

**A0M33EOA:
EAs for Real-Parameter Optimization.
Differential Evolution. CMA-ES.**

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Many parts adapted or taken from
Kubalík, J. *Real-Parameter Evolutionary Algorithms*.
Lecture slides for A4M33BIA course. 2016



Introduction



EAs for real-parameter optimization

Phenotype:

- Representation that the fitness function understands and is able to evaluate.
- Vector of real numbers.

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Genotype?

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Genotype?

- Representation to which the “genetic” operators are applied.

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Genotype?

- Representation to which the “genetic” operators are applied.
- **Binary vector** encoding the real numbers.
 - Discretization. Finite space.
 - Discretized problem is not the same as the original one.
 - Can miss the real function optimum. Results depend on the chosen precision of discretization.
 - Requires encoding and decoding process.

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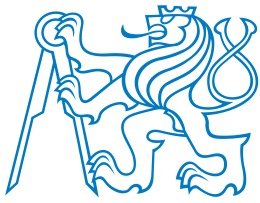
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- **Binary vector** encoding the real numbers.
 - Discretization. Finite space.
 - Discretized problem is not the same as the original one.
 - Can miss the real function optimum. Results depend on the chosen precision of discretization.
 - Requires encoding and decoding process.
- **Vector of real numbers** (genotype = phenotype).
 - *Infinite domain* (theoretically), even for space with finite bounds.
 - Opportunity to exploit *graduality* or *continuity* of the function (slight changes in variables result in slight changes of the function value).
 - No need for encoding/decoding.

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- Standard selecto-recombinative genetic algorithms with binary representation.
- Standard selecto-recombinative genetic algorithms with real representation.
- Evolution strategies.
- Differential Evolution.

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Standard EAs with Binary Encoding



Genotype-Phenotype Mapping

Mapping binary to real vector representation (2D example):

- 2D real domain, bound constraints $[x_l, x_r] \times [y_l, y_r]$.
- Using n bits to encode each parameter.

$$x_B = \begin{array}{|c|c|c|c|c|c|c|c|} \hline x_1 & x_2 & \dots & x_n & y_1 & y_2 & \dots & y_n \\ \hline \end{array}$$

- How to compute phenotype from known genotype?

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Genotype-Phenotype Mapping

Mapping binary to real vector representation (2D example):

- 2D real domain, bound constraints $[x_l, x_r] \times [y_l, y_r]$.
- Using n bits to encode each parameter.

$$x_B = \boxed{x_1 \quad x_2 \quad \dots \quad x_n \quad | \quad y_1 \quad y_2 \quad \dots \quad y_n}$$

- How to compute phenotype from known genotype?

$$x_R = \boxed{x_l + (x_r - x_l) \frac{\text{bin2int}(x_1, \dots, x_n)}{2^n - 1} \quad | \quad y_l + (y_r - y_l) \frac{\text{bin2int}(y_1, \dots, y_n)}{2^n - 1}}$$

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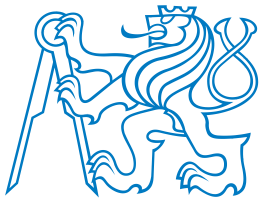
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- How to compute phenotype from known genotype?

$$x_R = \begin{array}{|c|c|} \hline x_l + (x_r - x_l) \frac{\text{bin2int}(x_1, \dots, x_n)}{2^n - 1} & y_l + (y_r - y_l) \frac{\text{bin2int}(y_1, \dots, y_n)}{2^n - 1} \\ \hline \end{array}$$

Where in the EA should we place the mapping?

Algorithm 1: Evolutionary Algorithm

```
1 begin
2   X ← InitializePopulation()
3   f ← Evaluate(X)
4   xBSF, fBSF ← UpdateBSF(X, f)
5   while not TerminationCondition() do
6     XN ← Breed(X, f) // using certain breeding pipeline
7     fN ← Evaluate(XN)
8     xBSF, fBSF ← UpdateBSF(XN, fN)
9     X, f ← Join(X, f, XN, fN) // aka ‘replacement strategy’
10  return xBSF, fBSF
```

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Genotype-Phenotype Mapping

Mapping binary to real vector representation (2D example):

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$$x_B = \begin{array}{|c|c|c|c|c|c|} \hline x_1 & x_2 & \dots & x_n & y_1 & y_2 & \dots & y_n \\ \hline \end{array}$$

- How to compute phenotype from known genotype?

$$x_R = \begin{array}{|c|c|} \hline x_l + (x_r - x_l) \frac{\text{bin2int}(x_1, \dots, x_n)}{2^n - 1} & y_l + (y_r - y_l) \frac{\text{bin2int}(y_1, \dots, y_n)}{2^n - 1} \\ \hline \end{array}$$

Where in the EA should we place the mapping?

