Estimation-of-Distribution Algorithms.
Continuous Domain.

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Last week. . .

Intro to EDAs

Black-box optimization

GA vs. EDA

- ✔ GA approach: select — *crossover* — *mutate*
- ✔ EDA approach: select — *model* — *sample*

EDA with binary representation

- ✔ the best possible (general, flexible) model: joint probability
  - ✘ determine the probability of each possible combination of bits
  - ✘ $2^D - 1$ parameters, exponential complexity
- ✔ less precise (less flexible), but simpler probabilistic models

Content of the lectures

Binary EDAs

- ✔ 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 $p(X = x|Y = y, Z = z, \ldots)$
  - ✘ Bayesian networks (BOA, EBNA, LFDA)

Continuous EDAs

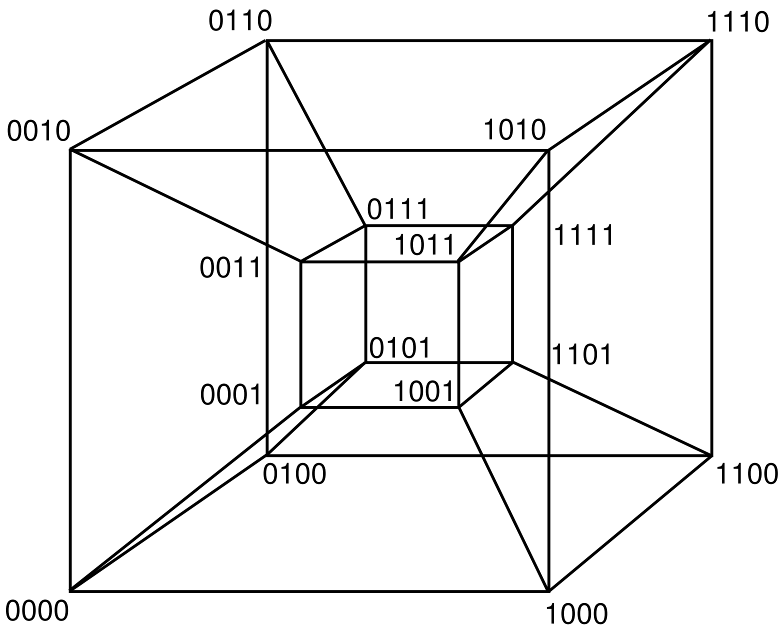
- ✔ Histograms, mixtures of Gaussian distributions
- ✔ Analysis of a simple Gaussian EDA
- ✔ Remedies for premature convergence
  - ✘ Evolutionary strategies
  - ✘ AMS, Weighting, CMA-ES, classification

Features of continuous spaces

The difference of binary and real space

Binary space

- ✔ Each possible solution is placed in one of the corners of *D*-dimensional hypercube
- ✔ No values lying between them
- ✔ Finite number of elements
- ✔ Not possible to make 2 or more steps in the same *direction*



Real space

- ✔ The space in each dimension need not be bounded
- ✔ Even when bounded by a hypercube, there are infinitely many points between the bounds (theoretically; in practice we are limited by the numerical precision of given machine)
- ✔ Infinitely many (even uncountably many) candidate solutions

Local neighborhood

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✔ . . . as a set of points that do not have the distance to a reference point larger than a threshold?

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- ✔ ...as a set of points that are closest to the reference point and their unification covers part of the search space of certain (constant) size?

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- ✔ . . . as a set of points that are closest to the reference point and their unification covers part of the search space of certain (constant) size?
  - ✘ The size of the local neighborhood rises with dimensionality of the search space
  - ✘ With increasing dimensionality of the search space the neighborhood is increasingly less local

Another manifestation of the **curse of dimensionality!**

Real-valued EDAs

Taxonomy

2 basic approaches:

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

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Again, classification based on the interactions complexity they can handle:

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  - ✘ UMDA: model is product of univariate marginal models, only their type is different
  - ✘ Univariate histograms?
  - ✘ Univariate Gaussian distribution?
  - ✘ Univariate mixture of Gaussians?

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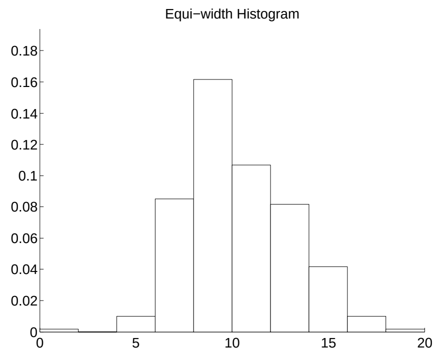
  - ✘ Univariate histograms?
  - ✘ Univariate Gaussian distribution?
  - ✘ Univariate mixture of Gaussians?
- ✔ Pairwise and higher-order interactions:
  - ✘ Many different types of interactions!
  - ✘ Model which would describe all possible kinds of interaction is virtually impossible to find!

UMDA: EDA with marginal product model $p(\boldsymbol{x}) = \prod_{d=1}^{D} p(x_d)$

Equi-width hist.



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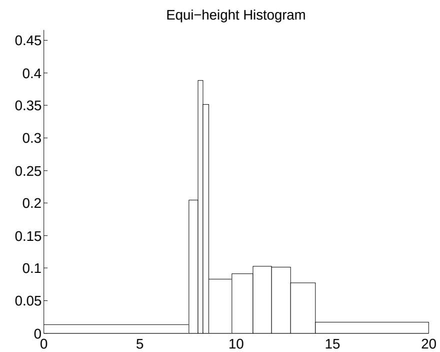
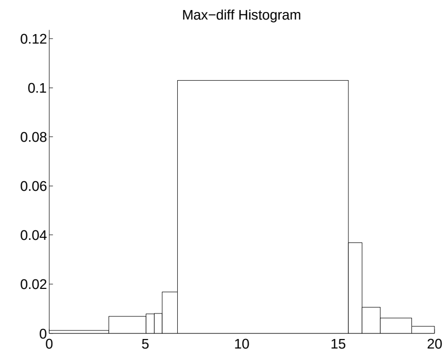
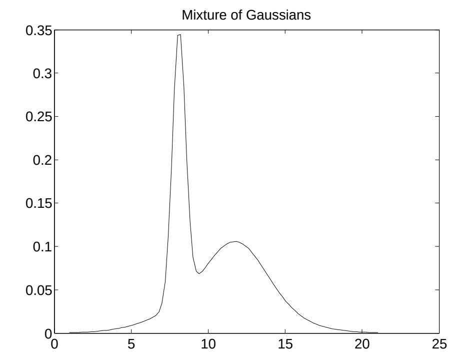


Max-diff hist.



Univar. mix. of Gaussians

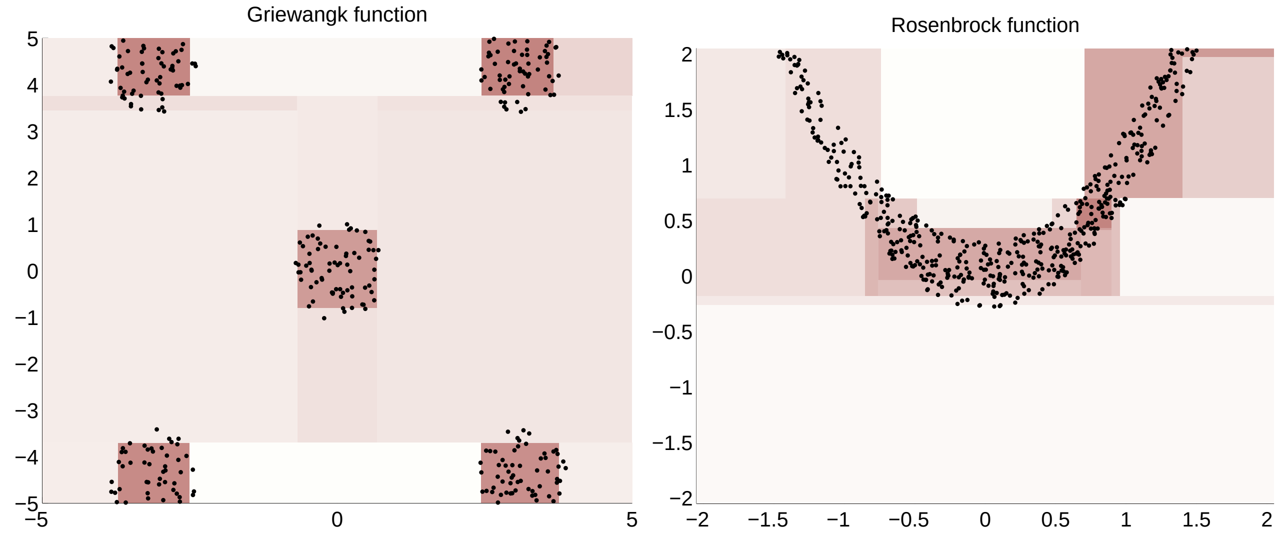


Lessons learned:

