genetic Algorithms GA vs EDA EDAs in Binary Spaces
- Agenda
- Personal History in EDAs
- State of the Art
- COCO Benchmarking

- 1. Personal history in the field of continuous EDAs:
 - ✓ how I used increasingly complex probabilistic models
 - only to learn that they do not work and that something else is fundamentally wrong,
 - ✓ and how I returned to the roots and study the simplest algorithms.
- 2. State of the art, current research directions
 - ✓ What is the best evolutionary algorithm for numerical optimization?
 - ✓ What are its competitors?
 - ✓ What design principles do they use?
- 3. COCO: benchmark to compare continuous optimizers
 - ✓ How do we judge which algorithm is the best?
- 4. Summary and future research directions

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Personal History in EDAs

Problems we face in real-valued EDAs

Situation shortly after Y2K

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- Transformations
- Non-linear global
- transformation
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- Premature convergence
- What happens on the slope?
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State of the Art

COCO Benchmarking

- ✓ Just started PhD
- ✓ Discrete (especially binary) EDAs well explored
- ✓ Not much research done in continuous EDAs
- ✓ A lot of space for further research
- ✓ Common belief:
 - "If EDAs work well in binary domain, they should work also in continuous domain, provided some sufficiently complex and flexible model is used."

EDAs in Continuous Spaces

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2 basic approaches:

- ✓ discretize the representation and use EDA with discrete model
- ✓ use EDA with natively continuous model

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2 basic approaches:

- ✓ discretize the representation and use EDA with discrete model
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Again, classification based on the interactions complexity they can handle:

- ✓ Without interactions
 - ✗ UMDA: model is product of univariate marginal models, only their type is different
 - ★ Univariate histograms?
 - ★ Univariate Gaussian distribution?
 - ★ Univariate mixture of Gaussians?

EDAs in Continuous Spaces

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 - ★ Univariate Gaussian distribution?
 - ★ Univariate mixture of Gaussians?
- ✓ Pairwise and higher-order interactions:
 - ★ Many different types of interactions!
 - ✗ Model which would describe all possible kinds of interaction is virtually impossible to find!

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No Interactions Among Variables

Histogram UMDA: Summary

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- Linear Coordinate
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COCO Benchmarking

Continuous UMDA [Poš03]

EDA with univariate marginal product model

$$p(\boldsymbol{x}) = \prod_{d=1}^{D} p(x_d) \tag{1}$$

The following univariate models were compared:

- ✓ Equi-width histogram
- ✓ Equi-height histogram
- Max-diff histogram
- ✓ Univariate mixture of Gaussians

Features:

- ✓ the most straightforward analogy with discrete histograms
- ✓ if any bin is empty, there is no way to create new individual in that bin



2D PDF using Equi-width Histograms



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Features:

- ✓ instead of fixing the bin width, fix the number of points in each bin
- no empty bins, always possible to generate any point in the hyperrectangle



2D PDF using Equi-height Histograms



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- ✓ Max-diff histogram
- ✔ Univariate mixture of Gaussians

Features:

- ✓ place the bin boundaries to the largest gaps between the points
- no empty bins, always possible to generate any point in the hyperrectangle



2D PDF using Max-diff Histograms



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✔ Univariate mixture of Gaussians

Features:

- ✓ built by the EM algorithm (probabilistic version of k-means clustering)
- ✓ more suitable for unbounded spaces



2D PDF using Marginal Mixtures of Gaussians



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The winner of comparison:

Equi-height histogram

- ✓ precise
- ✓ non-parametric



2D PDF using Equi-height Histograms



Histogram UMDA: Summary

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Suitable when

- ✓ the search space is bounded by a hyperrectangle
- ✓ there are no strong interactions among variables

Lessons learned:

- ✓ If a separable function is rotated, UMDA does not work.
- ✓ If there are nonlinear interactions, UMDA does not work.
- ✓ EDAs with univariate marginal product models are not flexible enough!
- ✓ We need EDAs that can handle some kind of interactions!

Distribution Tree

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Distribution Tree-Building Real-valued EA [Poš04]



Distribution-Tree model

- ✓ identifies hyper-rectangular areas of the search space with significantly different densities
- ✓ can handle certain type of interactions

Distribution Tree

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Distribution-Tree model

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- ✓ can handle certain type of interactions

Lessons learned:

- ✓ Cannot model promising areas not aligned with the coordinate axes.
- ✓ We need models able to rotate the coordinate system!