Algorithm 1: Evolutionary Algorithm with Genotype-Phenotype Mapping

```
1 begin
2   X ← InitializePopulation()
3   f ← MapAndEvaluate(X)
4   xBSF, fBSF ← UpdateBSF(X, f)
5   while not TerminationCondition() do
6     XN ← Breed(X, f) // using certain breeding pipeline
7     fN ← MapAndEvaluate(XN)
8     xBSF, fBSF ← UpdateBSF(XN, fN)
9     X, f ← Join(X, f, XN, fN) // aka ‘replacement strategy’
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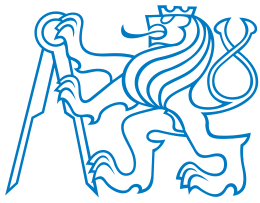
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Effect of bit-flip mutation

The neighborhood of a point in the phenotype space generated by an operation applied on the genotype.

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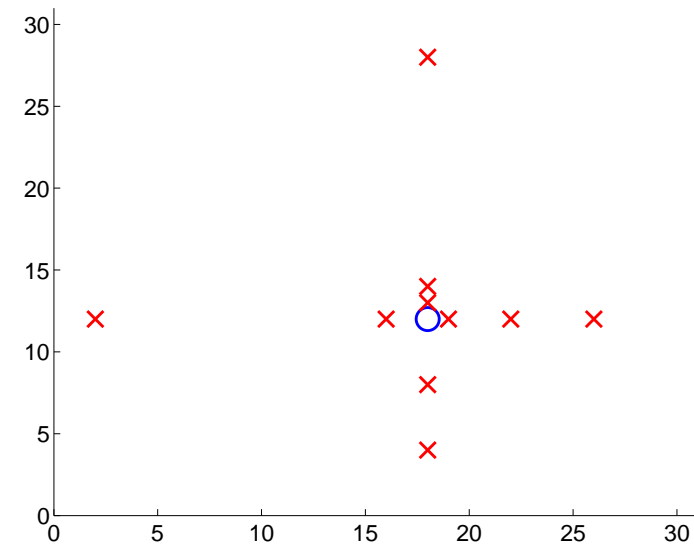
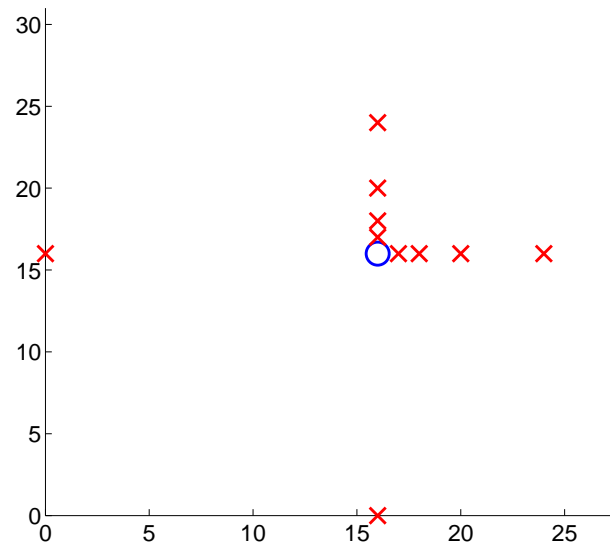
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- Genotype: 10bit binary string.
- Phenotype: vector of 2 real numbers (in a discretized space).
- Operation: “bit-flip” mutation.



A very common situation:

- Point which is locally optimal w.r.t. the phenotype is not locally optimal w.r.t. the genotype recombination operators. (**GOOD! An opportunity to escape from LO!**)
- Point which is locally optimal w.r.t. the genotype recombination operators is not locally optimal w.r.t. the phenotype. (**BAD: Even the best solutions found by EA do not have to correspond to the real optima we look for!**)



Effect of 1-point crossover

The neighborhood of a point in the phenotype space generated by an operation applied on the genotype.

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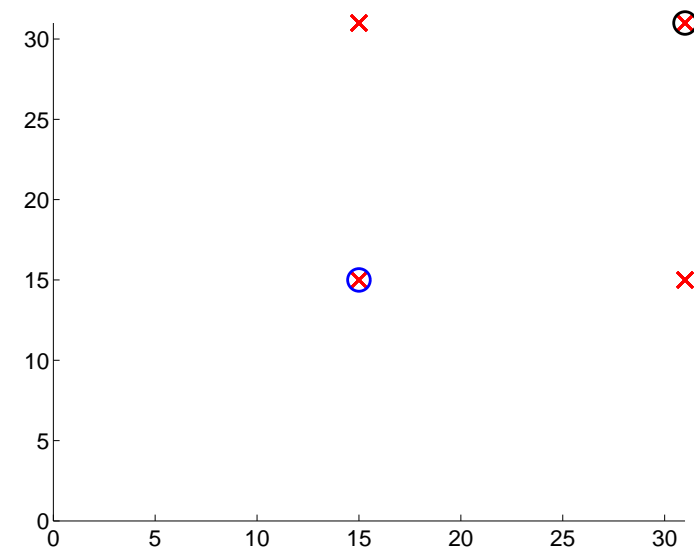
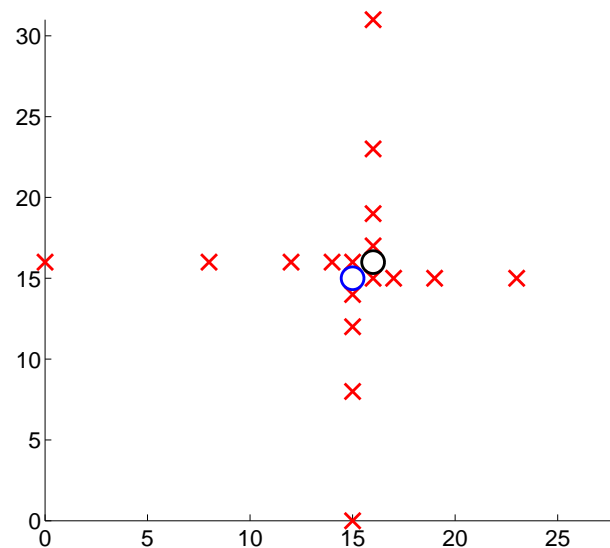
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- Genotype: 10bit binary string.
- Phenotype: vector of 2 real numbers (in a discretized space).
- Operation: 1-point crossover.





Effect of 2-point crossover

The neighborhood of a point in the phenotype space generated by an operation applied on the genotype.

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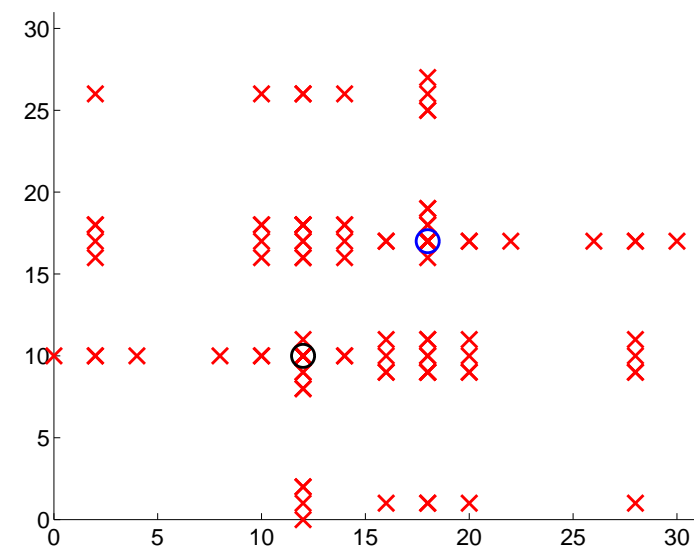
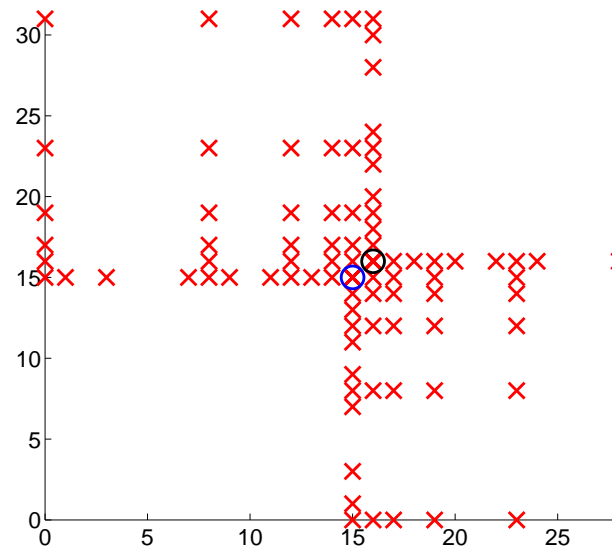
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- Genotype: 10bit binary string.
- Phenotype: vector of 2 real numbers (in a discretized space).
- Operation: 2-point crossover.





Summary

Binary encoding for real-parameter optimization:

- Results depend on the chosen discretization.
- The neighborhoods generated by binary crossover and mutation operators do not fit well to the “usual structures” of real-parameter functions.
- Can be useful for a rough exploration of the search space. (Then we can increase the resolution, or switch to real representation.)
- Using **Gray code** may help in certain situations, but does not solve the fundamental issues.

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Standard EAs with Real Encoding



Recombination Operators for ESs with Real Encoding

Genotype = Phenotype = Vector of real numbers!

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Recombination Operators for ESs with Real Encoding

Genotype = Phenotype = Vector of real numbers!

Standard mutation operators:

- Gaussian mutation
- Cauchy mutation

Standard recombination operators:

- Simple (1-point) Crossover: same as for binary strings
- Uniform Crossover: same as for binary strings
- Average Crossover
- Arithmetic Crossover
- Flat Crossover
- Blend Crossover BLX-(α)

Advanced recombination operators:

- Simplex Crossover (SPX)
- Unimodal Normal Distribution Crossover (UNDX)
- Parent-Centric Crossover (PCX)

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Binary EAs

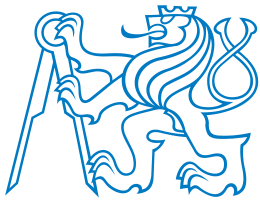
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Standard Recombination Operators for Real EAs

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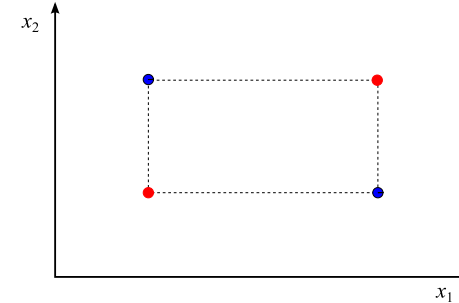
Summary

Assume that $x^1 = (x_1^1, \dots, x_n^1)$ and $x^2 = (x_1^2, \dots, x_n^2)$ are two parents.

- **Simple (1-point) Crossover:** a position $i \in 1, 2, \dots, n - 1$ is randomly chosen, and two offspring chromosomes y^1 and y^2 are built as follows:

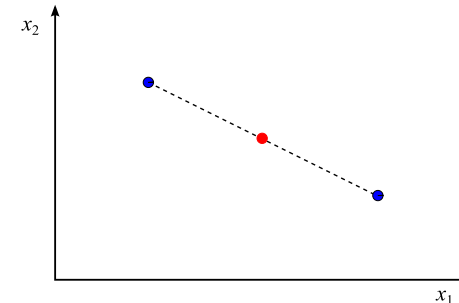
$$y^1 = (x_1^1, \dots, x_i^1, x_{i+1}^2, \dots, x_n^2)$$

$$y^2 = (x_1^2, \dots, x_i^2, x_{i+1}^1, \dots, x_n^1)$$



- **Average Crossover:** an offspring y is created as an average of the parents:

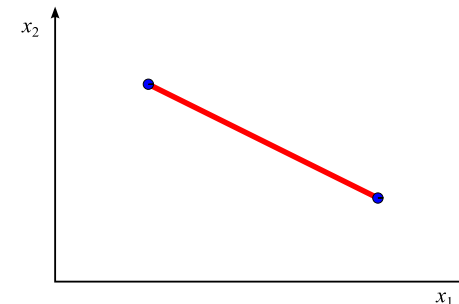
$$y = \frac{1}{2}(x^1 + x^2)$$

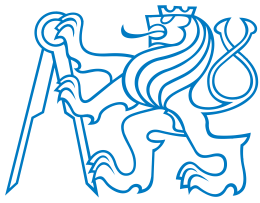


- **Arithmetic Crossover:** an offspring is created as a *weighted average* of the parents:

$$y = r \cdot x^1 + (1 - r) \cdot x^2,$$

where $r \in (0, 1)$ is a constant, or varies with regard to the number of generations made, or is randomly chosen.

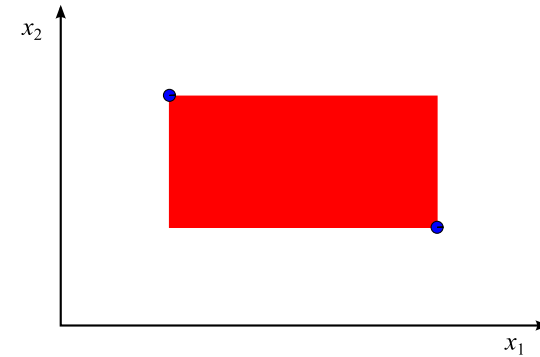




Standard Recombination Operators for Real EAs (cont.)

- **Flat Crossover:** an offspring $\mathbf{y} = (y_1, \dots, y_n)$ is created such that each y_i is sampled with uniform distribution from interval

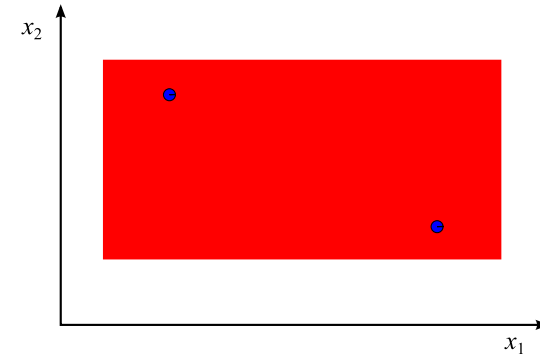
$$y_i \in [\min(x_i^1, x_i^2), \max(x_i^1, x_i^2)].$$



- **Blend Crossover:** an offspring $\mathbf{y} = (y_1, \dots, y_n)$ is created such that each y_i is sampled with uniform distribution from interval

$$y_i \in [c_{\min} - \alpha I, c_{\max} + \alpha I],$$

where $c_{\min} = \min(p_i^1, p_i^2)$,
 $c_{\max} = \max(p_i^1, p_i^2)$, $I = c_{\max} - c_{\min}$,
and $\alpha > 0$.



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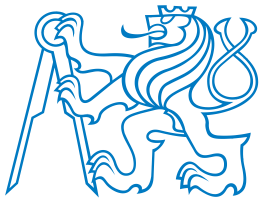
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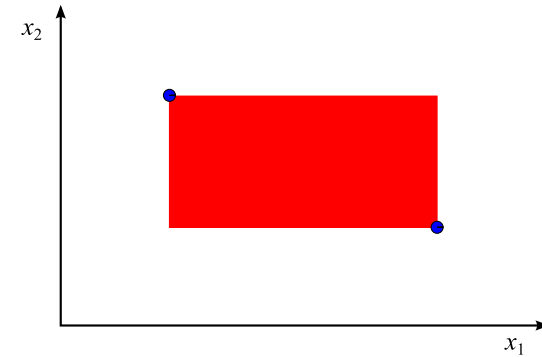
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- **Flat Crossover:** an offspring $\mathbf{y} = (y_1, \dots, y_n)$ is created such that each y_i is sampled with uniform distribution from interval

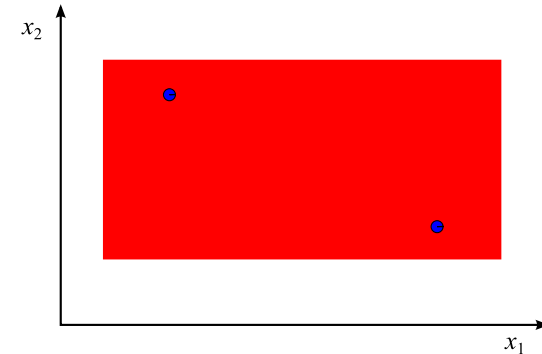
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- **Blend Crossover:** an offspring $\mathbf{y} = (y_1, \dots, y_n)$ is created such that each y_i is sampled with uniform distribution from interval