- ✔ 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

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

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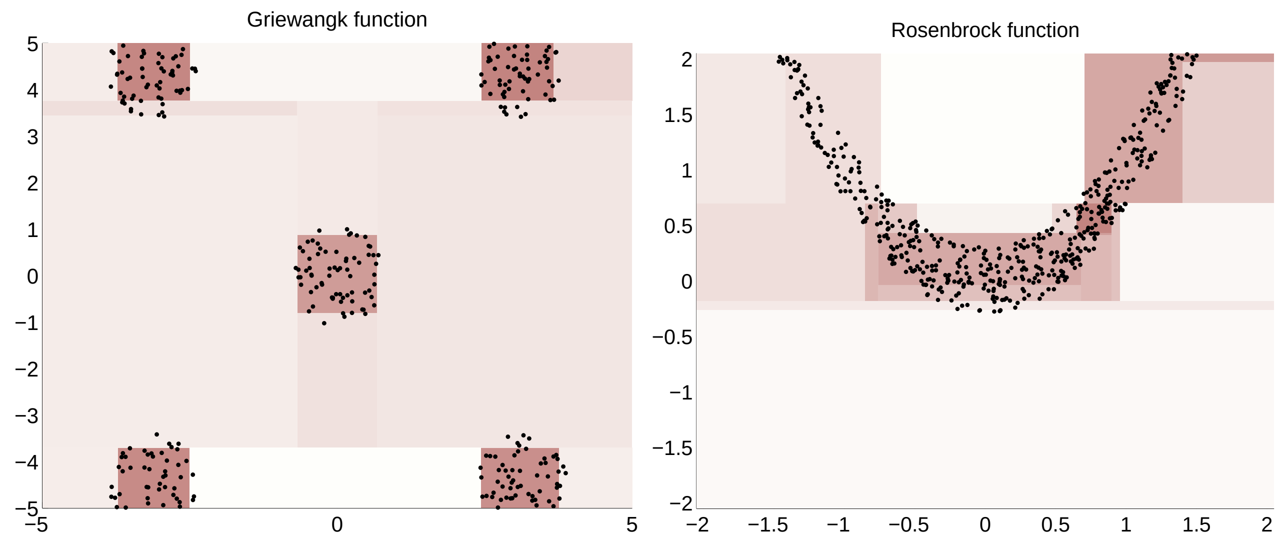

Distribution-Tree model

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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

Algorithm 1: EDA with global coordinate transformation

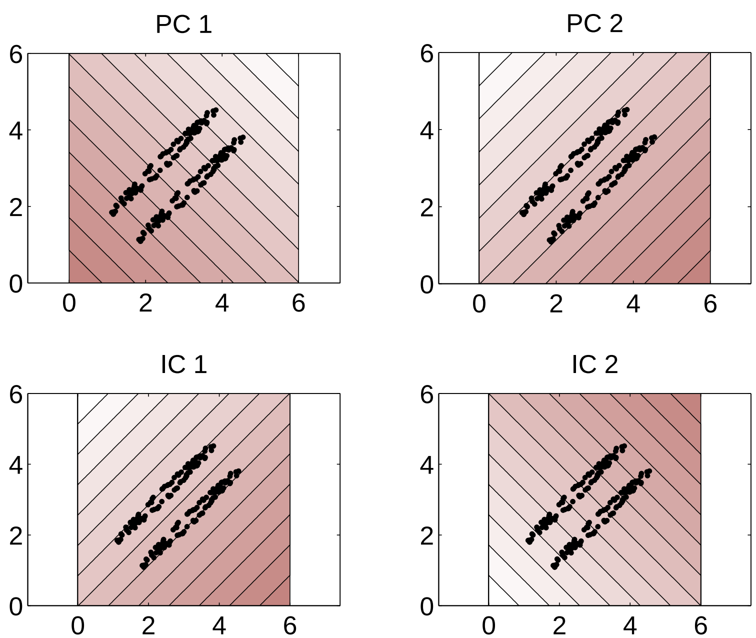
begin
  Initialize the population.
  while *termination criteria are not met* **do**
    Select parents from the population.
    Transform the parents to a space where the variables are independent of each other.
    Learn a model of the transformed parents distribution.
    Sample new individuals in 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).

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



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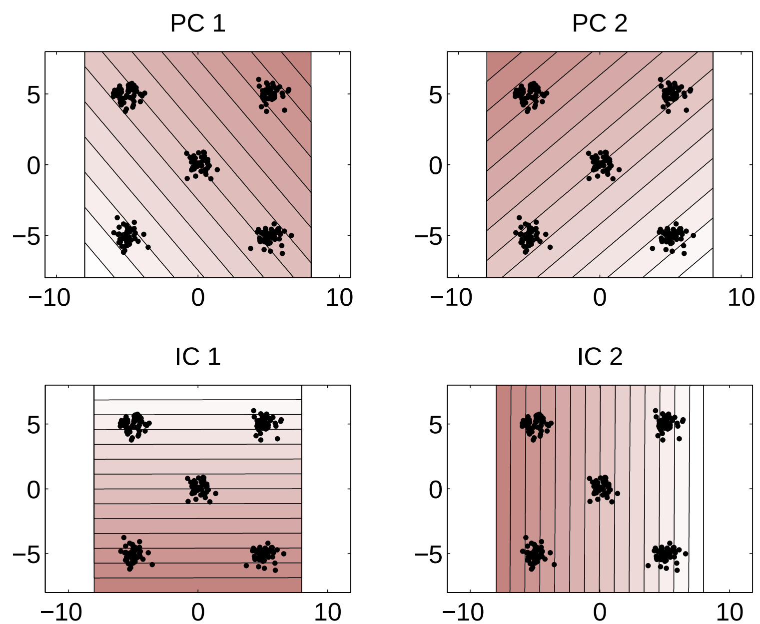

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Linear Coordinate Transformations

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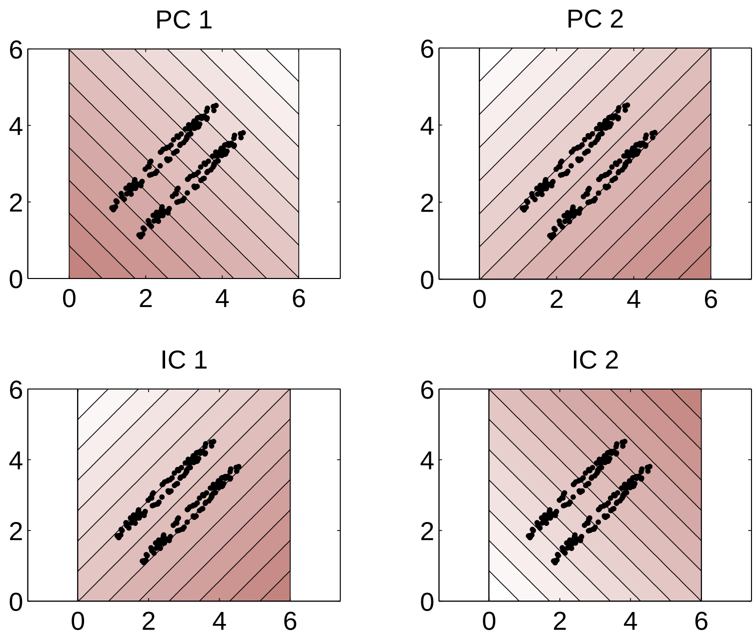

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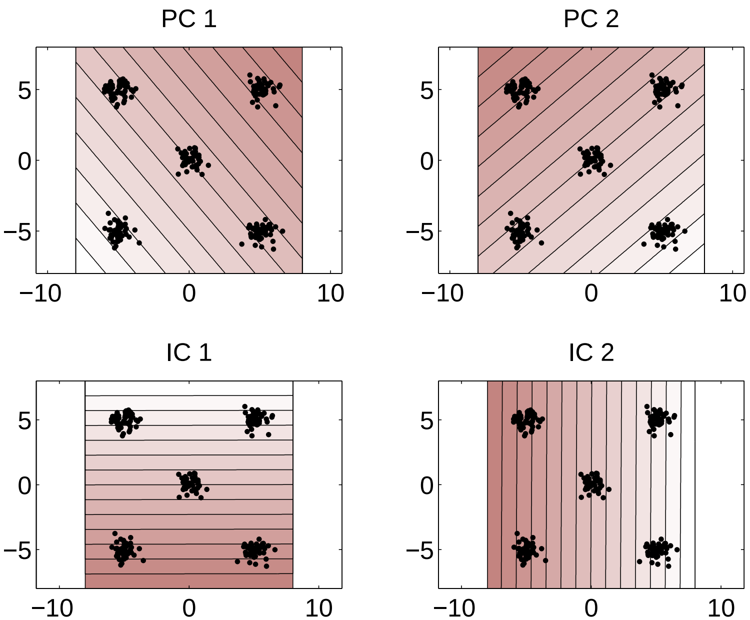


Different results: the difference matters!

Lessons learned:

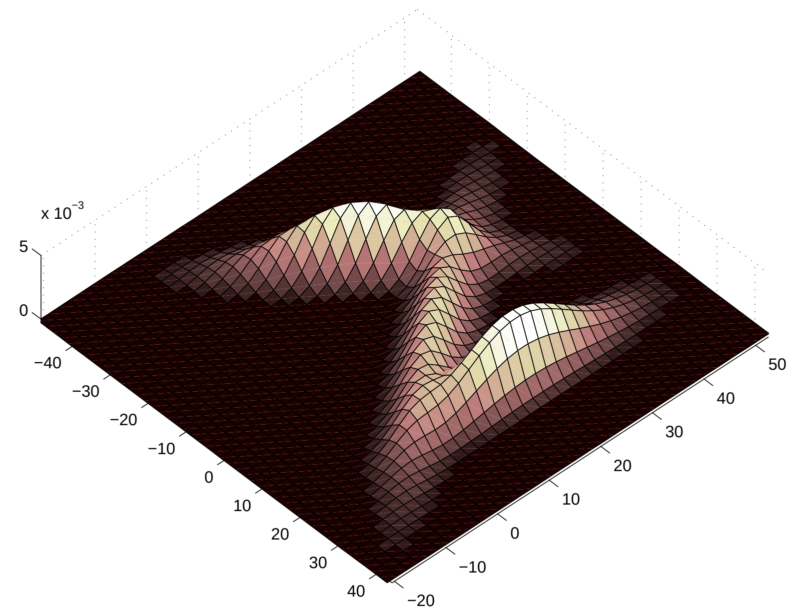
- ✔ The global information extracted by linear transformations was often not useful.
- ✔ *We need non-linear transformations or local transformations!!!*

[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.

Mixture of Gaussians

Gaussian mixture model (GMM):

$$P(x) = \sum_{k=1}^{K} \alpha_k \mathcal{N}(x|\boldsymbol{\mu}_k, \Sigma_k) \qquad (1)$$



Normalization and the requirement of positivity:

$$\sum_{k=1}^{K} \alpha_k = 1$$

$$0 \le \alpha_k \le 1$$

Model learned by EM algorithm.