[Poš04] Petr Pošík. Distribution tree–building real-valued evolutionary algorithm. In *Parallel Problem Solving From Nature — PPSN VIII*, pages 372–381, Berlin, 2004. Springer. ISBN 3-540-23092-0.

Global Coordinate Transformations

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Algorithm 3: EDA with global coordinate transformation

1 begin

2

3

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- **Initialize** the population.
- while termination criteria are not met do
 - **Select** parents from the population.
 - **Transform** the parents to a space where the variables are independent of each other.
 - Learn a model of the transformed parents distribution.
 - **Sample** new individuals in the tranformed space.
 - **Tranform** the offspring **back** to the original space.
 - **Incorporate** offspring into the population.

The individuals are

- ✓ evaluated in the original space (where the fitness function is defined), but
- ✓ bred in the transformed space (where the dependencies are reduced).

Linear Coordinate Transformations

UMDA with equi-height histogram models [Poš05]:

- ✓ No tranformation vs. PCA vs. ICA
- ✓ PCA and ICA are used to find a suitable rotation of the space, not to reduce the space dimensionality



Different results: the difference does not matter.



Different results: the difference matters!

Linear Coordinate Transformations

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Different results: the difference does not matter.



Different results: the difference matters!

Lessons learned:

- ✓ The global information extracted by linear transformations was often not useful.
- ✓ We need non-linear transformations or local transformations!!!

[[]Poš05] Petr Pošík. On the utility of linear transformations for population-based optimization algorithms. In *Preprints of the 16th World Congress of the International Federation of Automatic Control*, Prague, 2005. IFAC. CD-ROM.

Non-linear global transformation

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Kernel PCA as the transformation technique in EDA [Poš04]



Works too well:

- ✓ It reproduces the pattern with high fidelity
- ✓ If the population is not centered around the optimum, the EA will miss it

Non-linear global transformation

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- ✓ If the population is not centered around the optimum, the EA will miss it

Lessons learned:

- ✓ *Continuous EDA must be able to effectively move the whole population!!!*
- ✓ Is the MLE principle actually suitable for model building in EAs???
- [Poš04] Petr Pošík. Using kernel principal components analysis in evolutionary algorithms as an efficient multi-parent crossover operator. In IEEE 4th International Conference on Intelligent Systems Design and Applications, pages 25–30, Piscataway, 2004. IEEE. ISBN 963-7154-29-9.

Back to the Roots

Consider a simple EDA with the following settings:

Algorithm 4: Gaussian EDA

```
1 begin
           \{\mu^1, \Sigma^1\} \leftarrow \texttt{InitializeModel()}
2
           g \leftarrow 1
3
           while not TerminationCondition() do
4
                  \mathbf{X} \leftarrow \texttt{SampleGaussian}(\boldsymbol{\mu}^g, k \cdot \boldsymbol{\Sigma}^g)
5
                  f \leftarrow \texttt{Evaluate}(\mathbf{X})
6
                  \mathbf{X}_{sel} \leftarrow \texttt{Select}(\mathbf{X}, f, \tau)
7
                  \{\mu^{g+1}, \Sigma^{g+1}\} \leftarrow \texttt{LearnGaussian}(\mathbf{X}_{sel})
8
                  g \leftarrow g + 1
9
```

- ✓ Generational model: no member of the current population survives to the next one
- ✓ **Truncation selection**: use $\tau \cdot N$ best individuals to build the model
- ✓ Gaussian distribution: fit the Gaussian using maximum likelihood (ML) estimate

Back to the Roots

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                  g \leftarrow g + 1
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```

Gaussian distribution:

$$\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{\frac{D}{2}}|\boldsymbol{\Sigma}|^{\frac{1}{2}}} \exp\{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^{T}\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\}\$$

Maximum likelihood (ML) estimates of parameters

$$\mu_{\mathrm{ML}} = rac{1}{N} \sum_{n=1}^{N} x_n$$
, where $x_n \in \mathbf{X}_{\mathrm{sel}}$

- ✓ Generational model: no member of the current population survives to the next one
- ✓ **Truncation selection**: use $\tau \cdot N$ best individuals to build the model
- ✓ Gaussian distribution: fit the Gaussian using maximum likelihood (ML) estimate

$$\boldsymbol{\Sigma}_{\mathrm{ML}} = \frac{1}{N-1} \sum_{n=1}^{N} (\boldsymbol{x}_n - \boldsymbol{\mu}_{\mathrm{ML}}) (\boldsymbol{x}_n - \boldsymbol{\mu}_{\mathrm{ML}})^T$$

Premature convergence

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State of the Art

COCO Benchmarking

Using Gaussian distribution and ML estimation seems as a good idea... ...but it is actually very bad optimizer!!!