$$y_i \in [c_{\min} - \alpha I, c_{\max} + \alpha I],$$

where $c_{\min} = \min(p_i^1, p_i^2)$,
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and $\alpha > 0$.



Characteristics:

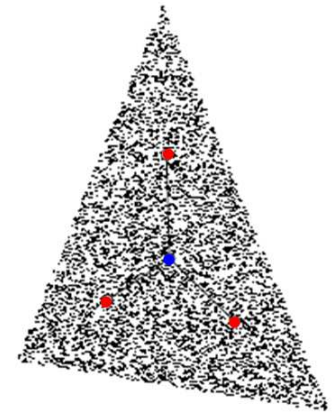
- Simple, and average crossovers are deterministic; arithmetic crossover does not introduce enough diversity either.
- Simple, flat, and blend crossovers are not rotationally invariant.



Advanced Operators

Simplex Crossover (SPX):

- Generates offspring around the mean of the μ parents
- with uniform distribution
- in a simplex which is $\sqrt{\mu + 1}$ times bigger than the parent simplex.



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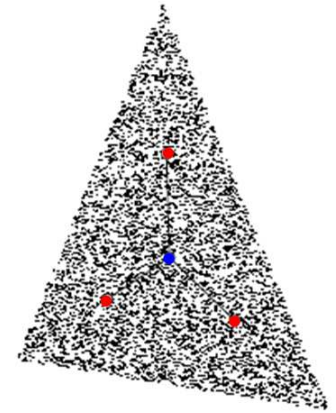
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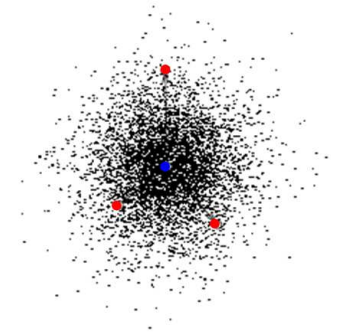
Simplex Crossover (SPX):

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Unimodal Normal Distribution Crossover (UNDX):

- Generates offspring around the mean of the μ parents
- with multivariate normal distribution.
- Preserves the correlation among parameters well.





Advanced Operators

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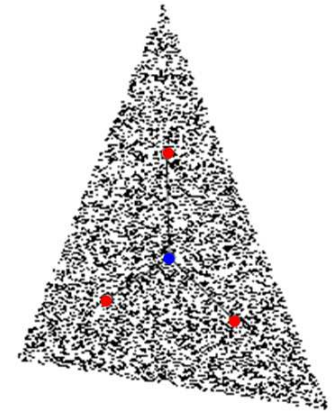
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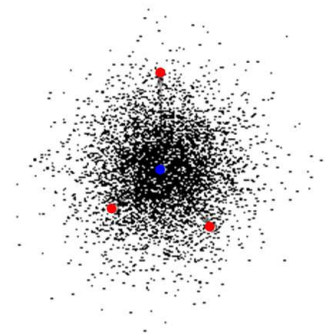
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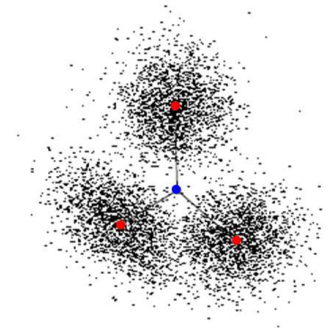
Unimodal Normal Distribution Crossover (UNDX):

- Generates offspring around the mean of the μ parents
- with multivariate normal distribution.
- Preserves the correlation among parameters well.



Parent-Centric Crossover (PCX):

- Generates offspring around one of the parents
- with multivariate normal distribution.
- The distribution shape is determined by the relative positions of the parents.
- Similar to adaptive mutation.





Generalized Generation Gap (G3) Algorithm

G3 [Deb05]: Elite preserving, steady-state, computationally fast. Special breeding pipeline and replacement operator.

1. From the population $P(t)$, select the best parent and $(\mu - 1)$ other parents randomly.
2. Generate λ offspring from μ parents using a recombination scheme.
3. Choose two parents at random from μ parents.
4. Form a combined subpopulation of chosen two parents and λ offspring, choose the best two solutions and replace the chosen two parents with these solutions.

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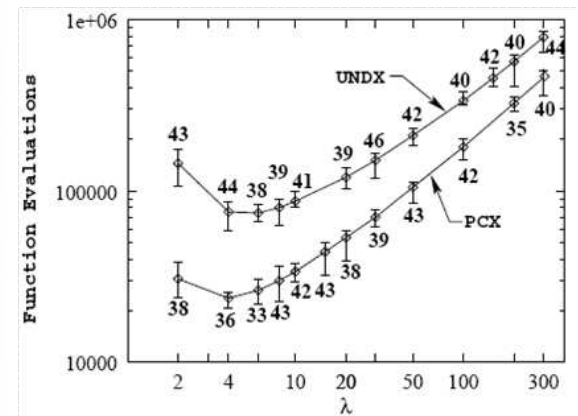
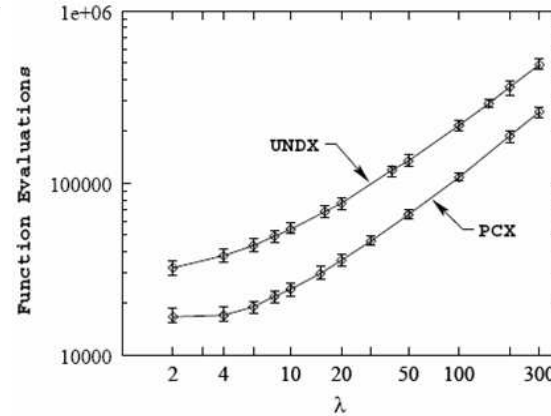
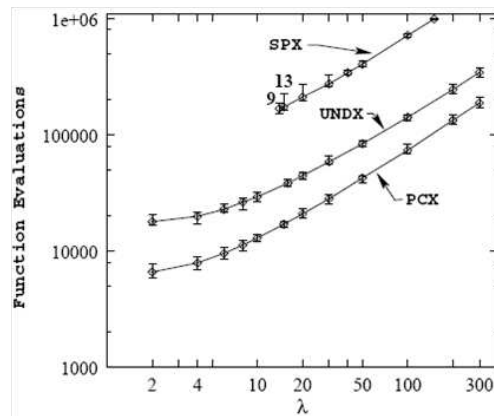


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Comparisons of UNDX, SPX and PCX with the G3 model on Ellipsoidal, Schwefel's, and Generalized Rosenbrock's functions for $D = 20$.



[Deb05] K. Deb. A population-based algorithm-generator for real-parameter optimization. *Soft Computing*, 9(4):236–253, April 2005.

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Selecto-recombinative standard EAs with real encoding

- often use the same algorithm and breeding pipeline as binary EAs,
- although a specialized pipeline can be designed (e.g., G3).
- They use different mutation and crossover operators.

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Binary EAs

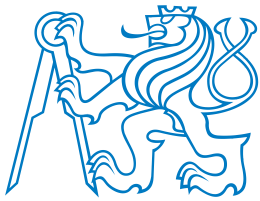
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Selecto-recombinative standard EAs with real encoding

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- although a specialized pipeline can be designed (e.g., G3).
- They use different mutation and crossover operators.

Operators for real encoding:

- Much wider range of possibilities than in binary space.
- Generally, there is no single best operator for all problems.
- Operators resulting in normal distribution of offspring usually work better for practical problems.

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- Standard ops
- Advanced ops
- Generalized Generation Gap (G3) Algorithm
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Evolution Strategies (ES)



Evolution Strategies: Introduction

“The European branch of Evolutionary Computation.”

- Originated in Germany in 1960's (Ingo Rechenberg and Hans-Paul Schwefel).
- ES use the natural representation of vectors in R^D as “chromosomes”.
- ES originally relied on *mutation and selection* only; recombination was added later.
- Mutation is performed by adding a random vector distributed according to multivariate Gaussian with covariance matrix $\sigma\mathbf{I}$, $\text{diag}(\sigma_1, \dots, \sigma_D)$, or general C .
- Special feature: *built-in* adaptation of mutation parameters!

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- Special feature: *built-in* adaptation of mutation parameters!

Notation: (μ^+, λ) -ES

- μ is the *population size* (and number of parents),
- λ is the *number of offspring* created each generation,
- + or , denote the *replacement strategy*:
 - , is *generational* strategy: old population is discarded, new population of μ parents is chosen from the λ generated offspring.
 - + is *steady-state* strategy: old population is joined with the new offspring, new population of μ parents is chosen from the joined $\mu + \lambda$ individuals.

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Notation: $(\mu/\rho^+\lambda)$ -ES

- *Recombination* (usually deterministic), choose ρ individuals out of μ parents, $\mu \geq \rho$.
- Sometimes, subscript to ρ is used to denote the type of recombination, e.g., ρ_I for intermediate recombination (average), or ρ_W for weighted recombination (weighted average). Other recomb. ops from Real EAs can be used in principle.

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Evolution Strategy Algorithm

ES use ordinary EA template (see lecture 1), with only slightly changed pipeline:

Algorithm 2: ES Breeding Pipeline

Input: Population X of μ individuals, with their fitness in f .

Number of parents ρ . Number of offspring λ .

Output: Population X_N of λ offspring.