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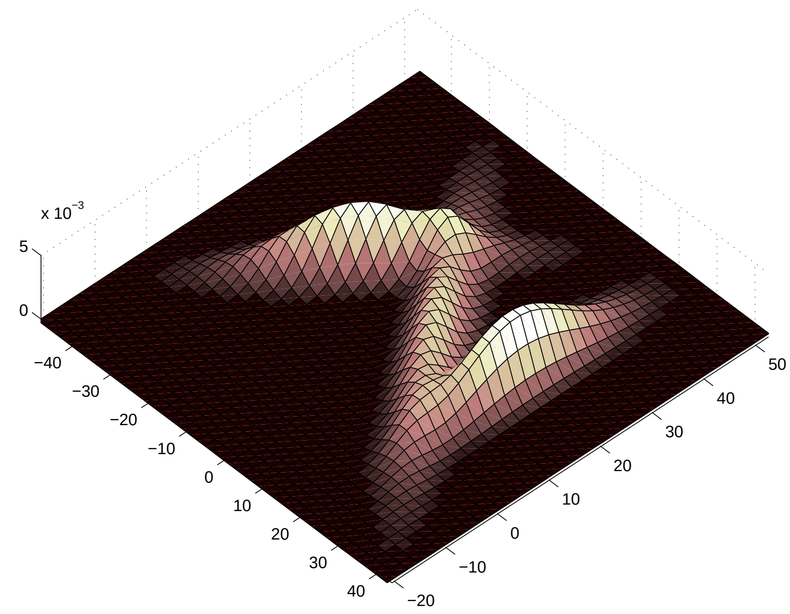
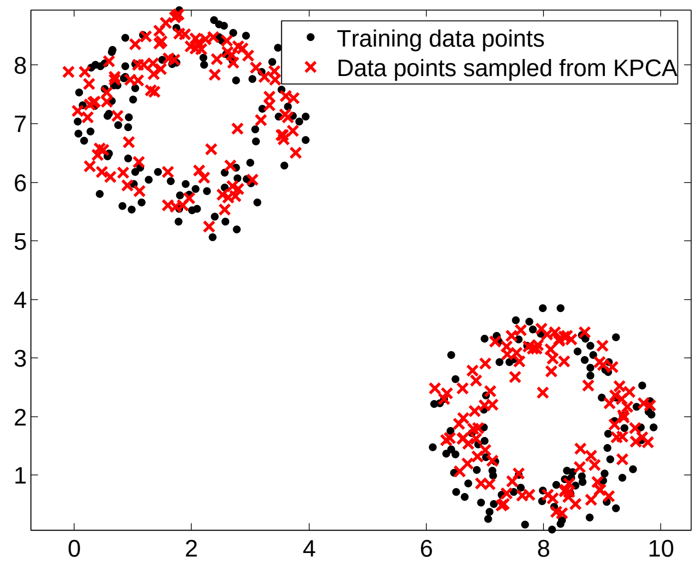


Lessons learned:

- ✔ GMM is able to model locally linear dependencies.
- ✔ We need to specify the number of components beforehand!
- ✔ If the optimum is not covered by at least one of the Gaussian peaks, the EA will miss it!

Non-linear global transformation

Kernel PCA as the transformation technique in EDA [Poš04]



Works too well:

- ✔ It reproduces the pattern with high fidelity
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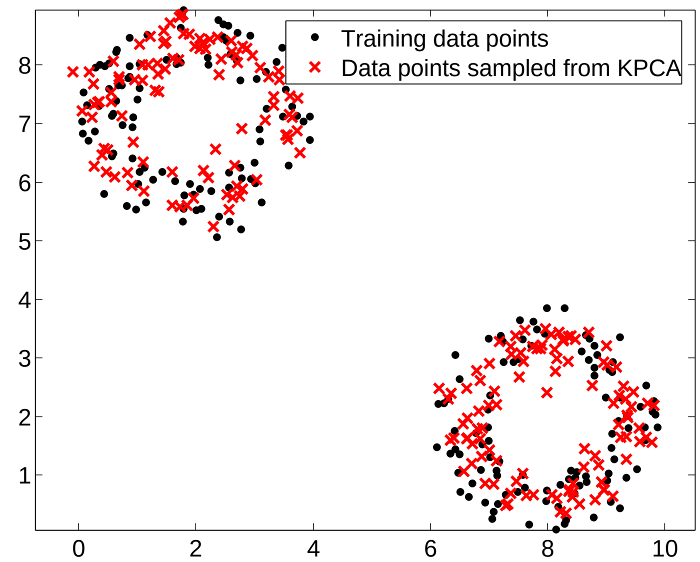

Works too well:

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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

Simple Gaussian EDA

Consider a simple EDA with the following settings:

Algorithm 2: Gaussian EDA

begin
  $\{\boldsymbol{\mu}^1, \boldsymbol{\Sigma}^1\} \leftarrow$ `InitializeModel()`
  $g \leftarrow 1$
  while not `TerminationCondition()` **do**
    $\mathbf{X} \leftarrow$ `SampleGaussian(`$\boldsymbol{\mu}^g, k \cdot \boldsymbol{\Sigma}^g$`)`
    $f \leftarrow$ `Evaluate(`$\mathbf{X}$`)`
    $\mathbf{X}_{\text{sel}} \leftarrow$ `Select(`$\mathbf{X}, f, \tau$`)`
    $\{\boldsymbol{\mu}^{g+1}, \boldsymbol{\Sigma}^{g+1}\} \leftarrow$ `LearnGaussian(`$\mathbf{X}_{\text{sel}}$`)`
    $g \leftarrow g + 1$

- ✔ **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

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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

$$\boldsymbol{\mu}_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} \boldsymbol{x}_n, \text{ where } \boldsymbol{x}_n \in \mathbf{X}_{\mathrm{sel}}$$

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

Premature convergence

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):

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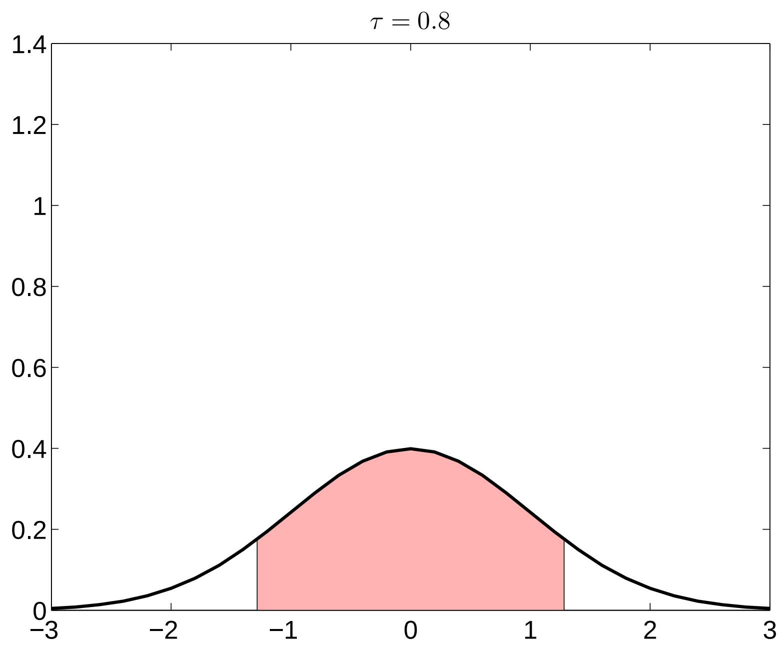

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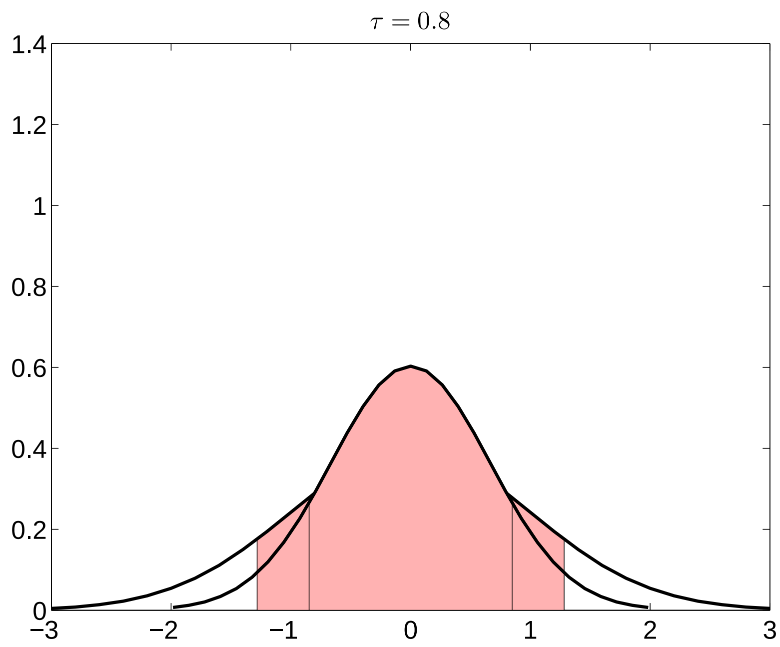