Two situations:

Population centered around optimum (population in the valley):

Population far away from optimum (population on the slope):

Premature convergence

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COCO Benchmarking

Using Gaussian distribution and ML estimation seems as a good idea... ...but it is actually very bad optimizer!!!

Two situations:

Population centered around optimum (population in the valley):



Population far away from optimum (population on the slope):

on the optimum

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the optimum is located

the algorithm *focuses* the population

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Two situations:

Population centered around optimum (population in the valley):



Algorithm works:

- ✓ the optimum is located
- ✓ the algorithm *focuses* the population on the optimum



- ✓ the optimum is far away
- ✓ the algorithm is not able to *shift* the population towards optimum

What happens on the slope?

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The change of population statistics in 1 generation:

Expected value:

where

$$\mu^{t+1} = E(X|X > x_{\min}) = \mu^t + \sigma^t \cdot d(\tau),$$

 $d(\tau) = \frac{\phi(\Phi^{-1}(\tau))}{\tau}.$

What happens on the slope?

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where

$$d(\tau) = \frac{\phi(\Phi^{-1}(\tau))}{\tau}.$$

Variance:

$$(\sigma^{t+1})^2 = \operatorname{Var}(X|X > x_{\min}) = (\sigma^t)^2 \cdot c(\tau),$$

where

$$c(\tau) = 1 + \frac{\Phi^{-1}(1-\tau) \cdot \phi(\Phi^{-1}(\tau))}{\tau} - d(\tau)^2.$$

What happens on the slope?

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Population statistics in generation *t*:

$$\mu^{t} = \mu^{0} + \sigma^{0} \cdot d(\tau) \cdot \sum_{i=1}^{t} \sqrt{c(\tau)^{i-1}}$$
$$\sigma^{t} = \sigma^{0} \cdot \sqrt{c(\tau)^{t}}$$

Convergence of population statistics:

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

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Geometric series

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The distance the population can "travel" in this algorithm is bounded!

Geometric series

Premature convergence!

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$$\lim_{t\to\infty}\sigma^{\iota}=0$$

The distance the population can "travel" in this algorithm is bounded!

Premature convergence!

Lessons learned:

- ✓ Maximum likelihood estimates are suitable in situations when model fits the fitness function well (at least in local neighborhood)
 - ★ Gaussian distribution may be suitable in the neighborhood of optimum.

Geometric series

- ★ Gaussian distribution is not suitable on the slope of fitness function!
- ✓ We need something different from MLE to traverse the slopes!!!

Variance Enlargement in a Simple EDA

What happens if we enlarged the MLE estimate of variance with a constant multiplier k? [Poš08]

- ✓ What is the minimal value k_{\min} ensuring that the model will not converge on the slope?
- ✓ What is the maximal value k_{max} ensuring that the model will not diverge in the valley?
- ✓ Is there a single value *k* of the multiplier for MLE variance estimate that would ensure a reasonable behavior in both situations?
- ✓ Does it depend on the type of the single-peak distribution being used?



- ✓ For Gaussian and "isotropic Gaussian", allowable *k* is hard or impossible to find.
- ✓ For isotropic Cauchy, allowable *k* seems to always exist...
 - ★ ... but this does not guarantee a reasonable behavior.

[[]Poš08] Petr Pošík. Preventing premature convergence in a simple EDA via global step size setting. In Günther Rudolph, editor, *Parallel Problem Solving from Nature – PPSN X*, volume 5199 of *Lecture Notes in Computer Science*, pages 549–558. Springer, 2008.

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Initially, high expectations:

- ✓ Started with structurally simple models for complex objective functions.
 - ✗ They did not work, partially because of the discrepancy between the complexities of the model and the function.

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Initially, high expectations:

- ✓ Started with structurally simple models for complex objective functions.
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- ✓ Used increasingly complex and flexible models.
 - ✗ Some improvements were gained, but even the most complex models did not fulfill the expectations.

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- ✓ Used increasingly complex and flexible models.
 - ✗ Some improvements were gained, but even the most complex models did not fulfill the expectations.
- ✓ Realized that a fundamental mistake was present all the time:
 - ✗ MLE principle builds models which try to reconstruct the points they were build upon.
 - ✗ This allows to focus on already covered areas, but not to shift the population to unexplored places.