```
1 begin
2    $X_N \leftarrow \emptyset$ 
3   for  $i \leftarrow 1, \dots, \lambda$  do
4      $X_S \leftarrow \text{SelectParents}(X, f)$  //  $\rho$  parents
5      $x_R \leftarrow \text{Recombine}(X_S)$  // usually only single offspring
6      $x_N \leftarrow \text{Mutate}(x_R)$ 
7      $X_N \leftarrow X_N \cup \{x_N\}$ 
8   return  $X_N$ 
```

- The `join()` operation then forms new population for the next generation by choosing the best μ individuals either from X_N (comma strategy) or from $X \cup X_N$ (plus strategy).
- Very often $\rho = \mu$, resulting in $(\mu/\mu^+, \lambda) - ES$. All offspring are then centered around a single vector x_R . Lines 4 and 5 can thus be removed from the `for`-loop and placed before it.

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Gaussian Mutation

Gaussian mutation: the mutated offspring y are distributed around the original individual x as

$$y \sim N(x, C) \sim x + N(0, C) \sim x + C^{\frac{1}{2}} N(0, I),$$

where $N(\mu, C)$ is a **multivariate Gaussian distribution** with probability density function in R^D

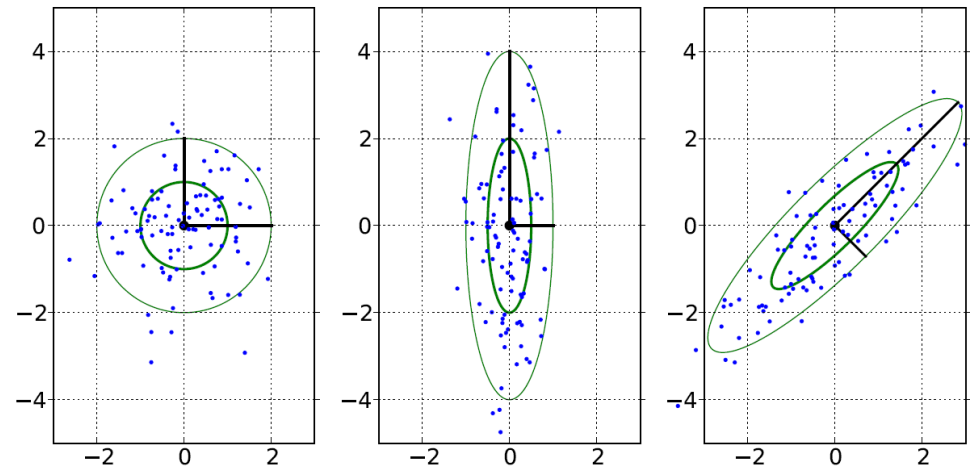
$$f_D(x|\mu, C) = \frac{1}{\sqrt{(2\pi)^D \det(C)}} \exp\left(-\frac{1}{2}(x - \mu)^T C^{-1}(x - \mu)\right)$$

Parameters:

- μ : location of the distribution. When used for mutation, $\mu = 0$ to prevent bias.
- C : Covariance matrix; determines the shape of the distribution:
 - **Isotropic:** $C = \sigma^2 I$
 - **Axis-parallel:** $C = \text{diag}(\sigma_1^2, \dots, \sigma_D^2)$
 - **General:** C positive definite

How many degrees of freedom (free parameters) do these have?

How to set up the parameters of covariance matrix?





Adaptation of Mutation Parameters

Adaptation of mutation parameters is **key to ES design!**

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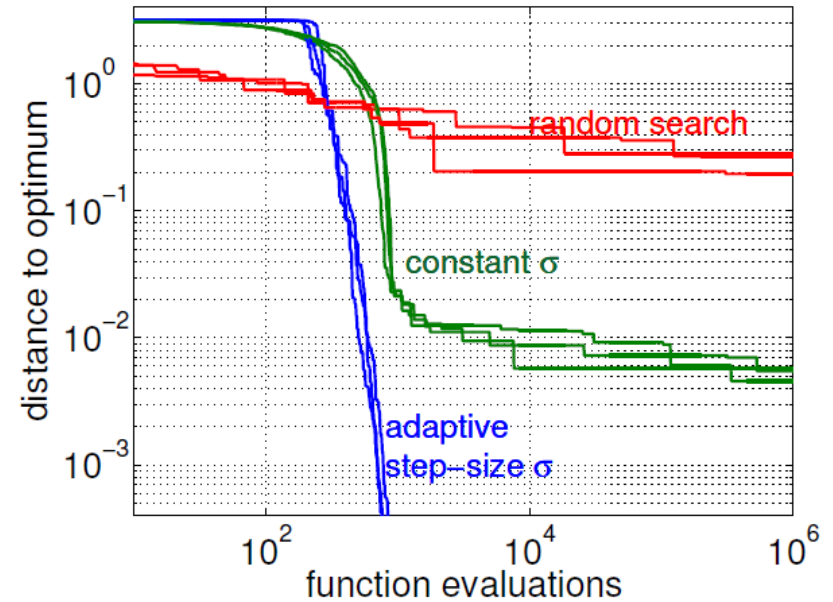
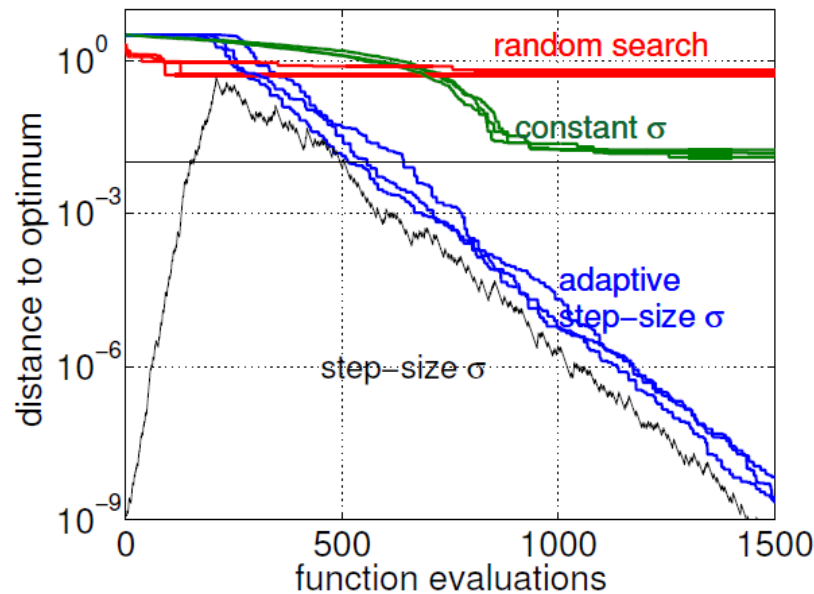


Adaptation of Mutation Parameters

Adaptation of mutation parameters is **key to ES design!**

Example: $(1 + 1)$ -ES (hill-climber) with isotropic mutation on Sphere function: $f = \sum_i x_i^2$

- Random search vs
- $(1 + 1)$ -ES with constant $\sigma = 10^{-2}$ vs
- $(1 + 1)$ -ES with σ adapted using $\frac{1}{5}$ -rule with $\sigma_0 = 10^{-9}$



- Random search: inefficient.
- Constant σ : initially too small value, appropriate value between 600 and 800 evals, too large value at the end.
- Adaptive σ : near-optimal value during (almost) the whole run!

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1/5 Success Rule

Progress rate φ : a ratio of the distance covered towards the optimum and the number of evaluations required to reach this distance.

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Summary

Rechenberg analyzed the behavior of (1+1)-ES on 2 simple functions:

- Corridor function: $f_1(\mathbf{x}) = x_1$ if $|x_i| < 1$ for $i \in (2, \dots, D)$, otherwise $f_1(\mathbf{x}) = \infty$
- Sphere function: $f_2(\mathbf{x}) = \sum_i x_i^2$



1/5 Success Rule

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Findings:

- In both cases, the optimal step size σ^{opt} is inversely proportional to the dimension of the space D (number of variables).
- The maximum progress rate φ^{max} is also inversely proportional to D .
- For the optimal step sizes, the following probabilities of a successful mutation were obtained:
 - $p_{S,1}^{opt} = 1/(2e) \approx 0.184$
 - $p_{S,2}^{opt} \approx 0.270$



1/5 Success Rule

Progress rate φ : a ratio of the distance covered towards the optimum and the number of evaluations required to reach this distance.

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 - $p_{S,1}^{opt} = 1/(2e) \approx 0.184$
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1/5 success rule: *To obtain nearly optimal (local) performance of the (1+1)-ES in real-valued search spaces, tune the mutation step in such a way that the (measured) success rate is about 1/5.*

- If it is greater than 1/5, increase the mutation step σ ; if it is less, decrease σ .

In practice, the 1/5 success rule has been mostly superseded by more sophisticated methods. However, its conceptual insight remain remarkably valuable.



(1+1)-ES with 1/5 rule

Algorithm 3: (1+1)-ES with 1/5 rule

Input: $D \in \mathbb{N}^+, d \approx \sqrt{D+1}$