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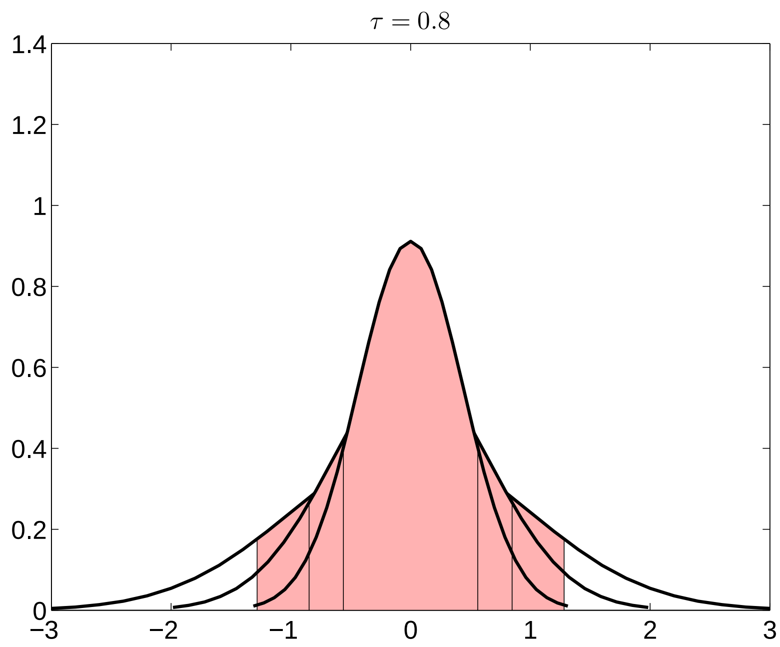

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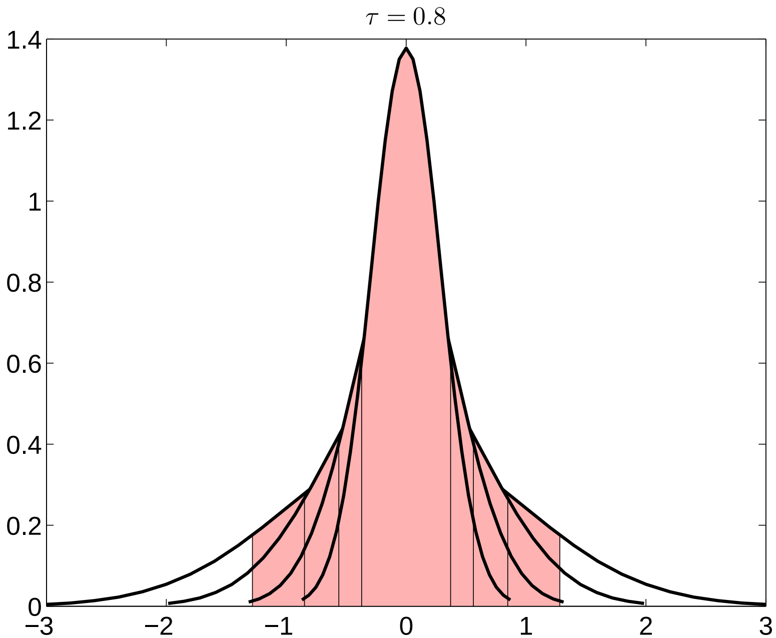

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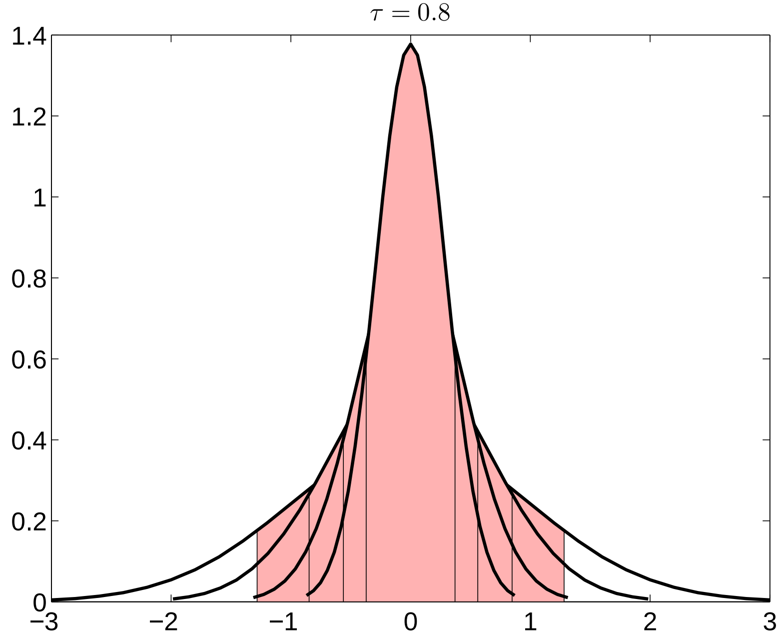

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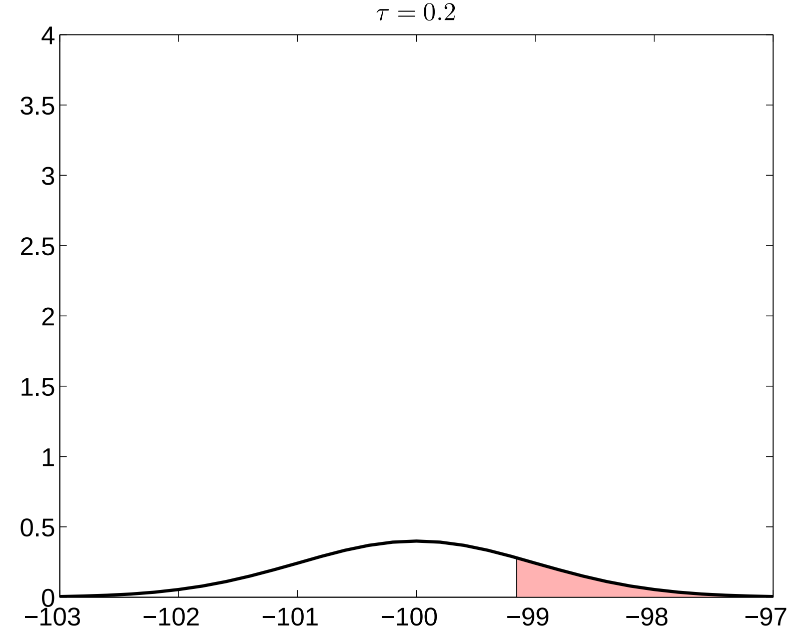

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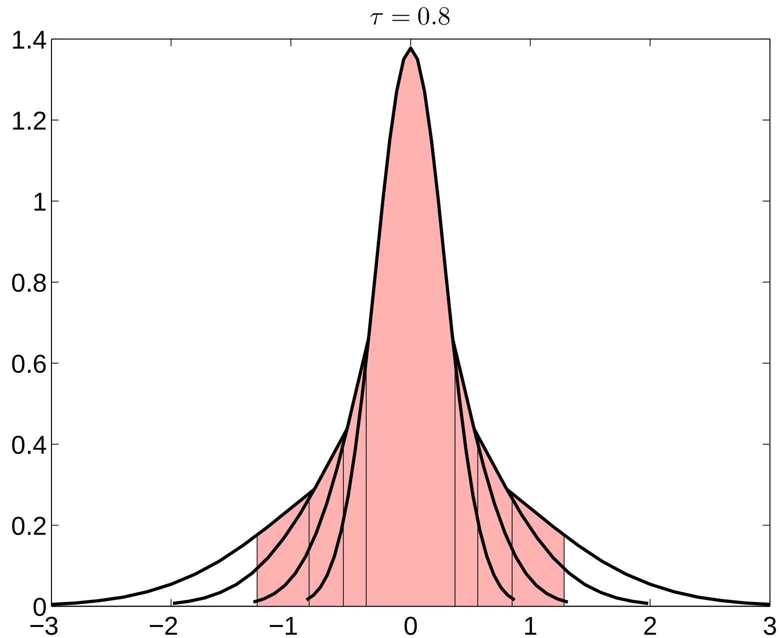

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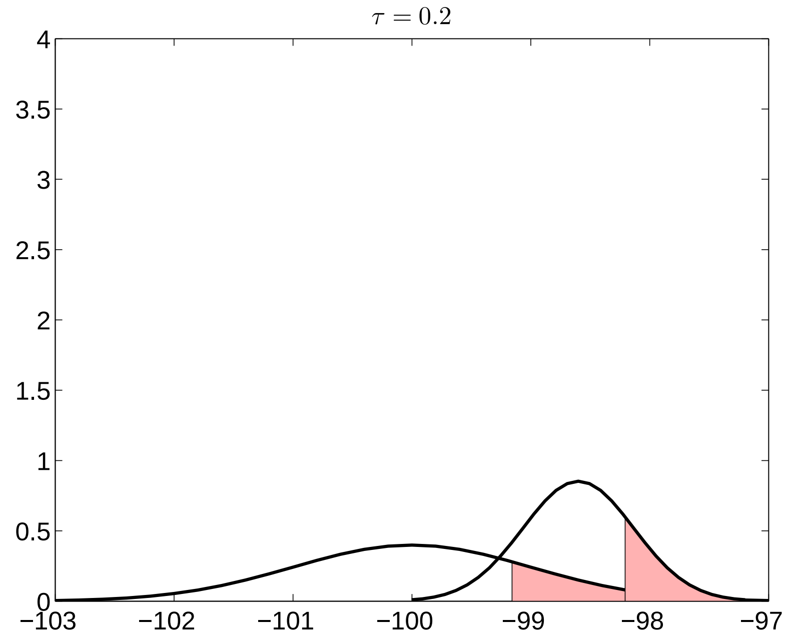

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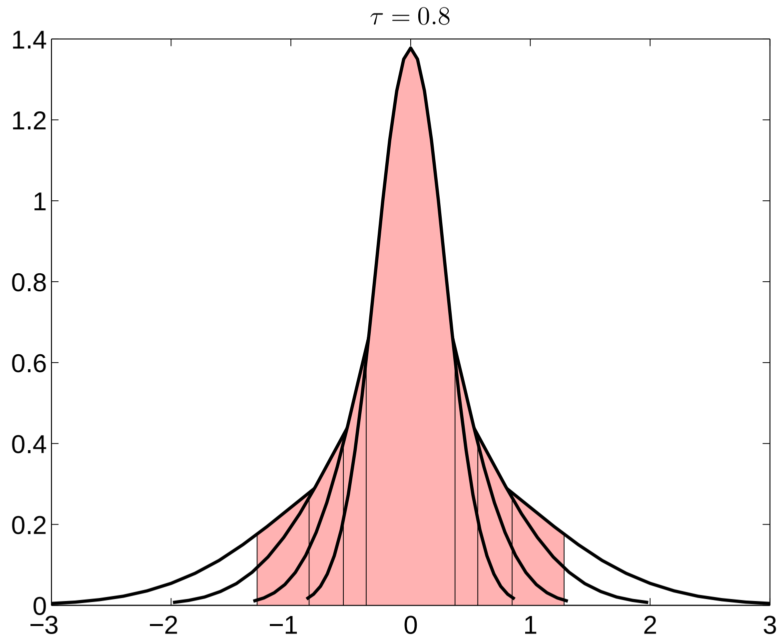