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 - ✗ This allows to focus on already covered areas, but not to shift the population to unexplored places.

My current work:

- ✔ Aimed at understanding and developing principles critical for successful continuous EDAs.
 - **✗** Studying behavior on simple functions first. **✗**
 - ✗ Using simple, single-peak models so that the resulting algorithm behave (more or less) as local search procedures.

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There's something about the population:

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There's something about the population:

✓ data set forming a basis for offspring creation

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There's something about the population:

- ✓ data set forming a basis for offspring creation
- ✓ allows for searching the space in several places at once

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There's something about the population:

- ✓ data set forming a basis for offspring creation
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There's something about the population:

- ✓ data set forming a basis for offspring creation
- ✓ allows for searching the space in several places at once (replaced by restarted local search with adaptive neighborhood)

Hypothesis:

- ✓ The data set (population) is very useful when creating (sometimes implicit) global model of the fitness landscape or a local model of the neighborhood.
- ✓ It is often better to have a robust adaptive local search procedure and restart it, than to deal with a complex global search algorithm.

Preventing the Premature Convergence

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- self-adaptation of the variance [OKHK04] (let the variance be part of the chromosome)
- ✓ adaptive variance scaling when population is on the slope, ML estimate of variance when population is in the valley
- ✓ anticipate the shift of the mean and move part of the offspring in the anticipated direction
- ✓ use weighted estimates of distribution parameters
- ✓ do not estimate the distribution of selected points, but rather a distribution of selected mutation steps
- ✓ use a different principle to estimate the parameters of the Gaussian

[OKHK04] Jiří Očenášek, Stefan Kern, Nikolaus Hansen, and Petros Koumoutsakos. A mixed bayesian optimization algorithm with variance adaptation. In Xin Yao, editor, *Parallel Problem Solving from Nature – PPSN VIII*, pages 352–361. Springer-Verlag, Berlin, 2004.

Adaptive Variance Scaling

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AVS [GBR06]:

- Enlarge the ML estimate of Σ by an *adaptive* coefficient c_{AVS}
- ✓ If an improvement was not found in the current generation, we explore to much, thus decrease c_{AVS} : $c_{AVS} \leftarrow \eta^{DEC} c_{AVS}$, $\eta^{DEC} \in (0, 1)$
- ✓ If an improvement was found in the current generation, we may get better results with increased c_{AVS} : $c_{AVS} \leftarrow \eta^{INC} c_{AVS}$, $\eta^{INC} > 1$
- ✓ c_{AVS} is bounded: $1 \le c_{\text{AVS}} \le c^{\text{AVS}-\text{MIN}}$

[GBR06] Jörn Grahl, Peter A. N. Bosman, and Franz Rothlauf. The correlation-triggered adaptive variance scaling IDEA. In *Proceedings of the 8th annual conference on Genetic and Evolutionary Computation Conference – GECCO 2006*, pages 397–404, New York, NY, USA, 2006. ACM Press.

AVS Triggers

With AVS, all improvements increase c_{AVS} :

- ✓ This is not always needed, especially in the valleys.
- ✓ Trigger AVS when on slope; in the valley, use ordinary MLE.

AVS Triggers

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Correlation trigger for AVS (CT-AVS) [GBR06]:

- ✓ Compute the ranked correlation coefficient of p.d.f. values and function values, $p(x_i)$ and $f(x_i)$.
- ✓ If the distribution is placed around optimum, function values increase with decreasing p.d.f., correlation will be large. Use ordinary MLE.
- ✓ If the distribution is on a slope, correlation will be close to zero. Use AVS.

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- ✓ If the distribution is on a slope, correlation will be close to zero. Use AVS.

Standard-deviation ratio trigger for AVS (SDR-AVS) [BGR07]:

- ✓ Compute $\overline{x^{\text{IMP}}}$ as the average of all improving individuals in the current population
- ✓ If $p(\overline{x^{\text{IMP}}})$ is "low" (the improvements are found far away from the distribution center), we are probably on a slope. Use AVS.
- ✓ If $p(\overline{x^{\text{IMP}}})$ is "high" (the improvements are found near the distribution center), we are probably in a valley. Use ordinary MLE.