```
1 begin
2    $x \leftarrow \text{Initialize}()$ 
3   while not TerminationCondition() do
4      $x_N \leftarrow x + \sigma \mathcal{N}(0, I)$  // mutation/perturbation
5      $b \leftarrow \text{BetterThan}(x_N, x)$  // Mutation successful?
6      $\sigma \leftarrow \sigma \left( \exp \left( \mathbb{1}(b) - \frac{1}{5} \right) \right)^{\frac{1}{d}}$  // 1/5 rule
7     if  $b$  then
8        $x \leftarrow x_N$ 
```

- $\mathbb{1}(b)$ is an indicator function:

$$\mathbb{1}(b) = \begin{cases} 1 & \text{iff } b \text{ is true,} \\ 0 & \text{iff } b \text{ is false.} \end{cases}$$

- Other implementations are possible.

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Self-adaptation

Self-adaptation:

- **Strategy parameters are part of the chromosome!** $x = (x_1, \dots, x_D, \sigma_1, \dots, \sigma_D)$
- Parameters undergo evolution together with the decision variables.
- Each individual holds information how it shall be mutated.

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Example: assuming axis-parallel normal distribution is used,

- mutation of $x = (x_1, \dots, x_D, \sigma_1, \dots, \sigma_D)$ creates an offspring individual

$$x' = (x'_1, \dots, x'_D, \sigma'_1, \dots, \sigma'_D)$$

by mutating each part in a different way:

$$\sigma'_i \leftarrow \sigma_i \cdot \exp(\tau \cdot \mathcal{N}(0, 1))$$

$$x'_i \leftarrow x_i + \sigma'_i \cdot \mathcal{N}(0, 1)$$

- Intuition: a “bad” σ' probably generates bad x' and is eliminated by selection.

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Remarks:

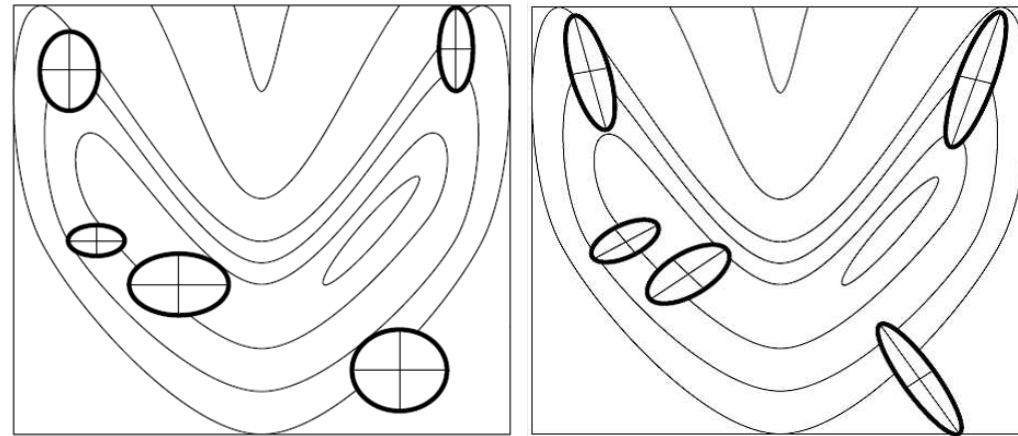
- An algorithm can adapt a global step size σ and coordinate-wise step sizes separately, such that the resulting coordinate-wise st. dev. is given as $\sigma \cdot \sigma_i$.
- The global step size may be adapted e.g. by the 1/5-rule.



Generalizations and issues

Generalizing from

- axis-parallel mutation distributions with D strategy parameters to
- general normal mutation distributions with full cov. matrix requires adaptation of $\frac{1}{2}D(D + 1)$ strategy parameters!



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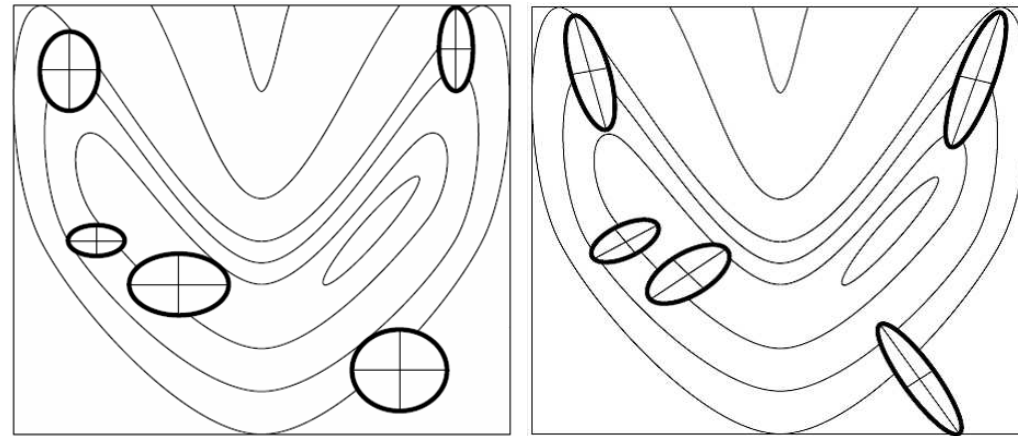
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Issues with self-adaptation: **selection noise** (the more parameters, the worse)!

- The intuition from the previous slide does not work much!
- A good offspring may be generated with poor strategy parameter settings (**poor setting survives**), or a bad offspring may be generated with good parameter settings (**good setting is eliminated**).

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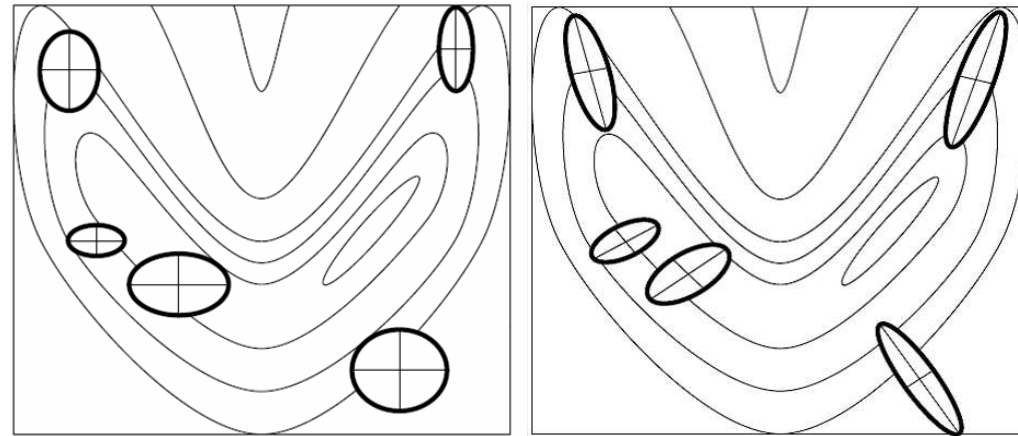
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- A good offspring may be generated with poor strategy parameter settings (**poor setting survives**), or a bad offspring may be generated with good parameter settings (**good setting is eliminated**).

Solutions: derandomization via

- reducing the number of mutation distribution: $(1, \lambda)$ -ES, $(\mu / \mu, \lambda)$ -ES, and
- accumulating info in time (evolution paths).

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CMA-ES

Evolutionary strategy with covariance matrix adaptation [HO01]:

- Currently, *de facto* standard in real-parameter optimization.
- $(\mu/\mu_W, \lambda)$ -ES: recombinative, mean-centric
- Offspring is created by sampling from a single normal distribution.
- Successful mutation steps are used to adapt the mean x and the covariance matrix C of the distribution.
- Accumulates the successful steps over many generations.

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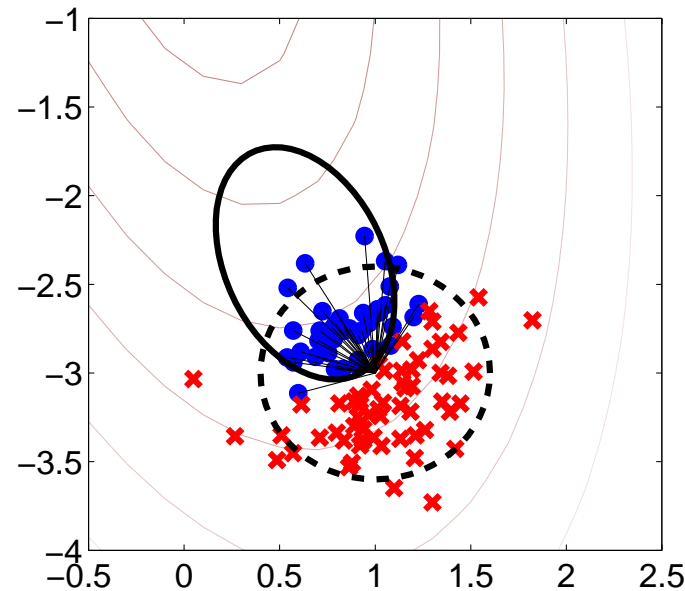
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[HO01] Nikolaus Hansen and Andreas Ostermeier. Completely derandomized self-adaptation in evolution strategies. *Evolutionary Computation*, 9(2):159–195, 2001.



CMA-ES Demo

CMA-ES on the Rosenbrock function:

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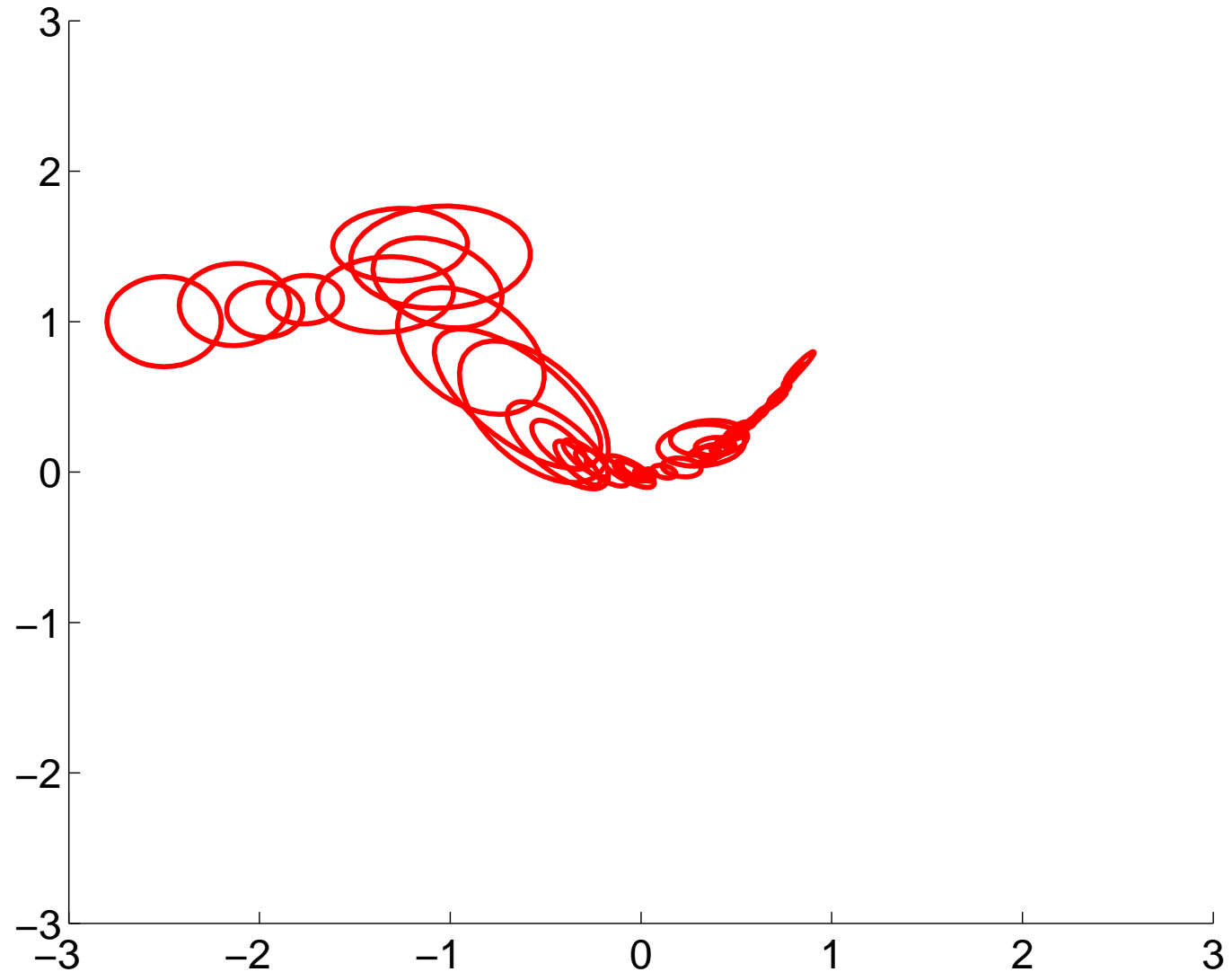
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CMA-ES Code (1)

CMA-ES is a **complex, but carefully designed** and tuned algorithm!

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CMA-ES Code (1)

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Really? It does not seem so from the pseudocode below...

Algorithm 4: CMA-ES