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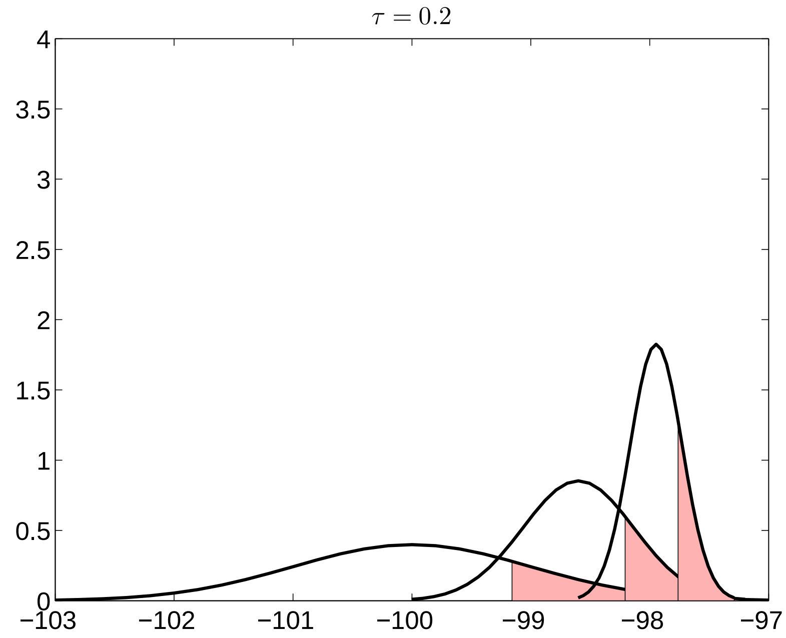

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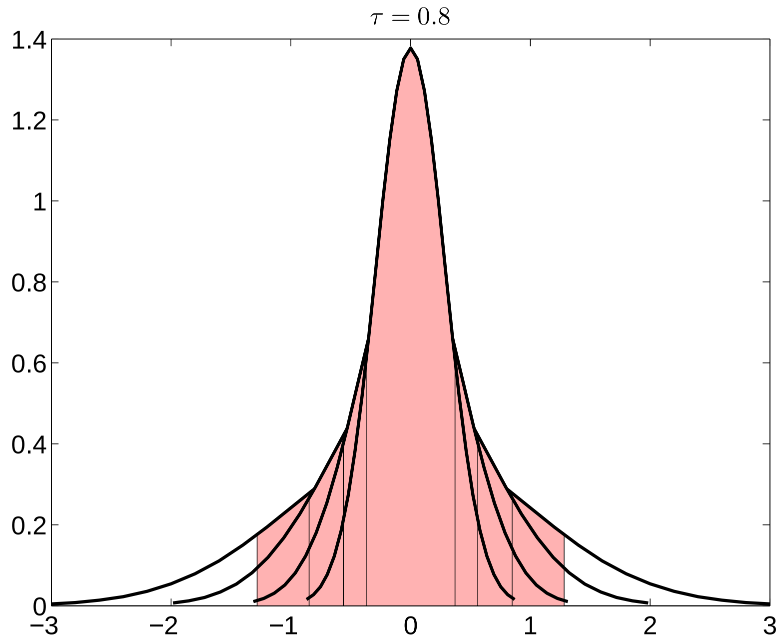

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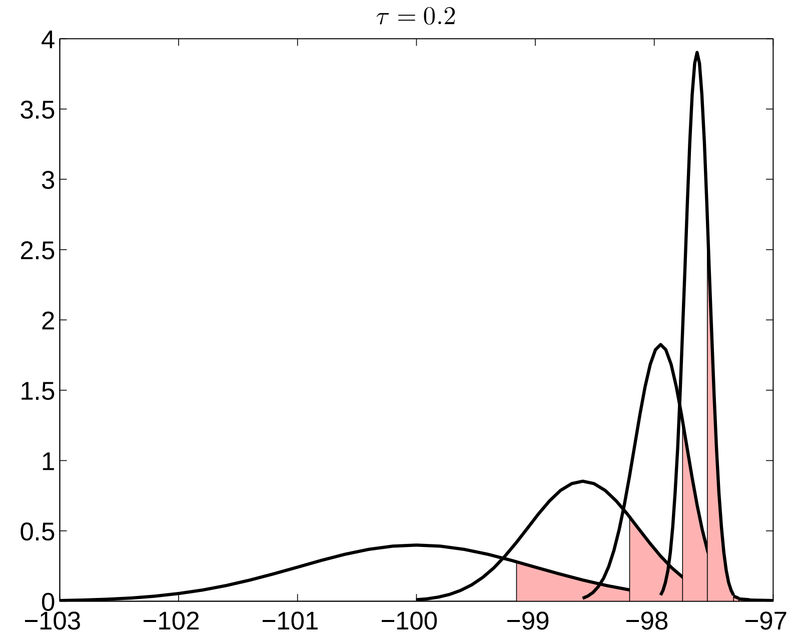

Algorithm fails:

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

What happens on the slope?

The change of population statistics in 1 generation:

Expected value:

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

where

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

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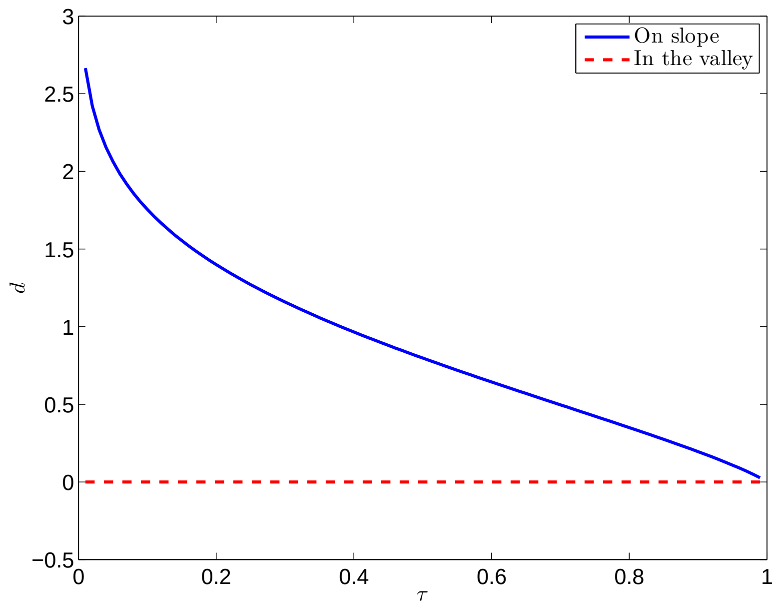

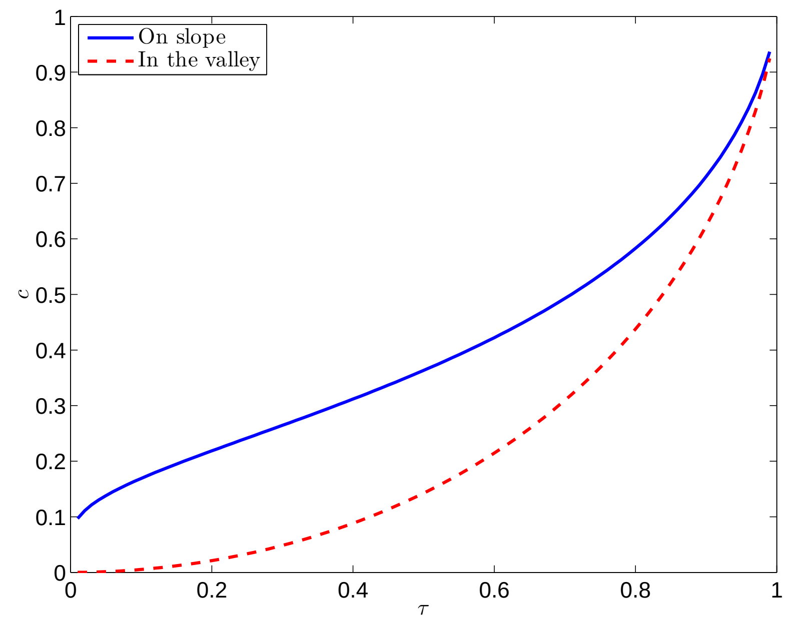

What happens on the slope (cont.)

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:

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

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

Premature convergence!

What happens on the slope (cont.)

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Geometric series

Convergence of population statistics:

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

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

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

Premature convergence!