[GBR06] Jörn Grahl, Peter A. N. Bosman, and Franz Rothlauf. The correlation-triggered adaptive variance scaling IDEA. In *Proceedings of the 8th annual conference on Genetic and Evolutionary Computation Conference – GECCO 2006*, pages 397–404, New York, NY, USA, 2006. ACM Press.

[[]BGR07] Peter A. N. Bosman, Jörn Grahl, and Franz Rothlauf. SDR: A better trigger for adaptive variance scaling in normal EDAs. In *GECCO '07: Proceedings of the 9th annual conference on Genetic and Evolutionary Computation*, pages 492–499, New York, NY, USA, 2007. ACM Press.

Anticipated Mean Shift

Anticipated mean shift (AMS) [BGT08]:

- ✓ AMS is defined as: $\hat{\mu}^{\text{shift}} = \hat{\mu}(t) \hat{\mu}(t-1)$
- ✓ AMS is an estimate of the direction of improvement
- ✓ 100α% of offspring are moved by certain fraction of AMS: $x = x + \delta \hat{\mu}^{\text{shift}}$

- ✓ When centered around optimum, $\hat{\mu}^{\text{shift}} = 0$ and the original approach is unchanged.
- Selection must choose parent from both the old and the shifted regions to adjust Σ suitably.



[BGT08] Peter Bosman, Jörn Grahl, and Dirk Thierens. Enhancing the performance of maximum-likelihood Gaussian EDAs using anticipated mean shift. In Günter Rudolph et al., editor, *Parallel Problem Solving from Nature – PPSN X*, volume 5199 of *LNCS*, pages 133–143. Springer, 2008.

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Weighted ML Estimates

Account for the values of p.d.f. of the selected parents X_{sel} [TT09]:

✓ assign weights inversely proportional the the values of p.d.f.



Weighted (ML) estimates of parameters

$$\boldsymbol{\mu}_{\mathrm{W}} = \frac{1}{V_{1}} \sum_{i=1}^{N} w_{i} \boldsymbol{x}_{i}, \text{ where } \boldsymbol{x}_{n} \in \boldsymbol{\mathrm{X}}_{\mathrm{sel}}$$
$$\boldsymbol{\Sigma}_{\mathrm{W}} = \frac{V_{1}}{V_{1}^{2} - V_{2}} \sum_{i=1}^{N} w_{i} (\boldsymbol{x}_{i} - \boldsymbol{\mu}_{\mathrm{ML}}) (\boldsymbol{x}_{n} - \boldsymbol{\mu}_{\mathrm{ML}})^{T}$$

where

$$w_i = \frac{1}{p(x_i)}$$
$$V_1 = \sum w_i$$
$$V_2 = \sum w_i^2$$

[TT09] Fabien Teytaud and Olivier Teytaud. Why one must use reweighting in estimation of distribution algorithms. In *GECCO '09: Proceedings of the 11th Annual conference on Genetic and evolutionary computation*, pages 453–460, New York, NY, USA, 2009. ACM.

CMA-ES

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Evolutionary strategy with cov. matrix adaptation [HO01]

- ✓ $(\mu/\mu, \lambda)$ -ES (recombinative, mean-centric)
- ✓ model is adapted, not built from scratch each generation
- ✓ accumulates the successful steps over many generations

Compare:

- ✓ Simple Gaussian EDA estimates the distribution of selected individuals (left fig.)
- ✓ CMA-ES estimates the distribution of successful mutation steps (right fig.)





NES

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Natural Evolution Strategies

- ✓ based on the idea of *Fitness Expectation Maximization* (FEM) [WSPS08]
 - ★ similar to weighted ML estimation, but more general
- ✓ recent incarnation: Exponential Natural Evolution Strategies (xNES) [GSY⁺10]
- ✓ the resulting implementation of NES and its behavior is very close to the behavior of CMA-ES

- [GSY⁺10] Tobias Glasmachers, Tom Schaul, Sun Yi, Daan Wierstra, and Jürgen Schmidhuber. Exponential natural evolution strategies. In *GECCO '10: Proceedings of the 12th annual conference on Genetic and evolutionary computation*, pages 393–400, New York, NY, USA, 2010. ACM.
- [WSPS08] Daan Wierstra, Tom Schaul, Jan Peters, and Jürgen Schmidhuber. Fitness expectation maximization. In Günter Rudolph, Thomas Jansen, Simon Lucas, Carlo Poloni, and Nicola Beume, editors, *Parallel Problem Solving from Nature – PPSN X*, volume 5199 of *Lecture Notes in Computer Science*, chapter 34, pages 337–346. Springer Berlin / Heidelberg, Berlin, Heidelberg, 2008.