```
1 begin
2   Initialize:  $x \in \mathbb{R}^D, \sigma \in \mathbb{R}_+^D, C = I.$ 
3   while not TerminationCondition() do
4      $\mathcal{M} \leftarrow \text{SampleDistribution}(\lambda, \mathcal{N}(x, \sigma^2 C))$ 
5      $\mathcal{P} \leftarrow \text{SelectBest}(\mu, \mathcal{M})$ 
6      $(x, \sigma, C) \leftarrow \text{UpdateModel}(x, \sigma, C, \mathcal{P})$ 
7   return  $x$ 
```

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```

Hm, ok, how is the Normal distribution actually sampled?

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CMA-ES Code (2)

CMA-ES with the distribution sampling step expanded:

Algorithm 5: CMA-ES

```
1 begin
2   Initialize:  $x \in \mathbb{R}^D, \sigma \in \mathbb{R}_+^D, C = I$ .
3   while not TerminationCondition() do
4     for  $k \in 1, \dots, \lambda$  do
5        $z_k \leftarrow \mathcal{N}(0, I)$ 
6        $x_k \leftarrow x + \sigma C^{\frac{1}{2}} \times z_k$ 
7        $\mathcal{P} \leftarrow \text{SelectBest}(\mu, \{z_k, f(x_k) \mid 1 \leq k \leq \lambda\})$ 
8        $(x, \sigma, C) \leftarrow \text{UpdateModel}(x, \sigma, C, \mathcal{P})$ 
9   return  $x$ 
```

Remarks:

- All individuals exist in 2 “versions”: z_k distributed as $\mathcal{N}(0, I)$, and x_k distributed as $\mathcal{N}(x, \sigma^2 C)$.
- x_k are used just as an intermediate step for evaluation!
- z_k are used for model update via the population of selected parents \mathcal{P} .

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CMA-ES Code (2)

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Algorithm 5: CMA-ES

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- x_k are used just as an intermediate step for evaluation!
- z_k are used for model update via the population of selected parents \mathcal{P} .

OK, that’s not that complex. What about the model update?

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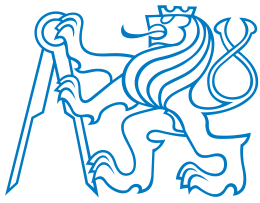
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CMA-ES Code (3)

CMA-ES with the model update step expanded:

Algorithm 6: CMA-ES