Lessons learned:

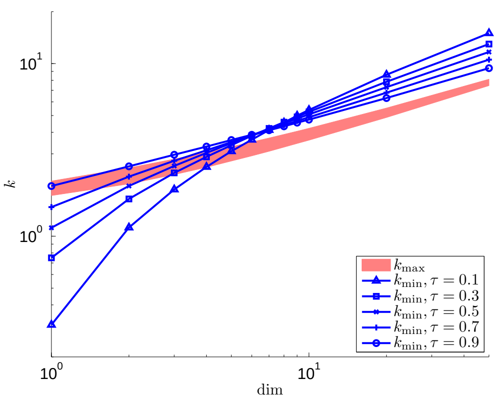
- ✔ Maximum likelihood estimates are suitable in situations when model fits the fitness function well (at least in local neighborhood)
  - ✘ Gaussian distribution may be suitable in the neighborhood of optimum.
  - ✘ Gaussian distribution is not suitable on the slope of fitness function!
- ✔ *We need something different from MLE to traverse the slopes!!!*

Variance Enlargement in a Simple EDA

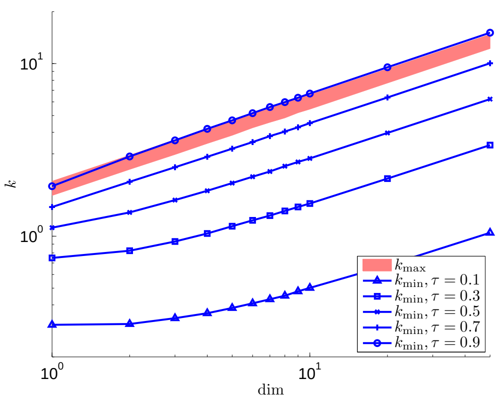
What happens if we enlarged the MLE estimate of variance with a constant multiplier k? [Poš08]

- ✔ 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?

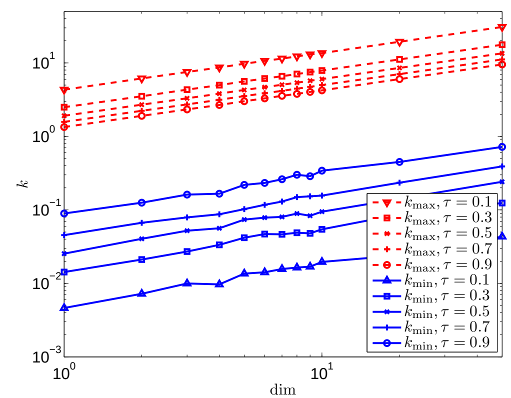
Gaussian



"Isotropic" Gaussian



"Isotropic" Cauchy



- ✔ 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.

Summary of Continuous EDAs So Far

Initially, high expectations:

- ✔ Started with structurally simple models for complex objective functions.
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- ✔ 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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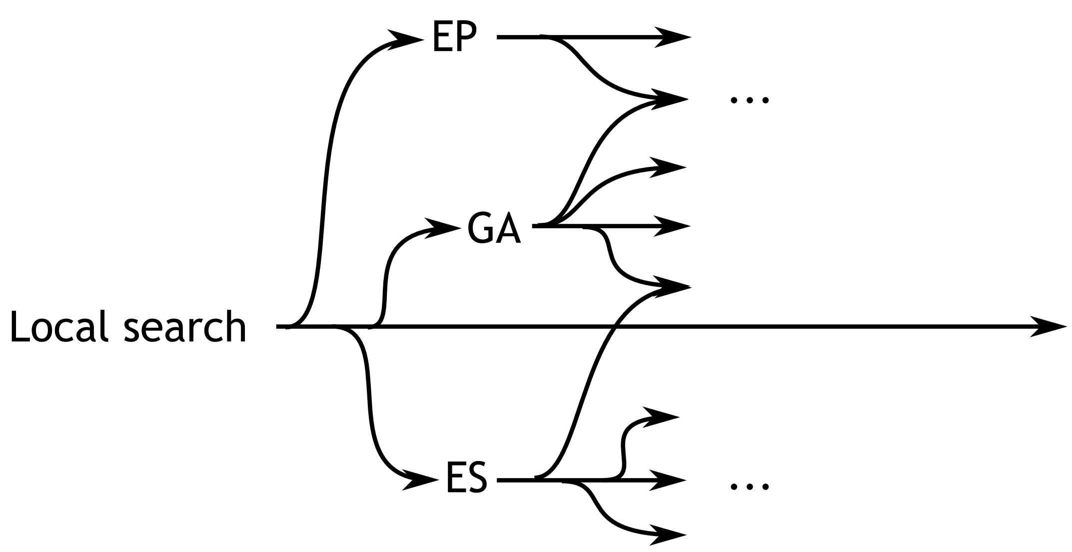
Current research directions:

- ✔ 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.

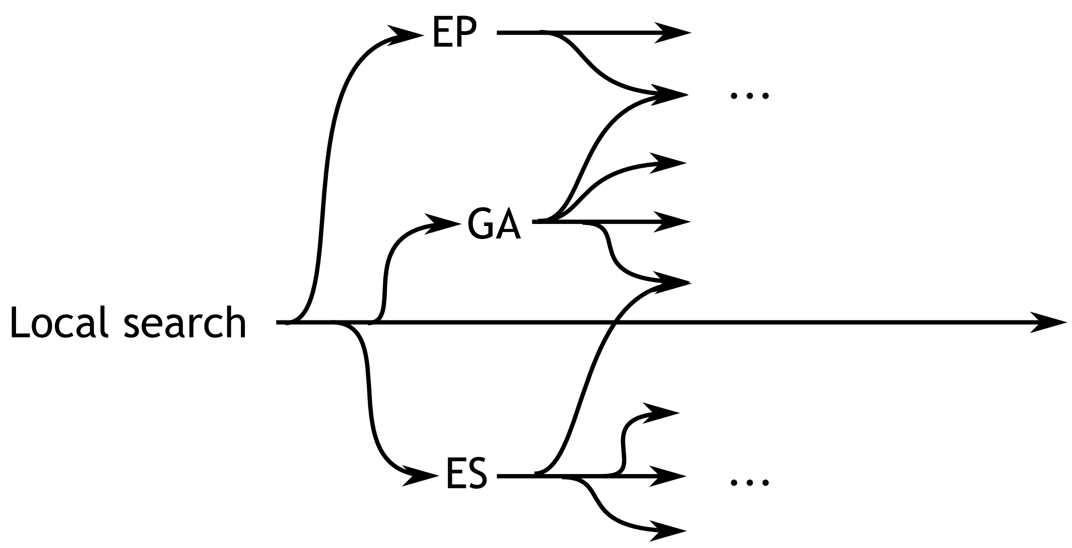
State of the Art

Current Trend: Population-based Adaptive Local Search



There's something about the population:

Current Trend: Population-based Adaptive Local Search



There's something about the population:

- ✔ data set forming a basis for offspring creation

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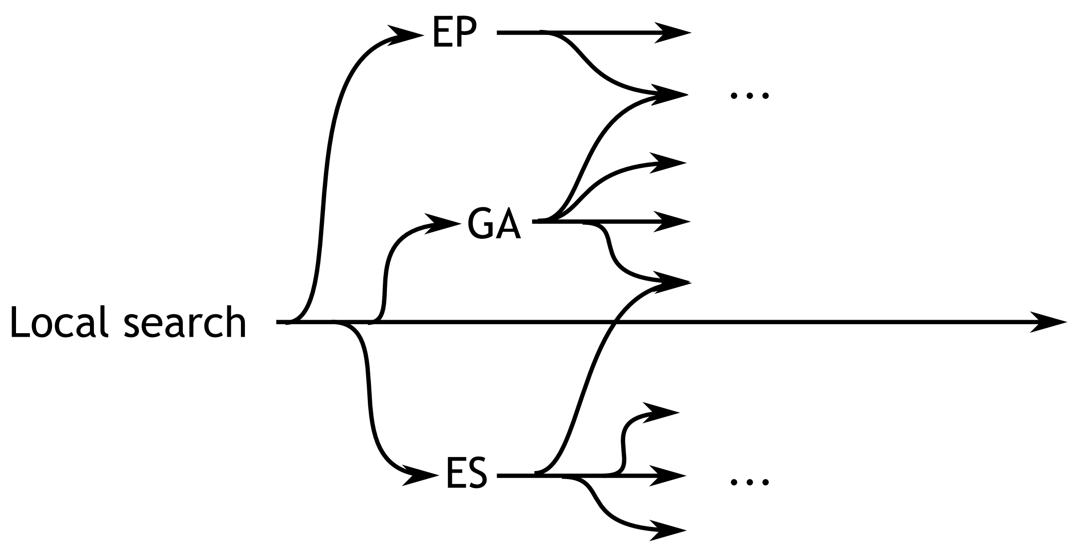

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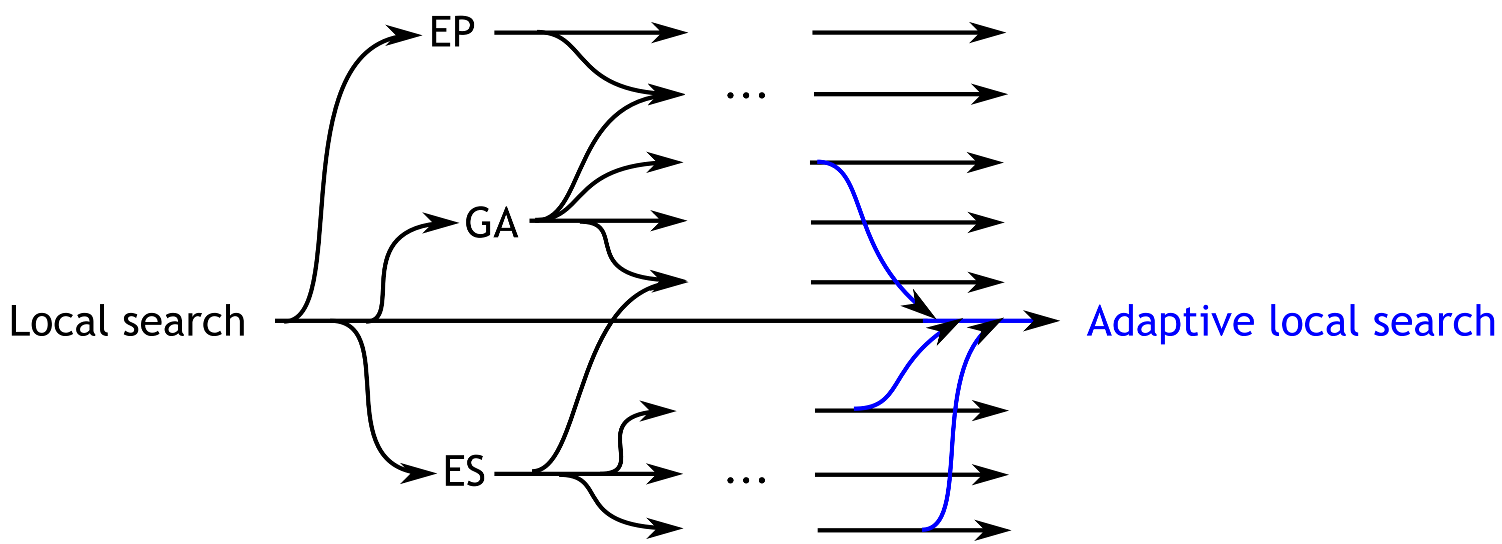