Optimization via Classification

Build a quadratic classifier separating the selected and the discarded individuals [PF07]



- Classifier built by modified perceptron algorithm or by semidefinite programming
- Works well for pure quadratic functions
- ✓ If the selected and discarded individuals are not separable by an ellipsoid, the training procedure fails to create a good model
- ✓ Work in progress; not solved yet



[PF07] Petr Pošík and Vojtěch Franc. Estimation of fitness landscape contours in EAs. In *GECCO '07: Proceedings of the 9th annual conference on Genetic and evolutionary computation,* pages 562–569, New York, NY, USA, 2007. ACM Press.

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- Many techniques to fight premature convergence
- ✓ Although based on different principles, some of them converge to similar algorithms (weighted MLE, CMA-ES, NES)
- ✓ Only a few sound principles; the most of them are heuristic approaches
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COCO and BBOB Expected Running Time and Its Distribution Example of comparison BBOB-2009 Final Summary and Future Trends Thanks for your attention

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Comparing Continuous Optimizers (COCO): http://coco.gforge.inria.fr/

 ✓ "… is a platform for systematic and sound comparisons of real-parameter global optimisers. COCO provides benchmark function testbeds and tools for processing and visualizing data generated by one or several optimizers."

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Black-box optimization benchmarking (BBOB) workshop:

- ✓ Held at GECCO conference in 2009 and 2010
- Organized by the COCO people
- ✓ Provides
 - ✗ benchmark functions (MATLAB/Octave, C, Java) with automatic storage of statistics,
 - ★ Python post-processing scripts for result tables and graphs,
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COCO and BBOB

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Comparing Continuous Optimizers (COCO): http://coco.gforge.inria.fr/

 ✓ "… is a platform for systematic and sound comparisons of real-parameter global optimisers. COCO provides benchmark function testbeds and tools for processing and visualizing data generated by one or several optimizers."

Black-box optimization benchmarking (BBOB) workshop:

- ✔ Held at GECCO conference in 2009 and 2010
- Organized by the COCO people
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- ✔ Benchmark functions
 - ★ 24 noiseless, 30 noisy (3 different types of noise)
 - ✗ separable, unimodal (moderate and high conditioning), multimodal (with adequate and weak global structure)

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 - ✗ separable, unimodal (moderate and high conditioning), multimodal (with adequate and weak global structure)
- ✓ Many already benchmarked algorithms to compare with!!! (Others on the way.)

COCO approach to benchmarking:

- \checkmark any incomplete algorithm can be restarted
- ✓ any restarted algorithm will eventually find a solution of the desired quality
- ✓ the expected running time (ERT) is the main measure of the algorithm efficiency
- ✓ comparisons based on empirical cumulative distribution functions (ECDF) of ERT

- ✓ set f_{target} and compare RTDs of the algorithms
- ✓ ... and add another f_{target} level ...



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This way we can aggregate RTDs of an algorithm *A* not only

- ✓ over various f_{target} levels, but also
- ✓ over different problems $\pi \in \Pi$ (!!!), of course with certain loss of information

- ✓ set f_{target} and compare RTDs of the algorithms
- ✓ ... and add another f_{target} level ...



Example of comparison

Workshop on black-box optimization benchmarking (BBOB) at GECCO conference:

all



unimodal, low cond.



unimodal, high cond.



separable



multimodal, structured



multimodal, weak structure



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Final Summary and Future Trends Thanks for your attention The page for BBOB-2009 workshop:

http://coco.gforge.inria.fr/doku.php?id=bbob-2009

A summary paper with the comparison of the 31 BBOB-2009 algorithms:

http://portal.acm.org/citation.cfm?id=1830761.1830790

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Empirical results:

- ✓ there is no best algorithm
- ✓ some are fast at the beginning, some can solve large proportion of problems in later stages
- ✓ there are algorithms which present a good compromise

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EDAs for continuous optimization:

- ✓ naive transfer of knowledge from the discrete domain does not work
- ✓ still far from perfect (many things can go wrong...)
- ✓ yet, algorithms of this class belong to the best algorithms for BBO

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Future trends:

- ✓ increasing efficiency of the current algorithms
- ✓ adaptivity (update previously used model, don't build it from scratch)
- ✓ search for general and unifying principles underlying the model building
- hybridization with global optimization methods of mathematical programming community

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Questions?