```

1 begin
2   Initialize:  $x \in \mathbb{R}^D, \sigma \in \mathbb{R}_+^D, C = I, s_\sigma = 0, s_c = 0.$ 
3   while not TerminationCondition() do
4     for  $k \in 1, \dots, \lambda$  do
5        $z_k \leftarrow \mathcal{N}(0, I)$ 
6        $x_k \leftarrow x + \sigma C^{\frac{1}{2}} \times z_k$ 
7        $\mathcal{P} \leftarrow \text{SelectBest}(\mu, \{z_k, f(x_k) \mid 1 \leq k \leq \lambda\})$ 
8        $s_\sigma \leftarrow (1 - c_\sigma)s_\sigma + \sqrt{c_\sigma(2 - c_\sigma)}\sqrt{\mu_w} \sum_{z_k \in \mathcal{P}} w_k z_k$  // search path for  $\sigma$ 
9        $s_c \leftarrow (1 - c_c)s_c + h_\sigma \sqrt{c_c(2 - c_c)}\sqrt{\mu_w} \sum_{z_k \in \mathcal{P}} w_k C^{\frac{1}{2}} z_k$  // search path for  $C$ 
10       $\sigma \leftarrow \sigma \cdot \exp^{c_\sigma/d} \left( \frac{\|s_\sigma\|}{\mathbb{E}\|\mathcal{N}(0, I)\|} - 1 \right)$  // update  $\sigma$ 
11       $C \leftarrow (1 - c_1 + c_h - c_\mu)C + c_1 s_c s_c^T + c_\mu \sum_{z_k \in \mathcal{P}} w_k C^{\frac{1}{2}} z_k (C^{\frac{1}{2}} z_k)^T$  // update  $C$ 
12       $x \leftarrow x + c_m \sigma C^{\frac{1}{2}} \sum_{z_k \in \mathcal{P}} w_k z_k$  // update  $x$ 
13  return  $x$ 

```

Remark: Two search paths, s_σ and s_c , are part of the algorithm state, together with x, σ , and C . They accumulate the algorithm moves across iterations.

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CMA-ES Code (3)

CMA-ES with the model update step expanded:

Algorithm 6: CMA-ES

```

1 begin
2   Initialize:  $x \in \mathbb{R}^D, \sigma \in \mathbb{R}_+^D, C = I, s_\sigma = 0, s_c = 0.$ 
3   while not TerminationCondition() do
4     for  $k \in 1, \dots, \lambda$  do
5        $z_k \leftarrow \mathcal{N}(0, I)$ 
6        $x_k \leftarrow x + \sigma C^{\frac{1}{2}} \times z_k$ 
7        $\mathcal{P} \leftarrow \text{SelectBest}(\mu, \{z_k, f(x_k) \mid 1 \leq k \leq \lambda\})$ 
8        $s_\sigma \leftarrow (1 - c_\sigma)s_\sigma + \sqrt{c_\sigma(2 - c_\sigma)}\sqrt{\mu_w} \sum_{z_k \in \mathcal{P}} w_k z_k$  // search path for  $\sigma$ 
9        $s_c \leftarrow (1 - c_c)s_c + h_\sigma \sqrt{c_c(2 - c_c)}\sqrt{\mu_w} \sum_{z_k \in \mathcal{P}} w_k C^{\frac{1}{2}} z_k$  // search path for  $C$ 
10       $\sigma \leftarrow \sigma \cdot \exp^{c_\sigma/d} \left( \frac{\|s_\sigma\|}{\mathbb{E}\|\mathcal{N}(0, I)\|} - 1 \right)$  // update  $\sigma$ 
11       $C \leftarrow (1 - c_1 + c_h - c_\mu)C + c_1 s_c s_c^T + c_\mu \sum_{z_k \in \mathcal{P}} w_k C^{\frac{1}{2}} z_k (C^{\frac{1}{2}} z_k)^T$  // update  $C$ 
12       $x \leftarrow x + c_m \sigma C^{\frac{1}{2}} \sum_{z_k \in \mathcal{P}} w_k z_k$  // update  $x$ 
13   return  $x$ 

```

Remark: Two search paths, s_σ and s_c , are part of the algorithm state, together with x, σ , and C . They accumulate the algorithm moves across iterations.

And what are all those c_1, c_h, c_μ, \dots ?

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CMA-ES Code

The full CMA-ES pseudocode:

Algorithm 7: CMA-ES

Given: $D \in \mathbb{N}_+$, $\lambda \geq 5$, $\mu \approx \lambda/2$, $w_k = w'(k) / \sum_{k=1}^{\mu} w'(k)$, $w'(k) = \log(\lambda/2 + 1/2) - \log \text{rank}(f(\mathbf{x}_k))$,
 $\mu_w = 1 / \sum_{k=1}^{\mu} w_k^2$, $c_\sigma \approx \mu_w / (D + \mu_w)$, $d \approx 1 + \sqrt{\mu_w / D}$, $c_c \approx (4 + \mu_w / D) / (D + 4 + 2\mu_w / D)$,
 $c_1 \approx 2 / (D^2 + \mu_w)$, $c_\mu \approx \mu_w / (D^2 + \mu_w)$, $c_m = 1$.