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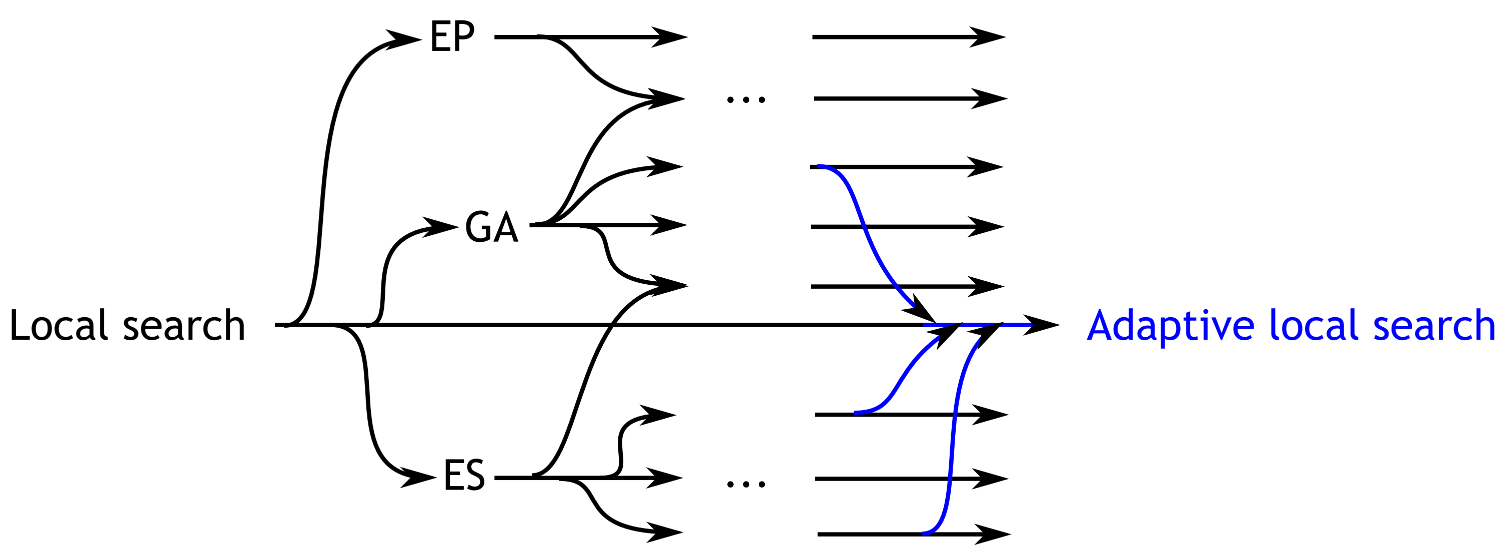

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Hypothesis:

- ✔ 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

- ✔ 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

AVS [GBR06]:

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

[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.

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

- ✔ Compute the ranked correlation coefficient of p.d.f. values and function values, $p(\boldsymbol{x}_i)$ and $f(\boldsymbol{x}_i)$.
- ✔ 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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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.

[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.

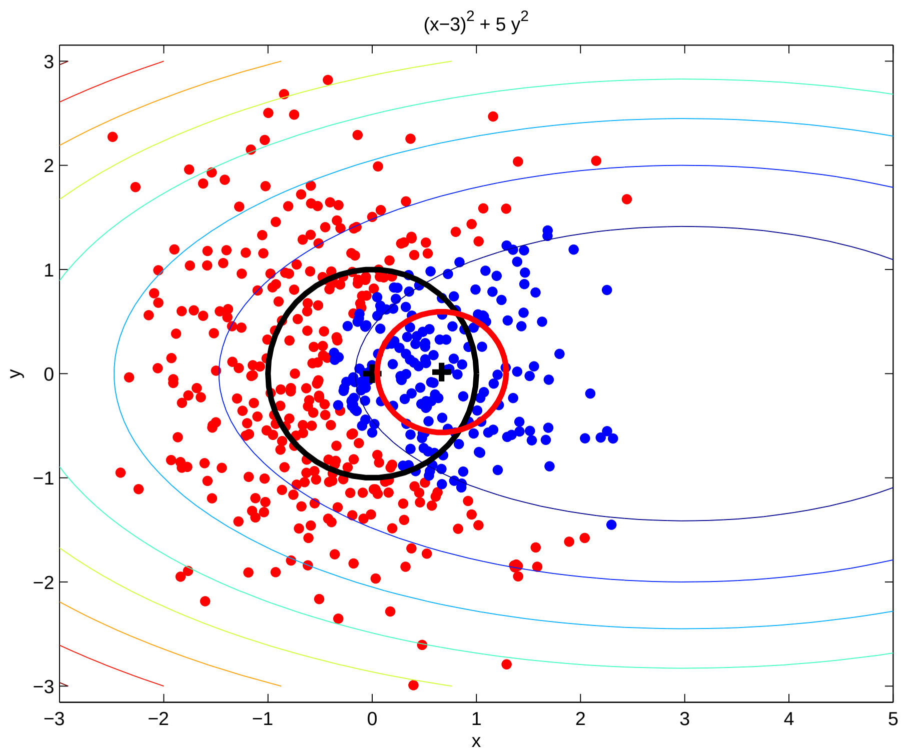
[GBR06] Jörn Grahl, Peter A. N. Bosman, and Franz Rothlauf. The correlation-triggered adaptive variance scaling IDEA. In *Proceedings of the 8th annual conference on Genetic and Evolutionary Computation Conference – GECCO 2006*, pages 397–404, New York, NY, USA, 2006. ACM Press.

Anticipated Mean Shift

Anticipated mean shift (AMS) [BGT08]:

- ✔ AMS is defined as: $\hat{\boldsymbol{\mu}}^{\text{shift}} = \hat{\boldsymbol{\mu}}(t) - \hat{\boldsymbol{\mu}}(t-1)$
- ✔ AMS is an estimate of the direction of improvement
- ✔ $100\alpha\%$ of offspring are moved by certain fraction of AMS: $\boldsymbol{x} = \boldsymbol{x} + \delta\hat{\boldsymbol{\mu}}^{\text{shift}}$
- ✔ When centered around optimum, $\hat{\boldsymbol{\mu}}^{\text{shift}} = 0$ and the original approach is unchanged.
- ✔ Selection must choose parent from both the old and the shifted regions to adjust $\boldsymbol{\Sigma}$ suitably.

MLE



[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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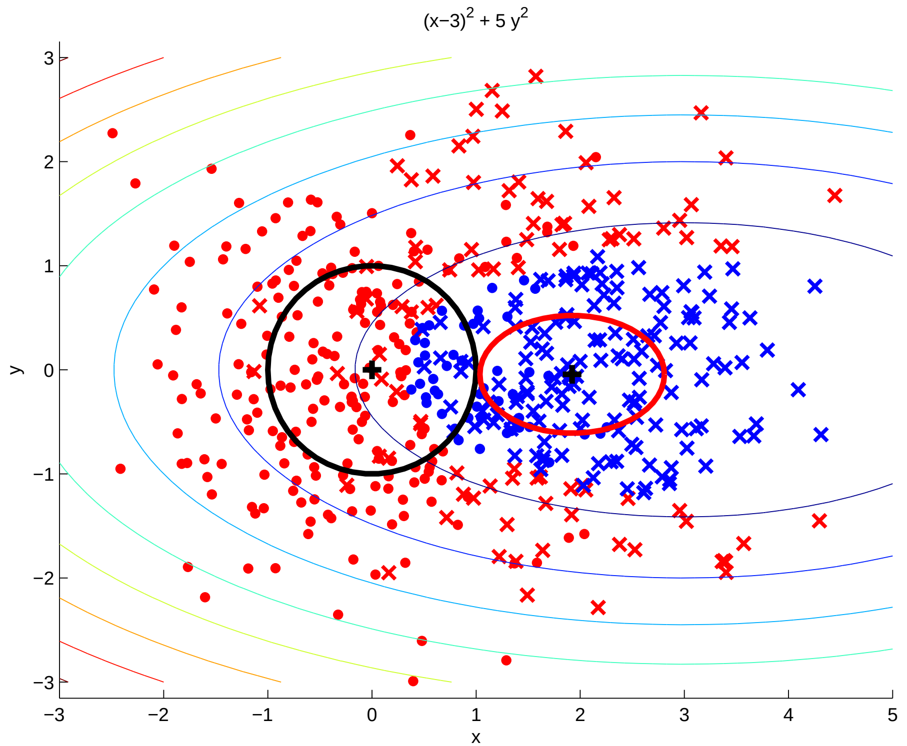
AMS: $\hat{\boldsymbol{\mu}}^{\text{shift}} = (1, 0)^T$