```

1  begin
2  Initialize:  $\mathbf{x} \in \mathbb{R}^D, \sigma \in \mathbb{R}_+^D, \mathbf{C} = \mathbf{I}, \mathbf{s}_\sigma = 0, \mathbf{s}_c = 0$ .
3  while not TerminationCondition() do
4      for  $k \in 1, \dots, \lambda$  do
5           $\mathbf{z}_k \leftarrow \mathcal{N}(0, \mathbf{I})$ 
6           $\mathbf{x}_k \leftarrow \mathbf{x} + \sigma \mathbf{C}^{\frac{1}{2}} \times \mathbf{z}_k$ 
7           $\mathcal{P} \leftarrow \text{SelectBest}(\mu, \{\mathbf{z}_k, f(\mathbf{x}_k)\} | 1 \leq k \leq \lambda)$ 
8           $\mathbf{s}_\sigma \leftarrow (1 - c_\sigma) \mathbf{s}_\sigma + \sqrt{c_\sigma(2 - c_\sigma)} \sqrt{\mu_w} \sum_{\mathbf{z}_k \in \mathcal{P}} w_k \mathbf{z}_k$  // search path for  $\sigma$ 
9           $\mathbf{s}_c \leftarrow (1 - c_c) \mathbf{s}_c + h_\sigma \sqrt{c_c(2 - c_c)} \sqrt{\mu_w} \sum_{\mathbf{z}_k \in \mathcal{P}} w_k \mathbf{C}^{\frac{1}{2}} \mathbf{z}_k$  // search path for  $\mathbf{C}$ 
10          $\sigma \leftarrow \sigma \cdot \exp^{c_\sigma/d} \left( \frac{\|\mathbf{s}_\sigma\|}{\mathbb{E}\|\mathcal{N}(0, \mathbf{I})\|} - 1 \right)$  // update  $\sigma$ 
11          $\mathbf{C} \leftarrow (1 - c_1 + c_h - c_\mu) \mathbf{C} + c_1 \mathbf{s}_c \mathbf{s}_c^T + c_\mu \sum_{\mathbf{z}_k \in \mathcal{P}} w_k \mathbf{C}^{\frac{1}{2}} \mathbf{z}_k (\mathbf{C}^{\frac{1}{2}} \mathbf{z}_k)^T$  // update  $\mathbf{C}$ 
12          $\mathbf{x} \leftarrow \mathbf{x} + c_m \sigma \mathbf{C}^{\frac{1}{2}} \sum_{\mathbf{z}_k \in \mathcal{P}} w_k \mathbf{z}_k$  // update  $\mathbf{x}$ 
13  return  $\mathbf{x}$ 

```

14 where $h_\sigma = \mathbb{1}(\|\mathbf{s}_\sigma\|^2 / D < 2 + 4 / (D + 1))$, $c_h = c_1(1 - h_\sigma^2)c_c(2 - c_c)$, and $\mathbf{C}^{\frac{1}{2}}$ is the unique symmetric positive definite matrix obeying $\mathbf{C}^{\frac{1}{2}} \times \mathbf{C}^{\frac{1}{2}} = \mathbf{C}$. All c -coefficients are ≤ 1 .

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CMA-ES Summary

CMA-ES is **quasi parameter-free**:

- It has a lot of internal parameters, but almost all of them are carefully set by the algorithm itself.
- The user has to specify only
 - initial solution \mathbf{x} ,
 - initial step size σ , and
 - the number of offspring λ (but even that can be set based on the search space dimension).

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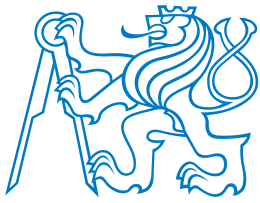
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CMA-ES is **quasi parameter-free**:

- It has a lot of internal parameters, but almost all of them are carefully set by the algorithm itself.
- The user has to specify only
 - initial solution x ,
 - initial step size σ , and
 - the number of offspring λ (but even that can be set based on the search space dimension).

CMA-ES Variants:

- Reducing the local search character of CMA-ES:
 - **IPOP-CMA-ES**: Restart CMA-ES several times, making the population twice as large each time.
 - **BIPOP-CMA-ES**: Restart CMA-ES many times in 2 regimes: IPOP, and small-pop (spend similar number of evaluations in IPOP and small-pop modes).
- Reducing the number of parameters to be adapted:
 - **L-CMA-ES**: Smaller memory requirements, suitable for high-dimensional spaces, limited adaptation.
- Learning from unsuccessful mutations:
 - **Active CMA-ES**: negative weights allowed during covariance update. Gotcha: C may lose positive definiteness!



Relations to other algorithms

Estimation of Distribution Algorithms (**EDA**):

- CMA-ES can be considered an instance of EDA.
- EDAs template: sample from probabilistic model, and update model based on good individuals (i.e., the same as CMA-ES uses).

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Relations to other algorithms

Estimation of Distribution Algorithms (**EDA**):

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Natural Evolution Strategies (**NES**):

- Idea: the update of all distribution parameters should be based on the same fundamental principle.
- NES proposed as more principled alternative to CMA-ES.
- Later it was found that CMA-ES actually implements the underlying NES principle.

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Relations to other algorithms

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- Idea: the update of all distribution parameters should be based on the same fundamental principle.
- NES proposed as more principled alternative to CMA-ES.
- Later it was found that CMA-ES actually implements the underlying NES principle.

Information Geometric Optimization (**IGO**):

- Framework unifying many successful algorithms from discrete and continuous domains.
- CMA-ES and NES (and many EDA variants, see the next lecture) can be derived as special instances of IGO.

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Differential Evolution

Developed by Storn and Price [SP97].

- Simple algorithm, easy to implement.
- Unusual breeding pipeline.

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Algorithm 8: DE Breeding Pipeline

Input: Population X with fitness in f .

Output: Offspring population X_N .

```
1 begin
2    $X_N \leftarrow \emptyset$ 
3   foreach  $x \in X$  do
4      $(x_1, x_2, x_3) \leftarrow \text{Select}(X, f, x)$ 
5      $u \leftarrow \text{Mutate}(x, x_1, x_2)$ 
6      $x_N \leftarrow \text{Recombine}(u, x_3)$ 
7      $X_N \leftarrow X_N \cup \text{BetterOf}(x, x_N)$ 
8   return  $X_N$ 
```

- Vectors x, x_1, x_2, x_3 shall all be different, x_1, x_2, x_3 chosen uniformly.
- For each population member x , an offspring x_N is created.
- x_N replaces x in population if it is better.

[SP97] Rainer Storn and Kenneth Price. Differential evolution – a simple and efficient heuristic for global optimization over continuous spaces. *Journal of Global Optimization*, 11(4):341–359, December 1997.



DE Mutation and Recombination

- Mutation and recombination:

$$\mathbf{u} \leftarrow \mathbf{x}_1 + F(\mathbf{x}_2 - \mathbf{x}_3), \quad F \in (0, 2)$$

$$x_{N,d} \leftarrow \begin{cases} u_d & \text{iff } \text{rand}_d \leq CR \text{ or } d = I_{\text{rand}} \\ x_{4,d} & \text{iff } \text{rand}_d > CR \text{ and } d \neq I_{\text{rand}} \end{cases}$$

- $\text{rand}_d \sim \mathcal{U}(0, 1)$, different for each dimension
- I_{rand} is a random index of the dimension that is always copied from \mathbf{u}
- $2^D - 1$ possible candidate points \mathbf{y}

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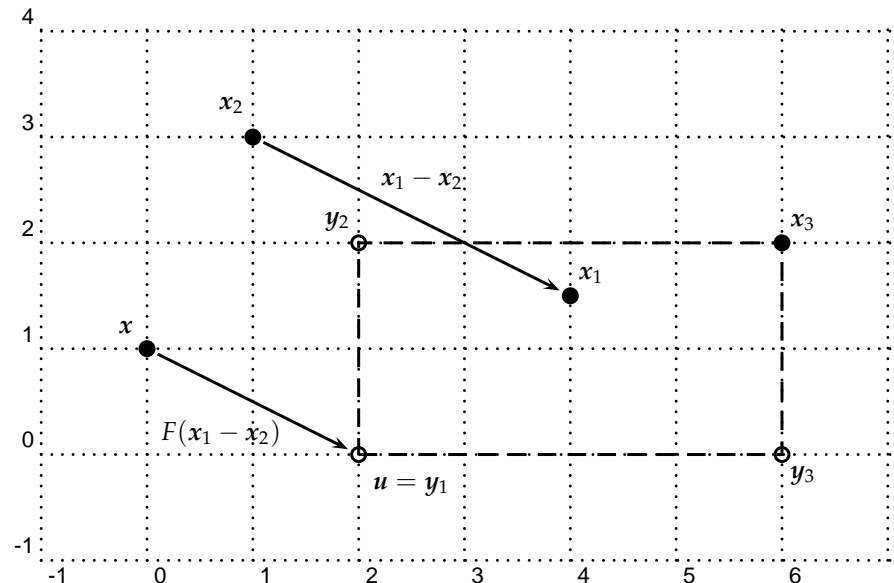
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DE Variants

Small variations of the base algorithm:

- DE/rand vs DE/best: the “best” variant uses the best of 4 parent vectors in place of x when generating the offspring.
- DE/./ n : n is the number of difference vectors taken into account during mutation.
- DE/././bin vs DE/././exp: binomial recombination (described above), exponential recombination (not described here)

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DE Variants

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- DE/./ n : n is the number of difference vectors taken into account during mutation.
- DE/././bin vs DE/././exp: binomial recombination (described above), exponential recombination (not described here)

Many adaptive variants: SaDE, JADE, ...

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Learning outcomes

After this lecture, a student shall be able to

- perform the mapping of chromosomes from binary to real space when using binary encoding for real-parameter optimization;
- describe and exemplify the effects of such a genotype-phenotype mapping on the neighborhood structures induced by mutation and crossover;
- give examples and describe some mutation and crossover operators designed for spaces of real number vectors;
- explain the main features of ES and differences to GAs;
- explain the notation $(\mu/\rho^+, \lambda)$ -ES;
- describe the differences between mutation with isotropic, axis-parallel, and general Gaussian distribution, including the relation to the form of the covariance matrix, and the number of parameters that must be set/adapted for each of them;
- explain and use two simple methods of mutation step size adaptation (1/5 rule and self-adaptation);
- write a high-level pseudocode of CMA-ES and describe CMA-ES in the $(\mu/\rho^+, \lambda)$ notation;
- implement DE algorithm;
- explain the basic forms of DE mutation and crossover.

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