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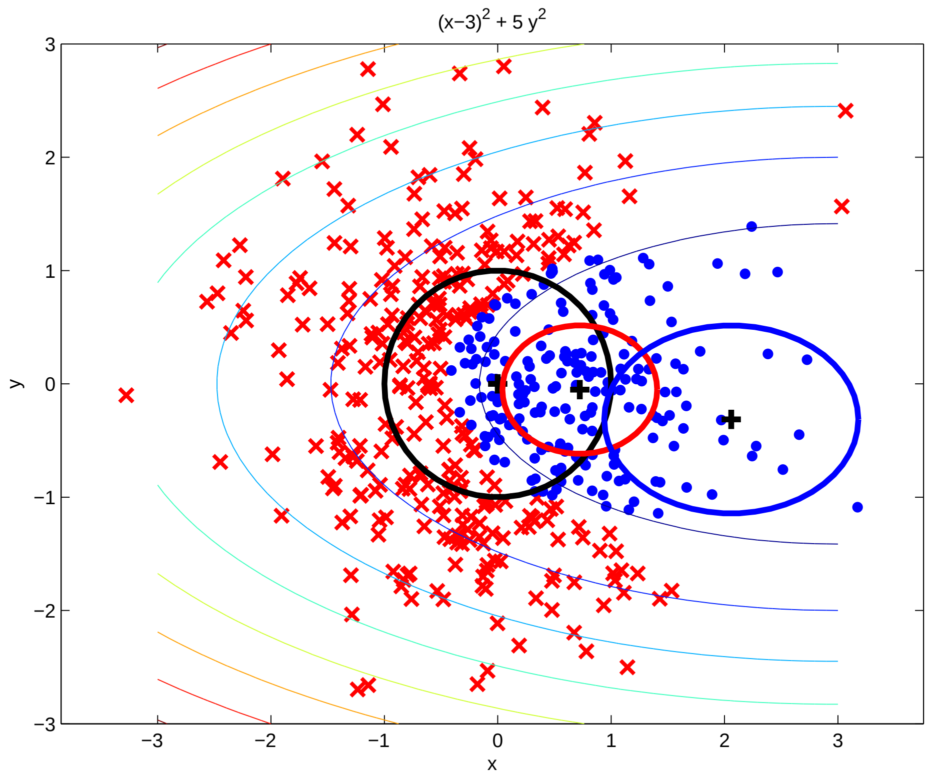
Weighted ML Estimates

Account for the values of p.d.f. of the selected parents $\mathbf{X}_{\text{sel}}$ [TT09]:

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



Weighted (ML) estimates of parameters

$$\boldsymbol{\mu}_{\text{W}} = \frac{1}{V_1}\sum_{i=1}^{N} w_i \boldsymbol{x}_i, \text{ where } \boldsymbol{x}_n \in \mathbf{X}_{\text{sel}}$$

$$\boldsymbol{\Sigma}_{\text{W}} = \frac{V_1}{V_1^2 - V_2}\sum_{i=1}^{N} w_i (\boldsymbol{x}_i - \mu_{\text{ML}})(\boldsymbol{x}_n - \mu_{\text{ML}})^T$$

where

$$w_i = \frac{1}{p(\boldsymbol{x}_i)}$$

$$V_1 = \sum w_i$$

$$V_2 = \sum w_i^2$$

[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.

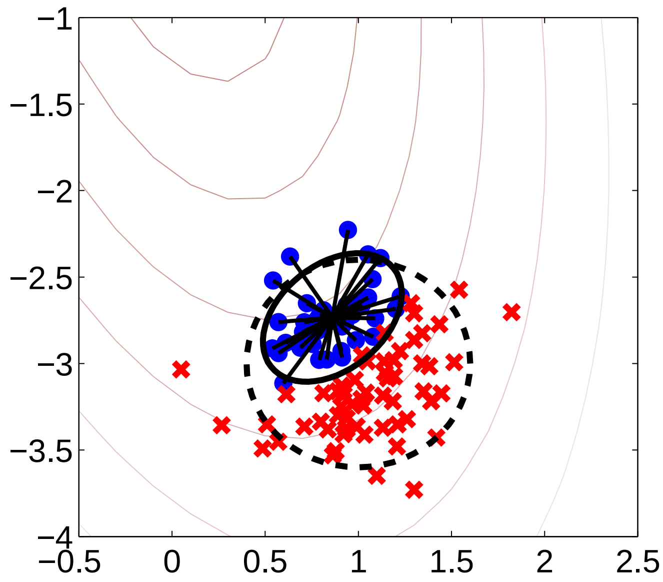
CMA-ES

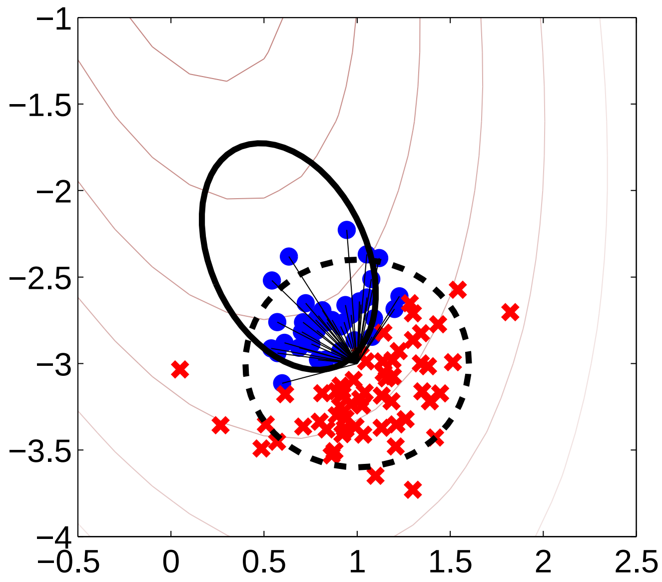
Evolutionary strategy with cov. matrix adaptation [HO01]

- ✔ $(\mu/\mu, \lambda)$-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.)

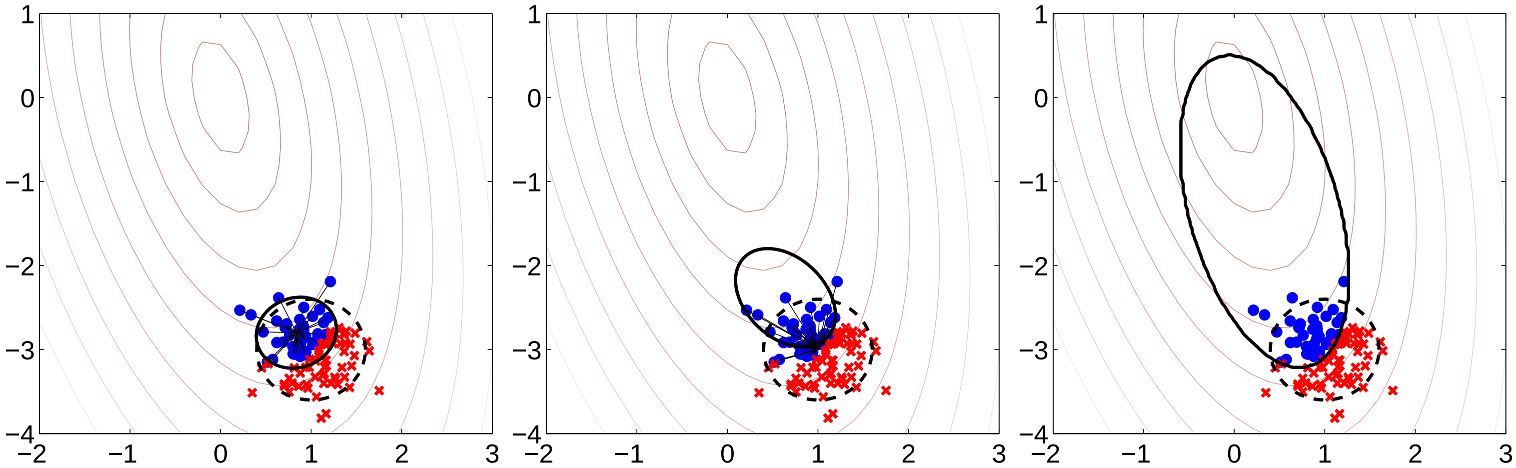




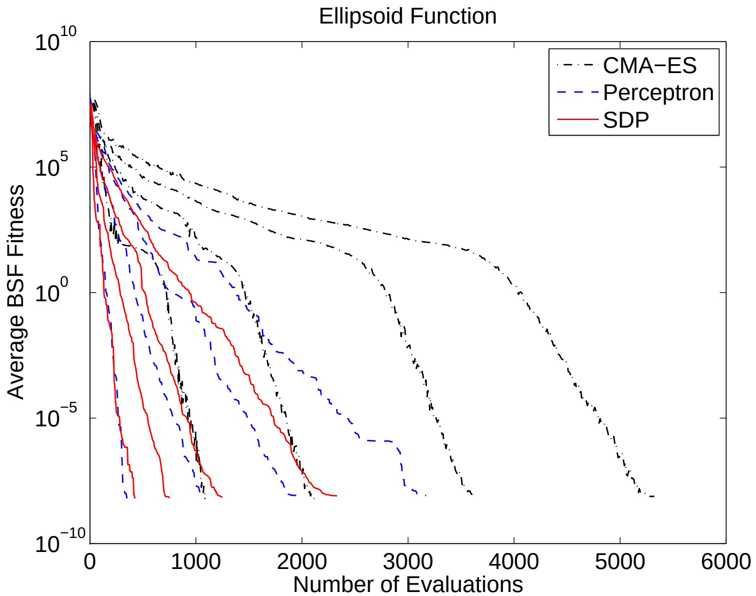
[HO01] Nikolaus Hansen and Andreas Ostermeier. Completely derandomized self-adaptation in evolution strategies. *Evolutionary Computation*, 9(2):159–195, 2001.

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.

Remarks on SotA

- ✔ 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

Summary

Real-valued EDAs

- ✔ much less developed than EDAs for binary representation
- ✔ the difficulties are caused mainly by
  - ✘ much more severe effects of the curse of dimensionality
  - ✘ many different types of interactions among variables
- ✔ Gaussian distribution used most often, but pure maximum-likelihood estimates are BAD! Some other remedies are needed.
- ✔ Despite of that, EDA (and EAs generally) are able to gain better results then conventional optimization techniques (line search, Nelder-Mead search, ...)